# 1. Advanced Combustion Engines

To strengthen national security, promote future economic growth, support American energy dominance, and increase transportation energy affordability for Americans, the Vehicle Technologies Office (VTO) funds earlystage, high-risk research. This research will generate knowledge that industry can advance to deploy innovative energy technologies to support affordable, secure, reliable, and efficient transportation systems across America. VTO leverages the unique capabilities and world-class expertise of the National Laboratory system to develop new innovations in electrification, including advanced battery technologies; advanced combustion engines and fuels, including co-optimized systems; advanced materials for lighter-weight vehicle structures and better powertrains; and energy efficient mobility technologies and systems, including automated and connected vehicles as well as innovations in connected infrastructure for significant systems-level energy efficiency improvement. VTO is uniquely positioned to address early-stage challenges due to its strategic research partnerships with industry (e.g., the U.S. DRIVE and 21st Century Truck Partnerships) that leverage relevant technical and market expertise. These partnerships prevent duplication of effort, focus DOE research on the most critical research and development (R&D) barriers, and accelerate progress. The partnerships help VTO focus on research that industry does not have the technical capability to undertake on its own—usually because there is a high degree of scientific or technical uncertainty or it is too far from market realization to merit sufficient industry emphasis and resources. At the same time, VTO works with industry to ensure there are pathways for technology transfer from government to industry so that Federally-supported innovations have an opportunity to make their way into commercial application.

The Advanced Combustion Engines (ACE) subprogram supports early-stage R&D to improve our understanding and ability to manipulate combustion processes, fuel properties, and catalyst formulations, generating the knowledge and insight necessary for industry to develop the next generation of engines and fuels for light- and heavy-duty vehicles. As a result, co-optimization of higher-efficiency engines and high performance fuels has the potential to improve light-duty fuel economy by 35% (25% from advanced engine research and 10% from co-optimization with fuels) by 2030 compared to 2015 gasoline vehicles. The subprogram supports cutting-edge research at the National Laboratories, in close collaboration with academia and industry, to strengthen the knowledge base of high-efficiency, advanced combustion engines, fuels, and emission control catalysts. The ACE subprogram will apply the unique facilities and capabilities at the National Laboratories to create knowledge, new concepts, and research tools that industry can use to develop advanced combustion engines and co-optimize with fuels that will provide further efficiency improvements and emission reductions. These unique facilities and capabilities include the Combustion Research Facility at Sandia National Laboratories (SNL), Advanced Photon Source at Argonne National Laboratory (ANL), Institute for Integrated Catalysis at Pacific Northwest National Laboratory (PNNL), detailed fuel chemistry expertise at the National Renewable Energy Laboratory (NREL), chemical kinetic modeling and mechanism development at Lawrence Livermore National Laboratory (LLNL), and the Spallation Neutron Source at Oak Ridge National Laboratory (ORNL), along with their high performance computing resources and initial work to utilize future exascale computing resources.

# **Project Feedback**

In this merit review activity, each reviewer was asked to respond to a series of questions, involving multiple-choice responses, expository responses where text comments were requested, and numeric score responses (*on a scale of 1.0 to 4.0*). In the pages that follow, the reviewer responses to each question for each project will be summarized: the multiple choice and numeric score questions will be presented in graph form for each project, and the expository text responses will be summarized in paragraph form for each question. A table presenting the average numeric score for each question for each project is presented below.

Table 1-1 - Project Feedback

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace001	Heavy-Duty Diesel Combustion	Mark Musculus (SNL)	1-7	3.83	3.67	3.83	3.33	3.69
ace004	Low-Temperature Gasoline Combustion (LTGC) Engine Research	John Dec (SNL)	1-11	3.13	3.13	3.38	3.00	3.14
ace005	Spray Combustion Cross- Cut Engine Research	Lyle Pickett (SNL)	1-16	3.80	3.70	3.90	3.70	3.75
ace006	Advanced Ignition for Gasoline Combustion	Isaac Ekoto (SNL)	1-21	3.38	3.38	3.50	3.38	3.39
ace010	Fuel Injection and Spray Research Using X-Ray Diagnostics	Christopher Powell (ANL)	1-25	3.60	3.50	3.50	3.40	3.51
ace012	Model Development and Analysis of Clean and Efficient Engine Combustion	Russell Whitesides (LLNL)	1-30	3.63	3.63	3.63	3.25	3.58
ace013	Chemical Kinetic Models for Advanced Engine Combustion	Bill Pitz (LLNL)	1-33	3.38	3.00	3.25	3.25	3.16
ace015	Stretch Efficiency for Combustion Engines: Exploiting New High- Dilution Combustion Regimes	James Szybist (ORNL)	1-37	3.40	3.30	3.20	3.40	3.33

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace017	Accelerating Predictive Simulation of Internal Combustion Engines (ICEs) with High- Performance Computing (HPC)	K. Dean Edwards (ORNL)	1-41	2.88	3.25	3.38	2.63	3.09
ace022	Joint Development and Coordination of Emissions Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination)	Josh Pihl (ORNL)	1-45	3.75	3.63	3.63	3.38	3.63
ace023	Fundamentals in Selective Catalytic Reduction (SCR), Filter, and Protocol	Yong Wang (PNNL)	1-50	3.00	3.25	3.00	3.00	3.13
ace027	Next-Generation Selective Catalytic Reduction (SCR)- Dosing System Investigation	Abhijeet Karkamkar (PNNL)	1-54	2.88	2.50	2.38	2.38	2.56
ace032	Cummins-ORNL Emissions Cooperative Research and Development Agreement (CRADA): NOx Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems	Bill Partridge (ORNL)	1-58	3.13	3.00	3.25	3.25	3.09
ace033	Emission Control for Lean Gasoline Engines	Vitaly Prikhodko (ORNL)	1-62	3.38	3.50	3.38	3.50	3.45
ace054	Rapid Compression Machine (RCM) Studies to Understand Autoignition Fundamentals	Scott Goldsborough (ANL)	1-66	3.00	3.00	3.33	3.17	3.06
ace056	Low-Temperature Oxidation	Yong Wang (PNNL)	1-69	3.13	3.38	3.00	3.00	3.22

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace084	Development and Validation of Simulation Tools for Advanced Ignition Systems	Riccardo Scarcelli (ANL)	1-73	3.20	3.30	3.70	3.20	3.31
ace085	Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization	Todd Toops (ORNL)	1-78	3.50	3.38	3.25	3.50	3.41
ace100	Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research - SuperTruck II	Justin Yee (Daimler Trucks North America)	1-82	3.70	3.60	3.40	3.60	3.60
ace101	Volvo SuperTruck II: Pathway to Cost-Effective Commercialized Freight Efficiency	Pascal Amar (Volvo Trucks North America)	1-86	3.40	3.40	3.20	3.40	3.38
ace102	Cummins-Peterbilt SuperTruck II	Jon Dickson (Cummins- Peterbilt)	1-90	3.70	3.70	3.70	3.70	3.70
ace103	Development and Demonstration of a Fuel- Efficient Class 8 Tractor and Trailer SuperTruck	Russell Zukouski (Navistar)	1-94	2.80	2.80	2.70	2.80	2.79
ace118	CLEERS Passive NOx Adsorber (PNA)	Janos Szanyi (PNNL)	1-99	3.63	3.25	3.00	3.38	3.33
ace119	Development and Optimization of a Multi- Functional SCR-DPF (Selective Catalytic Reduction-Diesel Particulate Filter) Aftertreatment System for Heavy-Duty NOx and Soot Emission Reduction	Ken Rappe (PNNL)	1-103	3.25	3.00	3.00	2.75	3.03
ace121	A High Specific Output, Gasoline, Low- Temperature Combustion Engine	Hanho Yun (General Motors)	1-108	3.75	3.88	3.50	3.63	3.77

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace123	Temperature-Following Thermal Barrier Coatings for High-Efficiency Engines	Tobias Schaedler (HRL Laboratories)	1-112	3.25	3.00	2.88	3.50	3.11
ace124	SuperTruck II - PACCAR	Carl Hergart (PACCAR)	1-116	3.33	3.25	3.17	2.92	3.22
ace125	Model Development of Fundamental Combustion Processes	Rainer Dahms (SNL)	1-121	3.13	3.38	3.00	3.13	3.23
ace126	Developing a Framework for Performing High- Fidelity Engine Simulations using Nek5000 Code for Exascale Computing	Muhsin Ameen (ANL)	1-125	3.30	3.40	2.90	3.00	3.26
ace127	Advanced Combustion Concepts for High- Efficiency Gasoline Engines	Scott Curran (ORNL)	1-131	3.75	3.50	3.50	3.50	3.56
ace128	Reduced Precious Metal Catalysts for Methane and NOx Emission Control of Natural Gas Vehicles	Michael Harold (University of Houston)	1-133	3.67	3.67	3.50	3.67	3.65
ace129	Design and Optimization of Structured Multi- Functional Trapping Catalysts for Conversion of Hydrocarbons and NOx from Diesel and Advanced Combustion Engines	Michael Harold (University of Houston)	1-136	3.50	3.25	3.63	3.25	3.36
ace130	Development of Passive Hydrocarbon/NOx Trap Catalysts for Low- Temperature Gasoline Applications	Mark Crocker (University of Kentucky)	1-140	3.33	3.50	3.50	3.67	3.48
ace131	Ducted Fuel Injection (DFI) for Heavy-Duty Engines	Charles Mueller (SNL)	1-143	3.70	3.70	3.50	3.50	3.65

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace132	Heavy-Duty Gasoline Compression Ignition	Chris Kolodziej (ANL)	1-147	3.38	3.38	3.50	3.13	3.36
ace133	Next-Generation Heavy- Duty Powertrains	Scott Curran (ORNL)	1-151	3.20	3.10	3.50	3.10	3.18
ace134	Multi-Mode Combustion in Light-Duty Spark-Ignition Engines †	Toby Rockstroh (ANL)	1-156	3.75	3.63	3.63	3.75	3.67
ace135	Development of Simulations Tools for Compression Ignition Engines †	Sibendu Som (ANL)	1-160	3.50	3.50	3.63	3.50	3.52
ace136	Medium-Duty Diesel Combustion †	Steven Busch (SNL)	1-164	3.75	3.50	3.63	3.38	3.56
Overall Average				3.40	3.36	3.35	3.28	3.36

<sup>†</sup> Denotes a poster presentation.

Presentation Number: ace001
Presentation Title: Heavy-Duty Diesel
Combustion
Principal Investigator: Mark Musculus
(Sandia National Laboratories)

Presenter Mark Musculus, Sandia National Laboratories

Reviewer Sample Size
A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer remarked that this continues to be an exceptional program that combines state-of-the-art optical diagnostics in a diesel engine environment with multi-dimensional engine simulations to understand the combustion behavior in both conventional and low-temperature combustion (LTC) modes. The reviewer said the project team is looking at issues of key interest to engine company engineers such as understanding how multiple injection pulses interact, how combustion system design choices affect soot formation, and so on. The reviewer noted that the new focus on

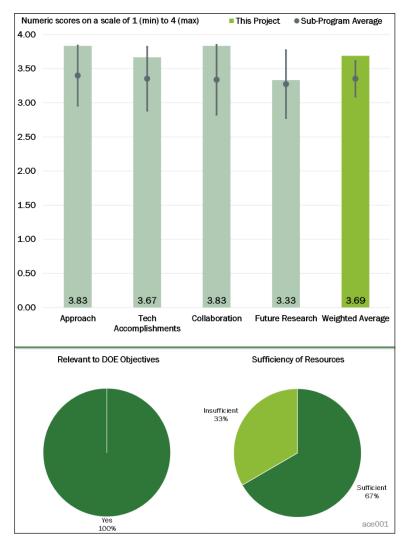


Figure 1-1 – Presentation Number: ace001 Presentation Title: Heavy-Duty Diesel Combustion Principal Investigator: Mark Musculus (Sandia National Laboratories)

heat transfer effects is particularly timely because the drive toward higher efficiencies over the past few years has led to a near obsession with heat transfer and how to manipulate it to further maximize efficiency. The reviewer said that some systematic research using appropriate experimental and analytical tools is definitely warranted and may aid combustion system developers in focusing on the right paths for further engine-efficiency improvements. The reviewer noted that it may be desirable and productive to add some more fundamental experiments to this research program to help isolate specific physical effects and reduce uncertainty where multiple physical phenomena come into play to affect the overall engine behavior. The reviewer said spray diagnostics come to mind for fundamental experiments, as do the various elements within the engine environment that affect heat transfer such as oil gallery cooling and others. According to the reviewer, it is understood that broadening the scope will mean either a dilution of the time and effort that can be devoted to individual topics or the need for increased funding and resources. Given the soundness of the overall approach and progress to date, the reviewer would certainly vote for the latter course of action.

## Reviewer 2:

The reviewer indicated that this project has been ongoing for a long time, but with continued focus on generating a science-based conceptual understanding of diesel combustion. The reviewer said the results presented continue to move the understanding at a good pace. The reviewer noted that publications and communications of the project results are easily found, indicating good knowledge transfer from this project to the engine combustion community. The reviewer stated that this project is one of the top U.S. Department of Energy (DOE) funded combustion projects and that it has direct and long-lasting relevance to the heavy-duty original equipment manufacturers (OEMs).

#### Reviewer 3:

The reviewer said that there is a growing interest in applying thermal barrier coatings (TBCs) for reducing the heat transfer. The reviewer noted that it will be beneficial for the engine community to learn from both experimental and computational approaches to using different types of TBC.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer observed that progress and accomplishments continue to be very strong. The reviewer indicated that this is particularly true regarding the recent focus on multiple injection behavior. The reviewer noted that the combination of optical engine data and computational results were combined to provide many useful insights. The reviewed stated that it would be interesting to see similar progress on understanding the barriers to high-load LTC operation and, even more importantly, exploring pathways to overcome barriers. The reviewer remarked that limitations of the current optical engine hardware to high-pressure operation was acknowledged as a pacing item by the project team. The reviewer stated that this, coupled with the new focus on heat transfer and the continued research on multi-pulse injection, seems to indicate the need for bringing in additional or perhaps even new facilities to provide the needed diagnostics environment. The reviewer asserted that on the computational front, it would be useful to learn more about how the capabilities of the computational fluid dynamics (CFD) tools that are being used for this research are being transferred to the commercial software tools available to engine developers. The reviewer asserted that this would ensure that the technologies being used to achieve these accomplishments are getting into the hands of the engineers tasked with developing new engines.

## Reviewer 2:

The reviewer stated that the completed milestones for this project show good progress. The reviewer said that the focus on heat transfer is key and is directly on point. The reviewer remarked that heat transfer is arguably one of the most difficult topics due to the spatial and temporal aspects. The reviewer summarized that the main thoughts surrounding this present heat flux effort have to do with how the heat flux measurements can be used to inform CFD simulations and how operating conditions translate to other relevant heavy-duty conditions (i.e., full load and density). The reviewer questioned if the project team has plans to model the impinging jet heat flux experiments in CFD or with similar tools to evaluate the heat flux increases before wall impingement or other similar situations. The reviewer indicated that this would help evaluate the hypotheses and identify gaps in engineering-level CFD wall modeling. The reviewer wanted more information on the surface thermocouples (TCs) and how the TC choice may bias the observations. The reviewer also questioned if the project team has plans to evaluate heavy-duty (HD)-relevant chamber densities and if the project team would expect the fundamental physics to substantially change with these more relevant conditions. The reviewer observed that the heat flux increase occurring before high-temperature gas wall impingement occurs generally right at top dead center (TDC), where there is strong squish flow in the piston channel and piston reversal. The reviewer questioned if these aspects relate to the observations of heat flux.

#### Reviewer 3:

The reviewer reported that the project team said 9 out of 13 TCs recorded data. The reviewer questioned if the project team knew why the four TCs failed and if the project team gained any insight from that failure. The reviewer wanted more information about whether the project's boundary layer compression is similar to the shock and boundary layer interaction in published literature.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

This reviewer said this project's approach is generally one of the benchmarks for collaboration, execution, and knowledge- sharing through papers, Advanced Engine Combustion (AEC) meeting, and direct collaborations. The reviewer requested that the project team continue leading this effort because it is bringing value to the spray combustion community. The reviewer stated that the project team's efforts are greatly appreciated.

## Reviewer 2:

The reviewer stated that collaboration and coordination between the diagnostics team at Sandia National Laboratories (SNL) and the CFD team at the University of Wisconsin (UW) appears to be outstanding. The reviewer noted this view was based on the presentations at the Annual Merit Review (AMR) and on presentations in other forums such as the bi-annual AEC and Memorandum of Understanding (MOU) meetings. The reviewer said it is a little less clear how the project's collaboration with Lund University on soot research or the Japanese team on "diesel and dual-fuel natural gas" research is progressing. The reviewer requested more details on what these interactions entail, what results have been achieved from these collaborations, and what the future plans are for collaboration. The reviewer suggested that this information be provided in future reports.

#### Reviewer 3:

The reviewer commented that the good dissemination of results indicate that this project has very good collaboration and coordination with industry and academia.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

According to the reviewer's experience, examining heat transfer in diesel and spark ignition (SI) engines is a challenging business, plagued by a lack of information because TC data on the piston surface are not enough. The reviewer continued that there is often perplexing behavior observed owing to a multitude of physical processes that are interacting and competing with heat-transfer pathways. The reviewer suspected that the project team will likely come to similar conclusions as the team continues to delve into this interesting, important, and often frustrating subject. The reviewer suggested that it might be worthwhile to look at bringing on additional expertise to the project team (e.g., from researchers who have focused on heat transfer in academia or other places with appropriate diagnostics and analysis techniques to make more progress here).

## Reviewer 2:

The reviewer stated that the plan for continuation of the experiments and simulations was clear and well organized. The reviewer petitioned for increased simulation priority to run in parallel with the engine experiments to help extract learning and provide back-and-forth progress. The reviewer noted that the fundamental aspects of the heat flux and multiple injection areas are very useful, but a concerted effort toward comparing this knowledge with what is modeled in state-of-the-art tools like CFD would greatly help to deliver value. The reviewer commented that a significant increase in funding would likely be required on the computational side to achieve this.

#### Reviewer 3:

The reviewer suggested that the proposed future research include a type of conjugate heat transfer (CHT) computer simulations to aid the research being done in this effort.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated that this project is extremely relevant for achieving the DOE's objectives, given the relationship to core engine combustion fundamentals that impact efficiency in heavy-duty engines.

#### Reviewer 2:

The reviewer said that this project supports the overall DOE objective because the study focuses on fundamentals of engine heat transfer.

#### Reviewer 3:

The reviewer remarked that increasing efficiency and reducing emissions still appear to be the overriding DOE objectives in the engine world and that this project addresses both, in terms of research to date and proposed future research. The reviewer inquired whether the team could devise a way to bring batteries and fuel cells into the picture.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer remarked that the resources on the experimental side seem reasonable for the desired deliverables. The reviewer petitioned for a significant increase in funds to support the CFD and simulation efforts (likely to match the magnitude of the experimental side of the project) to leverage the most value from existing efforts.

#### Reviewer 2:

As proposed, the resources appeared sufficient to the reviewer. The reviewer said, however, if some of the shortcomings previously noted (e.g., overcoming high-load LTC barriers, bringing in complementary focused experiments to isolate phenomena, utilizing additional diagnostics and analysis techniques for better understanding of heat transfer, etc.) are addressed, then more resources may be needed.

#### Reviewer 3:

The reviewer indicated that more computational resources may be necessary for this project since the high-fidelity simulations involving detailed chemical kinetics are computationally expensive.

Presentation Number: ace004
Presentation Title: Low-Temperature
Gasoline Combustion (LTGC) Engine
Research
Principal Investigator: John Dec
(Sandia National Laboratories)

## Presenter

John Dec, Sandia National Laboratories

## Reviewer Sample Size

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer observed nice experimental work and commented that the project shows that 2-ethylhexyl nitrate (EHN) can be used to apply reactivity-controlled compression ignition (RCCI) to gasoline LTC. The reviewer said that this establishes the bounds and performance benefits and that it can be coupled with other control techniques, like dual injection. However, the reviewer asked to what extent the effort should be extended to demonstrating control systems. So far, the work is within the bounds of fundamental investigation, namely investigating a hypothesized control

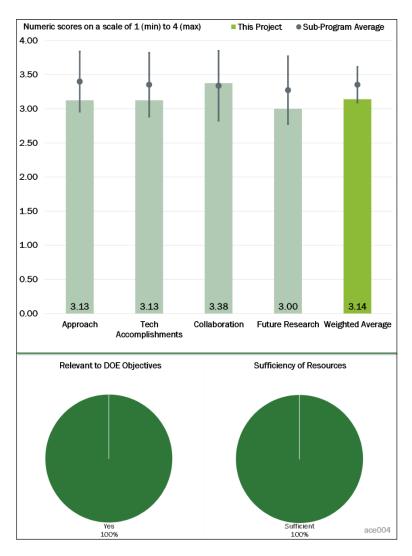


Figure 1-2 – Presentation Number: ace004 Presentation Title: Low-Temperature Gasoline Combustion (LTGC) Engine Research Principal Investigator: John Dec (Sandia National Laboratories)

system and if there is reason to believe it can be developed. The reviewer noted that at some point it will be industry's responsibility to develop the control strategy if industry thinks that the approach of adding EHN is a technical path to be followed. The reviewer suggested that the control system be developed only to the point that transients experiments can be run in the lab. The reviewer also asked when the project team could expect to start the optical engine work.

#### Reviewer 2:

The reviewer noted a modest efficiency gain over diesel, but also a reduced cost of ownership from cheaper components and less diesel exhaust fluid (DEF). The reviewer also noted additive mixing fuel injection for operating control and partial fuel stratification. The reviewer said that combining metal and optical engine experiments is a robust method for a comprehensive understanding. The reviewer commented that inclusion of collaborative capabilities for modeling, simulation, and kinetic mechanism development are appropriate. The reviewer stated that the project aims to address extremely relevant topics of low-temperature gasoline combustion (LTGC) load control, load range expansion, and transient control.

#### Reviewer 3:

The reviewer remarked that the approach is sound, given the partners and history of this work. The reviewer commented that the technical detail is very high and the results are thorough. The reviewer said, however, the approach is certainly more geared toward light-duty (LD) application, but there are several boundary conditions that make this work difficult to translate to heavy-duty application. The reviewer stated that 60°Celsius (C) intake is not something HD engine manufacturers would find reasonable due to warranty, durability, and other factors, which leaves either additive-mixing fuel injection (AMFI) or double direct injection (DDI)-partial fuel stratification (PFS) as levers to control ignition and combustion phasing. The reviewer indicated that light-duty OEMs have been very clear in expressing their desire for stoichiometric engine combustion systems without lean aftertreatment requirements. The reviewer concluded that this project appears to be a bit mismatched with the project goals and the target market.

## Reviewer 4:

The reviewer provided a summary of noted barriers. The first barrier noted was the rapid combustion timing control for LTC. While the AMFI system is unique, the reviewer was not sure if it is a significant improvement over RCCI, which also offers rapid combustion timing-control options. A real injector would still require, effectively, two injectors located in one body in order to meter both fuels. The reviewer further commented that with the constraints on packaging, cooling, and so on, it was uncertain whether the AMFI system would offer any real cost improvement over a direct injection-port fuel injection (DI-PFI) combination system. The consumption of the additive is lower on a volumetric basis, which may help consumer acceptance, but it is still not seamless (or as easy as plugging into a charger, which is the new competition for simplicity).

The second barrier this reviewer noted was improved low-load operation and efficiency. The reviewer observed good progress on this barrier and commented that the part-load efficiency looks quite good even though it is not too different from Delphi's gasoline compression ignition (GCI) numbers. The reviewer was unsure if one can call that low-load operation good unless the engine is also emissions compliant. The reviewer reported that project results shown indicate the oxides of nitrogen (NOx) emissions are just under the 2010 HD NOx limit, but asserted that this is no longer a relevant metric. The reviewer explained that the U.S. Environmental Protection Agency (EPA) Tier 3 and California Low Emission Vehicle (LEV) III Rulemakings, as well as the upcoming California Air Resources Board (CARB)/EPA HD NOx regulations, are around an order of magnitude lower, and that emissions measurements on dilute exhaust are at 1 parts per million (ppm) average over the test cycle. The reviewer concluded that unless there is a path to address the NOx emissions and particulate number (PN), which are assuredly not zero, then there is still a massive barrier here.

The third barrier identified by the reviewer was cold start, which is a very interesting and challenging aspect of engine combustion in general and probably more so for LTC. The reviewer would have preferred to see more work on this project just on this and to extend cold start down toward 0°C. The reviewer suggested that the lessons learned there would probably translate to other LTC projects, which would magnify the benefit.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

## Reviewer 1:

The reviewer remarked that there has been substantial technical progress on this project. The reviewer noted lots of excellent collaboration with simulation and other National Laboratory projects, particularly at Lawrence Livermore National Laboratory (LLNL). The reviewer stated that results show significant progress to understanding fuel influence, intake temperature, and additive effects upon ignition and combustion phasing. The reviewer indicated that it will be critical to see how this project adjusts as Hyundai Kia America Technical Center (HATCI), Inc., becomes more involved in the practical application of AMFI and/or DDI-PFS, and asked whether an automotive OEM is truly supportive of a lean-burn system versus electrification.

## Reviewer 2:

The reviewer remarked that this is very nice experimental work. The reviewer said that the project team was successfully meeting their objectives and time lines. The reviewer said that the techniques being pursued to control crank angle position where 50% of the heat is released (CA50) and control load have been described in the literature years ago including: multiple injections with different quantities of fuel, timing, and dwell between the injections; RCCI; temperature variation; exhaust gas recirculation (EGR); and so on. The reviewer noted that this work integrates those approaches nicely. The reviewer expressed the most interest in seeing optical probing of these in-cylinder approaches. The reviewer further noted that, for years, using metal and optical engines to gain a fundamental understanding of LTGC has been listed in the technical approach slide. The reviewer would like to know if there will be optical work to see soon.

#### Reviewer 3:

The reviewer noted that additive-mixing fuel injection reduces the amount of residual heat required for LTC; the project team is currently using EHN in a gallon-sized reservoir for 7,000-mile range. The additive costs \$20 and saves \$150 in gasoline. The reviewer also noted the extension of low load to 2 bar Indicated Mean Effective Pressure (IMEP). The reviewer commented that dual-direction injection, partial fuel stratification was used to conduct a 30% load change transient while maintaining CA50 appropriately without violating 2010 NOx requirements, even with the thermal stratification and additive injection.

The reviewer said that the proposed charge heating does reduce the amount of additive required, but it appears to remove load sensitivity. The reviewer questioned how complex the control problem will become (e.g., map-based, open loop, feedback, model-based). The reviewer stated that traditional map-based control with feedback should be enough. The reviewer indicated that additive makes the fuel "equivalence ratio sensitive," which can be obtained in combination with fuel stratification shown on Slide 13. The reviewer reported that cold start has been obtained with the AMFI system down to  $20^{\circ}$ C. The reviewer stated trends of additive consumption with boost and temperature will be required for feedback control and suggested that EGR and additives can both be utilized for CA50 control and used nearly interchangeably. The reviewer remarked that while soot may be immeasurable for a smoke meter, the particulate count will undoubtedly be greater than zero for a DI combustion scheme. The reviewer stated that nitrogen carried with the additive becomes a major source relative to the Zeldavich  $NO_x$ . The reviewer asserted that another additive with less carried nitrogen would be important (cost, density, etc., are all important).

## Reviewer 4:

The reviewer expressed a view on the key barriers that this program is uniquely addressing is a bit different from what is probably the focus of the project team. The reviewer stated that there has been reasonably good demonstration of the control range of the AMFI system and the use of DDI-PFS. A key question the reviewer wanted to understand is what is markedly different from other LTC combustion approaches. The reviewer said that in a broad sense these are similar tools to the reactivity stratification of RCCI or the fuel stratification of most homogeneous charge compression ignition (HCCI) and GCI approaches. The reviewer wanted to have a better explanation of how the work presented on this project fits into the findings from the broader spectrum of LTC projects.

The reviewer got the feeling that many questions of the work's practical implications are a bit divorced from the real-world constraints that an OEM will face in making an engine. The reviewer agreed that the AMFI system could be engineered to be a next-cycle response system so there was less reason for concern. However, demands for transient speeds and loads are really challenging in a real engine, and the restrictions on the sensors that are available for an acceptable cost and power consumption are severe. The reviewer concluded that these findings are scientifically interesting, but the project results should show some pathway toward higher technology readiness levels (TRLs). This reviewer was not able to see a real path forward.

## Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer praised the project for an excellent team of collaborators and support organizations, including General Motors (GM), the State University of New York (SUNY), and LLNL. The reviewer remarked that the challenge will be if either AMFI or DDI-PFS, or potentially both, can be made robust, durable, and low cost enough to compete with electrification and assist an automotive OEM in meeting greenhouse gas (GHG) and fuel economy targets. The reviewer commented that electrification along with LTGC are not likely compatible for cost reasons, especially in LD application.

#### Reviewer 2:

The reviewer said that the collaboration with relevant stakeholders is excellent.

#### Reviewer 3:

The reviewer remarked that the modeling interaction is good and expressed interest in seeing more modeling using a range of computational tools to bring more analysis to the experimental results. The reviewer would also like to see more bi-directional interaction with other engine projects, both to put the project work into the context of other LTC systems, and into the context of engines that can run over the full speed and load range.

#### Reviewer 4:

The reviewer observed adequate collaboration between the project team.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer commented that improved low-load performance and enhancing the actuation time of the AMFI were worthy pursuits.

#### Reviewer 2:

The reviewer mostly liked the proposed future research. The reviewer referenced prior comments and noted a need for analysis, experimentation, and/or something that ties the work here to real-world issues on emissions under the current regulatory regime and/or to full-range engine operation and similar topics and themes.

## Reviewer 3:

In referencing prior comments, the reviewer stated that the researcher's renown is from optical measurements. It seemed to the reviewer that the work is focusing on taking the metal engine work to a point of actual handoff to industry. The project team demonstrated that controlling transients looks feasible. The reviewer questioned if it is necessary to continue development of the control system. The reviewer personally wanted to see a more aggressive movement toward optical engine work.

## Reviewer 4:

It was very unclear to the reviewer if this approach will work within the cost and reliability constraints of the automotive sector in an age of increased electrification. Although the reviewer noted that it is good OEMs are participating, this reviewer pointed out that even Delphi tried to use intake air heating in its fairly successful GDCI project, and the intake air heater was met with significant resistance from other automotive OEMs. The reviewer said that for automotive companies, the race is about which technology will meet the fuel efficiency (FE), GHG, and other emissions targets at the lowest cost. The reviewer commented that electrification, full battery electric vehicles (BEVs), and LTC are competitors in this field and that whichever one delivers at the most predictable lowest cost will likely win. The reviewer said additional fluids in light-duty AMFI and EHN or something unknown to DEF in HD, may be major barriers to overcome in the future.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer said that this work is providing an important understanding of a combustion mode that, if perfected, could yield an improvement in engine efficiency and emission aftertreatment simplification.

#### Reviewer 2:

The reviewer commented that the methodologies to introduce advanced combustion strategies certainly support the DOE objectives.

## Reviewer 3:

The reviewer remarked that this project certainly supports DOE's overall objectives. The reviewer stated that the project has shown significant technical progress and has provided a much better understanding of the boundary conditions of this type of combustion system. The reviewer indicated that the challenge is to translate this work into more practical application. The reviewer suggested that it would be helpful to work with an OEM or a different lab to assist with the practical application of the results of this work.

#### Reviewer 4:

The reviewer was unsure if the specific project objectives are very relevant in the current age of hybridization and rapidly improving SI engine combustion. However, the reviewer noted that the project fits pretty well under the current objectives.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer observed sufficient resources for the proposed work product.

#### Reviewer 2:

Resources appear sufficient to continue progress from this reviewer's perspective.

#### Reviewer 3:

The reviewer noted that the project team appears to have adequate resources to achieve the milestones.

#### Reviewer 4:

The reviewer stated the project team is making good progress and do not appear to be hindered by lack of resources.

Presentation Number: ace005 Presentation Title: Spray Combustion Cross-Cut Engine Research Principal Investigator: Lyle Pickett (Sandia National Laboratories)

Presenter Scott Skeen, Sandia National Laboratories

Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer said the work is a productive and collaborative effort with many collaborators. The reviewer noted that the project leverages multiple measurement systems and simulation approaches and addresses important fundamental questions associated with sprays, combustion, and emission-formation processes. The reviewer commented that the data bases being generated are used extensively by industry.

#### Reviewer 2:

The reviewer commented that the project team used the constant volume

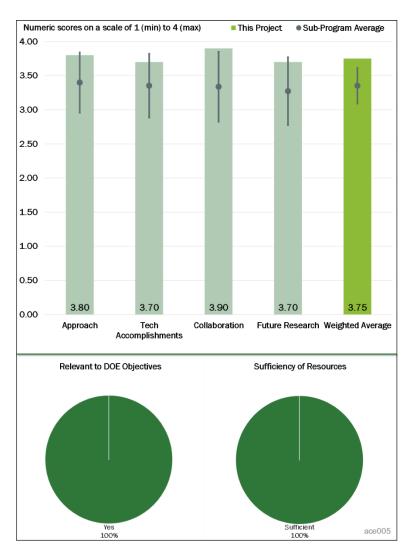


Figure 1-3 – Presentation Number: ace005 Presentation Title: Spray Combustion Cross-Cut Engine Research Principal Investigator: Lyle Pickett (Sandia National Laboratories)

combustion vessel to investigate spray injection and combustion under different conditions. The reviewer noted that advanced laser diagnostic methods have been applied to investigate the physical processes. The reviewer said, even more, a crowdsourcing platform was established through the Engine Combustion Network (ECN), which attracts resources worldwide to investigate the similar spray processes. The reviewer said simulations have been incorporated into the studies to help reveal some physical mechanisms.

## Reviewer 3:

This reviewer remarked that the project approach is generally the benchmark for collaboration, execution, and knowledge sharing through the ECN. The reviewer said that the combination of experiments and capabilities has offered unique information and knowledge generation. The reviewer commented that most of the milestones and deliverables seem to be completed or can be feasibly completed. The reviewer said it is excellent to see that more support for CFD is being used to help understand the experiments. The reviewer suggested that a place for approach improvement would be to strengthen the connection between the gained knowledge and understanding and its impact on the engine system efficiency trade-offs. The reviewer said this would enhance the effectiveness of the effort applied to the specific knowledge area.

## Reviewer 4:

The reviewer indicated that improving the shortcomings of CFD models by collaborations with the ECN is a great approach. The reviewer said multiple injections to limit liquid penetration is an important mechanism for gasoline direct injection (GDI) soot and the reviewer was glad to see it in this research. The reviewer commented that understanding sprays in vessels is an important first step but questioned how the flow field influences spray in an engine. The reviewer asked if the flow field makes the engine robust to variations in the spray.

## Reviewer 5:

The reviewer stated that the ongoing effort has been very valuable to the direct injection engine development community throughout the years. Much insight concerning cavitation, fuel temperature, and dynamic injection rate has been developed over that time. According to the reviewer, findings from this effort are important for fuel system suppliers and engine manufacturers in addressing future fuel consumption and emissions goals.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that the technical accomplishments are extensive. The reviewer said that new understandings have been developed for the following: impact of nozzle temperatures; elasticity and air ingestion into the sac on the initial rate of injection (ROI); and impacts of vanishing surface tension on liquid behavior for supercritical conditions, especially under conditions when chemical reactions are occurring. The reviewer remarked that working on understanding the effect of wall impingement on mixing enhancement promoting particulate oxidation is also a nice addition to the knowledge base. According to the reviewer, this is a very productive project.

## Reviewer 2:

The reviewer observed a lot of progress made in the past fiscal year (FY), and stated that the effects of needle and nozzle elasticity on sac volume and trapped gas have been investigated using finite element analysis (FEA) and X-ray, which help to explain the gas ingestion phenomena. The reviewer indicated that temperature-dependent injector deformation influences ROI at the startup, which is critical for spray development and ignition. The reviewer noted that the effects of injector temperature on early stage ROI and penetration were illustrated in shadowgraph imaging. The reviewer commented that the corresponding mechanism has been explained. The reviewer noted that preliminary results of supercritical spray were presented, showing potential capability for such extreme conditions. The reviewer also noted that sooting near the wall film has been quantitatively measured. The reviewer said the three-dimensional (3D) liquid volume fraction of GDI spray has been measured using tomographic reconstruction. The reviewer noted that simulations of impinging GDI spray have been conducted to evaluate the current models.

## Reviewer 3:

The reviewer stated that completed milestones for this project show good progress and expressed no concerns on the accomplishments or progress. Now that the high-flow vessel is running, the reviewer expected that the data throughput should increase further.

## Reviewer 4:

The reviewer said the tomography of fuel sprays should provide insights.

#### Reviewer 5:

The reviewer found that good progress was made during the last year and noted that the work on the impact of initial needle opening time period is very insightful along with the impact of nozzle temperature on the spray-formation process. The reviewer would have liked to see more focus on the impact of dwell on soot formation, given that the presented results were very limited and did not include the impact of load or overall injection duration on dwell and soot formation.

## Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer praised the ECN and said it is the most remarkable research collaboration group in the engine and combustion community. The reviewer said that there are many groups worldwide, many measurement techniques, and CFD codes with different models that have gotten involved. The reviewer noted that the ECN has generated outstanding outcomes in spray combustion. The reviewer commented that the monthly meeting has become the primary platform to show the latest achievements in spray combustion.

#### Reviewer 2:

This reviewer said this project approach is generally the benchmark for collaboration, execution, and knowledge sharing through the ECN. The reviewer urged continued leadership in this effort to bring value to the spray combustion community. The reviewer said that the project team's efforts are greatly appreciated.

## Reviewer 3:

The reviewer commented that the ECN continues to be a great example of collaboration.

#### Reviewer 4:

The reviewer remarked that the entire project is built around collaboration to leverage and take advantage of the wide range of capabilities, both experimental and computational, within the international technical community.

#### Reviewer 5:

According to the reviewer, there was excellent collaboration based on the vision Lyle and others had a decade ago. It is excellent work.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that the proposed research plan covers multiple critical problems in engine combustion, including quantitative soot measurement of combusting GDI spray, sooting from wall film, and flame-wall film interaction. The reviewer commented that improvements and developments of diagnostic methods such as soot imaging and near-wall spray imaging have been included. According to the reviewer, all the proposed topics are valuable and are worth being investigated.

#### Reviewer 2:

The reviewer noted a very well thought out research plan. The reviewer asked if it were possible to assess how the changing temperature and pressure environment in an engine cylinder might impact the relative magnitude, or prevalence of the spray and mixing phenomena, that have been identified in this work in constant volume and pressure vessels.

## Reviewer 3:

The reviewer remarked that the future proposed direction on spray-wall interactions, soot formation, and oxidation are probably the most relevant topics on which this project could focus. The reviewer noted that these two areas greatly affect engine combustion system design, development, limitations, efficiency, and heat transfer. The reviewer also commented that these two areas are also some of the most difficult to understand and model. The reviewer suggested that the project team prioritize these two areas if possible.

#### Reviewer 4:

The reviewer was glad to see multiple injections and liquid penetration for reduced wall impingement. The reviewer said that this is a key source of GDI soot during cold start. The reviewer remarked that methods to reduce impingement or enhance evaporation of impinged fuel is needed work.

#### Reviewer 5:

The reviewer thought the future work outlined was excellent and aggressive in nature but requested that the project team consider the load impact on multiple injections and the dwell impact on soot and projected indicated specific fuel consumption (ISFC).

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that this project is extremely relevant for achieving DOE's objectives. Most all high-efficiency IC engines utilize sprays for combustion and emissions control. The reviewer said fundamental spray combustion understanding and validation data are critical for industry to cost effectively advance product efficiency and performance. The reviewer remarked that the most effective way to improve powertrain efficiency is to enable core IC engine-efficiency improvements, even with hybrid powertrains.

## Reviewer 2:

The reviewer said that the problems addressed by this project including injector, spray, and resulting combustion/emission are the most critical problems for engine combustion. The reviewer remarked that the outcomes of this project provide high-fidelity data for validation of CFD models. The reviewer commented that the project reveals essential physical mechanisms of some phenomena, which offer guidance to mathematical model development.

#### Reviewer 3:

The reviewer responded affirmatively and stated that the project indirectly supports DOE goals by providing insight on the spray-formation process in direct-injection (DI) engines that is important toward developing dilute and more standard high-efficiency engines.

#### Reviewer 4:

The reviewer noted spray fundamentals that are very relevant to developing combustion systems.

#### Reviewer 5:

The reviewer referenced prior comments.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer said that the project team are making tremendous strides with the available resources. The reviewer did not get the impression that the project's progress was hindered by a lack of resources. The reviewer noted that no comments were made as to what would be done if more resources were available.

#### Reviewer 2:

The reviewer said the current facility is good for the project team to accomplish most of the tasks. The reviewer suggested that further improvements and developments of diagnostic methods may require additional resources.

## Reviewer 3:

The reviewer commented that the budgets look sufficient, given the addition for the soot efforts.

## Reviewer 4:

The reviewer said the resources were sufficient.

## Reviewer 5:

The reviewer noted that funding has been very strong over the years and appeared to still be sufficient.

Presentation Number: ace006
Presentation Title: Advanced Ignition for Gasoline Combustion
Principal Investigator: Isaac Ekoto (Sandia National Laboratories)

Presenter Isaac Ekoto, Sandia National Laboratories

Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer really appreciated the project team's responsiveness to reviewers and the effort to compare closely with conventional ignition systems. The reviewer said the link to modeling looks good too, although it is too early to fully evaluate the details of the model. The reviewer said that the results are showing some very interesting and promising improvements on combustion under challenging conditions, which is encouraging for the technology direction. The main thing the reviewer would like to see is more instrumentation and analysis to quantify the engine-level energy balance. The

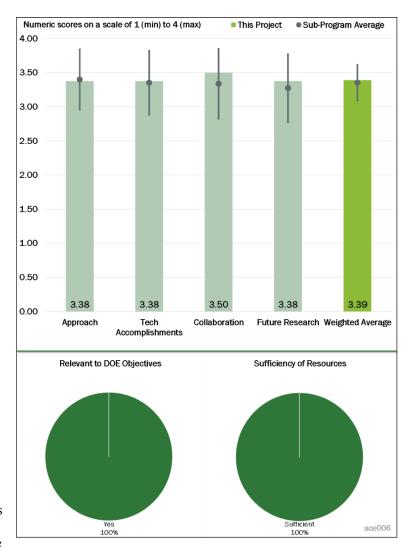


Figure 1-4 – Presentation Number: ace006 Presentation Title: Advanced Ignition for Gasoline Combustion Principal Investigator: Isaac Ekoto (Sandia National Laboratories)

reviewer noted that some way of estimating or measuring the primary energy requirement is key, and explained that this is because ultimately the engine has to generate that power to run the system and the benefits of the system to efficiency will have to show a net positive. The reviewer said that knowing where the technology stands with respect to that right now will be valuable for focusing the future research and development (R&D) efforts. The reviewer commented that from a combustion side, it would also be good to investigate the links between the faster reaction rates seen with the advanced ignition technologies and how that translates to brake-specific fuel consumption (BSFC) and brake thermal efficiency (BTE) for both conventional SI and spark-assisted compression ignition (SACI) combustion systems. The reviewer commented that the faster heat release rate should be good for improving the closed-cycle efficiency and for enabling higher dilution. The reviewer wanted to know how that impacts knock at higher loads and other real-world factors.

## Reviewer 2:

The reviewer noted that the project team is taking a systematic approach by categorizing milestones according to discharge, ignition, and engine combustion.

#### Reviewer 3:

The reviewer remarked that the technical barriers for the project have been well defined regarding fundamental understanding of low-temperature plasma (LTP) ignition and its application toward enabling multi-mode engines. The reviewer said that the project is relevant to the DOE current scope of interests. The reviewer commented that the project presents a unique experimental facility that is able to study the phenomena regarding LTP ignition, and that its feasibility and credence has been justifiably demonstrated in the current review meeting. The reviewer noted that experimental results demonstrate the advancement that LTP igniters can achieve to improve flame-kernel development toward leaner and more dilute conditions. The reviewer commented that experiments demonstrate good agreement with numerical initiative and collaborators at Argonne National Laboratory (ANL), which further demonstrates strength of the approach taken. The reviewer said that redesign of electrodes for optimization in actual engine applications demonstrated the completion of milestones on schedule to achieve the overall objective. The reviewer commented that the results presented were preliminary, but the technical approach seems to be working toward understanding and identifying optimal designs. The reviewer said that progress thus far demonstrates unique methods to minimize stream discharges. The reviewer commented that the project also looked at demonstrating the validity of LTP ignition in actual engines to bridge the gap between fundamentals and applications. The reviewer mentioned that this is a natural extension of the project and the approach is required.

#### Reviewer 4:

The reviewer asked if the project team could be more specific on benefits if improved ignition is attained. The reviewer recommended that the project team continue to focus on approaches with a strong pathway to commercialization, namely stoichiometric, highly dilute combustion.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer observed lots of promising results and referenced prior comments that apply here and provide opportunities for some additional technical accomplishments that would fill out the full story that the project is telling.

## Reviewer 2:

The reviewer noted good progress.

#### Reviewer 3:

The reviewer said that the project demonstrated advancements that can be made using an LTP-igniter system as compared to existing technologies in terms of extending dilution limits and establishing faster burn rates. The reviewer noted that engines studies demonstrated the kinetic enhancement that can facilitate ozone kinetics on the combustion. The reviewer indicated that results were also corroborated with numerical kinetic studies to instigate LTC chemistry. The reviewer commented that FY 2019 milestones that were set have been achieved, and the project looks like it is on track to completion for the remaining year. The reviewer said numerical collaboration for ozone kinetics has been deferred for FY 2020 but the reviewer was not able to discern the reason for this deferral.

## Reviewer 4:

The reviewer acknowledged that the project team responded to previous year reviewer comments and added more engine experiments and comparisons with conventional ignition systems. One concern the reviewer expressed is the durability of these ignition systems, as noted in the findings of project ACE121. The reviewer would like to know how ignitor durability affects the possible combustion models that can be explored and how that subsequently affects the project goals. The reviewer said, in addition, there was not much discussion on the pre-chamber work in this presentation even though it is listed on Slide 5.

## Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer noted good collaboration spanning National Laboratories, OEMs, universities, and suppliers.

#### Reviewer 2:

The reviewer said that efforts to collaborate with industry (e.g., small businesses, OEMS, and start-ups), academia, and other National Laboratories is evident. The reviewer indicated that all efforts are complementary to one another and further commented that this facilitates the collective efforts to advance LTP technologies for commercialization.

#### Reviewer 3:

The reviewer indicated that this topic is very challenging. The reviewer said the project team has sought feedback from many perspectives, as noted in Slide 16.

## Reviewer 4:

The reviewer said that this may be more an issue of communication of links in the short presentation time. The reviewer said that it is clear there is a good link between the ANL simulations and the SNL experiments. It was not clear to the reviewer how much coordination there is with some of the outside partners who are either supplying equipment or are on the commercial side of things. The reviewer observed a great list of collaborators, but was unclear how those collaborations are impacting progress of this specific project.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer remarked that the project team has proposed a natural extension to its current research scope and has established realistic milestones and schedules.

#### Reviewer 2:

The reviewer was glad to see catalyst heating modes included in future plans. The reviewer noted that any complete combustion system needs to support this mode.

## Reviewer 3:

The reviewer stated that the proposed future research work is relevant and extensive, but it was not explicitly clear from the material how the future work is prioritized. The reviewer would have liked to see more experimental efforts to answer the questions regarding energy consumption versus benefit of the groundless dielectric barrier discharge (GDBI) system and noted that this does not currently look like part of the planned work. Beyond that, it is critical to get a more detailed study of the ozone (O<sub>3</sub>) generation feasibility and performance of the GDBI system as well as the resulting combustion effects. The reviewer recommended both in terms of using the O<sub>3</sub> generation for autoignition tuning and dilution tolerance extension for conventional SI combustion. The reviewer said that in the short- to mid- term, this work is far more likely to see technology transfer potential if it can improve high EGR combustion that leverages conventional aftertreatment systems. For example, if the O<sub>3</sub> generation can extend the EGR tolerance of an engine, it could be a significant intermediate step toward kinetically controlled combustion systems. The reviewer noted these systems still have significant technology gaps for practical aftertreatment.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer said that project looks to meet DOE targets by improving ignition, which can enable a 25% increase in engine efficiency, lower pollutant emissions, and more reliable cold start.

## Reviewer 2:

The reviewer continued to see ignition as a critical barrier for any high-efficiency premixed combustion system. The reviewer remarked, that while Delphi has shown excellent results with a GCI system, the most feasible path to impacting the light duty market is to evolve the SI system toward higher efficiency combustion systems. The reviewer said that path is highly limited by ignition-system performance under high dilution. The reviewer commented that this project can uniquely, within the current VTO portfolio, provide solid scientific foundations for understanding how the advanced ignition systems available can provide a path toward higher engine efficiency.

#### Reviewer 3:

The reviewer commented on the important need for this type of work to enhance CFD models, as noted in the collaborative work with ANL.

#### Reviewer 4:

The reviewer said enhanced ignition is needed to support commercialization of highly dilute, stoichiometric combustion modes

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer stated that the budget looks quite good for the work path proposed and under execution.

#### Reviewer 2:

The reviewer remarked that the resources provided are sufficient to support the proposed future research.

#### Paviower 3

The reviewer indicated that all experimental equipment and personnel are at the disposal of the project team to carry out the tasks established.

#### Reviewer 4:

The reviewer observed sufficient resources.

Presentation Number: ace010
Presentation Title: Fuel Injection and
Spray Research Using X-Ray
Diagnostics
Principal Investigator: Christopher
Powell (Argonne National Laboratory)

#### Presenter

Christopher Powell, Argonne National Laboratory

# Reviewer Sample Size A total of five reviewers evaluated this

A total of five reviewers evaluated thi project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer described this laboratory's diagnostics facilities as virtually unique for studying behavior inside and outside injectors to observe phenomena such as flash-boiling, cavitation, and nozzle erosion. The reviewer stated that the project team has provided much useful information to both understand what is going on and provide support for CFD simulations, particularly high-fidelity analyses that are being used to develop better physical models for injector and engine design purposes. The reviewer commented that the project team involved has sought out and built

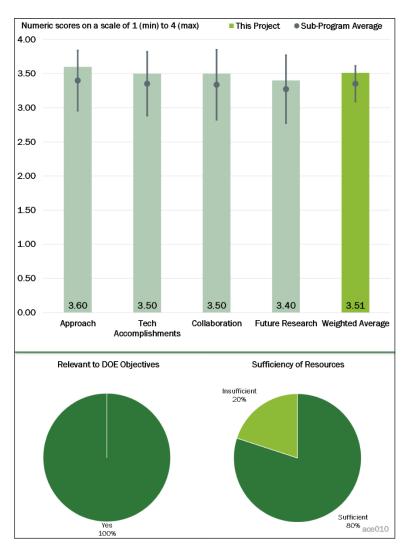


Figure 1-5 – Presentation Number: ace010 Presentation Title: Fuel Injection and Spray Research Using X-Ray Diagnostics
Principal Investigator: Christopher Powell (Argonne National Laboratory)

meaningful collaborations with other groups including other National Laboratories, universities, and industry.

#### Reviewer 2:

The reviewer stated that this project has had a history of excellent progress in uncovering fundamental physics of sprays. The summary shown this year of combining measurements of the internal geometry of an injector nozzle, the in-nozzle cavitation response to that geometry, and the resulting spray non-uniformity is an excellent example of this. Additionally, the work extending to GDI sprays is starting to uncover behavior specific to that combustion system. The reviewer pointed out that any scoring reduction here is a result of the next steps being less clear. Although some interesting tasks are proposed for the upcoming year to move to realistic hardware, a re-evaluation of the technical barriers may be necessary so that the project can be properly focused in coming years.

#### Reviewer 3:

The reviewer remarked that the project team used a unique diagnostics method to investigate the physical process inside the nozzle and near-nozzle spray, which offers rich information about the injector and the resulting spray. The reviewer commented that the methodology is getting mature and is being applied to more

complex phenomena such as flash boiling and cavitation. The reviewer said semi-3D results of X-ray tomography are perfect for CFD model validation and development. The reviewer indicated that measured surface area of the flashing spray is a perfect, quantitative dataset for validation of flash boiling.

#### Reviewer 4:

The reviewer said that the approach of this project is clear and seems to be in very good shape. The reviewer commented that breaking tasks into light-duty (LD) and HD areas seems pertinent and helps to orient and align collaborators and output. The reviewer noted that the technical barriers to multi-hole nozzle internal-flow visualization and cavitation erosion seem substantial. The reviewer would like the project team to clearly lay out what is needed to overcome these barriers, so an accurate assessment of project budget and resources can be made.

#### Reviewer 5:

The reviewer remarked that the approach of working with measurement of qualitative cavitation inside the nozzle, quantitative fuel density near the nozzle exit, and plume-to-plume interaction by flash boiling is good for computational validation.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer remarked that significant and important progress has been made under this project to increase knowledge of injector internal and near-nozzle external behavior in conditions such as cavitation, nozzle erosion, and particularly flash boiling. This knowledge has driven and is driving the development of better simulation capabilities. This reviewer is aware of engine development programs that have already been positively impacted by the flash-boiling models developed, in part, based on this project's experimental results.

## Reviewer 2:

The reviewer said that this year's accomplishments of Spray G under flash-boiling conditions and HD geometry effects on cavitation, fuel distributions, and breakup are very good and look complete. This fuel injection and spray knowledge and validation data are extremely valuable and allow progress in critical areas. The reviewer indicated that industry sees the value and greatly utilizes these unique data and stated that the project team knows a great deal about one or a couple of unique geometries. This is great for validation data of real devices. Likely, there is a real variation in devices to which good simulation models should be correctly predictive and sensitive. Subsequently, this reviewer asked whether there is an aspect of this project to build a more a statistically confident validation and knowledge database, and whether this is even needed. The reviewer asked how this relates to single- versus multi-hole nozzle thinking and what the technical barriers may be.

## Reviewer 3:

Although this reviewer would love to see even more results year over year because of impatience, the findings both for the HD and LD sprays are really interesting and should provide enough data to keep the model developers busy for a long time. The reviewer said there may be a point here where the technical accomplishments may need to start vectoring back toward tying the fundamental spray physics under examination to typical production issues with sprays—deposits, erosion, part variability, etc.—so that the results can be correlated to what industry is facing and to guide future tasks to address outstanding questions.

#### Reviewer 4:

The reviewer commented that the technical progress and accomplishments on this project are good. The reviewer said, however, it appears that CFD work does not suggest any specific sub-models to support the phenomenon occurring in the vicinity of nozzle exit other than validation specification. The reviewer did not see any feedback information from the CFD results to the experiment except varying the parameters. It was

also unclear that the uncertainty of measurements near the nozzle will influence how the downstream spray changes. The reviewer asserted that the uncertainty of experiments should be provided, and the effect should be compared with a sensitivity analysis of CFD.

#### Reviewer 5:

The reviewer commented that the near-nozzle behaviors of ECN Spray G under flash-boiling conditions have been visualized and compared with the ones under non-flash-boiling conditions. The reviewer said the X-ray tomography has been applied to visualize the cavitation phenomena of the internal nozzle flow of ECN Spray C. The reviewer commented that 3D CFD simulations have been conducted on the same spray and compared to X-ray measurements.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer said that collaboration on this project can be represented as excellent by the active involvement with ECN, industry, and computational researchers. The reviewer remarked that everyone wants Advanced Photon Source (APS) spray and injector experimental data for relevant spray, cavitation, and combustion work. The reviewer praised the project as one of the top DOE funded combustion-spray projects that has direct and long-lasting impact for engine and fuel system OEMs. The reviewer requested continued, strong support and resource commitment to this work.

#### Reviewer 2:

The reviewer observed great links to the ECN and requested to see more comparisons with other diagnostics. The CFD and X-ray comparisons are great, but the different diagnostics show different aspects of the spray; so, there may be some interesting knowledge to be found there. The reviewer noted that the project has a great link to the modeling community and that it also looks like the project has solid links to industry for technology transfer.

#### Reviewer 3:

The reviewer remarked that collaboration and coordination are quite evident, not just in the provided project documentation but by the reviewer's personal observation of the team in action at other meetings. The reviewer said, however, it would be interesting to see more collaboration between this research team and the neutron imaging team at Oak Ridge National Laboratory (ORNL), since the two facilities appear to have many complementary capabilities that might be leveraged to further increase the value of each. The reviewer commented that other researchers that collaborate with this team have started to examine combustion as an extension of the spray and internal injector diagnostics being done here, and that this will also be exciting work that promises to further multiply the importance of the research being done here.

## Reviewer 4:

The reviewer said that the project team is deeply involved in ECN activities. The reviewer commented that the unique X-ray measurements introduced valuable and insightful results into the ECN dataset. The reviewer said it is evident that the project team has collaborations with SNL, universities, and other teams in ANL that lead to higher productivities of this project. The reviewer recommended that more collaborations with industry will further enhance the productivity.

#### Reviewer 5:

The reviewer said the collaboration level seems to be okay.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that cavitation erosion physics understanding and validation data under HD engine and injector relevant conditions are a great direction. The reviewer commented that multi-hole HD injector measurements are also a clear need and a clear step toward real injectors. The reviewer referenced prior comments on the need for increased geometry variation and sensitivity understanding, as these areas may be extremely useful for model physics development. The reviewer said that the focus of LD spray-wall interactions also seems like a very relevant direction and recommended that the project team continue these directions.

## Reviewer 2:

The reviewer said that looking into the details about the nozzle erosion using X-ray is great. The reviewer noted that parametric study of flash boiling is also very good topic. The reviewer said that the project team may want to use the X-ray to reveal more details about the early stage of flash-boiling processes, and more results of flash boiling that are good for comparison with simulations are expected from this project.

#### Reviewer 3:

The reviewer liked the proposed tasks for FY 2020, but observed signs that the project needs to go back, evaluate fundamental barriers for improved engine efficiency and reduced emissions, and then determine how the project tasks need to evolve to address barriers that the field currently faces. The reviewer said that there is some value in the project also just generating data for the community – it is not the same kind of R&D, but given the unique capability of the diagnostics, there could be tremendous value in building a library of nozzle geometries that represent different aging factors, different manufacturing factors, and so on. The reviewer commented that the community does not understand any of those things at the level needed for the brave new world of modeling the community is entering, and that this project may be the only current means of providing the required measurements.

#### Reviewer 4:

The reviewer said that the planned research appears sound and follows in a logical manner from previous work and the needs of the engine community. As referenced in a previous response, the reviewer noted that building some collaboration with the emerging neutron diagnostics capability at ORNL and better folding in the diagnostics being done here with engine combustion studies would be also desirable. The reviewer stated that further examination of multi-hole injectors, which is in the plan, will be very important to injector and engine makers.

#### Reviewer 5:

The reviewer remarked that the future plan seems to be the extension of the current work with the production of a large amount of data and the project team's comparison with CFD model. The reviewer noted that no specific sub-models are used to bridge the gap between experiment and CFD performances, which the reviewer suggested. The reviewer would have liked to see how the project team handles the large amount of experimental data together with simulation data and the method to reduce the computational time.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer commented that better understanding of the injection process has a direct impact on better understanding engine combustion and emissions. The reviewer said that the understanding this project provides has direct impacts in the drive toward higher efficiencies and lower emissions, which are both key DOE objectives.

## Reviewer 2:

This reviewer indicated that project research focuses on fuel injectors, which are essential for engine combustion. Tiny details inside the injector will result in big different in spray dynamics, mixing, ignition, combustion, and emissions.

#### Reviewer 3:

The reviewer remarked that this project clearly supports the DOE objectives, because it enables science-based understanding of injection systems and sprays that are fundamental to engine efficiency and emissions reduction.

## Reviewer 4:

The reviewer noted that the project is relevant to DOE goals and that X-ray measurement seems to be the mature technique for the spray measurement. The reviewer believed development of the X-ray technique is needed to measure transient spray and cavitation.

## Reviewer 5:

The reviewer stated that the community has come a long way in terms of understanding spray physics over the past decade or two, but that there are still lots of things that are not understood, especially when looking at smaller time and spatial scales. The reviewer said that this project provides valuable measurements for continuing to develop the physics and engineering of these spray systems.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer commented that this project could achieve even more with an expanded budget. The reviewer explained that that would, to some extent, depend on beamline-access time but that additional funding could enable building a library of different nozzles and that could really benefit the community in terms of understanding real injector variability.

#### Reviewer 2:

The reviewer commented that the project likely has sufficient resources to complete the proposed future research, but said that it is not clear how much effort the difficult aspects, like cavitation erosion, will really need. Additionally, the resource limitation may not be something that can be easily increased (i.e., funding can be increased, but beam time may not be able to). The reviewer recommended that DOE consider evaluating and increasing resources as needed for this valuable project.

#### Reviewer 3:

The reviewer said that resources appear adequate for the presented plan.

## Reviewer 4:

The reviewer remarked that the project team has the access to the APS that provides light source for X-ray study. The reviewer said the current resource should be sufficient for the project team to accomplish the project.

## Reviewer 5:

The reviewer said that the project team has sufficient resources.

Presentation Number: ace012
Presentation Title: Model
Development and Analysis of Clean
and Efficient Engine Combustion
Principal Investigator: Russell
Whitesides (Lawrence Livermore
National Laboratory)

#### Presenter

Russell Whitesides, Lawrence Livermore National Laboratory

## Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer commented that this project is very important in that it is trying to solve computation time issues with chemistry solvers. The reviewer said that having the computation time as a linear function of the number of species is a very attractive solution especially for engine CFD simulations.

## Reviewer 2:

The reviewer said that the approach of a hybrid mechanism without compromising accuracy with reduced turnaround time is promising and it will have a big impact on industry adapting simulations for engine development.

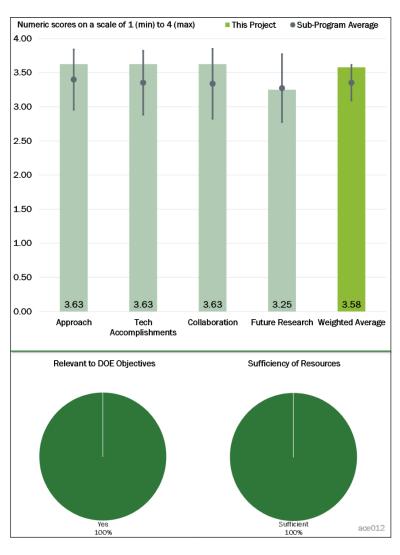


Figure 1-6 – Presentation Number: ace012 Presentation Title: Model Development and Analysis of Clean and Efficient Engine Combustion Principal Investigator: Russell Whitesides (Lawrence Livermore National Laboratory)

## Reviewer 3:

The reviewer remarked that the project had a nice approach to reduce simulation time, but that some more context and examples would be helpful.

#### Reviewer 4:

The reviewer said that the project is well focused on the barriers. The reviewer noted that the main project focus is on improving computational models and accelerating calculation speed. The reviewer indicated that turbulence-kinetics interaction is supposed to be the key understanding for engine combustion, while this project addresses only the kinetics side.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer said that the demonstration of Zero-Order Reaction Kinetics (Zero-RK) graphics processing unit (GPU) capability developed through this project for an actual engine project collaboration with GM and ORNL is significant.

#### Reviewer 2:

The reviewer pointed out the tremendous improvement in computation time for solving chemistry that has been achieved since the last AMR. The reviewer said that is project is on target and is performing very well.

#### Reviewer 3:

The reviewer commented on very nice progress and said that there is nothing to criticize.

#### Reviewer 4:

The reviewer observed nice work on sooting gasoline flames; more is needed.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer found excellent collaboration between various team members. The reviewer noted that GM collaboration is also a plus. The reviewer recommended that the project team collaborate with other OEMs as well, as the Zero-RK is a very powerful tool for CFD simulations and can be applied extensively in industry for analysis-led design exercise for engines.

#### Reviewer 2:

The reviewer commented that industry, academia and National Laboratories are well represented in this project for accomplishing the technical goals.

## Reviewer 3:

The reviewer commented on the good organization of collaboration.

#### Reviewer 4:

The reviewer said it is especially useful to collaborate across Co-Optima projects.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer indicated that the use of machine learning and data science and making Zero-RK platform flexibility are good topics for future research. The reviewer noted that coupling of Zero-RK to exa-scale ready CFD codes and adaptation of large eddy simulation (LES) for turbulence will hopefully provide more insight without adding too much computational burden.

## Reviewer 2:

The reviewer remarked on the good proposal, but said it needs more elaboration on the necessity of the exascale computing. The reviewer wanted information from the project team on what more improvement is expected with it and what is missing with the current approach. The reviewer said that the presented material shows nice agreement with the measurement. The reviewer noted that the backup slide shows the performance scaling saturates quickly with mechanism reduction already.

#### Reviewer 3:

The reviewer said an outline of the approach to incorporate machine learning would be useful.

#### Reviewer 4:

The reviewer recommended that the project team validate the reduced chemistry mechanisms for high-pressure laminar flames (greater than 20 bar). The reviewer suggested that some of the data, although not the yield sooting index (YSI), are available in the literature and that this will make more sense for comparing engine-like conditions. The reviewer said that the project team should also evaluate multi-component surrogates, such as primary reference fuel (PRF), toluene reference fuel (TRF), and others for simulating gasoline and diesel combustion not only from an ignition delay standpoint but also sooting tendency.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer remarked that this is exactly the kind of work DOE must be supporting. The reviewer stated that this will not be pursued by private investments or OEMs. The reviewer commented that this work is excellent from that standpoint. The reviewer said that speed-up in mechanism reduction is a great tool for industry to use for realistic CFD engine simulations.

## Reviewer 2:

The reviewer said that this project is very relevant to DOE objectives, which are to advance the state-of-the art in combustion simulation and impact industry-relevant problems. The reviewer noted that working to have high-fidelity models tangible to industry and academic users will definitely help further understand high-efficiency clean combustion (HECC).

#### Reviewer 3:

The reviewer remarked that this project addresses the most important question regarding reducing computation time for chemical kinetics without compromising the accuracy.

#### Reviewer 4:

The reviewer commented that simulation speed is a top priority.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer suggested that more computational resources may be needed from DOE to run various training machine learning algorithms.

#### Reviewer 2

The reviewer stated that resources are just sufficient.

#### Reviewer 3:

The reviewer commented that the resources seem to be sufficient and in the right proportion for executing this work.

## Reviewer 4:

The reviewer reported a substantial budget increase across the past three years.

Presentation Number: ace013
Presentation Title: Chemical Kinetic
Models for Advanced Engine
Combustion
Principal Investigator: Bill Pitz
(Lawrence Livermore National
Laboratory)

#### Presenter

Bill Pitz, Lawrence Livermore National Laboratory

# Reviewer Sample Size

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

This reviewer observed that the project team is taking an approach founded on fundamentals, which includes validation with ignition delay measurements.

## Reviewer 2:

The reviewer said that the approach is sound but recommended that the project team highlight how the next-generation fuels are being dealt with. The reviewer requested clarification of whether "advanced compression ignition" on Slide 5 includes GCI.

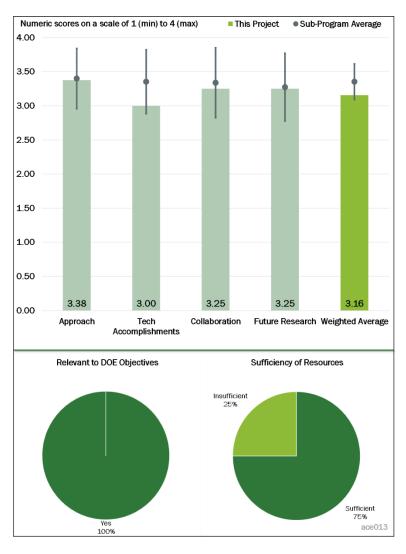


Figure 1-7 – Presentation Number: ace013 Presentation Title: Chemical Kinetic Models for Advanced Engine Combustion Principal Investigator: Bill Pitz (Lawrence Livermore National Laboratory)

#### Reviewer 3:

The reviewer remarked that the overall approach seems solid. The reviewer said that further understanding of the specific technical barriers of fuel-surrogate development would be a useful addition. It was unclear why specific hydrocarbon components were selected to be part of the surrogates, including those of specific focus for the activity in the previous year. The reviewer stated it would be useful to understand the key reasoning behind the components selected.

#### Reviewer 4:

The reviewer commented that the work is well worth doing; however, insufficient resources are being committed in view of the scale (compounds and conditions) and competitive efforts (fuel testing) needed to have a direct impact.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that progress shown on enhancing mechanisms is evidenced by citations in recent publications. It was very encouraging that this work was used to assist SNL engine experiments. The reviewer said it was mentioned during the AMR, however, that SNL has made some improvements to the mechanism used in Dec's HCCI engine. The reviewer would like to know if feedback from SNL has been incorporated into the final published mechanism.

#### Reviewer 2:

The reviewer observed good progress made this year, focusing on several different kinetic models relevant to gasoline and diesel fuels. Given the focus on improved kinetic models, however, it is not fully clear what the scale of improvement to the models is over the prior forms. The reviewer suggested it would be helpful to understand how a model's ability to represent kinetics has changed from previous iterations.

#### Reviewer 3:

The reviewer stated that the technical accomplishments and progress toward the overall project seem okay. Referencing Slide 6, it was hard for this reviewer to judge progress made against performance indicators. The reviewer thought the performance indicators should be clearly stated and where the project is relative to them. The reviewer comments about Slide 4 noted that cyclohexane was delayed until Quarter 4 (Q4), which seems to indicate the project is behind schedule even though the issue appears to be minor. The reviewer recommended that the project team state the beginning and end of FY 2019 with actual dates because there is a wide variety of FY definitions.

#### Reviewer 4:

The reviewer remarked that progress is as expected in the short term.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer observed solid collaboration in all areas. Of note is collaboration with Argonne National Laboratory for rapid compression machine (RCM) experiments, the Advanced Engine Combustion Working Group, SNL (John Dec and Magnus Sjöberg) on SACI engines, Jim Syzbist at ORNL, and Sibendu Som at ANL on CFD simulations. The reviewer asserted that all key players are there.

## Reviewer 2:

The reviewer indicated that the project team demonstrates strong collaborations with universities and National Laboratories on model development in addition to in-house LLNL work to develop advanced solvers. The reviewer said that the work is extensively cited in the literature and referenced by commercial CFD codes.

#### Reviewer 3:

The reviewer said there was good collaborations across the project team, utilizing experimental data for a variety of sources to help validate the models. The reviewer would have liked to see more detailed examples of other groups utilizing the models developed within this program.

## Reviewer 4:

The reviewer thought that DOE engineering groups are not collaborating enough with basic science groups within DOE. The reviewer said, for example, this expertise can be easily found in ANL.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that a focus on understanding how kinetic models perform in combustion environments with EGR is good step forward since most future engine platforms, both gasoline and diesel, are expected to utilize EGR in some capacity. The reviewer commented that understanding model performance under these conditions is therefore very relevant, as is understanding why certain model changes are made to yield improved behavior under these conditions. The reviewer encouraged the project team to look at behavior of kinetic models in relation to variability across experimental data. According to the reviewer, models may improve, but are still validated and compared against experiments, and at some point, refinement to the chemical mechanisms may move beyond the experimental data used to validate. The reviewer asserted that understanding this point would be useful.

#### Reviewer 2:

The reviewer remarked that improvement of the kinetic mechanisms with varying levels of EGR is important for advanced combustion work. The reviewer said that, additionally, kinetic models and flame-speed table studies relevant to cold start and engine knock conditions should be considered. The reviewer pointed out that the project team did not mention work to support the advanced low temperature, plasma, and pre-chamber ignition work being done at ANL and SNL. The reviewer questioned if the chemistry for these applications was already comprehended by the current work.

#### Reviewer 3:

The reviewer described future work on Slide 18 as good and expressed interest in knowing whether hydrogen (H<sub>2</sub>) could be included in EGR for engines running rich or a dedicated EGR case. Additionally, it would be good for the project team to state if future work includes kinetic models for renewable fuels.

#### Reviewer 4:

The reviewer stated that more emphasis is needed on complex fuel mixtures, which means that more chemical compounds need to be covered individually and fundamentally. The reviewer indicated that random models are a waste of effort. For example, surrogate mixtures need to be properly defined for a particular engine platform and there needs to be proper correlation between the chemical kinetics for each individual component before these definitions are established. The reviewer noted that the reaction pathways will define global properties such as ignition delays, soot formation, knock properties, etc. The reviewer asked to what extent all this information is transferable to a variety of engine platforms.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

Although very clear that this work is relevant to DOE objectives of having good kinetic models, it was not quite clear to this reviewer how next generation fuels are being addressed.

## Reviewer 2:

The reviewer commented that this work is absolutely relevant to DOE objectives. There is increasing program focus on modeling and simulation, and kinetic mechanisms underpin all of the combustion simulations. Therefore, the reviewer asserted that improvements here are crucial to the success of numerous other projects.

#### Reviewer 3:

The reviewer remarked that fundamental understanding of combustion phenomena must certainly be a key DOE objective.

## Reviewer 4:

The reviewer commented on the important need for this type of modeling activity to guide engineering level CFD codes.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer observed sufficient resources provided to support the proposed future research.

#### Reviewer 2:

The reviewer said that unless the engineering groups reach out to basic science groups, the real impact on combustion efficiency will not be seen in a timely fashion and make a sensible contribution to national problems.

#### Reviewer 3:

The reviewer had the impression that resources are okay, but indicated that it is hard to judge without a project plan with clear a beginning and end as well as progress achieved so far.

#### Reviewer 4:

Increased funds for this project were made available in FY 2019, but it was not clear to the reviewer how this increased the project team's ability to complete efforts. Additionally, if project output is limited by the availability of data from collaborative partners to support component model development, then it does not seem like additional funds would aid this effort.

Presentation Number: ace015
Presentation Title: Stretch Efficiency
for Combustion Engines: Exploiting
New High-Dilution Combustion
Regimes
Principal Investigator: James Szybist
(Oak Ridge National Laboratory)

#### Presenter

James Szybist, Oak Ridge National Laboratory

## Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

Overall, the reviewer commented that the approach should help answer some fundamental steady-state questions concerning the possible use of reforming to generate combustion-affecting species that enable very dilute combustion in spark ignition (SI) engines. One suggestion from the reviewer was to consider at some point in the future a possible real-world air system for cylinder two through four, including a possible different compression ratio in cylinder one.

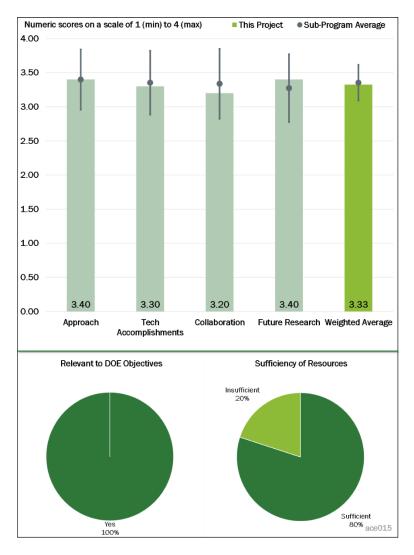


Figure 1-8 – Presentation Number: ace015 Presentation Title: Stretch Efficiency for Combustion Engines: Exploiting New High-Dilution Combustion Regimes Principal Investigator: James Szybist (Oak Ridge National Laboratory)

#### Reviewer 2:

The reviewer appreciated the focus on experimental results at this stage of the project.

## Reviewer 3:

The reviewer noted that methods to increase stoichiometric combustion will have strongest path to commercialization.

#### Reviewer 4:

The reviewer noted that the project follows a solid approach, with good analyses being performed along each step of the process and that the combination of engine experiments and exhaust flow reactor studies is crucial for understanding and improving this type of engine concept. The reviewer stated that using stoichiometric conditions makes it more readily applicable for light-duty automotive applications, and commented that it was good to see that exhaust temperatures were being monitored with an eye toward maintaining three-way catalyst viability. The reviewer noted that the modeled 40% turbocharger efficiency is reasonable for a single point, but may not be achievable across a wider range of conditions. The reviewer remarked that it would be useful to

have information on how turbocharger performance impacts operation and efficiency across a wider range of operating conditions.

#### Reviewer 5:

The reviewer observed that the use of a load-balanced cylinder is good from a practical perspective, but asked if an enriched cylinder would instead provide better results. The reviewer expressed concerns about fuel oil dilution and possible complicating factors due to fuel injection within the cylinder itself.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer stated that the project is addressing key barriers to commercialization including expanded load range and appreciated the deep understanding and explanation of efficiency gains and losses.

#### Reviewer 2:

The reviewer noted that one to two efficiency points over the entire operating range, while maintaining stoichiometric operation, is an encouraging conclusion for translation of these benefits.

#### Reviewer 3:

The reviewer asked if indicated mean effective pressure (IMEP) balancing between cylinders is a calibration or control barrier.

## Reviewer 4:

According to the reviewer, much understanding of this engine concept was been generated during the last two years though there still remain a number of questions to address, as pointed out by the PI during their presentation. One of them is long-term sulfur impact on the catalyst(s) arrangement of cylinder one.

## Reviewer 5:

Good progress was achieved with results coming from primarily catalyst experiments, according to the reviewer, though there were some engine results produced as well. The reviewer was disappointed to see the only milestone for the program occurred in Quarter 4 (Q4), which hampers the reviewer's ability to understand and judge progress.

**Ouestion 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

At some point in time, the reviewer said that it would be helpful for this project to see more industry interaction and collaboration. There did not appear to the reviewer to be a strong element of industry interest based on the presentation and possibly this is not the case.

#### Reviewer 2:

The reviewer said that the project collaboration was good.

#### Reviewer 3:

The reviewer noted that the project moves forward based on the close collaboration of Umicore, Precision Combustion, University of Michigan, and Oak Ridge National Laboratory (ORNL).

## Reviewer 4:

The reviewer commented that additional catalyst formulations and approaches may be key and that this area needs to be accelerated.

## Reviewer 5:

Though there was an expansive group of collaborations across industry, academia, and National Laboratories, the number of the collaborations are described merely as "discussions," according to the reviewer.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

Higher engine compression ratio, sulfur deactivation studies, and efficiency-increase limitations of molar-expansion ratio effects are appropriate future goals, according to the reviewer.

#### Reviewer 2:

The reviewer expressed interest in future molar-expansion work efforts as well as various catalyst formulation results.

#### Reviewer 3:

The proposed future research is very good though the reviewer suggested performing a real-world air system assessment of cylinders two through four. Also, the reviewer suggested exploring and considering the possibility of modifying the experimental setup for transient work if at all possible.

#### Reviewer 4:

The reviewer reported that the project has a solid approach moving forward. Future work focuses on directly addressing several remaining technical barriers. The reviewer would have liked to see a wider sweep of engine operating conditions to understand better the performance opportunities of the concept.

## Reviewer 5:

The reviewer observed that investigating the knock mitigation benefits addresses another key barrier of higher efficiency. The reviewer asked if the principal investigator (PI) has considered the cold start and catalystheating implications of the set-up and if there are benefits or additional barriers.

Question 5: Relevance—Does this project support the overall DOE objectives?

## Reviewer 1:

The reviewer said that the project addressed dilute combustion.

#### Reviewer 2:

Increasing efficiency by multiple points is certainly in line with U.S. Department of Energy (DOE) goals, the reviewer noted.

## Reviewer 3:

The reviewer remarked that the program focuses on a concept to improve engine efficiency and also addresses key areas of the U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability (U.S. DRIVE) Roadmap for dilute combustion, thus supporting overall DOE objectives for reduced fuel consumption.

#### Reviewer 4:

According to the reviewer, considering the modest \$300,000 budget—by comparison with other DOE- funded research—this project addressed relevant barriers to higher efficiency.

## Reviewer 5:

The reviewer indicated that this research project is another approach at enabling dilute high-efficiency gasoline engine technology toward meeting U.S. Department of Energy (DOE) efficiency goals. It does support DOE goals. One concern the reviewer had is projected transient capability of this concept though maybe this item will be addressed at some point in the future.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer thought that \$300,000 for a potentially very important path for stoichiometric dilute combustion is too low.

## Reviewer 2:

The reviewer indicated that the PI did not present any comments indicating a shortage of funding though the funding level for this project was noticeably lower than other projects on day one of the internal combustion (C) engine review.

## Reviewer 3:

According to the reviewer, the team has all the necessary resources to conduct the proposed research—engine, catalysts, custom manifolding, etc.

#### Reviewer 4:

The funding level seemed appropriate to this reviewer.

Presentation Number: ace017
Presentation Title: Accelerating
Predictive Simulation of Internal
Combustion Engines (ICEs) with HighPerformance Computing (HPC)
Principal Investigator: K. Dean
Edwards (Oak Ridge National
Laboratory)

## Presenter

K. Dean Edwards, Oak Ridge National Laboratory

## Reviewer Sample Size

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

## Reviewer 1:

The reviewer stated that the project helps to address technical barriers for developing more fuel efficient and cleaner engines. The real value of this project in the reviewer's opinion was providing a computational test bed for software development and its applications.

## Reviewer 2:

The reviewer found the approach of working with collaborators to be okay through high performance computing (HPC) capabilities at National Laboratories. Because the

computational fluid dynamics (CFD) platform is limited to the commercial code, the reviewer suggested that it would be good to have an open-platform CFD.

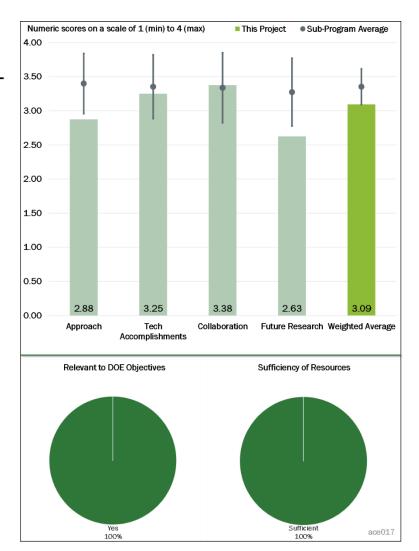


Figure 1-9 – Presentation Number: ace017 Presentation Title: Accelerating Predictive Simulation of Internal Combustion Engines (ICEs) with High-Performance Computing (HPC) Principal Investigator: K. Dean Edwards (Oak Ridge National Laboratory)

#### Reviewer 3:

The rationale behind running detailed conjugate heat transfer (CHT) simulations for accurate emissions predictions was not very clear to the reviewer but this work has established that the emissions results are relatively insensitive to heat-transfer simulations.

#### Reviewer 4:

The Approach presented was valuable for making simulations more relevant to the engine development and providing insight, according to the reviewer. However, the CHT approach presented did not address the boundary-condition specification on the piston (oil side, rings, and skirt) and its influence on the heat transfer. The reviewer was not sure whether the engine had an oil squirter on the back side of the piston but oil flow and its impact on the heat transfer is important. The reviewer also noted that original equipment manufacturers

(OEMs) are evaluating thermal barrier coatings for reducing the heat transfer and that accurate CHT methodology is very valuable for the industry for optimization of composition of the coatings.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that the milestones have been accomplished as per the schedule.

#### Reviewer 2:

The reviewer observed excellent progress with all the relevant accomplishments. A concern is that this may lead to advertising a commercial software, which is something about which to be careful.

## Reviewer 3:

The reviewer noted that the large eddy simulation (LES) mesh resolution and number of cycles are limited due to the allocation of HPC time, but was not really sure whether those results added value to the overall project. Published work in the literature suggests at least 50 cycles for LES simulations to predict cycle-to-cycle variability.

#### Reviewer 4:

The reviewer said that the technical progress and accomplishment on this project were okay; however, it appeared that the CFD work results showed significant difference compared with the measurement, particularly for the carbon monoxide (CO) and particulate matter (PM) prediction. The CHT model for thermal boundary conditions did not properly predict and this reviewer did not see the future plan to mitigate this challenge. Additionally, the reviewer would have liked to see progress on accuracy and speed because those were part of the project objectives.

**Ouestion 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

The reviewer commented that it was an ideal set-up for model validation and development as there seems to be no problem in collaboration within the arrangement.

## Reviewer 2:

The reviewer observed that there was really good collaboration among team members with a good mix of industry, National Laboratory, and CFD provider collaboration.

## Reviewer 3:

The collaboration level seemed to be adequate, according to the reviewer.

#### Reviewer 4:

The reviewer suggested that collaboration with more commercial OEMs, such Cummins and Caterpillar, would also be beneficial for the overall diesel engine development.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

For validation of CHT results, the reviewer recommended comparing fast thermocouple temperature data from experiments with simulation data. The reviewer suggested that possible coordination with Musculus etc. at Sandia National Laboratories' study on heat transfer would be beneficial for fundamental understanding of the heat transfer and provide insight due to boundary-layer compressing etc.

#### Reviewer 2:

To the reviewer, the future plan did not seem to be concrete in a way that the performance is relying on the CONVERGE platform too much. The reviewer noted that one of the future plans may generate a tremendous amount of data, but there is no method to handle the data with faster throughput and computation time speed-up. The reviewer believed that future success depends on the collaboration with experimental efforts for a new calibration method as well as the work to create a minimum tuning parameter model with fast turnaround of computation time.

## Reviewer 3:

The reviewer found the future work plan to be a little weak as it seemed that all the planned work was missing some novelty. The reviewer asked if there is any plan to further improve the software or correlation method. This, again, has a chance to end up just trying combinations of existing methodologies in commercial software on the Summit cluster.

#### Reviewer 4:

Future research plans were a bit unclear to the reviewer, who stated that it has been established through this work that the emissions predictions cannot be improved using detailed CHT models. The reviewer noted that there needs to be better validation of the CHT results to ensure accuracy before writing them off completely. The reviewer asked about experimental measurements of piston temperature and heat flux under motoring and firing conditions and using them for the simulations. The reviewer wanted to know whether doing this in a single-cylinder engine would help simplify the problem. This reviewer also inquired whether the CO discrepancy is attributed to crevice CO and whether the temperatures near the crevices are predicted correctly. Some validation with CO measurements (e.g., those collected at Sandia National Laboratories) may allude to some clues.

Question 5: Relevance—Does this project support the overall DOE objectives?

## Reviewer 1:

The reviewer remarked that the project supported the overall DOE objectives by using HPC resources for development of efficient engines to improve fuel economy and reduce emissions.

## Reviewer 2:

This project was relevant to DOE objectives in terms of providing a platform for accelerated model development and correlation with experiments, noted the reviewer. This will help further develop better engine combustion concepts and designs.

## Reviewer 3:

The reviewer commented that accurate model development for engine simulations should be indeed a DOE effort because it will not likely be funded by OEMs and others.

#### Reviewer 4:

The project is relevant to DOE's goal, noted the reviewer. In order to improve their model, it needs experimental data, especially the temperature profile on the piston surface for the CHT model.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer commented that project resources appear to be adequate.

#### Reviewer 2:

The funding seems to be enough to keep the current level of work, according to the reviewer.

## Reviewer 3:

The reviewer deemed the resources to be sufficient for the work proposed.

## Reviewer 4:

According to the reviewer, CHT simulations with detailed chemistry are very expensive. Simulations done with LES are very limited done to date due to lack of central processing unit (CPU) resources. The reviewer suggested that allocation of more computational resources (HPC allocation) for this project will be beneficial to make progress and have more impact.

Presentation Number: ace022
Presentation Title: Joint Development and Coordination of Emissions
Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination)
Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

Presenter
Josh Pihl, Oak Ridge National
Laboratory

Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer has monitored Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) since its inception around 2001 and was impressed. What was meant to be mainly emission-control modeling has now grown to include engines (gasoline, diesel, and natural gas [NG]), systems considerations, testing, pre-competitive research and development (R&D) and a bridge of connection among National Laboratories, industry, and academia. While CLEERS has been up against a diverse, large spectrum of needs of

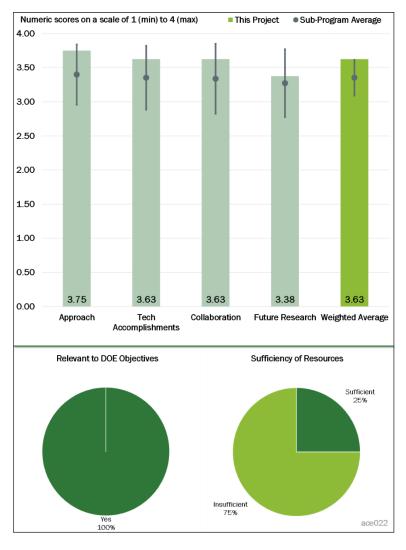


Figure 1-10 – Presentation Number: ace022 Presentation Title: Joint Development and Coordination of Emissions Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination) Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

interest to the emission control community, the reviewer remarked that it has nevertheless done a very good job managing the challenges and maintaining momentum in tackling serious questions of interest to the emission control communities. Its interface with industry, other National Laboratories and academia is impressive. According to the reviewer, its workshop has effectively become a good filler for the now-absent Directions in Engine-Efficiency and Emissions Research (DEER) conference. In all, it is becoming an indispensable component of our community.

## Reviewer 2:

In the reviewer's opinion, CLEERS is one of the most important and influential programs that Oak Ridge National Laboratory (ORNL) runs. It has strong impact on the industry, National Laboratories, and academia. The coordination of the CLEERS effort, teleconferences, and workshops is a key activity that is supported by DOE.

The reviewer appreciated the clarity with which the ORNL CLEERS activities were presented. The presenter did an outstanding job of organizing ORNL's various roles and showing how they fit together (literally speaking, the reviewer liked the use of puzzle pieces for illustrating concepts). The reviewer commented that this project is very well designed and really gets to the heart of the technical barriers faced by the industry with respect to emissions control.

#### Reviewer 3:

The reviewer remarked that the project team did a great job in coordinating the annual CLEERS conference, the monthly audios, and the annual survey. The reviewer said that the conference is always a great forum for people working in emissions and catalysis. Regarding the passive oxides of nitrogen (NO<sub>x</sub>) adsorber (PNA) work, the reviewer suggested assessing the PNAs on multiple consecutive cold-start simulations. The reviewer noted that perhaps the greatest challenge today for palladium (Pd)/zeolite PNAs is the gradual deterioration of the storage efficiency on back-to-back tests. Deactivation is exacerbated by high CO levels, and some diesel engines can emit as high as 3,000 parts per million (ppm) and even 5,000 ppm CO during the cold start.

#### Reviewer 4:

As noted by the reviewer, the CLEERS organization, as in past years, continues to advance the understanding and development of novel catalytic materials for automotive aftertreatment by conducting work in this area, hosting an annual CLEERS workshop, monthly teleconferences, and participating U.S. DRIVE working groups. All these venues function to better disseminate information related to advanced aftertreatment materials and technology directions. Also, through their annual survey, the reviewer stated that research areas of high importance to the light-duty (LD) and heavy-duty (HD) aftertreatment communities are summarized for the general membership and conveyed to DOE to align research and development (R&D) activities for greater effect. Interpreting the results of the survey, according to the reviewer, should weigh the responses of the OEM more heavily to help ensure proper focus.

The reviewer commented that the current research efforts reported out in this project is focused on characterizing the adsorption and desorption mechanisms of a supplier-developed PNA. Much of the findings are known from previous characterizations of this material. Therefore, the reviewer said, the focus should then turn more to ways of modifying this material for further optimizing its capture-and-release characteristics and developing a mechanistic model that is consistent with observations.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer indicated that there was very strong synergy among CLEERS mission, activities, and gains to those of DOE. CLEERS could be characterized as one of the most effective scientific and technical outreach programs that DOE has rolled out into the emission control and combustion community, which it simply cannot do without.

## Reviewer 2:

According to the reviewer, once again, ORNL has done a fantastic job in CLEERS coordination and analysis of samples by generating excellent protocols and data that allow for benchmarking between materials and Laboratories. The strong monthly participation by the industry in the calls shows how important and relevant the CLEERS work is.

#### Reviewer 3:

The reviewer remarked on the systematic investigation on the effects of CO level and water  $(H_2O)$  level on the  $NO_x$  storage efficiency. The reviewer had not observed the relatively poor storage performance seen when nitric oxide (NO) and CO are co-fed together, so investigating the reasons for that occurrence would be interesting. The reviewer was gratified that  $NO_x$  storage on  $Pd^{2+}$  sites were included in the model. Some have

claimed that  $Pd^{2+}$  does not store  $NO_x$ , but the performance is always maximized after a hot lean oxidation, where presumably lots of  $Pd^{2+}$  can be found.

It appeared to the reviewer that the model PNA needs over  $400^{\circ}$ Celsius (C) to release all the stored  $NO_x$ . Catalyst modifications that can result in the release of the stored  $NO_x$  at lower temperatures, preferably below  $300^{\circ}$ C, need to be explored since that is often the maximum temperature of the PNA during city driving. According to the reviewer, diesel exhaust temperatures only exceed  $400^{\circ}$ C under high-load conditions; even the US06 drive cycle only generates about  $350^{\circ}$ C.

## Reviewer 4:

According to the reviewer, the accomplishments of this project can be divided into two distinct areas. The first is CLEERS-related activities that have been proven highly valuable to the catalyst community for advancing the knowledge and development of novel catalytic aftertreatment materials. The second area is clearly focused on characterizing a developed PNA material.

With respect to the CLEERS activities, the reviewer noted that three accomplishments stand out: successfully hosting the annual CLEERS workshop; providing guidance and content in U.S. DRIVE aftertreatment characterization protocols for standardizing test practices of multiple catalyst technologies; and analyzing their annual aftertreatment survey for future trends and needs of catalyst R&D. These activities are performed very well.

With respect to current work to characterize a supplier PNA, the reviewer stated that progress was not as great. The PNA adsorption and release modeling efforts are somewhat redundant with other, prior work, but do reveal important information related to NO bonding sites that is useful. The reviewer suggested improving the capacity and release characteristics by novel methods and addressing ways of controlling those features. Thought should also be given to how PNAs will function in an integrated system.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The collaboration aspect of the work was excellent and included both the industrial partners and the research centers of several universities and National Laboratories, according to the reviewer.

#### Reviewer 2:

CLEERS received great remarks from this reviewer by doing an excellent job on integrating others and coordinating its activities with external entities, such as industry, National Laboratories, academic institutions, and others.

#### Reviewer 3:

The reviewer acknowledged good collaboration between ORNL and University of Virginia (UVA) and was pleased that the principal investigator (PI) was consulting with Hai-Ying at Johnson Matthey (JM).

## Reviewer 4:

The reviewer was very happy to see the collaboration on the coordination by using the advisory board on which three academics participate, and really liked the new university collaboration on the analysis side. The reviewer thought that there could still be more.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

In the reviewer's opinion, the CLEERS activities were generally fine, but the PNA work should focus on novel materials that are not part of another lab effort. The reviewer suggested combining efforts to reduce redundancy and develop a "best of both worlds" material with greater capabilities.

#### Reviewer 2:

The reviewer noted that, over the years, CLEERS has been flexible to redirect itself according to the shifting priorities in the field and industry, such as stronger focus on PNA and hydrocarbon traps. In the process, however, a couple of focused activities—such as ammonia (NH<sub>3</sub>) storage—were sacrificed. Given the project team's expertise, the reviewer recommended that the project receives more resources to tackle further challenges in broader sense; CLEERS is a worthwhile "bang for the buck."

## Reviewer 3:

The reviewer reiterated that the greatest challenge for PNAs is the gradual loss of  $NO_x$  storage performance on repeated cold-start tests, particularly with high CO levels and low maximum temperatures during the cycle. For instance, diesel engines can emit as high as 3,000-5,000 ppm CO during the cold start, although the steady-state levels are usually only around 500 ppm. According to the reviewer, solutions to this deactivation need to be studied for this technology to go forward.

#### Reviewer 4:

The reviewer was concerned that the future work section seemed light due to the projected budget for the activity. While the focus on PNAs and HC traps is important, those are not the only challenges facing the industry. The future works plans in the reviewer's opinion were strong and relevant, but just weak in content.

Question 5: Relevance—Does this project support the overall DOE objectives?

## Reviewer 1:

CLEERS broadly supports overall DOE objectives, according to the reviewer. It is a low-cost to value ratio undertaking with good returns for DOE and the energy and the emission control community (industry, academia, and others). Its broad impact makes it unique and irreplaceable.

## Reviewer 2:

According to the reviewer, both the CLEERS coordination activity and the analysis work directly supported DOE objectives. CLEERS exemplifies how industry-lab-academia interactions can work and be mutually beneficial and its objectives were clearly defined at the beginning of the presentation.

## Reviewer 3:

The reviewer stated that all the efforts supported the need for materials active at low temperature for emissions reduction to meet stringent Tier 3 and low-emission vehicle level III (LEVIII) standards and the introduction of more fuel-efficient powertrains.

## Reviewer 4:

The reviewer noted that PNAs will be needed to allow fuel-saving lean-burn engines with low exhaust temperatures to meet low NO<sub>x</sub> emission standards such as the Tier 3 standards.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer advocated for an increase in budget for the CLEERS activity as it provides fantastic work that is relevant to the industry while supporting Laboratory and university missions. The reviewer also noted that the CLEERS workshop provides a unique opportunity for the aftertreatment community to interact across industry, Laboratories, and universities. The limited size of the CLEERS workshop allows for meaningful interactions and fosters a sense of community in the people who work in that area.

#### Reviewer 2:

Among ORNL, UVA, and JM, the reviewer observed that resources were sufficient for the time being. Resources may need to be increased in the future to study the cold-start deactivation problem and to assess methods to release all the stored  $NO_x$  at temperatures that are representative of low-load operation (e.g.,  $300^{\circ}$ C) on the vehicle, such as city driving.

#### Reviewer 3:

The reviewer found the CLEERS organization resources to be somewhat insufficient because the focus was split between its activities and research efforts. The research efforts, in the reviewer's opinion, would benefit from additional personnel with formulation and modeling experience.

#### Reviewer 4:

The reviewer noted that there is still work to be done; urea selective catalytic reduction (SCR) is here to stay and for a long time. Low-temperature SCR, especially on the catalyst formulation side, is a demanding task needing pre-competitive work (everybody knows it is important, but few publicly discuss it). There are also other needs, which the reviewer said were highlighted in Slides 5, 6, 7, and 20. Given CLEERS' wide spectrum of activities and long-ranging impact, it could use more resources, including for catalyst characterization or for low-temperature SCR of NO<sub>x</sub>. Though the work was impressive, it appeared to the reviewer that the team is stretched thin across various activities; it is hard to do fundamental work having long-term impacts removed from the opportunity to have sufficient focus. Overall, the project appears underresourced given the broad activities of the project and its untapped needs.

Presentation Number: ace023
Presentation Title: Fundamentals in
Selective Catalytic Reduction (SCR),
Filter, and Protocol
Principal Investigator: Yong Wang
(Pacific Northwest National
Laboratory)

#### Presenter

Yong Wang, Pacific Northwest National Laboratory

## Reviewer Sample Size A total of four reviewers evaluated this

project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

#### Reviewer 1:

The reviewer commented that the approach of looking at a variety of catalysts to improve low-temperature SCR activity is useful. It was unclear whether downselecting promising candidates is in the project scope, in which case the reviewer wanted to know what the strategy is for rapid screening of candidates. The reviewer also asked if the focus is only on examining the fundamentals of a low-temperature (T) SCR mechanism. The reviewer noted that it would be useful to also consult with a substrate and filter manufacturer

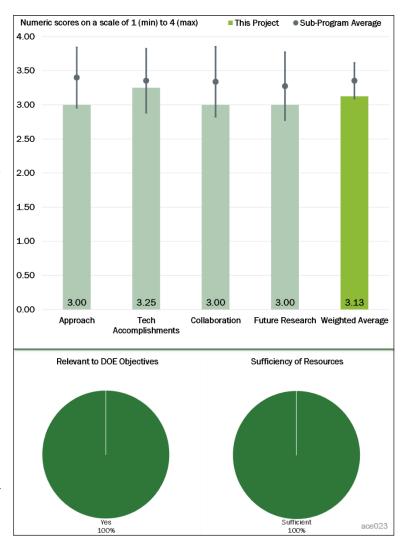


Figure 1-11 – Presentation Number: ace023 Presentation Title: Fundamentals in Selective Catalytic Reduction (SCR), Filter, and Protocol Principal Investigator: Yong Wang (Pacific Northwest National Laboratory)

to ensure that any addition of co-cations is compatible with the substrates.

#### Reviewer 2:

The reviewer remarked the work on SCR catalysts is very good, as is the work on the test fixture for measuring wall permeability in a small particulate filter sample. The reviewer was disappointed that the micro-computed tomography (CT) measurements of pore diameter were not aggregated because the aggregate number is most useful for model development.

### Reviewer 3:

The reviewer noted the presentation covers multiple projects carried out at Pacific Northwest National Laboratory (PNNL) and includes work from prior funding periods. While each individual work addressed an interesting question, it was unclear to the reviewer how the work interrelates, other than that it contributes to the knowledge base for SCR and multifunction devices, thus making it difficult to evaluate as a single project.

#### Reviewer 4:

The reviewer noted that this project investigates both advanced SCR catalysts and soot filtration via wall-flow monoliths. Regarding the SCR catalyst part, iron (Fe)-based catalysts are being investigated after having completed the study on copper (Cu)-based SCR catalysts. Although Fe SCR catalyst performance can be significantly enhanced by fast SCR, the reviewer was unsure that Fe-based SCR catalysts are better candidates for meeting the  $150^{\circ}$ C Challenge than state-of-the-art Cu-based SCR catalysts. It would be instructive for the investigators to provide compelling reasons why focusing on Fe-based SCR catalysts as the next step would make sense. This reviewer explained that one advantage of using Fe SCR catalysts instead of Cu SCR catalysts is lower nitrous oxide ( $N_2$ O) emissions. Regarding the filtration part, new techniques developed for measuring local permeability and pore-scale catalyst-coating characterization can provide useful information necessary for proper interpretation and understanding of the performance characteristics of multi-functional exhaust filters, such as SCR/diesel particulate filters (DPFs) and three-way catalyst (TWC)/gasoline particulate filters (GPFs). As currently set up, however, these two parts of the project (SCR catalyst and soot filtration) are being pursued independently without considering potential interactions between SCR performance and filtration efficiency.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that the improvement in low-T SCR conversion with sodium (Na) co-cation is impressive and that it will be useful to extend the work to look at the impact under practical engine conditions such as conversion under fast SCR, etc.

The reviewer remarked that the progress on using CT for coating distribution is great and that applying it to a broader data set and analyzing it statistically would come up with an error margin on this technique with respect to predictions of filter scale properties like washcoat-loading distribution, backpressure, and conversion, etc.

## Reviewer 2:

The reviewer noted timely completion of the SCR catalyst and multi-functional device tasks, as well as protocol development work with U.S. DRIVE, the Advanced Combustion Engine & Emission Control (ACEC) tech team, and the low-temperature aftertreatment (LTAT) group.

#### Reviewer 3:

On average, the projects appeared to be progressing on schedule, according to the reviewer, because the milestones have either been met or are on target to be met. It was unclear to the reviewer if any progress has been made on multi-function devices during the current funding period.

## Reviewer 4:

The reviewer stated that the low-temperature SCR NOx conversion was below target (90% conversion at 150°C), but the current performance of 60% NOx conversion at 160°C was promising. Assessing the silicon to aluminum ratio (Si:Al) and Na:Cu ratios in the Cu/SSZ-13 with Na<sup>+</sup> co-cations was good, but according to the reviewer, it would have helped to emphasize the design space survey and constituent optimization in the review presentation. It also was not clear to the reviewer how the water will be kept from interacting with copper in Cu/SAPO-34 to prevent degradation because exhaust will always have water in it, especially if that degradation happens at room temperature. The reviewer remarked that the team needs to continue tying together the X-ray CT particulate filter micro-structure with macroscopic properties of the filter.

## Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

There was good collaboration and coordination with multiple institutions and industrial partners, according to the reviewer.

## Reviewer 2:

The reviewer noted that collaboration across both experimental and modeling techniques looks excellent. There are several papers in recent literature that show enhanced SCR activity at low temperature and also enhanced stability at high temperature (e.g., JM presentation at Gothenburg Symposium, Honda Motor Company [HMC] paper on low-temperature aftertreatment [LTA]). The reviewer suggested that it would be useful to look at these and other papers to see if there is any synergy.

#### Reviewer 3:

The reviewer noted that the PNNL team has several external collaborators, but no external partners on this program. The team is actively engaged with Oak Ridge National Laboratory and the LTAT subgroup, though.

#### Reviewer 4:

The collaboration was evident in CLEERS work, protocol development, and prior work involving micro X-ray CT. Otherwise, the work appears to be carried out primarily by PNNL.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that the proposed future work lines up fairly well with the remaining challenges.

#### Reviewer 2:

The reviewer commented that the future research plans were built upon the technical accomplishments so far and PNNL's strong fundamental science base.

## Reviewer 3:

The reviewer was unclear as to why Fe catalysts were chosen for future SCR work, and asked why the team would not continue exploring further improvements with Na co-cation. Regarding the CT-scan work, it will be good to extend to filter scale and show a validation with SCR pressure drop and SCR activity. The reviewer noted that an important input to filter-scale models is the coating amount, distribution, and location, and that it would be good to see a validation on those metrics. This is in proposed future work and is important.

#### Reviewer 4:

According to the reviewer, a key question is how to make nitrogen dioxide ( $NO_2$ ) at low temperatures to support the  $NO_x$  conversion target. The reviewer said that the team needs to work out how to distinguish the three main aging mechanisms discussed in the review presentation. Lastly, the reviewer suggested that the team needs to develop detailed SCR-DPF and TWC-GPF system models, especially those that tie together the microscale measured properties with macroscopic behavior.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that this set of projects contributes to the fundamental understanding of materials and mechanisms that will hopefully contribute to meeting the 150°C challenge.

## Reviewer 2:

According to the reviewer, improving low-T SCR conversion is critical for achieving the Tier 3 and LEV III emission limits; developing models that enable good catalyst design is equally critical for faster development.

## Reviewer 3:

The project supports the goal of meeting Tier 3 bin 30 emissions at full useful life, especially the low-temperature conversion goal of greater than 90% NO<sub>x</sub> conversion at 150°C, according to the reviewer. The team should also consider strategies for managing CO and hydrocarbon emissions at low temperature.

#### Reviewer 4:

The reviewer noted that the project is aimed at developing highly efficient low-temperature SCR catalysts and multi-functional device to control NO<sub>x</sub> and soot emissions from fuel-efficient diesel engines.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The project appeared to have sufficient resources to complete the stated milestones in a timely manner, according to the reviewer.

#### Reviewer 2:

The reviewer said the resources and budget available seem appropriate for scope of work.

#### Reviewer 3

The reviewer noted that the projects appear to be sufficiently funded for the time being.

#### Reviewer 4:

The reviewer indicated that resources seemed sufficient. For the CT permeability modeling work, it would be good to use tens of samples to get statistical correlations and would be useful to get closer collaboration with catalyzers and substrate manufacturers.

Presentation Number: ace027
Presentation Title: Next-Generation
Selective Catalytic Reduction (SCR)Dosing System Investigation
Principal Investigator: Abhijeet
Karkamkar (Pacific Northwest
National Laboratory)

#### Presenter

Abhijeet Karkamkar, Pacific Northwest National Laboratory

## **Reviewer Sample Size**

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer noted that the approach of screening various materials using coupled experiments and theory is a good approach. The metrics for evaluation such as capacity, temperature, energy requirement, and safety are correct in their opinion.

## Reviewer 2:

The reviewer remarked that investigators recently switched efforts to porous metal oxides as candidate NH<sub>3</sub> storage materials. Although some of the computational and experimental techniques are in the process of being

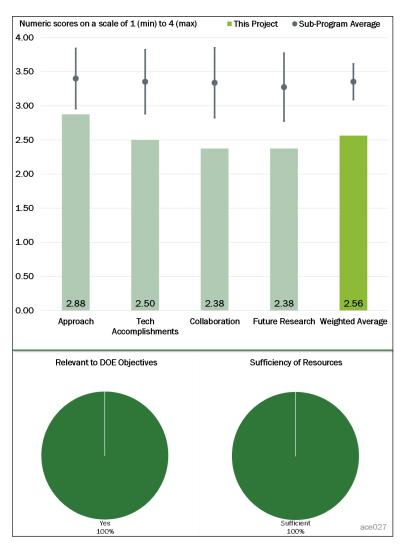


Figure 1-12 – Presentation Number: ace027 Presentation Title: Next-Generation Selective Catalytic Reduction (SCR)-Dosing System Investigation Principal Investigator: Abhijeet Karkamkar (Pacific Northwest National Laboratory)

implemented now, the stated approach to perform the work seems reasonable and logical overall.

## Reviewer 3:

The indicated that the goal is to find ways to mitigate issues with diesel exhaust fluid (DEF) dosing while still using NH<sub>3</sub>-SCR. The preference is to use other ammonia carriers or sources on vehicles. The project, then, is to screen materials that can store ammonia on board the vehicle, according to the reviewer, according to the reviewer.

#### Reviewer 4:

While the project addressed the barriers of ammonia storage and low-temperature ammonia delivery, the project felt somewhat unfocused to the reviewer. This may be indicative of the project's early stage (in that the current focus is rapid screening of materials), but it was unclear from the presentation whether the end goal of the project is material selection or systems development. There is also some question as to whether gaseous ammonia delivery is the right path forward for low-temperature  $NO_x$  abatement given the market share of Amminex or similar technologies and the existing infrastructure for DEF/urea water solution.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

Due to the fact that the research efforts have recently shifted to porous oxide materials, only some preliminary results have been reported during the review, noted the reviewer.

## Reviewer 2:

The project appears to be progressing on schedule, although it was unclear to the reviewer from Slide 18 whether or not the milestones and go-no go decisions are on track for September 2019.

#### Reviewer 3:

The reviewer asserted that it would be very useful to put the results generated so far into context by comparison with the current state of the art. The NH<sub>3</sub> adsorption studies on various materials are difficult to judge unless compared to the targets set by commercial applications (such as how much NH<sub>3</sub> is needed over a drive cycle or through urea delivery via DEF today). The computations work seemed very preliminary to the reviewer and not quite connected with experiments. It may be pragmatic to focus on one to two promising materials and optimize through theory, validate through experiments, and demonstrate the techniques before moving to screening a wide class of materials. The reviewer also suggested showing a path to couple the models and experiments.

#### Reviewer 4:

The reviewer noted that the team surveyed several potential  $NH_3$  carriers, but many are chloride salts that generate hydrochloric acid (HCl) gas in exhaust. In doing so, PNNL is giving up on halide salts as a storage medium, which is a sensible move. The reviewer mentioned that other suppliers are not wild about ammonium carbamate ( $[NH_4]_2CO_3$ ).

The reviewer commented that project team looked at NH<sub>3</sub> adsorption on (porous) zeolites and that the substituted metals were Brønsted acids that adsorbed NH<sub>3</sub> readily. Alkaline earth compounds in Zeolite Y look best, but release temperatures were high. Layered titanate (lepidocrete) was also a candidate, although the synthesis is tricky. All of the materials need an increased effective surface area to improve NH<sub>3</sub> storage capacity.

Computational modeling to screen materials has identified a few candidate ammonia sorbents. The reviewer also noted that the work had started, but more needs to be done. A fundamental issue with the ammonia-absorbing materials is that they still need to be replenished with anhydrous ammonia, and if that is the case, the reviewer asked why ammonia storage tanks are not used.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

Additional collaborators, including some industrial partners, on the team would be desirable in the reviewer's opinion.

## Reviewer 2:

The project team includes PNNL and the United States Council on Automotive Research (USCAR) although it was not clear to the reviewer how USCAR is contributing to the project team. They are looking for additional partners for the program, but with budgets already set, the reviewer asserted that this will be difficult to accomplish.

#### Reviewer 3:

Collaboration, to the reviewer, appeared to be limited to a series of meetings and teleconferences with USCAR. While the OEMs were indicated on Slide 5, there is no indication of how they are involved. The reviewer noted that perhaps their role will become apparent once systems-level implementation commences.

#### Reviewer 4:

Solid sorbents have been around for a while now. The reviewer recommended consulting with the industry for advice on what materials have already been studied and what needs to be avoided so as not to repeat prior work. Collaboration between theory and experiment is not quite clear and needs to be clarified, according to the reviewer.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The stated milestones seemed reasonable to the reviewer. In addition to examining  $NH_3$  storage capacity, it is critically important to investigate in detail  $NH_3$  release characteristics (temperature required, kinetics of  $NH_3$  release, and energy requirement) for promising candidate materials to ensure that sufficient amounts of  $NH_3$  reductant can be delivered in response to rapidly changing engine-out  $NO_X$  emissions under actual driving conditions.

#### Reviewer 2:

The reviewer said the materials considered must bind ammonia but not water, which is important because there is invariably water in an exhaust system. Given the direction to focus on ammonia-storage compounds, the reviewer found the next steps to be consistent. There is a need to actively consider the "status quo" options of the DEF tank and the anhydrous ammonia tank on a vehicle. The target ammonia-release temperature is 100°-150°C, if not lower, from these new materials.

## Reviewer 3:

The reviewer said that an upcoming milestone in September 2019 is selection of next-generation storage material, which does not seem to have been completed. Neither is a clear pathway to getting there soon, according to the reviewer. The modeling completion of high throughput screening in December 2019 also seems unlikely. The reviewer stated that it would be useful to have a clear path on addressing the above.

#### Reviewer 4:

The reviewer said that the go/no-go decision points in the presentation are not well defined. "Down selection of ammonia storage materials for high throughput screening" does not indicate that a yes/no decision is being made or what the criteria for that decision might be. The various tools that will be used to select a next-generation ammonia storage material are clear, but the structure (the plan) was not clearly apparent to the reviewer.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

This reviewer stated yes, low-temperature  $NO_X$  abatement is an important area of development, and low-temperature ammonia delivery (combined with low-temperature active SCR) is one possible pathway toward this goal.

## Reviewer 2:

The reviewer stated that low-temperature delivery of ammonia is important, when coupled with improved low-temperature SCR activity. The overall importance is to reduce NO<sub>X</sub> emissions for meeting tighter regulations.

## Reviewer 3:

The reviewer remarked that this project supports opportunities for lower temperature  $NO_X$  conversion, especially with ammonia SCR.

## Reviewer 4:

The reviewer commented that this technology can potentially provide  $NH_3$  at temperatures below 180°C to low-temperature SCR catalysts, so that significant  $NO_X$  conversion can be obtained in the low-temperature regime where urea does not decompose to  $NO_X$ .

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer stated that there are sufficient resources to perform the work stated.

## Reviewer 2:

This reviewer said the project appears to be sufficiently funded.

#### Reviewer 3

The reviewer noted that the resources look sufficient, but the team needs to speed up the work.

## Reviewer 4:

This reviewer remarked that there appears to be just enough budget for materials screening, but not for systems-level evaluations.

Presentation Number: ace032
Presentation Title: Cummins-ORNL
Emissions Cooperative Research and
Development Agreement (CRADA):
NOx Control and Measurement
Technology for Heavy-Duty Diesel
Engines, Self-Diagnosing
SmartCatalyst Systems
Principal Investigator: Bill Partridge
(Oak Ridge National Laboratory)

Presenter
Bill Partridge, Oak Ridge National
Laboratory

Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer stated that this is a nice approach for using the conversion inflection (CI) to improve the NO<sub>X</sub> conversion on a temporary basis. Also, it is a nice approach for studying the rates of the half cycles to understand the mechanism behind the CI. The reviewer asserted that it will be interesting to see how field aging and low-temperature formulations affect the reduction half cycle (RHC) and oxidation half cycle (OHC) compared to the de-greened baseline catalyst.

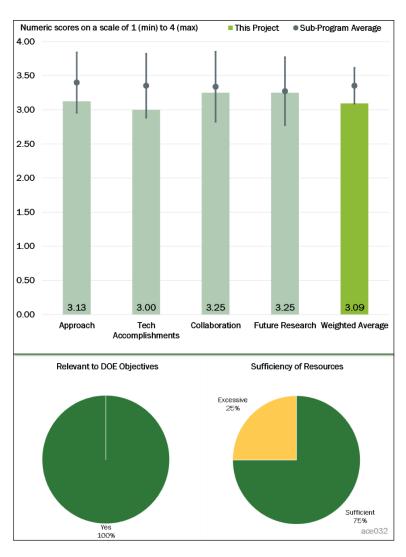


Figure 1-13 – Presentation Number: ace032 Presentation Title: Cummins-ORNL Emissions Cooperative Research and Development Agreement (CRADA): NOx Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems Principal Investigator: Bill Partridge (Oak Ridge National Laboratory)

## Reviewer 2:

The reviewer said the development of novel and cost-effective approaches for diagnosing the state of a catalyst is valuable to OEMs. The conversion-inflection phenomenon exploited in this activity to determine the aged state of an SCR catalyst is a unique diagnostic tool. However, according to the reviewer, field-aged SCR catalysts can be a compilation of multiple aging mechanisms. Being able to separate and quantify the contributions from each of the aging mechanisms on the CI phenomenon will be very challenging. Also, if this technique is meant to be an in-situ diagnostic method, the reviewer commented that determining the best way to use a NO<sub>X</sub> sensor to obtain this information requires additional development.

### Reviewer 3:

The reviewer stated that the approach to performing the work is based on a mix of modeling, testing, and analysis of field-aged SCR catalysts (outlined in Slides 7-13). Analysis of field-aged catalysts will prove to be more difficult than outlined here: if things stay simple, reduced activation will be simply due to temperature

exposures (thermal and hydrothermal aging); however, that rarely turns out to be the case. Additional impacts on lubricants, exhaust gas recirculation (EGR) fouling by-products, and even possibly platinum group metals (PGM) drift (oxidizing NH<sub>3</sub>), among others, will complicate the picture. According to the reviewer, such additional (unwanted) complexities are a risk to this project, which needs further highlight and added focus, more than what has been outlined. The reviewer asserted that this risk by itself is even greater than the challenge of understanding the second component of the project (impact of lower temperatures on SCR).

## Reviewer 4:

Considering that this project is a continuation of a long-running cooperative research and development agreement (CRADA), the reviewer expressed surprise at the lack of progress despite the short timeline for this most recent incarnation. This reviewer asserted that this should have been a poster rather than an oral presentation this year; it seemed rather light on content. The reviewer indicated that the technical approach to the project seems appropriate and praised the nice job on Slides 12 and 13.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

## Reviewer 1:

The reviewer said that although this is the first year of the project, it is off to a good start and has made adequate progress: Characterizing the nature of the challenge, putting forward plausible hypotheses (to be proven) on what the driving mechanisms could be, and constituting initial testing and early modeling (RHC, OHC, half-cycle based model).

#### Reviewer 2:

This reviewer remarked that there is a commendable match between the model and the data. The reviewer asked if there is a way to capitalize on the CI by turning the  $NH_3$  off and on periodically, in order to improve the overall  $NO_X$  conversion. Of course, the reviewer noted that this will need to be done without causing  $NO_X$  slip issues while the  $NH_3$  is turned off.

#### Reviewer 3:

The reviewer referenced prior comments.

## Reviewer 4:

It appeared to the reviewer that a portion of the work presented at this review has already been reported previously. Although the approach is novel, the level of progress in the past year is less than expected. The process of field-aging catalysts, which is central to this technique, is time consuming and requires some planning. Knowing exactly what the catalyst was exposed to and the conditions it was aged under will need to be fully captured in order to produce relevant data. Therefore, the reviewer suggested that the effects of oil poisons, PGM poisons, and thermal aging will have to be taken into consideration. This will require reference catalysts aged with each of these contributors to deactivation.

Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

This reviewer remarked that the addition of Johnson Matthey Inc. to the project team was good.

## Reviewer 2:

The reviewer noted that there appears to be good collaboration between Oak Ridge National laboratory (ORNL) and Cummins, with input from General Motors (GM) and Johnson Matthey.

## Reviewer 3:

The reviewer found the collaboration for this work to be very appropriate and should help advance this project. However, including a sensor and catalyst supplier would benefit the project and should provide greater insight

on how to accurately measure the  $NO_x$  and  $NH_3$  in a vehicle application and to characterize the catalyst appropriately.

#### Reviewer 4:

The reviewer noted the team is currently composed of ORNL, one major engine manufacturer, and a major Tier 1 supplier, which makes a strong team. However, this reviewer indicated one concern that the team is up against the major challenge of "decoding" the complexity of field-aging mechanisms (significantly more complex than lab-based aging) and further coupling such observations and findings with modeling. The modeling phase of this will be more complex than anticipated. That said, there is only one person (from Cummins) with modeling background in this project. In the opinion of this reviewer, more modeling capability is needed for such complex modeling.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

This reviewer said the future work (fiscal year [FY] 2020 and FY 2021) is planned with clear steps (Slide 14). FY 2020 will focus on aging and FY 2021 on low-temperature performance. The reviewer suggested that the team consult "early" on the existing SCR aging modeling literature in order to pave its road to some of the anticipated complexities of aging mechanisms and deactivation.

#### Reviewer 2:

The reviewer said this is a good plan to investigate field-aged samples and low-temperature formulations. It will be interesting to see how actual field aging affects the CI that the team is observing with de-greened catalysts. The reviewer asked if there is a plan to look at the effects of sulfur poisoning and high temperature aging on the CI.

## Reviewer 3:

This reviewer stated that to determine the merit of the CI phenomenon, the characterization of aged catalysts should proceed more quickly. Understanding the differences between field and laboratory aged catalysts will be important to derive useful information. Providing a matrix of characterization efforts would be helpful to better plot out a course of action.

#### Reviewer 4:

The reviewer noted that, based on the comments about general applicability that the PI made during the talk—and in response to a question posed during the presentation—this project seems to be very specific to the Cummins application and materials. This reviewer questioned the broader impact and value of this work.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer said that diagnostic tools are very useful to automotive OEMs for ensuring in-use compliance of their vehicle fleets. Software-based tools, which take advance of currently available sensors, are cost effective as well.

## Reviewer 2:

The reviewer stated that higher  $NO_X$  reduction is synonymous with fuel economy; better SCR catalyst performance would mean more efficient engines having lower fuel consumption. As such, the reviewer indicated that this project does support the DOE objective of more efficient engines as well as lower temperature catalyst performance.

## Reviewer 3:

The reviewer remarked that improving durability and investigating aging mechanisms are of interest to the general community.

## Reviewer 4:

The reviewer noted that this work can improve the performance of catalysts in the field, which will allow the engine to be tuned for better fuel economy.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The resources at ORNL and Cummins seemed to be sufficient to the reviewer.

#### Reviewer 2:

This reviewer noted that the team overall has access to engines, test equipment, microreactors, and modeling capabilities (the latter needs a closer look, stronger resource).

#### Reviewer 3:

This reviewer suggested that adding a sensor supplier may benefit this work.

#### Reviewer 4:

Due to the very specific nature of the work, this reviewer expressed surprise that DOE continues to invest in this CRADA. T the reviewer commented that this could be restructured as a Work for Others (WFO) project, and highlighted that this CRADA has been going on for nearly 20 years, if not longer.

Presentation Number: ace033
Presentation Title: Emission Control for Lean Gasoline Engines
Principal Investigator: Vitaly
Prikhodko (Oak Ridge National Laboratory)

#### Presenter

Vitaly Prikhodko, Oak Ridge National Laboratory

## **Reviewer Sample Size**

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The overall approach to the program seemed good to the reviewer. Test results from the new engine will definitely improve the quality of the results.

## Reviewer 2:

The reviewer noted that this project is looking at ways to improve both fuel economy and criteria pollutants simultaneously. The work also includes expanding the lean operation map, which is important for improving fuel economy.

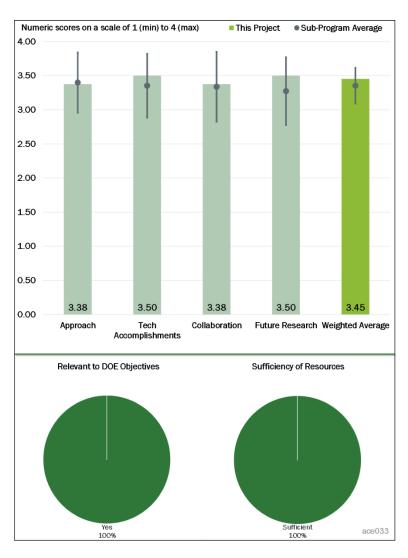


Figure 1-14 – Presentation Number: ace033 Presentation Title: Emission Control for Lean Gasoline Engines Principal Investigator: Vitaly Prikhodko (Oak Ridge National Laboratory)

### Reviewer 3:

This reviewer said the project appears to be well designed and feasible. The technical barriers are well addressed. It will be interesting to see how the system performs with the new engine. The only aspect of concern for the reviewer is the increasing system complexity, although this may be addressed by combining cans or the use of multi-function devices if possible.

#### Reviewer 4:

This reviewer stated that the system-level (i.e., catalyst plus engine) as well as the iterative flow reactor plus engine study approaches in this project helped achieve 8.3% fuel economy improvement while meeting the Tier 3 NO<sub>X</sub> plus non-methane organic gas (NMOG) 30 milligrams (mg)/mile standard. However, the reviewer commented that this requires a five-function catalyst system containing 5 grams (g) PGM/ liter (L) engine displacement. This translates into 10 PGM usage for the 2-L BMW engine used in the study, and with the possible addition of an air pump, the cost of the emission-control system has become too high to be practical. Additionally, the reviewer indicated that proper thermal management of such a multi-component emission-control system on actual vehicles would be very challenging. Perhaps, the project team should look for another breakthrough catalyst technology that requires lower PGM usage and simpler exhaust-system architecture.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

This reviewer observed that the project has achieved an 8.3% fuel-economy improvement while meeting Tier 3 standards; procured a new, improved lean-burn engine; and completed analysis of sulfur impact on NH<sub>3</sub> production as well as water gas shift (WGS) and steam reforming (SR) reactions.

#### Reviewer 2:

The reviewer said it will be useful to see performance evaluated on a certification test cycle (Federal Test Procedure [FTP], US06, etc.) and include cold-start emissions. For future catalyst architectures, the reviewer asked whether a TWC and  $NO_X$  storage component (NSC)—or other ways to downsize and also to reduce PGM—can be combined, given that the latest system requires a significant increase in PGM.

#### Reviewer 3:

The reviewer stated that the 8.3% fuel-consumption benefit from upgrading the exhaust aftertreatment system from TWC-SCR only to TWC plus NSC minus GPF minus SCR plus clean-up catalyst (CUC) is impressive, although it would be helpful to try to quantify the cost per mile per gallon (mpg) improvement (or cost per g CO<sub>2</sub>/mile [mi]) from the additional hardware.

The reviewer urged the project team to please consider using a modern, bi-functional CUC that includes both oxidation catalyst and SCR functions because that should improve the CUC selectivity for nitrogen over  $NO_X$  at the tailpipe.

The reviewer recognized that the current configuration is useful for development purposes, but would like to have seen a more compact aftertreatment system that shows the pathway toward a production system. For example, the reviewer asked if the CUC function can be coated on the back of the SCR monolith to combine that into one can.

#### Reviewer 4:

The reviewer found that good progress is being made toward the long-term goals. The reviewer had some concern about the cost effectiveness of the system if there are significant increases in the price of Pd.

**Ouestion 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

The reviewer stated that the project appears to be well coordinated across a broad range of collaborators.

## Reviewer 2:

It looked to the reviewer like there are good all-around contributions from all aspects of the project.

#### Reviewer 3:

The reviewer highlighted the fact that the team has recently expanded the network of collaborators.

#### Reviewer 4:

This reviewer remarked that the team of ORNL, GM, Umicore, and the University of South Carolina seems good and well engaged. The reviewer would have preferred more direct involvement from GM and Umicore than "guidance and advice." This reviewer also appreciated the coordination with CLEERS and other stakeholders.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said the future work, including jet ignition engine, is an excellent direction. It will be important to demonstrate the performance on the FTP cycle and emissions under cold start. Current data only show warmed-up emissions. The reviewer suggested that vehicle-level simulations should be included and compared with other leading concepts.

#### Reviewer 2:

This reviewer noted that the future research plan will primarily involve application of the catalyst technology developed so far to a new engine.

#### Reviewer 3:

The reviewer stated that future work addresses the primary barriers to achieving Tier 3 compliance, namely CO slip and NH<sub>3</sub>/NO<sub>X</sub> slip (with some tradeoff between the two).

#### Reviewer 4:

This reviewer found the planned future work to be appropriate and sensible. Changing to the MAHLE engine adds risk, since the engine is new to ORNL, and it is a research engine. That said, the reviewer understood the need to retire the aging BMW 120i lean SI engine from active use. The reviewer asked what the strategy is to mitigate CO during rich operation.

Question 5: Relevance—Does this project support the overall DOE objectives?

## Reviewer 1:

This reviewer said that improving fuel economy is an important objective aligned with VTO. Lean gasoline is seen as an important pathway to improve fuel economy. Also, in the United States, gasoline engines dominate the market so this is the right pathway.

#### Reviewer 2:

The reviewer stated that low-temperature aftertreatment performance is an enabler of more efficient and less-polluting engines.

## Reviewer 3:

This reviewer commented that viable emission-control catalyst system development is an enabler for fuel-efficient lean gasoline engines.

#### Reviewer 4:

The reviewer noted that this project seeks to provide a pathway to a significant increase in fuel economy by providing a cost-effective means of treating lean burn, gasoline engine exhaust.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

This reviewer stated that sufficient resources are available to achieve the stated milestones in a timely manner.

#### Reviewer 2:

The project appeared well funded from this reviewer's perspective.

## Reviewer 3:

The reviewer remarked that the team has the new engine, and the partners are supplying aftertreatment system hardware.

## Reviewer 4:

The reviewer said the resources are sufficient for the objectives as stated. For adding more testing on FTP or for vehicle simulations, more resources may be needed.

Presentation Number: ace054
Presentation Title: Rapid
Compression Machine (RCM) Studies
to Understand Autoignition
Fundamentals
Principal Investigator: Scott
Goldsborough (Argonne National
Laboratory)

Presenter Scott Goldsborough, Argonne National Laboratory

Reviewer Sample Size
A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

This reviewer stated that the focus on gasoline is appropriate for LD engine research.

#### Reviewer 2:

The reviewer noted that the PI addressed the auto-ignition mechanisms of different fuels, including surrogate blends under the engine-like operating conditions. The fuel-air mixture is premixed to isolate the kinetics from other effects (including flow and mixing). The measurements have been compared with the numerical results of

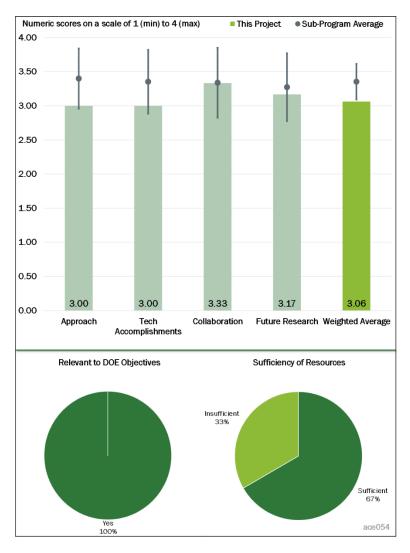


Figure 1-15 – Presentation Number: ace054 Presentation Title: Rapid Compression Machine (RCM) Studies to Understand Autoignition Fundamentals Principal Investigator: Scott Goldsborough (Argonne National Laboratory)

"adiabatic core" model with Lawrence Livermore National Laboratory (LLNL) gasoline surrogate mechanisms. According to the reviewer, the outcomes of this project are critical for development of kinetic models for different fuels. Low-temperature combustion (LTC) and the negative temperature coefficient (NTC) are critical for auto-ignition. Meanwhile, their measurements exhibit strong uncertainties. Quantification of these uncertainties in heat-release measurements will be of great importance for kinetic model development. The reviewer suggested that the team consider more detailed and realistic simulations to have an apples-to-apples comparison with the measurements. If the facility permits, more diagnostics and fast visualization about the ignition process will be valuable for future model validations.

## Reviewer 3:

The reviewer stated that the methodology is fine, but the end success will be defined by the goals. The quality of data might not fulfill such goals entirely.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer found the progress of this project to be good. The PI has finished measurements of primary reference fuel 90 (PRF90), 2-methyl-2-butene (2M2B) and its blends with toluene, and conducted analysis accordingly. Two tasks about multi-component surrogate blends, ethanol blends, and full boiling range gasoline are ongoing.

## Reviewer 2:

The reviewer suggested that leveraging the Rapid Compression Machine (RCM) Workshop to identify and understand facility influences should be a high priority. Unexplained variations in measurements make the results less useful.

#### Reviewer 3:

This reviewer emphasized that the project seems back loaded.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

This reviewer said the sharing of data and techniques is at an appropriate level.

## Reviewer 2:

This reviewer remarked that the collaborations with other teams from DOE National Laboratories, universities, and the European Union are great. More results generated by such collaborations will be very helpful to highlight the impact of the present work. Coordination of the International RCM Workshop is very important to have a broader impact to the whole international community.

#### Reviewer 3:

This reviewer said the data acquired needed to be evaluated against other experimental approaches, such as shock tubes and flow reactors.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer found that the proposed future research plan is reasonable. Besides testing different fuels, targeting at LTC and EGR conditions is of great importance for industry. Adding gas sampling will reveal more insights of the ignition process and generate more valuable data for model validation. The reviewer commented that it was unclear from the presentation and available material how uncertainty quantification (UQ) and global sensitivity analysis (GSA) will be integrated into the whole project.

#### Reviewer 2:

This reviewer strongly encouraged research that can be applied to highly dilute, stoichiometric combustion efficiency and emissions.

#### Reviewer 3:

The reviewer said it would be very beneficial if product species could be detected somehow to confirm the trends shown. Certainly, the models utilized need to be updated because the fits show very little correlation.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated that the present project addresses the auto-ignition behavior of different fuels for engine combustion. The outcomes of this project are very important for improving understanding of auto-ignition processes, fuel optimization, and reaction mechanism development.

#### Reviewer 2:

The reviewer indicated that fuel chemistry fundamentals are important to understanding combustion and improving models.

## Reviewer 3:

The reviewer noted that auto-ignition fundamentals are crucial to understand combustion efficiency.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

This reviewer observed sufficient project resources.

#### Reviewer 2:

The reviewer said the current RCM facility at Argonne National Laboratory (ANL) should be sufficient for this project. Additional resources should be added when gas sampling is considered.

## Reviewer 3:

The reviewer emphasized that the models have not been updated. Historically, reproducibility of RCM results is an issue

Presentation Number: ace056
Presentation Title: Low-Temperature
Oxidation
Principal Investigator: Yong Wang
(Pacific Northwest National
Laboratory)

#### Presenter

Yong Wang, Pacific Northwest National Laboratory

# Reviewer Sample Size A total of four reviewers evaluated this

A total of four reviewers evaluated thi project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer commented that the project is off to a good start; so, the approach being used seems reasonable.

#### Reviewer 2:

The reviewer stated that the project is looking at the right targets—improving methane conversion, stability, and resistance to water inhibition. The focus is on palladium (Pd)-based catalysts, but the approach to selecting the various catalysts chosen so far was unclear to the reviewer, who asked what connects the various catalysts. The reviewer identified the cost of Pd-based catalysts

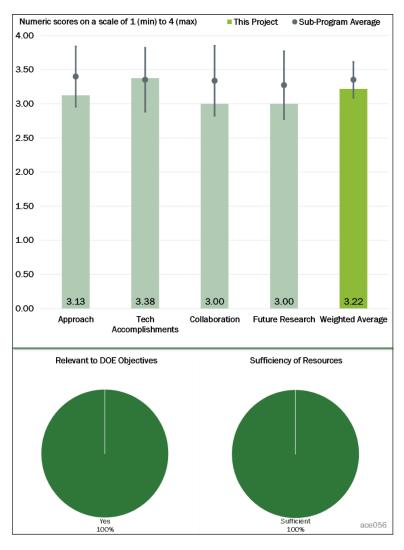


Figure 1-16 – Presentation Number: ace056 Presentation Title: Low-Temperature Oxidation Principal Investigator: Yong Wang (Pacific Northwest National Laboratory)

as one of the technical barriers; it will be good to address this.

### Reviewer 3:

The reviewer noted that several interesting catalyst design concepts are explored in this project. However, different test conditions were used to demonstrate the validity of each concept, which makes it difficult to ascertain the "best overall" catalysts for low-temperature (T) methane (CH<sub>4</sub>) oxidation. This project has focused on lean conditions, but given the literature reports that maximum  $CH_4$  conversion can be obtained under slightly rich conditions, the reviewer suggested that it would be worth examining the effect of feed stream stoichiometry (air-fuel ratio) on  $CH_4$  conversion. In addition, oxides of nitrogen (NO<sub>x</sub>) emissions from compressed natural gas (CNG) vehicles are generally of significant concern as well. Thus, it makes sense to address  $NO_x$  emission control in addition to  $CH_4$  emission control. So far in this project, mechanistic understanding has largely been inferred from kinetic measurements; the reviewer said that it would be desirable to strengthen catalyst characterization efforts in order to get more direct information on the catalyst performance-property relationship.

## Reviewer 4:

The reviewer indicated that the focus on palladium creates the potential for risk based on the increasing price of palladium. This is mitigated somewhat by the intention to maximize the efficiency of palladium used. The market size of natural gas vehicles (NGVs) in the United States is also quite small (approximately 225,000 out of about 270,000,000 vehicles).

The reviewer also noted the impression that this is a collection of related projects with their own hypotheses (support hydrophobicity increases stability, double confinement increases activity relative to single confinement, single atom palladium/rhodium-cerium oxide [Pd/Rh-CeO<sub>2</sub>] shows high activity at low temperature) as opposed to one unified project. The integration of some of these concepts is proposed in the future work.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

According to the reviewer, excellent methane conversion was demonstrated (greater than 80% at 350°Celsius [C]). Also, the project team shows pathways to improve stability and water resistance. The reviewer stated that it will be useful to show the sulfur tolerance and also demonstrate performance on engine testing. Also, the impact on NO<sub>x</sub>/carbon monoxide (CO) conversion should be shown.

#### Reviewer 2:

The project team appeared to the reviewer to have found a good palladium-zeolite catalyst for methane oxidation at relatively low temperatures and is making good progress with evaluating it and related options. The doubly-confined Pd/ceria catalyst also looked promising to the reviewer, but the materials did not make clear how that would be loaded onto a monolith support for automotive use.

## Reviewer 3:

The reviewer commented that several interesting catalyst design concepts to develop CH<sub>4</sub> oxidation catalysts with improved activity and stability have been proposed and tested and validated in this project.

#### Reviewer 4:

The reviewer noted that technical milestones have been met or are on track. It was somewhat unclear to the reviewer how the individual milestones contribute to the overall goal of 95% methane conversion at 350°C or less.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

Collaboration looked good to the reviewer, who said that it will be good to see a baseline activity on state-of-the-art catalyst included through working with catalyzer.

## Reviewer 2:

The reviewer remarked that the project team is Pacific Northwest National Laboratory (PNNL), Oak Ridge National Laboratory (ORNL), Cummins, Johnson Matthey (JM), and General Motors (GM). The team communicates regularly and is actively collaborating on new catalyst formulations for the project.

#### Reviewer 3:

Collaborative communication seemed sufficient to the reviewer. PNNL is doing most of the heavy lifting.

#### Reviewer 4:

According to the reviewer, stronger "pull" from (and/or more active participation by) vehicle and engine manufacturers and catalyst suppliers would help generate results of more practical value, thereby increasing the chances of actual implementation of the technology developed here.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The proposed future work seemed reasonable to the reviewer. The project team may examine stoichiometric conditions or the oxidation of small ( $C^{2+}$ ) hydrocarbons in the future. The reviewer recommended performance in stoichiometric conditions since that is still a common natural gas engine configuration.

#### Reviewer 2:

The reviewer said that future work covers sulfur resistance and cyclic operation. It will be important to include some level of engine testing and also testing at varying space velocity to examine mass transfer limitations. Also, the reviewer suggested that measurements of conversion of other species, such as CO and, NO<sub>x</sub>, be included.

#### Reviewer 3:

Each of the catalyst design concepts pursued so far in this project seemed to the reviewer to be aimed at addressing or mitigating a specific issue or a potential barrier (such as water inhibition effect mitigation, Pd active site stability, etc.) related to development of low-T CH<sub>4</sub> oxidation catalysts. It was not clear to the reviewer, however, that the proposed future research plan is a logical outgrowth of what has been learned from the previous work in this project.

## Reviewer 4:

A number of technologies are being evaluated, but it is was unclear to the reviewer how each individual technology contributes to the overall goal or whether they can be used in concert. It also appeared to the reviewer that there are no intermediate milestones currently planned between now and the end of the project.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated that natural gas engines are gaining market share in the heavy-duty sector and it is important to reduce methane emissions due to its high contribution to greenhouse gas (GHG) emissions.

## Reviewer 2:

The reviewer stated that yes, this project supports the overall DOE objectives through support of improved warm-up strategies and low-temperature pollutant conversion.

## Reviewer 3:

Low-T CH<sub>4</sub> oxidation catalyst development for CNG vehicle emission control was stated by this reviewer.

#### Reviewer 4:

The reviewer observed that this project addresses barriers to the adoption of natural gas vehicles, specifically the inability of current aftertreatment technologies to convert methane emissions at sub-400° C. This is especially important as methane is regulated as a greenhouse gas under a cap of 30 milligrams (mg)/mile and anything above this cap will count against fuel economy. The reviewer warned that this becomes more important as fuel economy regulations become more stringent.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer said that \$1.2 million over 3 years is \$400,000 per year, which seems suitable given the experimental work being performed.

## Reviewer 2:

The project appeared to the reviewer to be sufficiently funded.

## Reviewer 3:

Resources looked sufficient to the reviewer for the scope as defined. But, the reviewer added, that if engine testing is to be included (it should), then probably the resources are insufficient.

## Reviewer 4:

The reviewer stated that resources seem sufficient assuming that this project continues to focus on novel catalyst synthesis and testing in the laboratory (with no plans for engine tests), as described in the presentation.

Presentation Number: ace084
Presentation Title: Development and
Validation of Simulation Tools for
Advanced Ignition Systems
Principal Investigator: Riccardo
Scarcelli (Argonne National
Laboratory)

#### Presenter

Riccardo Scarcelli, Argonne National Laboratory

# Reviewer Sample Size A total of five reviewers evaluated this

project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewed asked that the project goal be clearly stated (e.g., model heat release rate within 20% of experimental data at a computational cost two times higher than the current approach). The reviewer wanted to see the geometry and conditions (engine speed and loads) that will be modeled and further stated that practical engine conditions (including high load) are important for industrial applications. The reviewer commented that the choice of topics is excellent, the topics are very relevant for industry, and the slides are clear and easy to understand.

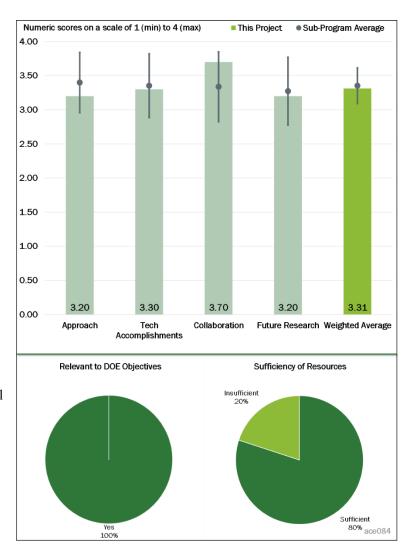


Figure 1-17 – Presentation Number: ace084 Presentation Title: Development and Validation of Simulation Tools for Advanced Ignition Systems Principal Investigator: Riccardo Scarcelli (Argonne National Laboratory)

#### Reviewer 2:

The reviewer said that the goal of translating research-level understanding of a range of different ignition strategies into a commercial code is excellent—it is exactly the point of programs like this and the collaborations the principal investigators (PIs) have established are great for that. The reviewer found the approach to be sound—the strategy of building up from fundamental understanding using tools like VizGlow to CONVERGE, in collaboration with people developing better chemistry, is good.

According to the reviewer, the drawbacks of the approach are that the focus of the current project is very broad, possibly too broad to allow the PI and the project team to dig into many of the important details in each topic. The project considers three modes of ignition—traditional spark ignition, low-temperature plasma, and pre-chamber jet ignition. These three topics are quite different and the bottleneck problems are likely very different among the three, meaning that the "efficiency" of the project is decreased. The reviewer indicated that gains in one area will not necessarily translate to others. Further, only one of the topics was covered in depth in the presentation, and so it was hard for the reviewer to judge the progress in the other topics.

The reviewer said the idea of properly capturing plasma generation chemistry and then predicting ignition and burning rate is a daunting one due to the uncertainty in all aspects of this analysis. It was clear to the reviewer that the plasma predictive chemistry is heavily lacking; thus, this area needs much attention. The reviewer said that it would be fair to ask if the project team could experimentally reduce some of this uncertainty with a cleverly designed experiment. The reviewer said that without this piece of the puzzle, this project is unlikely to make such overall progress.

#### Reviewer 4:

The project looked to the reviewer to advance the current state of the art of numerical simulations combustion ignition related to high-energy spark, low-temperature plasmas, and pre-chamber ignition. The approach relies on using current de facto computational tools to simulate these phenomena using CONVERGE computational fluid dynamics (CFD) and takes an interesting approach to couple plasma simulation (VizGlow) with standard CFD simulations. These represent the state of the art in terms of simulation tools, and is the reviewer expected that the approach is valid.

Considering the dearth of plasma-ignition fundamental material, the reviewer indicated that the work is making progress in trying to elucidate fundamental understanding of low-temperature plasma (LTP) ignition. The plasma-assisted combustion (PAC) community needs to collectively make further progress on offering further insight to the kinetics associated with PAC in order to progress and facilitate numerical studies such as these. The reviewer suggested that developing PAC mechanisms for Co-Optima relevant fuels should be a topic of future DOE funding initiatives.

#### Reviewer 5:

The reviewer proposed that large eddy simulation (LES) should be the next step and added that it would be nice to have seen some preliminary comparisons with LES at the Annual Merit Review (AMR). The reviewer acknowledged that this is a very tough challenge to tackle, which includes plasma chemistry, combustion chemistry, fluid dynamics, and turbulence interaction. There are a lot of questions left to be answered in this topic of research.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer indicated that substantial progress has been made in this project and milestones are on track to be completed. Of the milestones presented, more than 50% of the goal has already been achieved for Fiscal Year (FY) 2019. FY 2020 goals and milestones reflect the natural transition that this project should take and seem viable targets that can be met. Most goals entail simulation for relevant advanced compression ignition (ACI) and cold-start conditions.

#### Reviewer 2:

The reviewer found Slides 5 and 6 to be clear. The progress is good and the choice of topics is excellent.

#### Reviewer 3:

The reviewer remarked that great progress has been made toward the goals of the low-temperature plasma work. The collaborations with Sandia National Laboratories (SNL), industry software developers, and suppliers have helped support the progress. The PIs should continue to dig into some of the issues limiting the progress, particularly in the CONVERGE simulation. The plans outlined in the presentation were good, particularly in the area of plasma chemistry. However, it seemed to the reviewer as though there may be a fundamental limit to capturing these physics with a code like CONVERGE, and the solution to this issue was not addressed.

The reviewer remarked that the project team has made very good attempts to better understand the idea of accurately modeling ignition and combustion phenomena for advanced diluted engines. The reviewer noted that qualitatively the project has made progress, but quantitatively it is lacking, due to the difficulty of plasma chemistry predictions and subsequent ignition and combustion rate predictions.

#### Reviewer 5:

The reviewer found that good progress has been achieved relative to the goals in the project but a lot of additional work and progress needs to be made to simulate advanced ignition strategies.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer commented that the collaboration is excellent with Sandia and Michigan Technological University for experimental results, CONVERGE for the CFD software, Transient Plasma Systems (TPS), and original equipment manufacturers (OEMs).

#### Reviewer 2:

The reviewer indicated that there was excellent collaboration among team members, including National Laboratories, advanced ignition system providers, and OEMs.

#### Reviewer 3:

Efforts to collaborate with industry (small businesses, OEMS, and start-ups), academia, and other National Laboratories were evident to the reviewer. All efforts are complementary to one another, which facilitates the collective efforts to advance simulations tools for commercialization.

#### Reviewer 4:

The reviewer found great collaborations across the National Laboratories, software developers, and suppliers. The reviewer encouraged the PIs to continue to develop relationships with academia, particularly in the area of plasma chemistry. Collaboration with Lawrence Livermore National Laboratory (LLNL) will be good for integrating with neutral chemistry, but there is a lot of expertise in the academic community for plasmas that should be leveraged more heavily.

## Reviewer 5:

The reviewer said that there appears to be significant collaboration with universities, industry, and specialty engine modeling companies.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer stated that the topics of future work are very relevant to the need of industry (plasma and fuel kinetics, thermal plasma solver, spark-assisted compression ignition [SACI], low-temperature plasma advanced compression ignition [LTP-ACI], and pre-chamber advanced compression ignition [PC-ACI]).

## Reviewer 2:

The reviewer said that the project has proposed a natural extension to its current scope of research and has established realistic milestones schedules.

Given the progress so far, the reviewer found the future work plan to be sound and follows a logical path from the current state of the project. The reviewer encouraged future collaborations with experiments, particularly the measurements of plasma chemistry at SNL, as they may help identify pathways for better capturing important physics and chemistry in the models for the low-temperature plasma. The path forward for the other two topics was less clear to the reviewer, particularly the pre-chamber ignition work.

#### Reviewer 4:

The reviewer commented that the project team plans to improve the current of plasma predictions, particularly oxygen (O), as well as subsequent ignition and combustion rate predictions. The reviewer said that these efforts appear to be all analytical and said it would be great and incredibly helpful if the project team could generate a clever experiment to aid in the former plasma constituent predictions.

#### Reviewer 5:

The reviewer observed significantly more outstanding questions in this project. The disparity between CONVERGE CFD simulations and VizGlow is of concern but is expected as these are comparisons from two completely different tools with different governing equations. However, the reviewer thought that the research will benefit with additional experimental data in terms of whether actually a shockwave is seen, e.g., schlieren (or is it a numerical wave in VizGlow). Additional non-intrusive temperature and species field data using optical diagnostics may be helpful in VizGlow model validation (is 3500 Kelvin [K] observation really true). Once this is established, CFD work may be beneficial. The reviewer thought that it is too premature to use detailed CONVERGE simulations at this point. Perhaps only LES in CONVERGE may allude to some results (less diffusion). Additionally, wherever experimental data cannot be acquired, the reviewer recommended investigating whether direct numerical simulations (DNS) will yield any data that can be used for VizGlow validation.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1

The reviewer praised the work as this is exactly the fundamental work that DOE should supporting. Fundamental models such as these will not be pursued by industry. It is a good use of taxpayer dollars.

#### Reviewer 2:

According to the reviewer, having a project focusing on ignition modeling greatly supports the overall goals of the Vehicle Technologies program. The processes that occur during ignition are fundamentally different from those in typical combustion, and so the directed modeling effort in this area allows for deeper investigation of these issues. The reviewer found that it is also good that this modeling effort is directly connected to both commercial codes and implementations of these models into those codes, as well as the manufacturers of ignitors to aid in design.

## Reviewer 3:

The project looked to the reviewer to meet DOE targets by improving ignition, which can enable a 25% increase in engine efficiency, lower pollutant emissions, and more reliable cold start. This is also relevant to assess the current state-of-the-art plasma modeling capabilities and areas where they can be improved.

#### Reviewer 4:

The reviewer asserted that yes, this project does support overall DOE objectives. The objectives are clearly stated on Slide 3, while Slides 4, 5, 6, and 21 clearly show how objectives will be met. The reviewer asked for clarification on Slide 6 (top right on the plot) of what the experimental and simulated data are for all symbols.

#### Reviewer 5:

The reviewer said that the project does indeed support DOE goals of developing future high-efficiency engines for transportation purposes. The reviewer noted that one such area is diluted engines that offer high thermal

efficiency and low emissions, and that this project is an enabler for such engines. The reviewer indicated that one worry is that the inability to predict the plasma composition is insurmountable; thus, this project will have minimal impact to DOE goals.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

According to the reviewer, Slide 5 seems to indicate that resources are okay. This project is well worth funding.

## Reviewer 2:

The reviewer said that all simulation resources, computational power, software, and personnel are at the disposal of the PI to carry out the tasks established.

#### Reviewer 3:

The reviewer stated that the resources allocated for the project are reasonable given the personnel of the project. The project covers a number of disparate topics and so it was unclear to the reviewer how all of them are connected and how much progress is being made on each one. It seemed to the reviewer like the low-temperature plasma is the highest priority, and if this is the case, then the resources are sufficient.

## Reviewer 4:

The reviewer said that funding appears to be enough for completing the various proposed tasks for this particular project.

#### Reviewer 5:

We are just barely scratching the surface of these advanced ignition CFD simulations. The reviewer believed that some additional funding will be beneficial in advancing the science and improving the plasma and CFD models. Additional investment from DOE is warranted for this work.

Presentation Number: ace085
Presentation Title: Low-Temperature
Emission Control to Enable FuelEfficient Engine Commercialization
Principal Investigator: Todd Toops
(Oak Ridge National Laboratory)

## Presenter

Todd Toops, Oak Ridge National Laboratory

# Reviewer Sample Size A total of four reviewers evaluated t

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

## Reviewer 1:

The reviewer remarked that the earlystage development and characterization of fundamentally different approaches to achieve high CO and HC oxidation performance are an important phase of the process to finding viable catalyst solutions in a timely manner to meet future emissions requirements of highly efficient powertrains. For instance, the work developing highly dispersed Pd and platinum (Pt) catalysts to achieve low-temperature light-off of CO and hydrocarbons (HC) supports the need of these low-temperature aftertreatment (LTAT) technologies to meet the OEM requirements during cold start and for

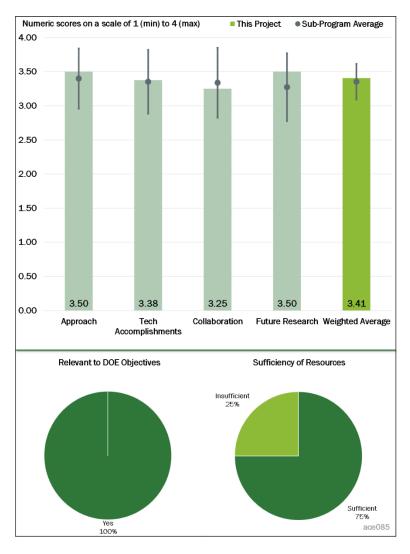


Figure 1-18 – Presentation Number: ace085 Presentation Title: Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization Principal Investigator: Todd Toops (Oak Ridge National Laboratory)

low-temperature portion of drive cycles. The reviewer indicated that this approach is strongly supported by the United States Council for Automotive Research (USCAR) engine and aftertreatment objectives to meet future Tier 3 and low-emission vehicle level III (LEVIII) emissions standards. However, the performance of the catalyst must be able to survive in an exhaust environment for many years, so ensuring the innovative material is robust to thermal and chemical poisons should be addressed at a very early stage to be viable. Additionally, the reviewer said that consideration should be given to the manufacturability of the materials. If the material cannot be produced cost effectively, then it is not a viable solution.

## Reviewer 2:

According to the reviewer, 90% conversion of regulated species at 150°C is a challenging target and pushes the kinetic limits, for which the reviewer said that we will wait and see. It was a nice approach to tackling the challenge and a good mix of material consideration, testing approach, and capitalizing on prior work. The reviewer found this to be good milestone setting for three years. While both hydrocarbon traps (HCTs) and diesel oxidation catalysts (DOCs) are viable technologies, the reviewer stated that the selection process ("why not other technologies") could be more optimal. Selection criteria could be a mix of impact factor (degree of

impact on market or to what extent a newer technology is unknown, etc.) Given that this is the first year of this undertaking, the reviewer commented that it may be fair to argue there may be some ambiguity, needing time to reach its optimal. The audience could benefit from more visible selection criteria.

#### Reviewer 3:

The reviewer stated that this project attacks one of the key barriers to implementing high-efficiency, low-temperature combustion strategies. The 150°C challenge has long been identified as an important issue for the industry, as are issues of durability and poison tolerance. The approach taken in this work—investigating oxidation catalysts, passive NO<sub>x</sub> adsorbers (PNAs), HC traps, and combinations of them—is the logical way to address these issues, according to the reviewer.

The reviewer highlighted one issue that should be addressed, which another reviewer discussed during the live session—for the aging protocol currently being used, 800°C seems overly aggressive for these materials, as compared to what temperatures they may see in use. It would be interesting to the reviewer to have seen the effect of a temperature sweep (between 700°C-850°C, every 25°C) on the material—to understand how sensitive the materials are to temperature excursions—and how much the aging temperature impacts the results shown in Slide 11. This is further underscored by the first bullet on Slide 31.

## Reviewer 4:

The reviewer asserted that low-temperature catalysts are definitely going to be needed for future engines that emit lower exhaust temperatures. It was commendable that the project team is using the catalyst testing protocols from the Advanced Combustion & Emissions Control (ACEC) Tech Team. There was a nice approach at investigating the size of the silicon dioxide (SiO<sub>2</sub>) at zirconium dioxide (ZrO<sub>2</sub>) particles to maximize activity and durability. Also, there was a good approach in including cerium (Ce) and Ce/zirconium (Zr) in the shell to provide some oxygen storage capacity (OSC), which will be needed for stoichiometric operation. For the PNA work, the reviewer suggested that the project team might consider a lower aging temperature than 800°C (e.g., 750°C) for diesel systems that use a downstream fuel injector and an exothermic catalyst for diesel particulate filter (DPF) regenerations. Pd-based PNAs will have a very difficult time surviving 800°C, according to the reviewer.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer stated that the oxidation catalysis work using a SiO<sub>2</sub> core shell foundation is showing improved results with respect to CO oxidation. The project team is making good progress toward the 150°C light-off goal after appropriate aging. This work in the area of highly dispersed Pt/Pd bimetallic catalysts shows promise for lean applications. Therefore, incorporating various versions of the SiO<sub>2</sub> core shell design to achieve improved aged CO and HC performance is desirable. Improving stability of the highly dispersed particles through increased support surface area would appear to be important for this work to be successful. Improving and stabilizing the small Pt and Pd particles would be critical to this work.

The reviewer noted that the catalysts under development for HC and  $NO_x$  trapping are not showing the same level of progress as the oxidation catalyst. It appeared to the reviewer that the materials developed so far for this work are not thermally stable or do not possess the required efficiency to be practical in a vehicle application. Other approaches have proven more successful at this stage and the reviewer suggested that a reevaluation of this work should take that into consideration for either improving this technology or moving to a new material.

#### Reviewer 2:

The reviewer said that there was good work and progress. Material selection is well designed and good progress has been made. The reviewer noted that It is however too early to make a reasonable judgment in regard to "meeting the goal." This is a very challenging problem.

The reviewer observed relevant and interesting technical accomplishments in all areas of the project, even if they were not always promising. The idea that unexchanged zeolites (Zeolite Socony Mobil - 5 [ZSM-5]) could be used as a passive HC trap (with some added thermal stability) is exciting and well poised for relatively quick deployment on the fleet. Referring to the Pd/SSZ-13 material, the reviewer stated that a 4-hour high-temperature regeneration does not seem like a reasonable approach for the application and asked why it was pursued. The reviewer asked how the project team will quantify loss of the Pd-ion exchange sites and whether there is a similar plan to investigate efficacy of the ion-exchange process. Regarding the combined system, the reviewer lacked understanding of why the project team does not see the same loss of the Pd-ion exchange sites.

#### Reviewer 4:

The reviewer was glad that the project team is investigating the gradual loss of performance on repeated tests with the PNAs as it is the greatest challenge today for PNAs. According to the reviewer, the project team may need to go out to 10, 20, or even 50 tests to demonstrate the consistency of the catalyst. Automated reactors are very helpful for this. Rapid cooling systems (e.g., fans and automatic opening of the oven door) can help minimize the cooling time, allowing more tests to be performed in a day.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer found really excellent emphasis on collaboration with university and industry partners.

#### Reviewer 2:

The reviewer indicated that the project team has successfully integrated academia, industry, and other National Laboratories in this project. Collaboration (Slide 8) is wide ranging.

#### Reviewer 3:

The reviewer commented that most of this work was in collaboration with only the University at Buffalo. Collaborations with PNNL and a supplier would have benefited the trapping material development and helped minimize overlap of efforts to produce a viable material.

## Reviewer 4:

Collaborations with Buffalo and Harvard were mentioned, but the reviewer did not see specific examples of these collaborations or other collaborations.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer was really interested in learning more about the approach to investigating the interaction between the support and platinum group metals (PGM) materials. The reviewer said there was significant improvement in the approach by incorporating chabazite and bimetallics.

## Reviewer 2:

The reviewer said that this is a three-year program; only the first year (materials focus and synthesis) has been completed. The goals for the next two years are well specified and stated to be a mix of further explorations, down-selection, and demonstration.

The reviewer commented that the future work proposed for the core shell work is a logical extension of that activity and should yield even better results. The trapping material development requires additional input from another source to yield a better material. Lastly, the reviewer indicated that more consideration should be given to the processing of the material and its viability for cost-effective production.

#### Reviewer 4:

The reviewer suggested that emphasis should be on the gradual deterioration of  $NO_x$  storage efficiency on repeated cold-start tests. Solutions to this deterioration need to be explored, either through catalyst changes or system modifications.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that the development of low-temperature catalysts is critical for allowing fuel-saving engine technologies that generate lower exhaust temperatures to satisfy stringent emission standards, such as Tier 3. HC traps and NO<sub>x</sub> traps will help lean-burn applications, such as diesel engines, to meet low-emission standards.

#### Reviewer 2:

The reviewer remarked that this is relevant, inception-stage research and consistent with the call for low-temperature aftertreatment by USCAR and the needs of the OEMs in general.

#### Reviewer 3:

The reviewer noted that thes project goal is well within the DOE goals, both for the project goal and in terms of good industry involvement in the project.

#### Reviewer 4:

The reviewer stated yes.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer found the project team to be broad and very capable. In all, at ORNL and collectively across the broader team, there appear to exist sufficient capabilities and resources.

## Reviewer 2:

The project team seemed sufficiently funded to the reviewer.

#### Reviewer 3:

The reviewer said that core shell work is proceeding well, but the trap material innovation could benefit from additional collaborators.

#### Reviewer 4:

The reviewer commented that resources may need to be increased to study and solve the cold-start deterioration problem with PNAs.

Presentation Number: ace100
Presentation Title: Improving
Transportation Efficiency through
Integrated Vehicle, Engine, and
Powertrain Research - SuperTruck II
Principal Investigator: Justin Yee
(Daimler Trucks North America)

#### Presenter

Derek Rotz, Daimler Trucks North America

## **Reviewer Sample Size**

A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer found the project to be aligned well to achieve the SuperTruck 2 (ST2) goals of 100% improvement in fuel economy (FE) and 55% brake thermal efficiency (BTE). Each sub-task is well coordinated with the whole project and appears feasible.

## Reviewer 2:

The reviewer was very impressed with the approach throughout this project. Utilizing the A-sample prototype for as much as the project team is doing is very good and makes the second prototype a more robust, mature concept

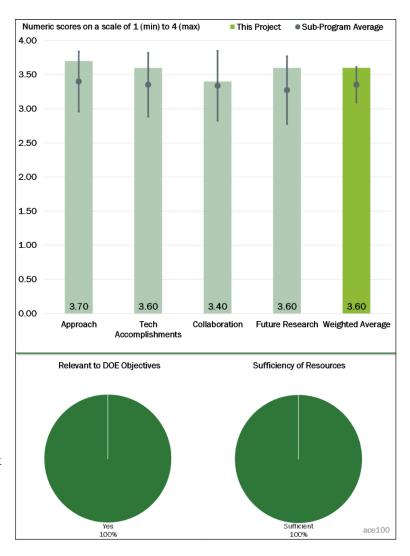


Figure 1-19 – Presentation Number: ace100 Presentation Title: Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research - SuperTruck II Principal Investigator: Justin Yee (Daimler Trucks North America)

than would have been otherwise. The reviewer said there was very good integration work across differing systems to make the necessary tradeoff decisions—good job.

## Reviewer 3:

The approach targets areas for efficiency improvement that the reviewer would expect, with the key challenges being not only advancing technology in each area but systems integration. The use of "main," "stretch," and "investigation" topics is a useful construct for both project design and outside review, according to the reviewer.

#### Reviewer 4:

The approach looked very good to the reviewer, but the vehicle freight-efficiency pathway was not laid out as clearly as that for the powertrain, so this may be just admitted confusion on the part of the reviewer. The ethanol-based phase-change cooling (PCC) system with elimination of the engine coolant circuit is novel and offers high potential, albeit with high risk.

The approaches taken on both vehicle (Slide 4) and engine (Slide 11) sides are impressive, covering all key technology areas, thus providing the best opportunity to achieve the program goals. With these road maps, it seemed to the reviewer that their vehicle goal at 115% would be too conservative, which is the same as the one achieved in SuperTruck1 program.

On the engine side, the reviewer observed that the approach taken with PCC on waste-heat recovery (WHR) and two independent cooling loops is something new and looks promising, although this can really make the system more complicated and may have packaging issues in the real vehicle assembly.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer indicated that the accomplishments are significant and on track for the next phase of making final design decisions and building the main prototype.

#### Reviewer 2:

Both the vehicle and powertrain sub-projects appeared to the reviewer to be progressing well, with hardware build evident toward testing of the first prototype of the final vehicle. The reviewer commended Daimler for pursuing an interesting new WHR system rather than continuing with the ST1 system or using a conventional organic Rankine cycle (ORC) approach. The reviewer hoped to see more detail on the performance and function of the system, particularly the phase-change points in the system (in the head or only in the exhaust gas recirculation (EGR) and exhaust heat exchanger components).

#### Reviewer 3:

The reviewer found that the graph of "Pathway to Reach Aerodynamic Target" on Slide 5 was not legible, even after zooming in. The reviewer assumed that it is the same as the previous graphic on Slide 4. It seemed to the reviewer that aerodynamics is the only area from this graph that has prototype validation completed, but the summary on Slide 2 indicates that phase 3 is 50% completed. According to the reviewer, there seems to be a lot of work remaining in the other areas to validate the simulations and the reviewer expected to see significant achievement in this area next year.

#### Reviewer 4:

Technical progress appeared to the reviewer to be good and advanced well beyond ST1. Powertrain control work appeared to the reviewer to be lagging behind other areas but the team indicated there was some personnel turnover, which is has identified and prioritized as a need.

## Reviewer 5:

It seemed to the reviewer that significant progress has been made on the vehicle side. Aerodynamic and exterior development are moving forward. Although development on dual tires are also coming along, the single-wide base tire would still offer the better opportunity to enhance the program goal. Similarly, this reviewer noted little progress made on model predictive powertrain controls since last year. The same figure has been used again, such as the figure for the intake manifold pressure versus time. It was unclear to the reviewer how this model control approach can help achieve the program goal, and how this program would be integrated with the vehicle and the engine control unit (ECU). The reviewer stated that this is more like a research and development (R&D) program without tangible return, and suggested that more description would be helpful.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer found the collaboration with all partners mentioned on Slide 20 to be excellent.

This reviewer indicated that the project appeared well coordinated with the expected collaboration.

#### Reviewer 3:

The reviewer had no particular issues with the coordination; Daimler is using a wide range of partners to address specific technical areas and the coordination is working well.

#### Reviewer 4:

This looked to the reviewer like a great team with suppliers, a trucking company, a trailer company, National Laboratories, and universities. The powertrain area did a really good job of explaining how these team members were coordinating, but this was not as clear on the vehicle side. Slide 8 could have made this clearer. The reviewer asked what role the National Renewable Energy Laboratory (NREL) has.

#### Reviewer 5:

The reviewer found strong evidence of work with universities and laboratories. The reviewer was a bit concerned that there was no mention of the partnering with the end-user fleet. The reviewer remarked that it would appear, given the requirements of commercialization analysis and finalizing prototype design, that the influence from the fleet would show up here.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The project appeared to the reviewer to be well on a path to meet the ST2 final performance targets, and some interesting new technologies will be brought to the final product assuming the current paths are maintained.

#### Reviewer 2:

The reviewer indicated that significant work to validate the simulated benefits of several technology areas is planned with the demonstrator unit on target.

#### Reviewer 3:

The reviewer noted that the project team is on plan—maybe even a bit ahead and well poised to deliver on the build and testing of the next phase.

## Reviewer 4:

Future projected work appears to be thought out with risk and unforeseen events properly considered. Alternative development pathways were not expressly discussed, but the presentation provided reasonable indications that results-based flexibility would guide future work.

## Reviewer 5:

The reviewer said that it would have been more helpful if the detailed summary and future work had been described in separate slides rather than just using one busy slide (Slide 18) for both engine and vehicle.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

According to the reviewer, achieving at least 115% improvement goal on the vehicle side plus 55% BTE on the engine would clearly support DOE objectives.

The reviewer indicated that the project meets the DOE goal by demonstrating 55% BTE and freight efficiency of 115% from baseline.

#### Reviewer 3:

The reviewer stated that SuperTruck 1 (ST1) and ST2 are addressing the biggest consumer of fuel, which is long-haul trucking.

#### Reviewer 4:

The reviewer stated yes, this work clearly supports DOE objectives by advancing efficiency-improving technologies and concepts. It is designed to reach the DOE-established goals and provides opportunities for rapid commercialization of some technologies or approaches.

#### Reviewer 5:

The reviewer had no particular comment.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

The reviewer commented that the budget breakdown on Slide 2 does not indicate any excess or shortages.

#### Reviewer 2:

Resources appeared to the reviewer to be in line with previous efforts and appropriate for the ST2 objectives.

#### Reviewer 3:

The reviewer said the project team has all it needs to achieve the program goals.

## Reviewer 4:

The reviewer was rather surprised that the Daimler Trucks North America (DTNA) and Detroit share is being maintained at the 50% of total project value level. The work performed looked to the reviewer like it would have required significantly more spend.

## Reviewer 5:

This reviewer described project resources as sufficient.

Presentation Number: ace101
Presentation Title: Volvo SuperTruck
II: Pathway to Cost-Effective
Commercialized Freight Efficiency
Principal Investigator: Pascal Amar
(Volvo Trucks North America)

#### Presenter

Pascal Amar, Volvo Trucks North America

## Reviewer Sample Size

A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

## Reviewer 1:

The reviewer praised the approach as outstanding, with much evidence of the team tackling some major systems-level decisions. They include such items as the continued decision to incorporate an aluminum frame and 19.5-inch tires.

## Reviewer 2:

The reviewer commented that the approach targets areas for efficiency improvement that the reviewer would expect, with the key challenges being not only advancing technology in each area but systems integration and tradeoffs.

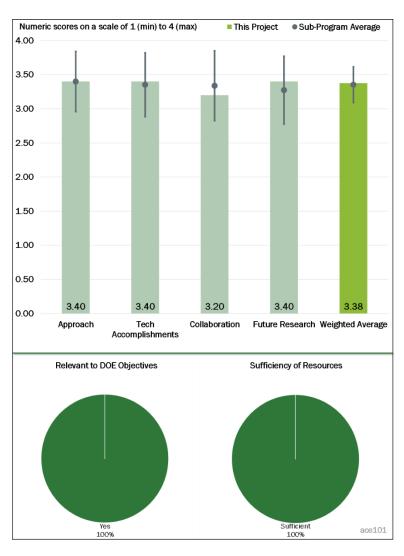


Figure 1-20 – Presentation Number: ace101 Presentation Title: Volvo SuperTruck II: Pathway to Cost-Effective Commercialized Freight Efficiency Principal Investigator: Pascal Amar (Volvo Trucks North America)

#### Reviewer 3:

The reviewer stated that a clear, multi-faceted approach was presented. According to the reviewer, it was good to see most of the technology in the 55% BTE demonstrations going into the vehicle freight-efficiency demonstrator.

#### Reviewer 4:

The reviewer indicated that the approaches taken on both vehicle and engine side are comprehensive, covering all key technology areas, thus providing the best opportunity to achieve the program goals. With these road maps, it seemed to the reviewer that the vehicle goal of 100% would be too conservative, even though 120% as a stretch goal was mentioned.

## Reviewer 5:

The program plan appeared to the reviewer to be designed to meet the ST2 performance targets. The reviewer found that there does not appear to be much effort into novel technologies that really leverage the DOE funding to go beyond fairly typical production technology paths though.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that technical progress was clearly laid out and looks great.

#### Reviewer 2:

The reviewer said that technical progress appears to be good and advanced well beyond ST1.

#### Reviewer 3:

The reviewer found that the accomplishments shared show good progress on meeting the program deliverables. Lack of any status on vehicle-level metrics is a big concern in that reviewers have no means to validate that the accomplishments are being made against the objectives required of the program. The reviewer expected that this was a minimum requirement of this review.

#### Reviewer 4:

The reviewer stated that it was impossible to really evaluate the technical accomplishments and progress. The vehicle design does show some good progress toward a first build and some interesting approaches to reducing weight (the structural element air tanks, for instance). Almost no real information on the hybrid benefit is noted, even from a simulation perspective. For the powertrain, the technical path appeared to the reviewer to be primarily an extension of the ST1 plan, and there are no real numbers to evaluate where the engine is at for BTE either from a simulation or experimental perspective. On the whole, the reviewer said that the project progress appears workmanlike but not particularly exciting relative to some of the reported progress from other ST2 teams.

#### Reviewer 5:

The reviewer indicated that significant progress has been made on the vehicle side, specifically on weight reduction, tires, and aerodynamic development. In addition, the demonstration vehicle is being built. On the engine side, it was again disappointing to the reviewer to see that there is no report on the BTE progress with a specific BTE number, making the reviewer wonder about the exact status. Although some progress has been made on thermal barrier coating and combustion, it was not clear to the reviewer how much these technologies can really help the BTE goal. It was not convincing to the reviewer why a pre-turbo catalyst is being used in the program where it can really build up back pressure, thus hurting engine performance for normal on-highway operation at high loads.

Ouestion 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1

The reviewer noted that the project appears to be well coordinated and with expected collaboration.

#### Reviewer 2:

This reviewer pointed out that there is a slide indicating what the various team members are responsible for, but they are not noted under any of the technical accomplishment slides. Subsequently, it was not possible for the reviewer to evaluate if they are really contributing anything toward the final work product or not.

## Reviewer 3:

The reviewer indicated that the Michelin, University of Michigan, Metalsa, Johnson Matthey, and Oak Ridge collaborations were very clear and look very good. Although listed on Reviewer-Only Slide 22, it was not clear to the reviewer what the rest of the collaboration team had contributed or how they were involved.

This reviewer observed solid evidence of collaboration across the universities and labs. During the presentation, there was reference to working with two fleets. Although more discussion or proof of those enduser discussions helping with key decisions was expected, this reviewer expected that they are occurring.

#### Reviewer 5:

The reviewer commented that it would have been helpful if one slide had been dedicated to the collaboration for all partners involved in this program, although this slide is actually shown in Slide 22 as the Reviewer-Only slide. Perhaps, the reviewer suggested, it would be helpful in the future if individual icons of each company or organization appear in any slides that are associated with their work or contribution.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer stated that the upcoming year was clearly laid out for each technical area.

#### Reviewer 2:

According to the reviewer, future work is planned and has a high likelihood of delivering success to the targets. The reviewer expects next year to see proof of freight efficiency and which decisions are influencing the outcomes by what percentage.

#### Reviewer 3:

The reviewer commented that future projected work appears to be thought out with risk and unforeseen events properly considered. Alternative development pathways were not expressly discussed but the presentation provided reasonable indications that results-based flexibility would guide future work.

#### Reviewer 4:

The reviewer was confident that the project will achieve the technical goals of ST2 on time, but there is a lot to be completed that is only very roughly defined in terms of what exactly the truck will look like or what contribution each element will provide toward the final result.

## Reviewer 5:

The reviewer found that no dedicated slides are used to summarize the future work, although the reviewers can get a vague sense from (Slide 3 on Schedule & Phasing).

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated yes, this work clearly supports DOE objectives by advancing efficiency-improving technologies and concepts. It is designed to reach the DOE-established goals and provides opportunities for rapid commercialization of some technologies or approaches.

## Reviewer 2:

This reviewer responded that yes, the project meets DOE goals by demonstrating 55% BTE and 100% freight-efficiency improvement.

## Reviewer 3:

According to the reviewer, achieving 100% improvement goal on the vehicle side plus 55% BTE on the engine would clearly support DOE objectives.

The reviewer indicated that ST1 and ST2 are addressing the biggest need—long haul trucking—which consumes the majority of all commercial vehicle fuel.

## Reviewer 5:

This reviewer stated no particular comment.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer commented that resources appear to be in line with previous efforts and appropriate for ST2 objectives.

## Reviewer 2:

The reviewer stated that the project team has all that is needed to achieve program goals.

## Reviewer 3:

The reviewer mentioned that FY 2019 funding was not included on Slide 2, but the project would seem to be on schedule for the total project.

#### Reviewer 4:

No particular comment was indicated by this reviewer.

## Reviewer 5:

This reviewer observed sufficient project resources.

Presentation Number: ace102
Presentation Title: Cummins-Peterbilt
SuperTruck II
Principal Investigator: Jon Dickson
(Cummins-Peterbilt)

Presenter
Jon Dickson, Cummins-Peterbilt

Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer indicated that using the new engine with numerous advanced technical features substantially increases the chance to meet the program goal at 55% BTE. On the vehicle side, it clearly shows the excellent approach and road map (Slide 18), demonstrating how the vehicle improvement goal could be achieved.

## Reviewer 2:

The reviewer mentioned that Cummins is indicating that they see a path to significantly exceed the ST2 targets and plan on demonstrating 55% BTE on the truck engine along with 125-150% FE improvement. The projections appeared

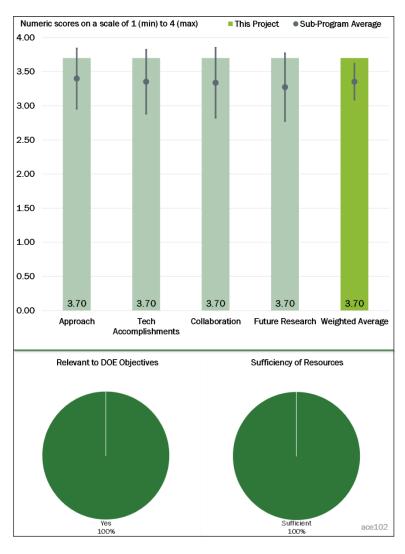


Figure 1-21 – Presentation Number: ace102 Presentation Title: Cummins-Peterbilt SuperTruck II Principal Investigator: Jon Dickson (Cummins-Peterbilt)

reasonable to the reviewer and this is a major jump over the targets of the program.

## Reviewer 3:

The approach targets areas for efficiency improvement that the reviewer would expect with the key challenges being not only advancing technology in each area but systems integration. This project team's approach appeared to the reviewer to be providing a slightly greater emphasis on technologies and opportunities for near-term commercialization. This can be a benefit to the ST2 effort as well as the individual team.

## Reviewer 4:

The reviewer found the graph on Slide 9 to be confusing. Without scales on the x or y axis, the reviewer was not sure what message should be taken away from it except that less engine work per mile is better and higher engine BTE is better. According to the reviewer, the rest of this year's presentation is short on the details of the approach compared to last year's presentation, which the reviewer clearly understood.

The reviewer praised the outstanding approach to engine and powertrain work, but questioned the vehicle-level work as there is not as much evidence of efforts. The reviewer suggested that possibly there was too much reliance on reducing weight against the baseline rather than improving fuel use through technologies to meet the goal.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer stated that a number of specific accomplishments have been noted in the program, which include numeric statements on their benefits. It was good for the reviewer to see hardware under test with results so early in the program so that there can be some confidence in reaching the ST2 goals without a final-hour thrash to finish testing and development. The reviewer noted that having the 50% BTE milestone achieved so early in the program is also good. Other teams indicated that they have done so as well, but did not document it or back it up with data.

#### Reviewer 2:

The reviewer observed that the Cummins-Peterbilt team is really overachieving in ST2. The reviewer said that it was exciting to see them pushing the limits up toward theoretical maximum efficiency.

#### Reviewer 3:

The reviewer found solid accomplishments. According to the reviewer, particularly noteworthy is that Cummins plans to install the 55% BTE engine into the final prototype.

#### Reviewer 4:

The reviewer remarked that technical progress appears to be good and advanced well beyond ST1.

## Reviewer 5:

It was impressive to the reviewer that 50% BTE goal has been already achieved. Slide 11 clearly quantifies how this was achieved. A lot of the progress has been made on many areas of the vehicle side. The demonstration vehicle is being built.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

Not only is there a long list of collaborators, which there must be for a project of this scope, but there were a number of callouts that noted specific successes with the collaborators and documented the achievements from the partnerships.

## Reviewer 2:

The reviewer found good evidence of collaboration across the universities, labs, component manufacturers, and end-user fleet.

## Reviewer 3:

The project appeared to the reviewer to be well coordinated and with expected collaboration.

## Reviewer 4:

The reviewer indicated that this is a great team with extensive working collaborators and market inputs. The reviewer still did not understand the purpose of having both Slides 25 and 26.

Although Slide 25 shows how the partners contributed to the program, the reviewer suggested that it would still be helpful in the future if individual icons of each company or organization appear in any slides that are associated with their work or contribution.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

It is very exciting for the reviewer to see the plan for the 55% BTE engine to be in the final demonstrator truck, which is a significant leap past the ST2 targets and what most predicted would be feasible. The projected weight savings and other developments leading to a higher than required FE gain are also very promising.

#### Reviewer 2:

The reviewer asserted that Slide 12 on Approach for 55% BTE provide a good sense on how the engine can achieve 55% BTE in the near future. In addition, Slide 28 summarizes what it needs to be done in order to achieve 55% BTE goal and 125% FTE improvement goal.

#### Reviewer 3:

Proposed work looked excellent to this reviewer. The Driver Environment (Slide 24) is puzzling as to how this work contributes to the DOE efficiency improvement other than the aerodynamic design impact on these features.

## Reviewer 4:

The reviewer stated that future projected work appears to be thought out with risk and unforeseen events properly considered. Alternative development pathways were not expressly discussed but the presentation provided reasonable indications that results-based flexibility would guide future work.

#### Reviewer 5:

The reviewer expressed concern about the breadth of vehicle-level work being done with this project.

Ouestion 5: Relevance—Does this project support the overall DOE objectives?

## Reviewer 1:

The reviewer emphatically praised that DOE objectives have been met and exceeded with greater than 55% BTE demonstration, 125% freight efficiency demonstration, and putting the 55% BTE engine system in the demonstration vehicle.

#### Reviewer 2:

Very much so was the response from the reviewer. Long-haul trucking consumes a great deal of fuel and ST1 and ST2 are making a huge difference across the industry.

## Reviewer 3:

The reviewer stated yes, this work clearly supports DOE objectives by advancing efficiency-improving technologies and concepts. It is designed to reach the DOE-established goals and provides opportunities for rapid commercialization of some technologies or approaches.

## Reviewer 4:

According to the reviewer, achieving 125% improvement goal on the vehicle side plus 55% BTE on the engine would clearly support DOE objectives.

The reviewer stated no particular comment.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

Budget and spending are on track, according to the reviewer.

## Reviewer 2:

The reviewer commented that resources appear to be in-line with previous efforts and appropriate for the ST2 objectives.

## Reviewer 3:

The reviewer remarked that the project team has all they need to achieve the program goals

## Reviewer 4:

The reviewer had no particular comment.

## Reviewer 5:

This reviewer observed sufficient project resources.

Presentation Number: ace103
Presentation Title: Development and
Demonstration of a Fuel-Efficient
Class 8 Tractor and Trailer
SuperTruck
Principal Investigator: Russell
Zukouski (Navistar)

Presenter Russell Zukouski, Navistar

Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer stated that the approach is very strong to deliver the objectives.

#### Reviewer 2:

The reviewer found that the approach is comprehensive and explores many aspects of the vehicle to achieve freight-efficiency targets, including those for the engine, trailer, and tractor. There was interesting use of the ST1 vehicle for development and testing, according to the reviewer, and a good introduction of a 48-volt (V) system for support. Selective catalytic reduction (SCR) optimization will have practical

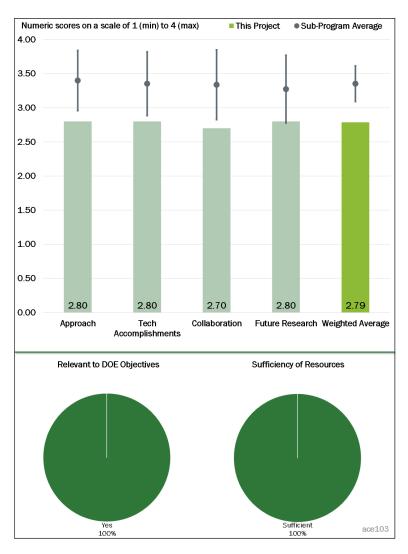


Figure 1-22 – Presentation Number: ace103 Presentation Title: Development and Demonstration of a Fuel-Efficient Class 8 Tractor and Trailer SuperTruck Principal Investigator: Russell Zukouski (Navistar)

benefits. The gasoline compression ignition (CI) work at Argonne National Laboratory (ANL) could produce interesting results but it did not seem to the reviewer to be a direct contributor to the main targets of the project.

## Reviewer 3:

The reviewer commented that the project may be doing better than it seems, but the slides presented provided almost no information or data to indicate that the technical barriers are being addressed or that the project is focused on technology development that would impact the final truck. According to the slides, the powertrain task looked to the reviewer like various engine changes are being tested and they sometimes show a benefit but sometimes do not. The vehicle side looked to the reviewer like it is farther along, but again there are no really solid metrics to see if the approach looks sufficient.

#### Reviewer 4:

The reviewer commented that the approach targets areas for efficiency improvement that the reviewer would expect, with the key challenges being not only advancing technology in each area but also systems integration. The project team approach was broader than others and included both diesel and gasoline technologies; this

supports ST2 goals. The reviewer noted that the team discusses how its approach identified and evaluated these concepts and then ultimately selected its ST2 truck pathway. The reviewer asked how the resources used to explore the technology pathways not selected provided insight of benefit to ST2, 21st Century Truck (21CT), and other DOE programs.

#### Reviewer 5:

The reviewer mentioned that the approach taken on the vehicle (Slide 15) side covers all key technology areas, thus providing a reasonably good opportunity to achieve the program goal. However, it was not clear to the reviewer why a gasoline engine is being used in this program. Although it can be still efficient in one single mode or even multiple points, the reviewer said that it is highly questionable if this engine can work well in a transient operation, not to mention how this engine would be integrated with the vehicle in achieving the program goal. The reviewer hoped that one or a few slides would be used in the future to address the reviewer comments from last year's review.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

Technical progress appeared good to the reviewer and advanced well beyond ST1.

#### Reviewer 2:

The reviewer found good progress on WHR, lightweighting designs, SCR improvement, and adaptive cruise control. The minimal success with a low heat-transfer cylinder liner was somewhat predictable, which the reviewer said was a good effort toward a long-standing unresolved barrier.

According to the reviewer, a shortcoming is lack of quantitative information, such as in the waterfall chart on Slide 15. It was difficult for the reviewer to assess progress or impact of steps in approach.

#### Reviewer 3:

The reviewer remarked that the presenter indicated that the project team had measured 50% BTE in the laboratory, but nothing was noted in the slides to document this. There is also no real documentation of either predicted or measured improvements in vehicle weight, aerodynamics, or anything else. The reviewer stated that it was really impossible to measure progress toward the goal.

## Reviewer 4:

There is evidence of progress against the goals for the engine, but not the total vehicle. Without a vehicle-level status to freight-efficiency targets, it was difficult for the reviewer to evaluate the progress of this project versus the overall goals. The reviewer expected that it is there, but unfortunate that it is not shared.

## Reviewer 5:

The reviewer indicated the PI provided a lot of details regarding progress on the vehicle side, such as aerodynamics, weight reduction, vehicle cooling, and cruise control, which seem to point toward the program goal. However, on the engine side, progress with the gasoline engine shown in Slide 12 only includes one mode point. The reviewer stated that the lack of performance data in the transient operation makes this program goal questionable. The aftertreatment device (Slide 13) seemed to use one long box in a sequence manner, which is not efficient packaging. Additionally, it was not clear to the reviewer whether the hardware of the WHR system is being procured or is just in the simulation stage; this is critical because of the long lead time to get the hardware and test it. More description would have been helpful to this reviewer.

## Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer said that partners were noted, but no real accomplishments or interactions with any of them was noted in the presentation aside from a slide on the gasoline compression ignition (GCI) engine. However, the presenter indicated that the GCI engine was being wound down and that it was not the prime path for the truck. It was also unclear to the reviewer that the GCI engine was in the running for the 55% BTE engine, so it was not clear that the partnership with ANL has provided any value to the project at all.

#### Reviewer 2:

Although a broad project team is named, the reviewer commented that the discussion and slides do not reveal a very dynamic team approach. The reviewer wondered if there is an aftertreatment supplier on board. Dana and Timken are mentioned, but the member roles are not all explained.

#### Reviewer 3:

The reviewer noted evidence of working with labs and universities. There is limited evidence of working with suppliers and no mention of an end-user fleet involved in this project at all, which is unfortunate because the reviewer expected that their input on major system and design decisions would be shared in this review.

## Reviewer 4:

Overall coordination is likely sufficient, but this reviewer observed some disconnect with regard to the development and de-selection of the gasoline alternative concept. It was not clear to the reviewer whether there was room for improved collaboration during the parallel diesel and gasoline development and selection-deselection process. All project team members should be aware of why alternatives are picked for exploration, how they are evaluated, how the work may have value beyond the ST2 truck, and why the team ultimately chose one pathway or another.

#### Reviewer 5:

Although Slide 3 shows all partnerships with the program, it was not clear to the reviewer how individual companies help in the program. Also, the reviewer suggested that it would be helpful in the future if individual icons of each company or organization appear in any sides that are associated with their work or contribution

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The future research and remaining challenges appeared to the reviewer to be well understood and are adequately included in the timeline for the project. The reviewer said that the gaps in quantitative results leave some question about potential success in reaching the project overall targets.

#### Reviewer 2:

Future projected work appeared to the reviewer to be thought out with risk and unforeseen events properly considered. The reviewer said that alternative development pathways were not expressly discussed but the presentation provided reasonable indications that results-based flexibility would guide future work.

## Reviewer 3:

The reviewer indicated that the plan going forward looks viable and strong, but not knowing the status against plans, it was difficult for the reviewer to have confidence in the future research plans.

The reviewer commented that the current work plan does not even indicate that any buildup will happen until year 4, so it was not clear to the reviewer how the current work plan will be successful since there are no intermediate milestones indicated to measure against.

#### Reviewer 5:

The reviewer noted that Slide 21 summarizes the proposed future research. However, the reviewer found nothing to address transient operation optimization with the gasoline engine if this engine were to be a backup engine.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated that achieving a 100% improvement goal on the vehicle side plus 55% BTE on the engine would clearly support DOE objectives.

## Reviewer 2:

The reviewer stated yes, this work clearly supports DOE objectives by advancing efficiency-improving technologies and concepts. It is designed to reach the DOE-established goals and provides opportunities for rapid commercialization of some technologies or approaches.

## Reviewer 3:

According to the reviewer, medium- and heavy-duty vehicle (MHDV) freight efficiency is critical to national economic competitiveness, reduced petroleum dependence, and reduced climate impact.

#### Reviewer 4:

The reviewer remarked that long-haul trucks consume a great deal of fuel and the focus of ST1 and ST2 is clearly delivering improvements in the industry.

## Reviewer 5:

No particular comment was indicated by this reviewer.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer noted that resources appear to be in line with previous efforts and appropriate for the ST2 objectives.

## Reviewer 2:

The reviewer said that resources are sufficient, but it was difficult to have a lot of confidence given the lack of information about vehicle-level status.

## Reviewer 3:

The resources seemed to be satisfactory to the reviewer for the project, who suggested that perhaps a higher budget could permit higher innovation. On the other hand, greater use of simulation and virtual testing could be advantageous for efficient use of resources.

#### Reviewer 4:

The reviewer indicated that resources may be sufficient on the vehicle side, but the reviewer was not sure resources would be sufficient on the engine side because of uncertainty about the use of the gasoline engine for this program and lagging development on WHR.

Teviewer 5:  To particular comment was stated by this reviewer.	

# Presentation Number: ace118 Presentation Title: CLEERS Passive NOx Adsorber (PNA) Principal Investigator: Janos Szanyi (Pacific Northwest National Laboratory)

#### Presenter

Janos Szanyi, Pacific Northwest National Laboratory

## Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-

#### Reviewer 1:

planned.

The reviewer remarked that the PNNL project team has focused on an important, emerging technology that holds promise for capturing cold-start  $NO_x$  emissions to achieve more stringent Tier 3 LEVIII standards for light duty vehicles. The reviewer said that it is desirable to see more resources placed on a smaller number of technologies that have demonstrated viability for vehicle powertrains. Since PNA catalysts are normally located upstream of complementary catalysts in an exhaust system, they must be both thermally stable and poison resistant. It

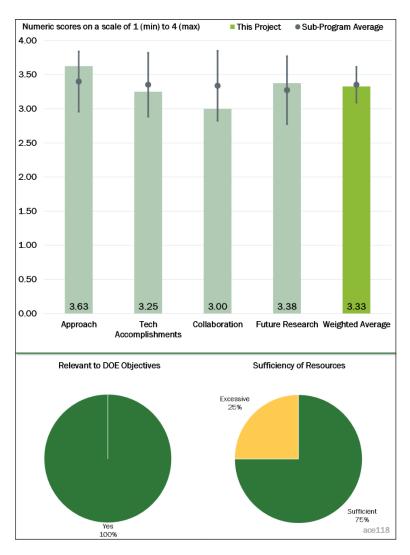


Figure 1-23 – Presentation Number: ace118 Presentation Title: CLEERS Passive NOx Adsorber (PNA) Principal Investigator: Janos Szanyi (Pacific Northwest National Laboratory)

appeared to the reviewer that this work is addressing those concerns as the team develops the PNA technology. Also, this team has incorporated a great degree of understanding of adsorption and release mechanisms as well as aging mechanisms. According to the reviewer, what the team has learned is critical to appropriately optimizing the catalyst formulation and approach. Additionally, new insight is provided with respect to larger pore zeolites and their benefits and drawbacks by team's systematic approach to characterizing this technology.

## Reviewer 2:

The reviewer offered that this was a nice approach to investigating the cause of deactivation of the Pd/PNA and thanked the project team for looking at the effect of sulfur dioxide  $(SO_2)$  poisoning proactively.

#### Reviewer 3:

The reviewer found this to be a very scientific approach along with sound testing and high-resolution analysis. It was a good mix of well-designed project fundamentals, evaluation, and test protocols. The reviewer said that it was a well-designed project and has clear milestones, good execution, and clear deliverables and timeline.

It somewhat surprised the reviewer that this is an Energy Efficiency and Renewable Energy Vehicle Technologies Office (EERE VTO) project rather than a Basic Energy Sciences (BES) project based on the approach taken in this work. The reviewer commented that the PNNL catalysis group does really awesome fundamental work—it just often seems rather far from application. This reviewer noted reviewer comments from previous years that reminded the project team to add water into the gas mixture when evaluating materials. The approach taken in this project does not really seem to be well aligned with the application or with that taken by the industry.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer praised the great job of improving the dispersion of the Pd in SSZ1-13 and achieving a NO/Pd ratio of 1.0. The reviewer highlighted the nice assessment of the effect of the silica to alumina ratio (SAR) on the durability of the SSZ-13 PNA and said that it was interesting that the lower SAR of 6 provided the best durability on Slide 9, as higher SARs (i.e., lower amounts of aluminum [Al]) usually provide greater thermal durability. Also, there was good work in improving the durability of the BEA passive NO<sub>x</sub> adsorber (PNA) with large crystalline size.

#### Reviewer 2:

The reviewer commented that there was very good progress on two fronts: understanding the effects of aging and the deactivation mechanisms; and improving the formulation and support for increased PGM utilization for nitric oxide (NO) trapping and preserving aged performance. According to the reviewer, this work has demonstrated impressive NO<sub>x</sub> storage per Pd atom, which suggests that the team understands how to prepare highly dispersed and active Pd catalysts that are stable. Continuing to optimize the capacity, PGM utilization, durability, and uptake and release characteristics should yield a viable technology. The reviewer suggested that careful consideration should be given, especially to sulfur tolerance and aging mechanisms.

## Reviewer 3:

The reviewer said that the accomplishments seem reasonable for the funding.

## Reviewer 4:

The reviewer found that good progress has been made but some details are missing. One of the goals is to "demonstrate greater than 95%  $NO_x$  adsorption within 3 mins at  $100^{\circ}$ C and release at greater than 200°C (go/no-go decision)," originally targeted by September 30, 2019 (Slide 5). According to the reviewer, this goal is a key differentiator. Although good progress has been made, sufficient information was unavailable to allow an objective assessment of whether adequate progress has been made to assess whether that goal would be met.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

According to the reviewer, partnering with a supplier that is actively developing this type of PNA is very appropriate. Coupling the supplier's formulation capability with the testing and characterization abilities of PNNL is an excellent combination of resources. However, the reviewer commented that there are other suppliers that are further along in developing this technology that might be more appropriate. Also, it appeared to the reviewer that ORNL is developing a similar technology. This is a case where there might be an opportunity to co-develop this technology to minimize overlap of effort and maximize resources.

## Reviewer 2:

The breadth of collaboration seemed reasonable (Slide 14) to the reviewer as 9 other entities are highlighted. However, only a list is provided; no detail is given (except for PNNL being the lead) on who is doing what (receiving information only, assisting with testing, with analysis, planning). A simple "responsible,"

"approving," "supporting," "informed," and "consulted" (RASIC) chart would have helped the reviewer quite a bit to highlight the role of each party in the overall project.

#### Reviewer 3:

The reviewer noted the collaboration with ORNL via Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS), but pointed out that it is unclear how PNNL is active in the organization of CLEERS. BASF came on as an industrial partner, which the reviewer said was promising, but it was hard to evaluate how much coordination and collaboration is occurring to date. The reviewer questioned the lack of OEM or academic partners. From the standpoint of meeting the VTO mission, it would be nice to see a pathway to application from this work (otherwise, it seems to be more BES than EERE) and university collaboration is always a plus.

## Reviewer 4:

Although collaboration with ORNL regarding coordination of CLEERS activities (annual conference and monthly conference calls) was mentioned, this reviewer saw no evidence of collaboration on technical matters.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

## Reviewer 1:

The reviewer mentioned that future work is well planned (Slide 16), and barriers are identified (Slide 15).

#### Reviewer 2:

The reviewer found that focusing on PGM utilization and increased dispersion is appropriate and desirable. Given the current environment of high precious metal costs, minimizing the use of Pd is of significant interest to automotive OEMs. However, the reviewer noted that incorporating large-pore zeolite development into the project may not be as desirable. HC effects on the zeolite and Pd sites may be detrimental to the activity of the catalyst for NO<sub>x</sub> trapping. The reviewer suggested that more consideration of the drawbacks of this approach and ways to overcome those potential pitfalls is needed.

#### Reviewer 3:

The reviewer highlighted the urgency of investigating the loss of NO<sub>x</sub> storage efficiency on repeated cold-start tests. It is the greatest challenge for PNAs today and is currently a barrier to implementing PNAs on production vehicles.

## Reviewer 4:

Again, from the standpoint of meeting the EERE VTO mission, the reviewer said that it would have been nice to see a pathway to application from this work (otherwise, it seems to be more BES than EERE). The reviewer continued to struggle to see the path toward application.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer found the project to be highly relevant for low-temperature  $NO_x$  remediation catalysts to meet cold-start emissions and to achieve Tier 3 LEVIII emissions standards going forward.

#### Reviewer 2:

The reviewer said that PNAs will be critical for meeting strict emission standards with advanced engine technologies that improve fuel economy but also produce lower exhaust temperatures.

At present, PNA appears to be a viable technology though the reviewer stated that it is hard to say at this point whether PNA will have the same wide-ranging impact as some other technologies did upon their introduction (e.g., DOC or DPF). It is the opinion of this reviewer that, when it is all done and good, PNA will have a rather limited range of applications and will not have such wide-reaching impacts as SCR, DPF, DOC, or other equipment. Nonetheless, the reviewer commented that it is fair to argue currently that exploring PNA potentials and efficiency would fall well within the DOE targets. While for now advances on PNA are well warranted, the reviewer remarked that progress in low-temperature SCR is however a competition and may prove PNA irrelevant in the coming years. This needs more time to become clear.

#### Reviewer 4:

Question 6: While the project supports overall DOE objectives, the reviewer commented that it does not necessarily support the EERE VTO goals. This project seems significantly more BES focused. When the reviewer looked at the listed "Relevance" bullet points, they fail to match relevance on all accounts. Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

This reviewer commented that project resources seemed to be sufficient.

#### Reviewer 2:

The reviewer indicated that the team, and especially those at the PNNL catalyst lab, have access to world-class instruments well suited to this undertaking. Further, this reviewer observed no apparent resource risk.

#### Reviewer 3:

Although resources are sufficient, the reviewer noted the project team would benefit from a collaboration with ORNL in developing this technology as long as project restrictions do not restrict technology information sharing.

#### Reviewer 4:

Referencing prior comments, this reviewer stated that it is unclear why PNNL funded for efforts that ORNL is leading in terms of CLEERS coordination. This is a BES project from this reviewer's perspective. Although the reviewer emphasized that it is very good work, it is significantly more fundamental. It is getting better in the proposed future work—more toward application

Presentation Number: ace119
Presentation Title: Development and
Optimization of a Multi-Functional
SCR-DPF (Selective Catalytic
Reduction-Diesel Particulate Filter)
Aftertreatment System for HeavyDuty NOx and Soot Emission
Reduction
Principal Investigator: Ken Rappe
(Pacific Northwest National
Laboratory)

#### Presenter

Ken Rappe, Pacific Northwest National Laboratory

## Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer found this to be an interesting approach at using an oxidation component within the SCR catalyst to generate NO<sub>2</sub> in situ for the fast SCR reaction while maintaining and using NO<sub>2</sub> from the DOC for soot oxidation.

#### Reviewer 2:

The reviewer indicated that this continued cooperative research and development agreement (CRADA) (this must be the second CRADA renewal as

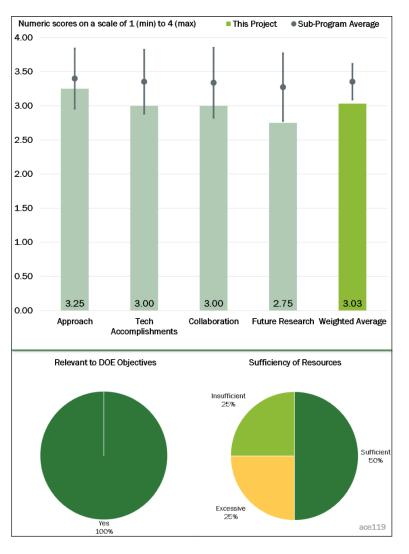


Figure 1-24 – Presentation Number: ace119 Presentation Title:
Development and Optimization of a Multi-Functional SCR-DPF (Selective Catalytic Reduction-Diesel Particulate Filter) Aftertreatment System for Heavy-Duty NOx and Soot Emission Reduction Principal Investigator: Ken Rappe (Pacific Northwest National Laboratory)

this project has been going on for a while) follows an interesting approach to integrating aftertreatment components in order to reduce the number of components used in the system. The project began back in approximately 2010 with a focus on combining the SCR and DPF by coating SCR catalysts onto a DPF, and now is working on changing the materials to encourage additional passive soot oxidation.

## Reviewer 3:

The reviewer commented that the use of multifunctional catalysts to reduce the aftertreatment footprint, while maintaining or improving thermal maintenance and emissions performance to meet more stringent standards, is highly desirable to OEMs. Incorporating SCR into a DPF is a logical and useful extension of this concept. Including a component-level understanding of the washcoat effects on the catalyst behavior, together with a systems approach, is valuable information for OEMs. However, the reviewer suggested that a thorough study of the effects of both thermal and chemical poisons on the catalyst performance is needed before a technology progresses too far down the development pathway to avoid wasting time and effort.

The presentation was somewhat confusing to this reviewer, who commented that slides better be limited to having one to two figures reflecting the key message; three to four figures on one slide does not help comprehension, and the bullet-point messages do not cut straight to the point. It was hard for the reviewer to follow a "coherent story."

Slide 10 includes graphs of standard and fast SCR (on left) and standard SCR again on the right. One can infer that the graph on the right is the same standard SCR turned into fast SCR due to selective catalytic oxidation (SCO); but, then, the reviewer asked why it is still yielding only approximately 40% conversion at about 300°C. The reviewer wanted to know about the efficiency or whether this is still work in progress. Additional information would have been helpful to the reviewer in highlighting the outcome.

If the project has been ongoing since 2016, the reviewer questioned why it is then only 68% complete. The reviewer also asked what the reasons are for what appears to be modest outcome relative to the existing state of the art as SCR-on-DPF has been in the works in the industry for more than 10 years by now.

The reviewer reported that Slide 9 displays 10% manganese dioxide (MnO<sub>2</sub>)-on-ZrO<sub>2</sub> in copper (Cu)-chabazite (CHA) yielding a 95% NO<sub>x</sub> conversion efficiency at approximately 220°C (impregnated or physically mixed). This was puzzling because commercial SCR catalysts do not yield such efficiency, let alone SCR-on-DPF. The reviewer stated that it then again begs the question about the benchmark to which the SCO-based formulation is being compared.

Because the project last year focused on using barium (Ba) to promote the storage of NO<sub>x</sub>, the reviewer wanted to know what happened to pursuing Ba as there was no information available to assess why that path appears discarded now. Another missing link or "room for improvement," is to have a solid "baseline." SCR-on-DPF is now a commercial product (especially on light-duty vehicles in Europe); subsequently, the reviewer questioned why a commercial product from a catalyst supplier was not used as a baseline so that performance of the SCObased SCR could be benchmarked. While the reviewer appreciated the complexity of the R&D stage, having a clear benchmark, metric of comparison, or "end target" is critical to knowing which direction the project and R&D must shoot for. That said, the reviewer commented that the concept of using manganese (Mn)/Zr in SCR to promote NO-to-NO<sub>2</sub> "in-situ" in SCR is a nice idea. Once this "newer" NO<sub>2</sub> is formed in-situ as proposed, it is unclear how one guarantees that it is still not consumed by ammonia. The reviewer explained that, kinetically, ammonia would not distinguish between the incoming NO<sub>2</sub> and the one formed in-situ. Despite this ambiguity and if seeing is believing, the reviewer indicated that whether this lab-based exploratory data has a message in it remains to be seen and further explored. Still, a clearer picture needs to be painted for the project structure; benchmarks; overall timeline; milestones; interim deliverables; warranting project streamlining; and removing apparent gaps in communicating the message and producing a clear blueprint for getting the project to the finish line. According to the reviewer, these are either missing or insufficiently clear to allow a clear assessment on how the project end-game is to be accomplished.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

## Reviewer 1:

The reviewer remarked that a single-wall model is on track for completion and there are ongoing studies regarding catalytic material. There has been progress in evaluating the activity of higher dispersion materials and an optimum chemistry has been developed for activity and durability. The reviewer found strong progress on density functional theory (DFT) modeling.

#### Reviewer 2:

The reviewer remarked that incorporating an understanding of catalyst mechanisms into the development of a novel washcoat material, as is done in this project, is very important to the development of an appropriate solution. Compensating for the loss of NO<sub>2</sub> depleted from passive NO<sub>x</sub> oxidation by incorporating a SCO

component to the catalyst is a logical and necessary step to preserve the  $NO_x$  reduction functionality of the SCR-on-DPF. The reviewer appreciated the level of characterization to optimize the material in this work. However, the reviewer suggested that the investigators should be presenting particulate matter (PM)/particle number (PN) performance as well to ensure the changes made to the washcoat do not adversely impact the filtration or back pressure functionality of the DPF. In addition, the negative effects of both thermal and chemical aging need to be addressed early on in the development process as well as monitoring nitrous oxide ( $N_2O$ ) and  $CH_4$  emissions that are also inventoried by the U.S. Environmental Protection Agency (EPA).

## Reviewer 3:

The reviewer found this to be a comprehensive look at the  $NO_2$  generation from the SCO phase for various catalyst formations and production methods. It appeared to the reviewer that the SCO-SCR catalyst has some durability concerns, as  $800^{\circ}$ C aging significantly decreased the  $NO_x$  conversion. It would have been nice to have seen some soot-oxidation results along with the  $NO_x$  conversion results to demonstrate that the soot is indeed continuously oxidized with the SCO-SCR catalyst.

#### Reviewer 4:

According to the reviewer, the concept as presented last year was focused on use of Ba/Zr oxide to promote  $NO_x$  reduction in SCR-on-DPF with "good results." This year's concept is shown to be focused on using oxides of manganese (MnO<sub>x</sub>); it was unclear what happened to change direction. Describing the reasons for an apparent discontinuation of pursuing Ba/Zr-oxide would have been very helpful to the reviewer. Data are presented now on the use of MnO<sub>2</sub>-on-ZrO<sub>2</sub> in the development, but there are gaps in the overall picture and project plan on where it has come, where it is going, along with why and how. The project approach may be "let's explore as we move ahead and see," for which there may be nothing wrong with this approach, in principle. However, this reviewer explained that this comes with high risks and lack of clarity on, ultimately, how many resources would be needed to reach the finish line. In short, the reviewer stated that a clearer R&D "game plan" is missing and highly warranted.

**Ouestion 3: Collaboration and Coordination Across Project Team.** 

## Reviewer 1:

The reviewer observed good collaboration between PNNL and the CRADA partner, who also brings in the substrate supplier and catalyst company.

#### Reviewer 2:

The reviewer said that there was very good collaboration with PACCAR.

## Reviewer 3:

According to the reviewer, this project is a good example of leveraging the strengths of PNNL's characterization and formulation abilities with the practical input of an OEM entity, such as PACCAR, for a diesel application. Adding a washcoat supplier that is a leader in SCR formulations would provide further insight into other options for improving the SCO-SCR-DPF washcoat.

#### Reviewer 4:

The reviewer remarked that this is a CRADA project between PNNL and PACCAR. According to Slide 16, the reviewer noted that PNNL is pursuing DFT modeling and PACCAR is pursuing SCO phase discovery, selective catalytic reduction on filter (SCRF) washcoat development, SCR phase development, and DPF optimization. Pursuit of the latter three activities were unclear to the reviewer as PACCAR is not a coater (an issue addressed by a reviewer last year that did not seem to be addressed). The reviewer said that it is possible that PACCAR may be working with a coater. According to the reviewer, most CRADA projects, especially when involving long-term exploration and industry impacts, include additional partners (i.e., beyond just the National Laboratory and one corporate partner). The reviewer wanted to know if there is a reason why another institution is not involved. It was further unclear to the reviewer what the "needs" are in the long term and how the resources are put in place for each need to be addressed and to tackle them all. Risks are not low in this

project. Should the project not display a major breakthrough soon, the reviewer was concerned that, in the end, it may result merely in a few patents with no ultimate commercial impact.

Ouestion 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer remarked that the proposed future activities are appropriate for this work. The use of Mn and similar species has shown drawbacks; therefore, appropriate aging is required.

## Reviewer 2:

The reviewer was very interested in the sulfur sensitivity and desulfation requirements and said that it will be very interesting to evaluate the potential of the combined system.

#### Reviewer 3:

The reviewer reported that there is a need to move up the sulfur work as Mn forms very stable sulfates that require very high temperatures (e.g., 800°C) to decompose under lean conditions. Also, there is a need to look at N<sub>2</sub>O emissions as NO<sub>2</sub> can react with ammonia (NH<sub>3</sub>) to form ammonium nitrate, which can decompose to N<sub>2</sub>O. Excessive N<sub>2</sub>O counts against fuel economy. The reviewer suggested examining and reporting on the soot-oxidation capability along with the NO<sub>x</sub> conversion results.

#### Reviewer 4:

This reviewer reported that Slide 18 outlines future work. The eventual transition from micro-reactor-based development (current stage) to full-size honeycomb and to engine testing (the ultimate demonstration), as well as their respective timelines are needed. For instance, the reviewer asked whether these future activities are 1year undertakings (unlikely) or will span over 3-5 years (more likely). That would mean a need for more funding and resources. If so, the reviewer asked what resources are needed and which would be at PNNL or PACCAR. The reviewer asked if the capabilities at these two entities are sufficient or if another partner or further capability is needed. Generally, while some needed steps are highlighted, other steps, a timeline, and resource planning are missing and ambiguous.

## Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer remarked that by using more of the feedgas NO<sub>2</sub> for oxidizing the soot, the frequency of DPF regenerations can be reduced, which saves fuel. This should also benefit the durability of the SCR catalyst as it will not be exposed to as many high-temperature soot regenerations.

## Reviewer 2:

The reviewer stated that reduction of soot accumulation in a filtration honeycomb is synonymous with reduced backpressure, which would result in fuel economy. Attempts to reduce NO<sub>x</sub> and soot accumulation in the SCRon-DPF, the ultimate goal of this project, is well within the DOE objectives.

## Reviewer 3:

The reviewer said that this project satisfies the need for more efficient aftertreatment systems to meet increasingly stringent emissions standards while improving fuel efficiency.

#### Reviewer 4:

The reviewer commented that the project is definitely relevant to DOE objectives.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

According to the reviewer, the resources between PNNL and PACCAR seem to be sufficient for this project.

## Reviewer 2:

The reviewer said that resources are sufficient.

#### Reviewer 3:

The reviewer stated that the greatest needs of this project include a clear timeline, recognition of its potential challenges and risks, and highlighting its interim milestones. At the present, the project appeared to the reviewer to be exploring by trying various pathways. The reviewer highly suggested that the technical team in this project bring in a "project planner" (a totally different skillset) to assist with developing a granular plan and the pathway ahead. The reviewer referenced previous comments on why the resources, as they appear at present, are deemed insufficient by highlighting the project risks.

#### Reviewer 4:

The reviewer indicated that this is significant funding that only benefits one entity. The reviewer had very mixed feelings about this.

Presentation Number: ace121
Presentation Title: A High Specific
Output, Gasoline, Low-Temperature
Combustion Engine
Principal Investigator: Hanho Yun
(General Motors)

Presenter Hanho Yun, General Motors

Reviewer Sample Size
A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer found this to be very nice work. The focus of this project is to integrate many of the advanced technologies that have been, and are being, investigated in VTO programs into a realistic, concept demonstration, mimicking production-type applications. According to the reviewer, this is an important activity that should be selectively undertaken. In the reviewer's opinion, this project is a good example of when this should be done.

# Reviewer 2:

The reviewer indicated that this project

has a solid approach, using 4 combustion strategies to cover the operating range of an engine to enable 16% improvement in fuel economy. The barriers of control and emissions aftertreatment are being addressed as well.



The reviewer noted that the approach is well designed to maximize potential for success. Barriers are well identified and addressed in the approach.

#### Reviewer 4:

The reviewer remarked that the approach was well laid out in the presentation, though some more discussion as to the difficulties for some key barriers may be valuable, especially for considering future work. The timeline shown was valuable and the reviewer looked forward to hearing about the results of the aftertreatment testing in the upcoming report.

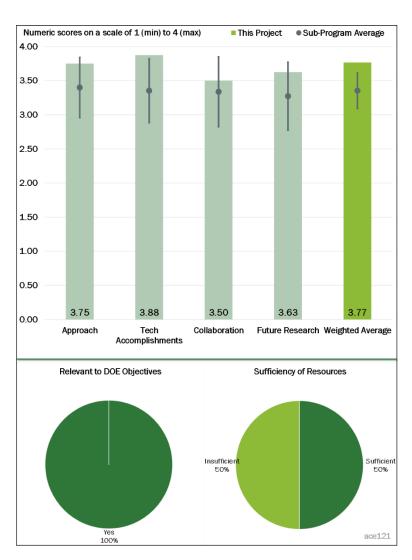


Figure 1-25 – Presentation Number: ace121 Presentation Title: A High Specific Output, Gasoline, Low-Temperature Combustion Engine Principal Investigator: Hanho Yun (General Motors)

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer indicated that the project is making excellent progress toward goals and is well aligned for the next phase of the project—transient demonstration. The accomplishments are impressive and align well with the technical barriers of the various combustion modes. The accomplishments are setting the stage for success in meeting the overall program objectives.

#### Reviewer 2:

This reviewer stated that work here lays the foundation for other work in low-temperature combustion (LTC). There has been much progress shown and the results indicate future paths that will need to be researched. There was good discussion on various R&D components (injection, injection timing, and EGR), how varying each component was evaluated, and the effect it had. Of particular interest to the reviewer was the spray pattern work. It may be interesting to continue with injector orientation variations to see if the LTC mode is sensitive to this characteristic.

#### Reviewer 3:

The reviewer commented that the project team is meeting its targets and providing valuable information regarding successes and remaining challenges of implementing the technologies that VTO has been investigating. The reviewer asked if it is possible for some of the detailed data on engine operating and incylinder conditions to be shared with the Co-Optima program. It might enable Co-Optima to evaluate their analysis capabilities relative to fuel properties as facilitators for engine operation in alternative combustion regimes and to explore whether the operating regimes identified in this work could be expanded with changes in fuel properties.

#### Reviewer 4:

The reviewer noted that the 4 combustion strategies being developed to enable 16% improvement in fuel economy have been identified to cover the entire map. It still unclear to the reviewer how the engine will transition between the adjacent modes in a real-world driving cycle so a great follow-on project would be to demonstrate this strategy in a vehicle.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer commented that GM has assembled a strong team of experts to help address the many technical challenges. Coordination of this team looks excellent in making progress toward the challenges.

#### Reviewer 2:

The reviewer observed that the project is GM-centric, but collaborations are still critical and have been effectively leveraged, namely with stakeholder suppliers.

#### Reviewer 3:

Though it was obvious that there were supporting partners who were well coordinated in this project, the reviewer believed that complex computing capabilities (which are newly available) would allowing expansion of this project into advanced combustion computing, leading to projections for future benefits in LTC.

#### Reviewer 4:

The Federal Mogul collaboration is well described on the groundless barrier discharge igniter (GBDI) system. The reviewer believed that the BASF work was covered in more detail in last year's AMR presentation. The Delphi interaction on the fuel-spray pattern optimization was also good, but the FEV role was not covered in much detail. The reviewer noted that no universities or National Laboratories were involved.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer indicated that progress so far has set the stage well for the proposed future work. The next stage is particularly exciting—demonstration of robust operation across the cold and warm Federal Test Procedures (FTPs). This will be an extremely exciting accomplishment for GM, DOE, and industry.

#### Reviewer 2:

The reviewer stated that the project is approaching the end date. The future plans are to finish the tasks laid out in the work statement.

#### Reviewer 3:

According to the reviewer, the discussion for future research centered around completing the tasks currently on the schedule for this project, which is good, but when those are complete and the results analyzed, work in this area will need to move forward and include additional "Co-Optima" team interaction to help determine future steps.

#### Reviewer 4:

The reviewer commented that a good deal of the future work is focused on transient operation and, more specifically, on mode changing. Cold starting will also be good to see. With the project ending at the end of 2019, it was not clear to the reviewer that these tasks can all be accomplished.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer said that the project aligns perfectly with DOE objectives toward significant improvements in engine efficiency and fuel economy while meeting emissions.

#### Reviewer 2:

The reviewer observed that this work directly aligns with DOE's mission to reduce fuel consumption through the use of novel internal combustion engine (ICE) strategies and the development of new components. This work is early TRL and should also help component suppliers as prototype ignitors are being tested and developed.

#### Reviewer 3:

The reviewer remarked that this project meets DOE objectives by demonstrating an approach and method to achieve a 15%-17% improvement in fuel economy.

#### Reviewer 4:

The reviewer asserted that evaluating the potential of integrating VTO-supported fundamental understanding into engine-operating strategies and hardware technologies for production-like engines is indeed relevant.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

The reviewer commented that the project is near its end, objectives are being met, and, based on the presentation, it is on budget.

#### Reviewer 2:

The reviewer had no comment as resources appear sufficient for the project and progress to date.

#### Reviewer 3:

The reviewer believed that this project should be extended and additional funding appropriated to include a vehicle demonstration.

#### Reviewer 4:

The reviewer indicated that, based on the accomplishments and potential impact of successful LTC combustion and aftertreatment characterization, this type of work will need to be continued and additional resources required to ensure proper collaboration is done upfront and a larger scope of work can be done to detect sensitivities to fuel, injector pattern, or other "in use" variations.

Presentation Number: ace123
Presentation Title: TemperatureFollowing Thermal Barrier Coatings
for High-Efficiency Engines
Principal Investigator: Tobias
Schaedler (HRL Laboratories)

#### Presenter

Tobias Schaedler, HRL Laboratories

#### **Reviewer Sample Size**

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer observed that this is a very innovative approach of using microspheres for low conductivity and low heat capacity. There are difficult challenges with sealing and joining to aluminum and apparently some patents.

#### Reviewer 2:

The reviewer stated that the researchers have a good approach to development of temperature-following thermal barrier coatings using novel, hollow nickelalloy microspheres. Various approaches have been tried and the project team has been resilient in seeking solutions to complex difficulties.

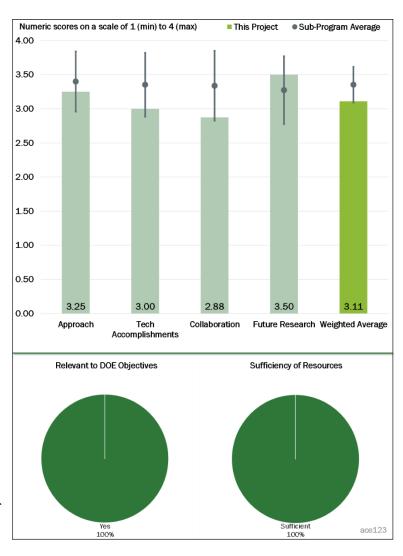


Figure 1-26 – Presentation Number: ace123 Presentation Title: Temperature-Following Thermal Barrier Coatings for High-Efficiency Engines Principal Investigator: Tobias Schaedler (HRL Laboratories)

#### Reviewer 3:

The reviewer remarked that this project is aiming to develop thermal barrier coatings. The approach being used—pursuing a coating with both low thermal conductivity as well as low thermal capacity to maximize the temperature-following behavior—is an approach that has a firm basis in thermodynamics. According to the reviewer, the project team has identified some promising candidate materials that can help to achieve this, specifically the use of high-porosity microspheres. Like some previous thermal barrier coating efforts, one of the main challenges to this technology appears integrating the technology in a durable way. Appropriately, this is where a lot of the focus of the project is being spent.

#### Reviewer 4:

The reviewer commented that the approach employed is on a good path and is reasonable as it could result in improved efficiency, if durable. Employing porosity is a clear path to reduce thermal conductivity and using a metal made a lot of sense. The reviewer was surprised that there was not more discussion with respect to coefficient of thermal expansion matching and thought that this could be a durability issue if not fully addressed. It would have been nice if the researchers had a firm list of techniques to try to add to the piston at

the beginning of the project. It seemed to the reviewer like the project team is coming up with ideas on the fly, which could be limiting. Moving to steel pistons that are of a similar weight as the aluminum pistons could be a good path forward.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that some progress has been made, but not as much as needed to reach success. It was a little surprising to the reviewer that more work with steel pistons has not been achieved. One might have expected bringing in new team members with complementary skills in materials joining.

#### Reviewer 2:

The reviewer observed that a significant portion of the presentation was the same as the presentation from the prior year. Specifically, the microstructure of the spheres and the findings about applying pressure during the sintering process were the same. It looked to the reviewer like most of the new results were associated with testing a number of different generations of coatings on the engine valves. This is important and good work. The reviewer looked forward to seeing more progress on the piston coating as this project progresses.

#### Reviewer 3:

With an operating budget of \$1.14 million in FY 2019, the reviewer would like to have seen more positive progress this year. The approaches on the valves and exhaust port seemed to go smoothly and looked promising to the reviewer. Hopefully, the steel piston transition will solve the issues with the piston coating, the most critical portion of the project. The reviewer understood that there have been delays with the piston manufacturer and hoped that there will be sufficient funds to make progress for the remaining year.

#### Reviewer 4:

The reviewer noted good progress made since last year's AMR, but the reviewer would like to have seen more progress on the steel piston approach. The use of steel pistons to overcome bonding issues was discussed last year.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer noted that HRL is working with GM and has also tapped other companies, such as Federal Mogul for pistons and 3M for microsphere production.

#### Reviewer 2:

According to the reviewer, good partners are involved here although it would be nice to have a piston supplier that was more responsive to the project needs.

#### Reviewer 3:

The reviewer found the evidence of collaboration from other members of the project team to be rather weak. The reviewer suggested that the team would benefit by participation of a laboratory (either private or government) having exceptional capabilities in joining and materials.

#### Reviewer 4:

The reviewer said that this project team is a very good one, with HRL producing the barrier materials and GM providing the engine support. The reviewer thought, though, that the delay in getting a steel piston coated shows a weakness in the collaborative partners. It would have been good to have a partner onboard who could develop the new piston design in a much faster way.

The reviewer indicated that there may also be opportunities to re-think the piston design with the thermal barrier coatings included that could be brought by a piston manufacturer. In particular, if there are thermal barrier coatings applied to the piston, the cooling jet and heat transfer through the piston is significantly reduced. The reviewer stated that there could also be more integral ways to design in the thermal barrier coatings. This may be premature, but it could also be a path to bring some enabling perspectives for this technology.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

Solutions to improve bonding and sealing appeared to the reviewer to be well thought out.

#### Reviewer 2:

Continuing to refine the thermal barrier coating on both the pistons and on the engine valves is the correct path forward for developing this technology, according to the reviewer.

#### Reviewer 3:

The reviewer stated that the future research was a good path forward to focus on steel piston and getting good coating before getting engine results.

#### Reviewer 4:

The reviewer found that future research tasks were on target to explore overcoming challenges to this unique approach. The use of steel pistons to (at least temporarily) overcome bonding of the thermal barrier coating (TBC) to the aluminum pistons is a wise move that can permit an on-engine performance assessment. If modeled improvements are proven out, then resolving aluminum bonding can be addressed.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer remarked that the approach and project address engine heat-transfer losses, which is among the most elusive longstanding barriers to higher engine efficiency.

#### Reviewer 2:

The reviewer reported that the application of temperature-swing thermal barrier coatings has a firm thermodynamic basis and, if successful, will help to enable more efficient engines.

According to the reviewer, improving efficiency is directly related to DOE goals and this project fits that.

#### Reviewer 4:

The reviewer commented that modeling shows the potential for real benefits if the coatings can be cheaply applied and durable over the life of the engine. This a high-risk, challenging enabling technology that has potential for high payoff if successful.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer stated that the award size is adequate for a strong effort, mostly in the laboratory (no major overthe-road demonstration).

#### Reviewer 2:

Resources for this project appeared to the reviewer to be sufficient.

#### Reviewer 3:

The reviewer said that resources appear to be adequate for the program.

#### Reviewer 4:

The reviewer indicated that there are sufficient funds to meet the goals as long as delays in manufacturing do not significantly impact progress.

Presentation Number: ace124
Presentation Title: SuperTruck II PACCAR
Principal Investigator: Carl Hergart
(PACCAR)

Presenter Carl Hergart, PACCAR

Reviewer Sample Size
A total of six reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer found the approach is very comprehensive and well focused. The path includes engine, powertrain, and many aspects of the vehicle architecture and operations. There is a suitable balance between technology risk and benefits.

#### Reviewer 2:

The reviewer noted that the approach targets areas for efficiency improvement that one would expect with the key challenges being not only advancing technology in each area but systems integration. The project team conveyed a strong emphasis on end-user (fleet)

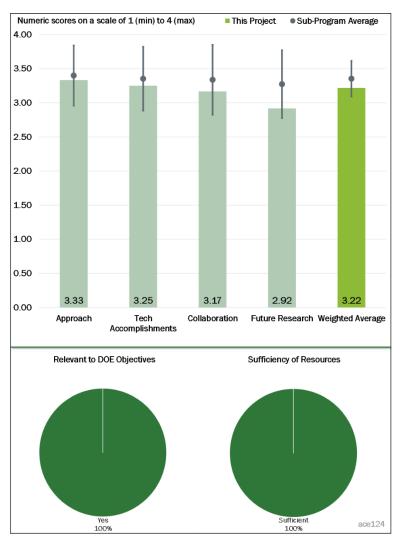


Figure 1-27 – Presentation Number: ace124 Presentation Title: SuperTruck II – PACCAR Principal Investigator: Carl Hergart (PACCAR)

input and tools used to facilitate fleet feedback at even the early stages of the project.

#### Reviewer 3:

The reviewer indicated that PACCAR is showing a sound approach for this stage of their program, looking at all possible options for their potential and viability.

#### Reviewer 4:

The work is a year behind the other ST2 participants, so this presentation needs to be reviewed in light of that. The current work does appear to be well crafted to address the technical barriers for meeting the ST2 targets and each of the technical areas looks reasonable.

#### Reviewer 5:

The reviewer said that this is a solid approach to plan the project. This team is 1 year behind the others and has a strong plan to meet objectives.

#### Reviewer 6:

According to the reviewer, the approach taken on the vehicle side (Slide 7) is way too simplified. For example, tires and weight reduction are missing and they have to be part of the plan or road map. It also seemed simplistic to the reviewer to show the path of how a baseline engine with 47% BTE can achieve 55% BTE (Slide 8). Because PACCAR would use its competitor's WHR system, the reviewer commented that it would be unlikely that PACCAR can get the best WHR system in this program from its competitor, thus making this program notably less innovative and unique compared to others. At the same time, the program has the same DOE funding as all others, which means that double funding is invested for the same or similar WHR technology and its application from the same company. The reviewer asserted that not only could it make the program less competitive and innovative, but also this could create an unfair playing field for other competitors.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

Considering late start, the reviewer found that the technical accomplishments are excellent. Many technology decisions have been locked in.

#### Reviewer 2:

The reviewer asserted that there are good accomplishments toward completing the project team's initial analysis and baselines for year 1.

#### Reviewer 3:

The reviewer said that technical progress appears to be good and on track to meet ST2 objectives and timelines.

#### Reviewer 4:

The reviewer said that accomplishments include the detailed plan and high-level assessment of opportunities along with making some high-level decisions.

#### Reviewer 5:

The reviewer noted that the high-level simulations indicate good progress on the technical path selection and the powertrain technology validation shows validation of many of the individual technologies. It was not clear to the reviewer which have been experimentally validated and which are via simulation. Nor was it clear if the technologies have all been tested in combination or if each one has been tested independently. However, the reviewer stated that the progress is consistent with the current time line of the project.

#### Reviewer 6:

The technology validation on the 55% BTE map (Slide 16) was puzzling to the reviewer because the efficiency-improvement road map has a huge jump with WHR. The reviewer asked if that is realistic, and inquired about the meaning of the numbers from 1 to 9 in the Slide 14bar chart. On the vehicle side, the reviewer commented that it is too vague to just put improvement numbers on Slide 29. For example, the reviewer questioned PACCAR's belief that a 25% tire coefficient of rolling resistance (Crr) improvement is achievable and that a 30% weight reduction can be achieved. More specific descriptions would be helpful.

#### Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

The reviewer said that the involvement and roles of the project team are evident in the progress being made and the decisions about technology to be used. The roles are concisely explained.

#### Reviewer 2:

The reviewer was very impressed with the noted collaborators and evidence of engagement by UPS, the fleet partner.

#### Reviewer 3:

The project appeared to the reviewer to be well coordinated and with the expected collaboration.

#### Reviewer 4:

The reviewer stated that the partnerships have been noted, and each has a specific technical task. However, it was not possible for the reviewer to tell from what has been presented if the coordination and collaboration are effective or not nor what the individual outputs are from each partner.

#### Reviewer 5:

According to the reviewer, Slide 33 shows the partnerships and collaborations. The reviewer suggested that it would be helpful in the future if individual icons of each company or organizations would appear on any sides that are associated with their work or contribution.

#### Reviewer 6:

The reviewer commented that this looks to be a good project team of very qualified collaborators and partners. It was interesting to the reviewer that Cummins is the waste heat recovery partner, as they have their own ST2 project. The reviewer noted that there are not any universities on this team who could probably help with some of the analysis and modeling in the early phase of the project.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

Future projected work appears to be thought out with risk and unforeseen events properly considered. Alternative development pathways were not expressly discussed, but the presentation provided reasonable indications that results-based flexibility would guide future work.

#### Reviewer 2:

The reviewer found that plan to be robust. It seemed to the reviewer that over 50% of the freight-efficiency improvement is due to lightweighting, here called "architecture," of the tractor and trailer. Although an acceptable action to meet the goals, the reviewer thought that commercialization of fuel-efficiency technologies should be a higher percentage.

#### Reviewer 3:

The reviewer said that the path toward ST2 goals is good. There is not much presentation of alternate pathways, nor of many technical aspects of the program that have significant research risk.

#### Reviewer 4:

The reviewer commented that the future research area is OK but does not have details. For example, a tire partner has been brought it and an aggressive target set, but there are no details on the technical approach to achieve improvement.

#### Reviewer 5:

According to the reviewer, the future work was presented in three separate sections, which the reviewer evaluated by section as follows: engine—this planned work is detailed, thorough, and looks good; powertrain—heavily focused on hybridization, which is an important part of the freight-efficiency plan for this team and a good plan, and (3) vehicle—seems to be lacking detail in this section as Slide 30 lists the

challenges and Slide 31 just repeats these as future work. The reviewer wanted to know what the challenges are of building the mule vehicle and commissioning it.

#### Reviewer 6:

The reviewer commented that no research and further development are needed on WHR in the engine proposed future plan in FY 2020, because its competitor WHR system is used. This could create an uneven playing field for other competitors.

Ouestion 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that the project affords an opportunity to explore improved freight efficiency with some higher risk approaches but with real-world vehicle systems.

#### Reviewer 2:

The reviewer commented that this project meets the objectives of DOE's Vehicle Technologies Office by demonstrating 55% BTE and 100% improvement in freight efficiency.

#### Reviewer 3:

The reviewer noted that DOE and industry investment in ST1 and ST2 are definitely making a difference in the real world. Long-haul trucking consumes a majority of the fuel in the United States and this is highly relevant.

#### Reviewer 4:

The reviewer stated yes, this work clearly supports DOE objectives by advancing efficiency-improving technologies and concepts. It is designed to reach the DOE-established goals and provides opportunities for rapid commercialization of some technologies or approaches.

#### Reviewer 5:

According to the reviewer, achieving the 100%-improvement goal on the vehicle side plus 55% BTE on the engine would clearly support DOE objectives.

#### Reviewer 6:

No particular comment was indicated by this reviewer.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer remarked that the breadth of technology approaches is significant for the available funding, but not inadequate.

#### Reviewer 2:

The reviewer stated that it was a little difficult to assess after 1 year, but progress seems appropriate for the funding level compared to the other teams.

#### Reviewer 3:

The reviewer said that evidence is there to assume that the resources are sufficient at this point.

#### Reviewer 4:

Resources appeared to the reviewer to be in line with previous efforts and appropriate for the ST2 objectives.

#### Reviewer 5:

The reviewer indicated that resources may be sufficient on the vehicle side, but was not sure that resources would be on the engine side due to lack of experience. Development cost can be significantly cut with the help

of the competitor's WHR, but at the same time, the risk would be high because of too much reliance on a competitor's WHR, which can hardly be the best available system.

#### Reviewer 6:

The reviewer had no particular comment.

# Presentation Number: ace125 Presentation Title: Model Development of Fundamental Combustion Processes Principal Investigator: Rainer Dahms (Sandia National Laboratories)

#### Presenter

Tuan Nguyen, Sandia National Laboratories

## Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer indicated that the PIs tackle the issues and problems in engine combustion by improving the fundamental mathematical models for the physical processes using asymptotic analysis and DNS. The models include a drag model and a turbulent combustion model, which are of great importance for engineering simulations of engine combustion. The reviewer noted that multiple gaps in the present popular spray and combustion models have been identified, including multi-zone model, tangential diffusion, etc. The models were validated by comparing with

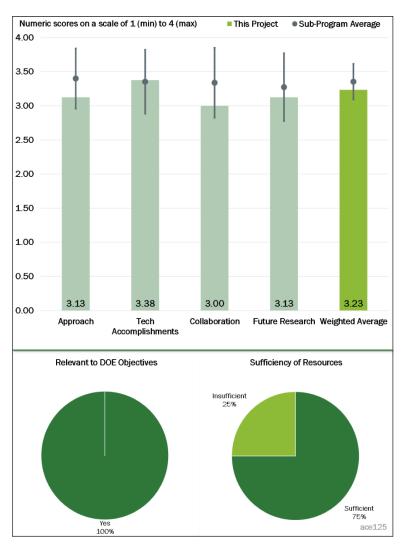


Figure 1-28 – Presentation Number: ace125 Presentation Title: Model Development of Fundamental Combustion Processes Principal Investigator: Rainer Dahms (Sandia National Laboratories)

conventional models, DNS results, and available experimental data. For the improved drag model, the reviewer said that the current test case is not a good case for validation since it contains too much noise, such as breakup. A case that can isolate drag from other processes (breakup, evaporation) will be ideal to validate the drag model only.

#### Reviewer 2:

The reviewer said that the project is trying to perform multiple different tasks (Lagrangian spray, TCI) to improve the overall accuracy of combustion simulations. The reviewer stated that the accuracy aspect was discussed but there was no mention of computational cost associated with the approach.

#### Reviewer 3:

The reviewer remarked that there are several sub-models that affect engine-combustion simulations (e.g., turbulence, near wall flows, etc.). The PIs have chosen to focus on spray drag modeling and combustion turbulent chemistry interaction (TCI). Although important, the reviewer asserted that the research team should explain how these areas were selected. The reviewer asked why a focus on primary atomization to tackle the

near-field, dense spray region was not included. The reviewer found value in the overall philosophy to leverage high-fidelity codes to improve engineering-level CFD models.

#### Reviewer 4:

According to the reviewer, the need to improve models for high-fidelity simulations of sprays is an important goal within the overall VTO portfolio of work. The two model improvements discussed in this project were (1) capturing the non-spherical shape of droplets and (2) developing better flamelet models for multiple-injection fueling strategies. From a high-level perspective, it was unclear to the reviewer how these two topics were chosen for further investigation; the analysis that showed that these were the two most critical elements to address in high-fidelity modeling was not discussed and the presenter did not answer the reviewer's question about this directly. This may have been because the presenter was not the PI —one of the PIs had since left Sandia—but it would have been helpful to have the other PI present the work instead of a post-doc to address these more programmatic questions. The reviewer commented that it would have been particularly nice to talk about this prioritization process this year since it was the first presentation of this particular project.

Given that these were the two topics chosen for analysis in this project, the reviewer found the approach on each topic to be sound. On the topic of non-spherical droplets, it was unclear to the reviewer how this model will be connected with models that necessarily come "upstream" of this issue, particularly the spray-breakup model. As these two topics are so coupled, the reviewer said that it would have been good to understand whether the "significant differences" the presenter showed with the new non-spherical droplet model will still be significant in the context of the breakup model. This goes back to the previous comment about overall prioritization. The second topic—improved flamelet models for capturing multiple-injection behavior—has a well-designed approach and the PI on the project has done work like this before and so has the expertise to make significant progress in this area.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

The reviewer commented that the project has been very productive during the past year. The team developed a new drag model. The model has been validated by comparing the standard model as well as part of experimental data. The results show improvements over the standard model. Asymptotic analysis showed that the Sage model partially included TCI. The reviewer said that the multi-zone model for combustion chemistry calculation has a deficiency that may lead to big errors in CFD. DNS of spray with multiple injection was conducted. A new flamelet model for multi-injection is under development.

#### Reviewer 2:

The reviewer indicated that a lot of technical accomplishments are mentioned, but it is better to focus on few major highlights and show the impact on overall engine-simulation predictive accuracy. For example, simulation results on the effect of drag prediction are mentioned, but the following slides discuss projected liquid volume (PLV) rather than whether the simulation is done with conventional CFD code or DNS code.

#### Reviewer 3:

The reviewer supported the focus on drag modeling for the spray simulations as this has been a concern for several years. The reviewer would like to have seen a component in the drag work that focuses on the correction of drop relative velocity due to the interspacing effect of the liquid droplets. Isolated droplet work is important but a spray consists of many closely spaced droplets in varying orientations. Additionally, the reviewer asked if breakup and collision had been turned off in Slide 12. Overall, the combustion and spray work should begin to place effort on gasoline-engine relevant fuels and conditions with focus on Spray G.

#### Reviewer 4:

On the first topic of non-spherical droplets, the reviewer observed that the technical accomplishments are good and the underlying science is sound. The comparisons with experiment are good, but it was unclear to the

reviewer what was happening in the rest of the simulation (particularly the spray-breakup model) and the relative importance of this particular model to the overall problem. The presenter noted that the goal was just to show that this new model "makes a difference, not that it matches the data," which was someone unclear to the reviewer since the ultimate goal should be to capture what is happening in the experiment. The slides show that there is better agreement with data, which is really good, but again the context is missing.

According to the reviewer, the technical accomplishments on the second topic of a better flamelet model for multiple injections are good. The progress on the model is quite good so far. The project team should continue to push it to more realistic conditions and begin to compare with experimental data to understand if the model is capturing more realistic processes.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer found good collaboration with multiple partners industry, academia and laboratories.

#### Reviewer 2:

According to the reviewer, collaboration with CONVERGE is a great step for the droplet modeling, and participation in the Engine Combustion Network is critical to increasing the impact of this work. Interaction between the high-performance computing activities and this project is also important. The reviewer suggested that the PIs also consider connecting the flamelet modeling with the Turbulent Non-Premixed Flame and/or Turbulent Premixed Flame workshops as these methods may be useful for the community in general. This would also help with increasing collaborations with the academic community.

#### Reviewer 3:

Comparing to other DOE projects, the reviewer said that the current project has fewer collaborations with other teams, which is normal since it is a model-development project. Given enough time, the impacts of this project on the whole community will show up.

#### Reviewer 4:

Given the effort on high-fidelity spray modeling, the reviewer was surprised that the research team is not working more closely to validate its work against the X-ray work at Argonne. If this activity is happening, it was not apparent to the reviewer from the presentation material. Additionally, the reviewer thought that the combustion focus of this work would benefit by closely linking itself to engine-combustion system hardware measurements from another Advanced Combustion Engine (ACE) project.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer noted that the future research plan, which targets multiple, big unsolved problems in engine-combustion modeling, is good. However, since Dr. Dahms left the team, it shades huge uncertainties for the future of this project. There is limited evidence that the project can be as productive as before, according to the reviewer.

#### Reviewer 2:

In the proposed research topics, the reviewer asked what the motivation is for implementing a Lagrangian spray framework in PeleLM. Given all the uncertainties in Lagrangian spray models, the reviewer asked the reason to put a "lower order" approach in a high-fidelity code. If the PeleLM is being written for exascale, the reviewer inquired whether the computer hardware exists to absorb a more accurate formulation.

#### Reviewer 3:

The reviewer saw multiple details regarding the liquid drop models, implicit TCI, and improved multi-injection modeling. As referenced in the reviewer's prior comments, the models will not be useful for OEMS if the accuracy is improved, but at very high computational cost.

#### Reviewer 4:

The reviewer found that the e future work plan is sound and the progress in the next year will make significant progress toward overcoming modeling barriers. The only point of the future plan that was not clear to the reviewer is the topic of "study film combustion," which is listed under the multi-injection combustion. It was not clear how this connects with the other goals of this sub-task and the plan to do this was not discussed.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer reported that the project addresses the most fundamental problems in engine-combustion simulations. The outcomes of this project are valuable for both fundamental research and industry applications. The improved models can be applied to analysis-based product development.

#### Reviewer 2:

The reviewer said that there is an important need for this type of work to enhance engineering-level CFD models leveraging high-fidelity simulations.

#### Reviewer 3:

The reviewer stated that this project focuses on engineering simulations whose coarser resolution needs accurate sub-models.

#### Reviewer 4:

The reviewer asserted that this model improvement, particularly for the turbulent combustion models, is highly relevant for achieving the goals of the Vehicle Technologies program. The reviewer suggested that the PIs should continue to work to connect these models with more realistic conditions with liquid fuels.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer reported that the resources provided are sufficient to support the proposed future research.

#### Reviewer 2:

The reviewer indicated that this project needs additional computational resources for making progress with DNS simulations.

#### Reviewer 3:

The reviewer commented that the project requires extensive computational resources, especially for the DNS studies. The computational resources at Sandia should be sufficient for this purpose.

#### Reviewer 4:

According to the reviewer, the project needs to find a second PI in order to continue the large scope of work outlined, particularly given the current PIs in other projects. If another PI is identified, then the project will be properly staffed and will have reasonable resources for achieving the goals.

Presentation Number: ace126
Presentation Title: Developing a
Framework for Performing HighFidelity Engine Simulations using
Nek5000 Code for Exascale
Computing
Principal Investigator: Muhsin Ameen
(Argonne National Laboratory)

Presenter Muhsin Ameen, Argonne National Laboratory

Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer asserted that the project certainly is well devised with an appropriate approach. The new code seems well suited as a platform for high-fidelity modeling. The validation plan looked good to the reviewer, too.

#### Reviewer 2:

According to the reviewer, the higher order spectral method mentioned to improve lower order methods is a valuable approach for improving overall acceleration of simulation technology for engine development. The reviewer

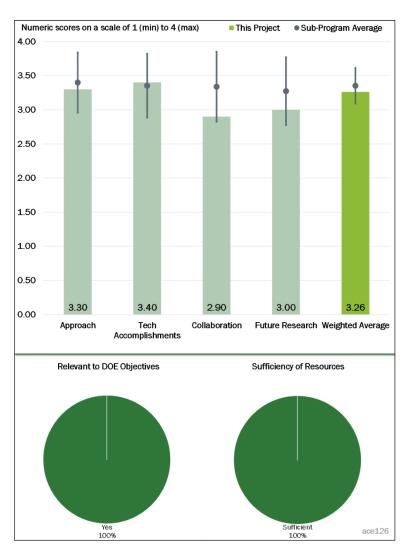


Figure 1-29 – Presentation Number: ace126 Presentation Title: Developing a Framework for Performing High-Fidelity Engine Simulations using Nek5000 Code for Exascale Computing Principal Investigator: Muhsin Ameen (Argonne National Laboratory)

said that it will be valuable if there is a study regarding the accuracy, element size, element type, and spectral element method Nth order relationship.

#### Reviewer 3:

The approach thus far seemed reasonable to the reviewer, given that the code is undergoing significant early development and proof-of-concept validation. Given the number of people working on code development, the reviewer urged the project team to use caution to ensure that the code is structured and maintained well and that strict version control is in place. The reviewer did not see any mention of this in the material. This is especially critical if the Argonne version of the code is to be released under an OpenFOAM framework.

#### Reviewer 4:

The reviewer found the approach to the work to be sound. For the prediction of in-cylinder flows, the use of overset meshing is a good approach. It was surprising to the reviewer that this technique had not been implemented in the past as overset meshes have been quite standard for many years now in other applications with difficult meshing geometries. However, according to the reviewer, the results that the PI has obtained

through this method are an improvement over previous methods, particularly in computational cost, and so this approach should be continued. In terms of the turbulent combustion modeling component, the implementation of these models into the Nek5000 code seems to be going smoothly.

The reviewer remarked that there does seem to be significant overlap in terms of the fundamental knowledge between this effort and others who are working on implementing turbulent combustion models into other simulation frameworks. It was somewhat unclear to the reviewer how this effort is unique beyond the code in which it is being implemented. The reviewer suggested that the unique contribution of this effort, as compared to others (at Argonne and Sandia), should be highlighted in future reports.

Finally, the PI mentioned the potential for use of machine-learning algorithms in future work as part of the collaboration with high-performance computing, but the plans for implementation were currently unclear to the reviewer. The direction is a promising one, but the PIs should articulate clearer plans on new directions in these presentations if this information is to be mentioned as a possible direction.

#### Reviewer 5:

It was unclear to the reviewer how developments from this program will be passed onto commercial code vendors for incorporation into the fully supported, production-engine simulation software needed by engine developers. As someone who has been involved in combustion CFD development and application over the past 30 years, the deadlines and pressures of developing combustion systems make utilization of open source research codes impractical in the extreme. This reviewer's firm was using a research code when he joined the organization over a decade ago, and the negative impact that had on solving code problems was substantial. The switch to commercial, fully supported software—as imperfect as it is—allowed this team to increase productivity several fold, making analysis-led design for today's high efficiency, low emission engines a practical reality. There is no doubt in the reviewer's mind that improved physical models are needed, but as proposed, it was not clear to the reviewer that these are the focus here. The reviewer reiterated that commercial software allows coupling injector internal flow with in-cylinder sprays and combustion, integrating conjugate heat-transfer calculations into engine-design simulations, automating bowl-and-port design into the simulation process, utilizing LES to study closed crankcase ventilation (CCV), performing multi-cylinder combustion analysis with large numerical models, etc., by driving code vendors to work with National Laboratories to incorporate better physics, numerics, etc. The reviewer asked what the plan is here to have such an immediate impact and, further, how this code development is different from or complementary to the work that Carrington, et al., have been pursuing for 30 years with KIVA. The reviewer wanted to know why KIVA has been, albeit historically, the de facto standard for open-source engine simulation and not NEK5000. The reviewer also asked whether the community would be better served by pooling resources and having one program for code development tightly linked with one or more commercial code development teams than two research code development programs that appear to be only marginally in communication with said vendors.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

Since this project is a new one, the reviewer said that there is nothing much to talk about. Making the three-dimensional (3D) calculation work seems a little challenging, but it is not likely to slip too much from the time schedule.

#### Reviewer 2:

According to the reviewer, the results of this year's efforts are encouraging. Improvement in simulation time and accuracy with the overset meshing will certainly lead to further improvements of prediction, particularly with applications to light-duty engines in the new Consortium. The reviewer encouraged the PIs to continue to reach out to others with well-characterized engines in order to test the method in a number of different geometries, operating conditions, etc., in order to ensure robustness. The results of the turbulent combustion-

modeling implementation are promising and meet standard benchmarks. It was unclear to the reviewer, however, how unique this contribution is relative to other simulation efforts across the National Laboratories. The connections with the high-performance computing resources are strong and should be continued.

#### Reviewer 3:

The project has just started, so it was difficult for the reviewer to judge progress against overall project goals. However, it was not clear to the reviewer that the stated goals will produce results that will have the maximum positive impact on the engine-development simulation community.

#### Reviewer 4:

Thus far, the reviewer noted that the team has performed validations on relevant problems having experimental measurement data. Numerically speaking, the reviewer asked if the project team has proved that the modeling results are consistent when running over different number of computer cores. Also, related to the "Milestones" slide, the reviewer assumed that the comparison of Nek5000 with Transparent Combustion Chamber (TCC-III) engine particle image velocimetry (PIV) measurements is forthcoming.

Meshing is key to any CFD code, especially when related to engine applications. The reviewer wanted to know if the project team has done an extensive study to ensure that the overset meshing strategy conserves mass. Other codes that use this approach have had difficulties in the past. Furthermore, the reviewer asked if there is any plan to look at wall-boundary layers to improve law-of-the-wall formulations. This type of analysis would be relevant, given the recent efforts in developing conjugate heat-transfer modeling approaches.

#### Reviewer 5:

The reviewer stated that comparison of velocity data from the spectral method with other, conventional finite volume approaches would be beneficial. It was not really clear whether NekNek overset is similar to Chimera type of overset meshing or not. The reviewer asked if the method is conservative or not and if there are any limitations with the NekNek type of meshing.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1

The reviewer found the current collaboration to be satisfactory as the PIs are working with the academic source of the code framework and a couple of colleagues from Argonne. The planned collaborations mentioned in the presentation are great potential directions and should be pursued. Details on the framework for these collaborations and the ultimate outcome were not clear to the reviewer and should be considered, particularly as many collaborations were proposed. The clearest and most impactful collaboration is the high-performance computing capability and the PIs should continue strong partnership with this group in order to ensure that the simulation framework is using the computing resources to the greatest extent.

#### Reviewer 2:

The reviewer remarked that this project is just beginning so it is understandable that the partner list is developing. The list of current and proposed partners consists of members from the university and National Laboratory community. The reviewer liked the inclusion of the KIVA 4 team from Los Alamos National Laboratory (LANL). However, the reviewer strongly suggested that the PI seek input from an industrial partner, even in this early stage of planning. An industrial partner will ensure that the scope of the work maintains a perspective relevant to product development. This perspective is important, given the dynamic changes occurring in the automotive industry.

#### Reviewer 3:

The reviewer indicated that collaboration with a company like Pointwise for mesh generation may be valuable for this effort. Also, including an engine OEM in the project collaboration would be beneficial.

#### Reviewer 4:

The reviewer noted that the current collaboration is only with some code development and implementation. Listed collaborators look strong, but they are designated as "potential." According to the reviewer, it would be nice to have more on the list for back up just in case.

#### Reviewer 5:

The reviewer responded that it was hard to say there is a list of collaborators, but no description of the collaboration actually achieved to date. It was curious to the reviewer that collaboration with the LANL development team is limited to mesh generation; surely Carrington, et al., have over the last decade or more made substantial developments warranting greater across-the-board collaboration. Under fast chemistry solvers, the reviewer said that collaboration with LLNL is indicated and asked about collaboration with ANL's own Sibendu Som, who has been working on a tabular chemistry approach. Testing by this reviewer's organization of the LLNL chemistry solver technology a few years back showed it did not provide tremendous speedup, while more recent testing of a tabular approach, albeit not Som's (although that is coming), did show that significant gains (100 times [100X]) were possible.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer remarked that the proposed work takes the project in a logical direction. The work with the direct injection spark ignition (DISI) engine is particularly interesting and will significantly enhance the new working group on light-duty engines. The reviewer commented that the scaling exercises are also quite important. While the implementation of the sub-models will be important for the overall function of this code, there are still questions about overlap with other projects happening concurrently. Finally, the reviewer stated that the idea of building a platform for collaboration and implementation of new sub-models is quite interesting and will significantly increase the impact of this work.

#### Reviewer 2:

The proposed future tasks made sense to the reviewer, although it is to set up a code development and validation environment. The sub-models to be chosen for implementation and/or to be improved were unclear to this reviewer. Also, a more detailed plan is needed on how to setup an interface allowing access to the code and results for industry, academia, and National Laboratories.

#### Reviewer 3:

The reviewer noted that there was no mention of spray-wall interaction models in the proposed research. According to the reviewer, wall heat-transfer models and how they perform with Spectral methods would have a significant impact on overall accuracy.

#### Reviewer 4:

The reviewer suggested that more thought on the "barriers" to producing software that commercial product teams can immediately, consistently, and quickly apply needs to be given and a plan for passing on what is learned in this program to those that can produce, maintain, and support that software needs to be developed. Hooking a research code to a production software is not a route that makes much sense to the reviewer, who suspected that the end-user would spend most of his time getting the research software to work properly or the interface between the software packages to work properly rather than designing new combustion systems.

#### Reviewer 5:

The reviewer observed that the research team is placing a significant focus on studying the CCV issue. Although interesting from a research perspective, it is not as immediately relevant to production engine work. The reviewer suggested that adding a component that does focus and validate available port-flow

measurements to ensure that the code is properly capturing the traditional charge motion versus air flow trade-off. Additionally, the reviewer asked whether Nek5000 properly predicts the breakdown of bulk tumble flow to turbulence to drive turbulence flame speed and how these results compare with a Reynolds-averaged Navier-Stokes (RANS) model. These types of issues are important to industry, given the heavily reliance on CFD to design engine ports and combustion chambers prior to prototype engine builds.

#### Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer asserted that this work links well with overall DOE objectives on a number of fronts. First and foremost, it links very well with the increased use of high-performance computing resources for addressing a range of both fundamental and practical problems. Second, the collaboration with the Advanced Light-Duty Combustion Consortium will boost a number of objectives in that space.

#### Reviewer 2:

The reviewer remarked that the new code platform is supposed to provide a more, in-depth look at the combustion physics in a high performance computing (HPC) environment. This will help further understanding of advanced combustion and develop more efficient engines.

#### Reviewer 3:

The reviewer indicated that there is an important need for this type of modeling activity to guide engineering-level CFD codes.

#### Reviewer 4:

The reviewer commented that yes, this project works on improving overall accuracy of lower order models with higher order codes, such as Nek5000, which is open-source code.

#### Reviewer 5:

In a roundabout fashion, the reviewer commented that improving software tools that aid combustion-systems designers to develop cleaner, more efficient engines certainly supports the DOE's objectives. However, as currently described, it appeared to the reviewer that this program will be producing a research tool that someone might later be able to develop into the kind of tool that engine makers need and the reviewer was not sure that the engine design community can wait that long.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

Resources appeared adequate to the reviewer for the project as currently formulated.

#### Reviewer 2:

The reviewer stated that the project resources should be sufficient, assuming that the high-performance computing resources are available. The PI notes in the presentation slides that proposals for more computing time are in the works. If those are not granted, however, it was unclear to the reviewer how this work will progress.

#### Reviewer 3:

The budget seemed to be enough to the reviewer. Depending on how the partner-collaborator build-up goes, the reviewer suggested that the budget may need to be revisited (either reduce or increase).

#### Reviewer 4:

The reviewer noted that more computational resources may be necessary to accomplish some of the goals mentioned in the future study.

#### Reviewer 5:

It was somewhat unclear to the reviewer about how the \$700,000 will be spent, given that this is an open-source code. The reviewer asked (1) if most of the money is directed toward contractual work for sub-model development, (2), additionally, if the PIs envision wide proliferation of their code to the modeling community, and (3) if so, ANL will provide technical support.

Presentation Number: ace127
Presentation Title: Advanced
Combustion Concepts for HighEfficiency Gasoline Engines
Principal Investigator: Scott Curran
(Oak Ridge National Laboratory)

#### Presenter

Scott Curran, Oak Ridge National Laboratory

#### **Reviewer Sample Size**

A total of two reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer commented that the three PIs use state-of-the-art experimental and advanced analysis methods to improve the understanding of advanced concepts for high-efficiency gasoline engines. The plan to overcome technical barriers is sound.

#### Reviewer 2:

The reviewer indicated that it would be helpful to have seen the surface, volume, and other characteristics of pistons with varying compression ratios (CRs) with the high stroke and bore layout.

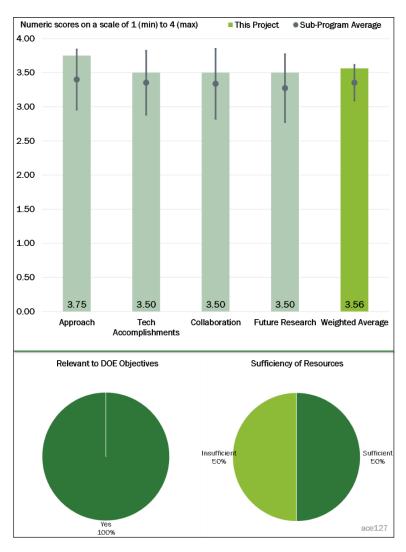


Figure 1-30 – Presentation Number: ace127 Presentation Title: Advanced Combustion Concepts for High-Efficiency Gasoline Engines Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that there were three different tasks associated with this project period and all three produced the expected results. Milestones for current year were met.

#### Reviewer 2:

The reviewer asked why the project team used 99 research octane number (RON) fuel instead of 91 RON 10% ethanol content gasoline (E10).

#### Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer observed that the project requires good coordination with both academia and industry. The results showed that the collaboration during this funding period was very good.

#### Reviewer 2:

The reviewer indicated that collaboration with an advanced ignition activity may help at the high dilution rates.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer stated that higher load experimental results will be the key for hybridization applications.

#### Reviewer 2:

The reviewer found that the plan for the proposed future research is sound. It continues the outstanding work that PI did in the past on advanced combustion strategies for gasoline engines in the past years.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer said that the project will improve the current understanding of combustion strategies for advanced gasoline engines, which is extremely important for DOE objective of designing the next generation of highly efficient and zero-pollution vehicles.

#### Reviewer 2:

The reviewer commented that the project is well matched to high dilution in the road map.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

According to the reviewer, current funding supports the objectives for current and next fiscal year.

#### Reviewer 2:

The reviewer recommended a substantial budget increase for further experimental results as the budget is quite small.

Presentation Number: ace128
Presentation Title: Reduced Precious
Metal Catalysts for Methane and NOx
Emission Control of Natural Gas
Vehicles

Principal Investigator: Michael Harold (University of Houston)

#### Presenter

Michael Harold, University of Houston

#### **Reviewer Sample Size**

A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer found that the project is a good combination of atomic level (DFT) modeling, reactor-level modeling, and experiment. The initial results are intriguing. The reviewer was interested to see the mechanistic conclusions regarding the influence of the spinel on performance during modulation (and why modulation can be tuned).

#### Reviewer 2:

The reviewer observed that the project looks at the problem of improving methane conversion comprehensively

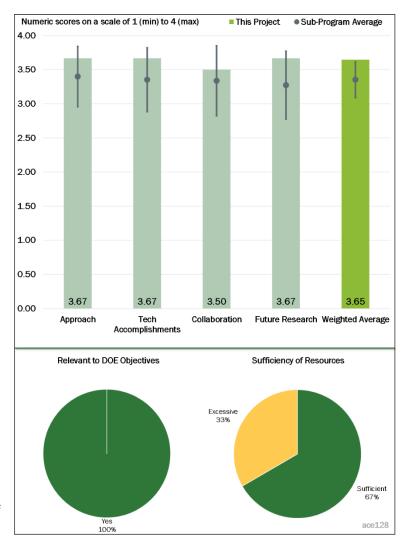


Figure 1-31 – Presentation Number: ace128 Presentation Title: Reduced Precious Metal Catalysts for Methane and NOx Emission Control of Natural Gas Vehicles Principal Investigator: Michael Harold (University of Houston)

through atomistic simulations for new materials discovery, flow-reactor studies for understanding the impact of lambda variations (as an example), and finally, engine studies. The project addresses the following barriers effectively: evaluation of new materials and lambda lean/rich cycling optimization is expected to provide a pathway to low-temperature methane conversion and the reduction of PGM usage; and the inclusion of sulfur impact, which is important for practical considerations.

#### Reviewer 3:

The overall approach seemed feasible to the reviewer. It is addressing the barrier to adoption of natural gasfueled vehicles of methane emissions out the tailpipe.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer said that everything appears to be progressing on schedule.

#### Reviewer 2:

The reviewer commented that the performance of a PGM-only versus a PGM and spinel material has been compared, with the latter shown to provide a much superior performance under lean and rich cycling. Cycling frequency and amplitude have been studied and also some mechanistic explanation is proposed. This should lead to further improvements in the future. The reviewer noted that DFT studies are helping to discover and assess new materials, although it is not clear how well these are integrated with the flow-reactor studies and if there is a rapid screening process in place for new materials.

#### Reviewer 3:

The reviewer observed that the goal is high methane-oxidation conversion with catalyst PGM loadings under 30 g/cubic foot and to do so by leveraging the project team's expertise with spinel compounds. The team has been able to get 50% methane conversion at 350°C and 10% at 300°C, which are promising but not yet at the target.

Ouestion 3: Collaboration and Coordination Across Project Team.

The project appeared to the reviewer to be well coordinated across the project team, with the University of Houston (UH) as the main driver.

#### Reviewer 2:

It looked to the reviewer like the project team is drawing well on the expertise that each partner organization provides.

#### Reviewer 3:

The combination of the DFT approach and flow reactor was not apparent to the reviewer, who inquired as to how many new materials were discovered through DFT and how many of those were tested through flow reactor studies. The reviewer noted that it will be good to see a scatter plot showing light-off temperatures on the flow reactor versus a DFT-based metric for various materials.

Ouestion 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer commented that the project plan is very clearly laid out across a range of activities; it is very nice work. The reviewer was excited to see where this goes.

#### Reviewer 2:

The reviewer remarked that the project team is proposing a lot of future work (Tasks 2.1 through 2.9 in the presentation), which seems very ambitious for the next year or two. The reviewer agreed that those tasks are necessary, especially to improve methane conversion below 300°C. According to the reviewer, it would be good to understand how spinel enhances the methane conversion, especially when cycling around stoichiometric conditions.

#### Reviewer 3:

The reviewer said that future work is well planned. Sulfur tolerance is in scope, not done yet, and it was encouraging to the reviewer to see this being done sooner rather than later as it is better to find out early if the material has serious degradation issues with sulfur. Also, the reviewer suggested that some hydrothermal aging should be included to assess end-of-life performance of the catalysts. Also, the reviewer stated that it will be good to include more spinel compositions in the study (the reviewer was not clear if the chosen one is optimum). This will be especially important and useful to further reduce the light-off temperature.

#### Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer responded positively. Given the regulation of CH<sub>4</sub> as a greenhouse gas and the natural gas production capacity in the United States, an effective and low-cost methane abatement method is necessary for the adoption of stoichiometric natural gas vehicles.

#### Reviewer 2:

The reviewer noted that natural gas engines are gaining market share, both for GHG emissions as well as low  $NO_x$  considerations on heavy-duty vehicles. Methane emissions are an issue with these engines and this needs to be addressed.

#### Reviewer 3:

The reviewer said that the program addresses barriers to adoption of heavy-duty (HD) natural gas engines that would replace HD diesel engines.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The project appeared to the reviewer to be sufficiently funded.

#### Reviewer 2:

The reviewer commented that the use of various tools—from DFT through to engines—is necessary for such projects and is being done effectively. It will be useful to screen more materials and this is one place where the resources may be in question. The reviewer recommended that the budget should be reviewed in a year.

#### Reviewer 3:

It looked to the reviewer like the total budget is \$2.5 million over 3 years (or roughly \$800,000 per year), which seems generous, especially since the year 1 budget was \$660,000. The reviewer wanted to know how the money will be spent and if there are more resources coming available to support the ambitious set of future tasks.

Presentation Number: ace129
Presentation Title: Design and
Optimization of Structured MultiFunctional Trapping Catalysts for
Conversion of Hydrocarbons and NOx
from Diesel and Advanced
Combustion Engines
Principal Investigator: Michael Harold
(University of Houston)

Presenter
Michael Harold, University of Houston

Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer indicated that the movement toward Tier 3 LEVIII emissions standards for vehicles requires the investigation of multiple novel approaches in order to ensure viable aftertreatment solutions are available. In particular, the most challenging emissions component of the certification drive cycle is the low-temperature, cold-start phase, and, potentially, the newly emerging requirements of off-cycle and on-road testing where the catalyst may "light out." The reviewer commented that conventional catalysts do not always

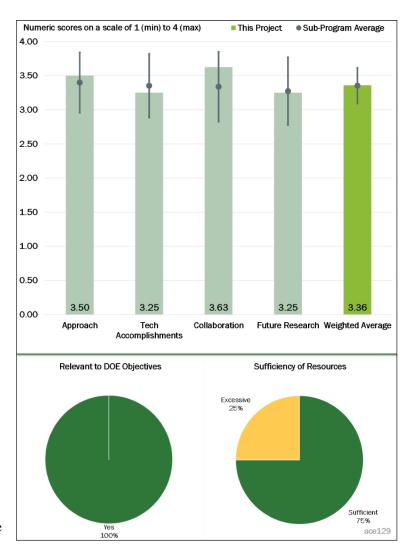


Figure 1-32 – Presentation Number: ace129 Presentation Title: Design and Optimization of Structured Multi-Functional Trapping Catalysts for Conversion of Hydrocarbons and NOx from Diesel and Advanced Combustion Engines Principal Investigator: Michael Harold (University of Houston)

have adequate capability to meet or remediate these emissions. Therefore, alternative, novel formulations or alternative approaches to remediating HC, CO, and NO<sub>x</sub> emissions must be developed. According to the reviewer, this work represents a novel solution by combining the functionality of both HC and NO<sub>x</sub> trapping at very low temperatures, along with an oxidation component in one catalyst for a lean application. The individual HC trapping and PNA materials are representative of technologies that have shown promise and are therefore reasonable starting points for further developing the combined functionality.

#### Reviewer 2:

The reviewer commented that this is a nice approach for combining an HCT, a PNA, and an oxidation catalyst to achieve both low HC and NO<sub>x</sub> emissions. The combination of reactor work and molecular modeling is commendable.

#### Reviewer 3:

The reviewer stated that the project team has a sensible approach to address emissions-control barriers to more efficient and less polluting engines.

#### Reviewer 4:

Overall, the reviewer said that a systematic approach is used in this project, which includes DFT and microkinetic and reactor-level modeling. However, one concern of the reviewer is that reactor-based evaluation of multi-component catalyst systems would not correctly capture the temperature gradients developed along the flow direction in actual exhaust systems, potentially generating overly optimistic results and conclusions. Immediately following an engine cold start, the reviewer indicated that the storage devices (HC and NO<sub>x</sub> traps) located upstream would be heated up first by the hot engine exhaust, but the conversion devices (oxidation catalyst [OC] and SCR) located downstream would remain cold. Such a temperature gradient along the flow direction would be expected to add further challenges to the common problem associated with many current storage catalyst systems, namely, premature release of the stored species before the conversion devices become operational. The reviewer suggested that simulating this adverse effect of thermal gradient in a realistic way in the laboratory reactor would be very difficult, and thus reactor-evaluation results should be viewed with caution. It would be worth exploring ways to integrate the conversion functions into the storage and release function in single devices in order to circumvent or mitigate the problem and thus increase the practicality of this project.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer found interesting modeling to explain the benefits of ethylene  $(C_2H_4)$  and CO on the  $NO_x$  storage efficiency. There is impressive agreement between the model and experimental results.

#### Reviewer 2:

The reviewer said that there was good progress according to the plan, with budget period 1 (BP1) milestones achieved.

#### Reviewer 3:

The reviewer said that investigating appropriate benchmarking of materials and appropriate feed compositions is a logical start to the project and will help guide the development of the most promising materials. This project team is also incorporating a thorough kinetic and mechanistic model into this development effort to provide the level of understanding necessary to optimize the catalyst formulations. The reviewer commented that making use of novel materials under development by members of this consortium, will help speed the process of providing a viable solution as long as appropriate thermal and chemical aging is performed quickly to adjust the material development pathway. Consulting established test protocols for these materials will be beneficial. Additionally, as the catalyst is being developed, the reviewer suggested that the investigators should consider how to diagnose the functionality of the combined catalyst since this is requirement of the OEMs for their aftertreatment.

#### Reviewer 4:

While the technical team has made good progress, the reviewer indicated that there are also some significant gaps. It looked to the reviewer like the overall progress is somewhat behind schedule. It appeared to the reviewer that the early progress was with PNA materials and HC oxidation. The work on HC traps is lagging, according to the reviewer.

#### Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The members of this project team are a very good combination of formulators, modelers, and OEMs to ensure the focus is in the correct direction and is addressing the needs of the end customer.

#### Reviewer 2:

It looked to the reviewer like each project team member company is substantially contributing to the program. Co-Investigator Bill Epling of the University of Virginia (UVa) has been leading HC trap work.

#### Reviewer 3:

The reviewer found good collaboration and coordination with UVa, ORNL, Southwest Research Institute (SwRi), and JM.

#### Reviewer 4:

According to the reviewer, there is excellent sharing of duties among UH, UVa, SWRI, and ORNL.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer stated that the proposed future activities are appropriate for this work.

#### Reviewer 2:

This reviewer noted that work on the HC traps needs to catch up to work on the PNA and HC oxidation catalysts. The reviewer inquired about the following: the best order of the functions; how to ensure that the net function is still what is desired, as EAS warms up; and if the functions can be layered into one monolith so that the thermal gradients are not an issue.

#### Reviewer 3:

The proposed future research seemed to the reviewer to focus on refinement, improvement, optimization, and integration of the BP1 milestones. The reviewer said that it would be worth exploring ways to integrate the conversion functions into the storage and release functions in single devices in the future in order to increase the practicality of the project.

#### Reviewer 4:

The reviewer called out a need to investigate PNAs over multiple tests performed consecutively. Higher CO levels cause more deactivation so multiple tests with different CO levels would be helpful. The reviewer indicated that efforts to minimize this deactivation on consecutive tests need to be included in the project as this is the greatest challenge for PNAs today.

#### Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer stated that this project satisfies the need for more efficient aftertreatment systems to meet increasingly stringent emissions standards, while improving fuel efficiency.

#### Reviewer 2:

The reviewer commented that the project is looking at new technologies to support faster criteria-pollutant removal from ICE exhaust, which supports lower fuel use during cold-start periods.

#### Reviewer 3:

The reviewer found that this project is aimed at developing multi-functional catalyst systems to control HC and  $NO_x$  emissions during cold-start periods.

#### Reviewer 4:

According to the reviewer, NO<sub>x</sub> and HC traps will be needed for fuel-efficient engines to achieve low-emission standards.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

It appeared to the reviewer that sufficient resources are available, especially with effective coordination and collaboration with the multiple partners involved.

#### Reviewer 2:

The reviewer said that resources among the different companies seem to be sufficient.

#### Reviewer 3:

The reviewer stated that resources are sufficient.

#### Reviewer 4:

The reviewer commented that \$2.35 million seems like a very generous budget for a program with this scope unless the materials and testing are considerably more expensive than the reviewer is estimating. It was not clear to the reviewer how the project team will be able to spend out its remaining budget to complete the BP2 milestones, given the current team size and resources.

Presentation Number: ace130
Presentation Title: Development of
Passive Hydrocarbon/NOx Trap
Catalysts for Low-Temperature
Gasoline Applications
Principal Investigator: Mark Crocker
(University of Kentucky)

#### Presenter

Mark Crocker, University of Kentucky

#### **Reviewer Sample Size**

A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer praised the project as a really strong combined modeling and experimental approach to understand the fundamental chemistry of PNA zeolites.

#### Reviewer 2:

The project utilizes a good mix of experimental and computational methods and appeared to the reviewer to be well designed.

#### Reviewer 3:

The reviewer stated that the approach of focusing on one class of materials—Pd/zeolite—and studying the fundamentals of NO adsorption and desorption is a good one.

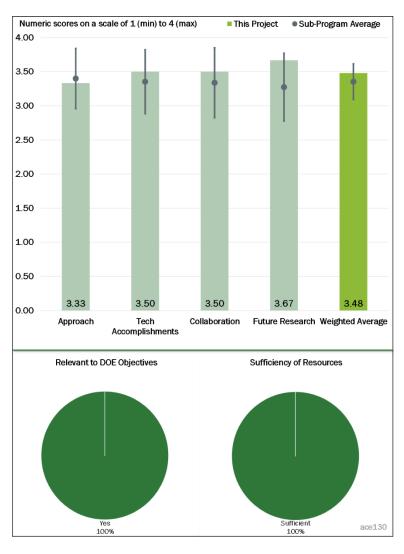


Figure 1-33 – Presentation Number: ace130 Presentation Title: Development of Passive Hydrocarbon/NOx Trap Catalysts for Low-Temperature Gasoline Applications Principal Investigator: Mark Crocker (University of Kentucky)

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer found strong progress to date. Years 1 and (the partial of) 2 were focused on understanding the framework, aluminum distribution, and SAR impact on NO adsorption and desorption behavior.

#### Reviewer 2:

The reviewer noted that identification of Pd species most active in NO adsorption is an important step. Also, identification of CHA as more effective than BEA or CeO<sub>2</sub>-ZrO<sub>2</sub> is an important step forward. Understanding the degradation mechanism and overcoming that will be useful, according to the reviewer.

#### Reviewer 3:

The project appears to be progressing well, though it was somewhat unclear to the reviewer whether the milestones are on track. For instance, the reviewer noted that the status of spectroscopic studies, which has a date in the past, is "Done/on-going." The reviewer asked whether this implies that the milestone has been met but additional work is being done in the area.

#### Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer commented that there is excellent collaboration that includes three universities, a National Laboratory, an OEM, and a catalyst company—a great team.

#### Reviewer 2:

The project appeared to the reviewer to be well coordinated across a broad set of collaborators.

#### Reviewer 3:

The reviewer said that this is a good partnership, including an OEM and a catalyzer on board.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer indicated that there are really strong, on-going and future work plans.

#### Reviewer 2:

The future work appeared to the reviewer to be well planned. The work on reactivation and prevention of degradation is especially important for practical application of this technology.

#### Reviewer 3:

The reviewer commented that the future work addresses some of the challenges identified and extensions to include the impact of CO and HC on NO adsorption. Engine testing is an important part of the future work and should be done, especially under certification test-cycle conditions. The reviewer said that it will be useful to look at the degradation mechanism identified in this work.

#### Ouestion 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that the project was very relevant to DOE and OEM interests.

#### Reviewer 2:

The reviewer observed that passive  $NO_x$  (and HC) adsorption is important to address cold-start emissions, which cannot be treated by traditional three-way catalysts (TWCs). This is important to meet the Tier 3 LEVIII regulated tailpipe limits for HC +  $NO_x$ .

### Reviewer 3:

The reviewer stated yes, and added that Passive NO<sub>x</sub> and HC adsorption is one of the possible pathways to reduce cold-start emissions. The focus on the largest market (stoichiometric gasoline) made sense to the reviewer.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer stated that resources look sufficient for the work done so far and planned.

## Reviewer 2:

The project appeared to the reviewer to be sufficiently funded.

#### Reviewer 3:

The reviewer remarked that funding levels look good.

## Presentation Number: ace131 Presentation Title: Ducted Fuel Injection (DFI) for Heavy-Duty Engines Principal Investigator: Charles Mueller (Sandia National Laboratories)

#### Presenter

Charles Mueller, Sandia National Laboratories

#### **Reviewer Sample Size**

A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

#### Reviewer 1:

The reviewer praised the project as exciting and potentially seminal work. It is being methodically done—working to understand the fundamentals and progressively increasing the scope of the work toward more realistic engine operation.

#### Reviewer 2:

The reviewer said that this project is directly addressing the barriers for soot reduction with a very novel idea. It leverages a unique and the best resource available—an optical engine—to identify soot formation and the reduction mechanism.

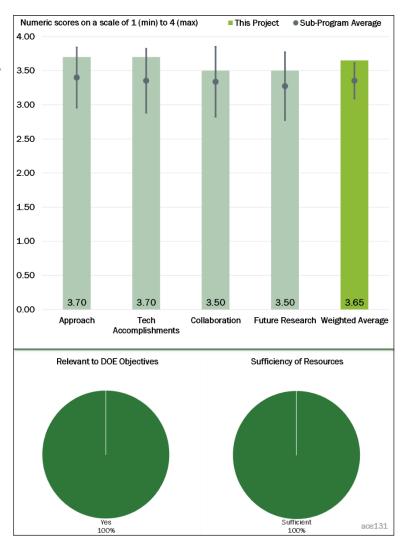


Figure 1-34 – Presentation Number: ace131 Presentation Title: Ducted Fuel Injection (DFI) for Heavy-Duty Engines Principal Investigator: Charles Mueller (Sandia National Laboratories)

#### Reviewer 3:

According to the reviewer, the project uses an optical engine to assess the ducted fuel injection (DFI) technology for diesel engines. Parametric studies of a variety of operating parameters were conducted to evaluate their impacts on emissions and efficiency. The reviewer said that more detailed analyses and incylinder imaging about the DFI will be helpful to improve the understanding of the physics.

#### Reviewer 4:

The programmatic approach seemed reasonable to the reviewer, with current work focused on understanding engine behavior with a simplified two-hole and duct system, then increasing system complexity as part of future work. Key technical questions are clearly understood, and the order of approach seemed appropriate to the reviewer to investigate each of them in turn.

#### Reviewer 5:

The reviewer found that the project is well designed to address the simultaneous reduction of engine-out  $NO_x$  and particulate emissions, which are one of the key research areas of highest priority for clean diesel

combustion. The primary focus of the results presented in this research so far has been based on burning all the fuel and burning it as fast as possible. With fuel stratification schemes more prevalent in diesel engine applications, the reviewer suggested that the investigators should make sure that they investigate how this combustion technology will be affected with multiple injections.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer found excellent progress. The experimental data, analysis, and interpretation are outstanding. There is no hype associated with the development of this concept—just statements of the facts and observations.

#### Reviewer 2:

The reviewer praised the fantastic progress made on this project, with clear demonstration of the simultaneous reduction of engine-out  $NO_x$  and particulate emissions albeit at a single-mode point of 1200-revolutions per minute (rpm) engine speed. The reviewer had a suggestion to please take images of the jet that comes out of the duct and include those in future presentations or reports.

#### Reviewer 3:

The PIs have successfully installed DFI into one optical engine at Sandia. Parametric studies of EGR, duration of injection (DOI), state of charge (SOC), injection pressure, intake manifold absolute pressure (IMAP), and intake-manifold temperature have been conducted. With DFI, two to three orders of magnitude reduction in soot is observed. Retarding SOC reduces NO<sub>x</sub> emissions but increases HC and CO emissions. Increased injection pressure leads to lower soot, HC, and CO. In-cylinder images from the optical engine are expected.

#### Reviewer 4:

The reviewer remarked that very solid accomplishments have been made to explore the concept. The DFI has shown clearly that it can break the  $NO_x$ -soot tradeoff. Various parameter sweeps tested help in characterizing the DFI performance as well.

#### Reviewer 5:

The reviewer noted that the program is making good overall progress, with the implementation of a two-hole and duct system and sweeps conducted of primary engine parameters to understand general performance and emissions trends. Given the timing, as a new program start for 2019, the reviewer said that good progress has been made thus far. There have been several publications, and quite a number of presentations on the work, within the past year.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer indicated that there is good collaboration and coordination with other institutions and industry partners through the CRADA. The reviewer suggested that the project team please continue to engage more industry partners that will help with overcoming barriers to commercialization of the technology in the long term. The reviewer applicated the work as well done.

#### Reviewer 2:

The reviewer commented that collaboration and stakeholder engagement have been beneficial for this project and are being leveraged to help design experiments and identify the fundamentals that could be better understood via simulation efforts.

# Reviewer 3:

The reviewer stated that the project is partially involved with Co-Optima. Collaborations with OEMs, including Caterpillar and Ford, have been established through a CRADA, which is very helpful for pushing the technology into the market.

#### Reviewer 4:

According to the reviewer, it was good to see the commercialization CRADA with Caterpillar and Ford. Recognizing the challenges of a new, unique technology and more active collaborations to support and accelerate advancement would be of value.

# Reviewer 5:

The reviewer found a very nice arrangement of collaboration across industry and academia. It would be nice to include a few more CFD groups to try RANS and DNS as well.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer noted that the proposed future research follows a logical progression of sequentially stepping toward more fundamental understanding of DFI under more realistic engine-operating conditions.

#### Reviewer 2:

The reviewer stated that there is a clear understanding of the remaining key technical barriers and proposed future work addresses them. Performance of ducted fuel injection at high loads and duct behavior when ducts are placed in close proximity are key questions that need to be addressed moving forward.

# Reviewer 3:

The reviewer indicated that the plan for future work has not been extensively laid out, with the next and only milestone identified being the sensitivity of DFI to operating condition and fuel-injection parameters. This is understandable since the research work is still in the exploratory phase. However, the reviewer asserted that reasonable effort was made to identify the remaining challenges and barriers as well as future research.

# Reviewer 4:

The reviewer remarked that the missing parts of the current project are mainly the lack of theoretical analysis and CFD, which have been included in the research plan. Potential risks, such as wall impingement on duct surface and deposit formation, have been considered.

#### Reviewer 5:

The reviewer said that studying the geometry effect relative to injector configuration (hole diameter, for example) would be critical future work. The reviewer suggested closely monitoring the fuel-conversion efficiency trend with load changes.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer praised this work as an ideal example of what a National Laboratory can do to meet the needs from DOE, industry, and the community. The long-lived NO<sub>x</sub>-soot trade-off is finally about to be broken, if successful.

#### Reviewer 2:

If successful, the reviewer remarked that this combustion technology will provide an in-cylinder solution for simultaneously reducing engine-out  $NO_x$  and particulate emissions that will eliminate the need for aftertreatment systems, with the end result being the availability of a low-cost, clean energy solution that can be commercialized.

#### Reviewer 3:

According to the reviewer, the major challenge with the modern diesel engine is to meet the emissions standard for particulate matter. This project explores a new technology that has the potential to reduce incylinder soot emissions, which is of great importance for diesel engines and aligns with DOE's mission.

#### Reviewer 4:

The reviewer said that cleaner diesel engines achieving the same or better efficiency is relevant work for DOE.

#### Reviewer 5:

The reviewer noted that the program supports DOE objectives for clean energy technologies for transportation.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer found great progress, with no indication that the work has been constrained by lack of resources.

#### Reviewer 2:

The level of funding seemed adequate to the reviewer and commensurate with achieving the stated remaining milestone, which is due on September 30, 2019.

#### Reviewer 3:

The reviewer said that the current facility at Sandia is sufficient for conducting this project. Advanced diagnostic tools available at Sandia should be sufficient for in-cylinder analysis of DFI.

#### Reviewer 4:

Program resources seemed sufficient to the reviewer, based on the program status as a new effort and progress thus far.

# Reviewer 5:

Considering that this project is split in two, the reviewer stated that the funding seems to be sufficient.

# Presentation Number: ace132 Presentation Title: Heavy-Duty Gasoline Compression Ignition Principal Investigator: Chris Kolodziej (Argonne National Laboratory)

#### Presenter

Chris Kolodziej, Argonne National Laboratory

Reviewer Sample Size A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer observed that the project uses a single-cylinder, heavy-duty diesel engine dynamometer to evaluate the GCI technology for heavy-duty applications. Additionally, endoscopic imaging was used to visualize the incylinder combustion process. Transmission electron microscopy (TEM) was used for characterization of soot-size distribution. X-ray was used to investigate the injector erosion. Onedimensional (1-D) and threedimensional (3-D) simulations helped to identify the conditions of liquid wall impingement. The reviewer noted that a few of the most representative speeds and loads have been focused on.

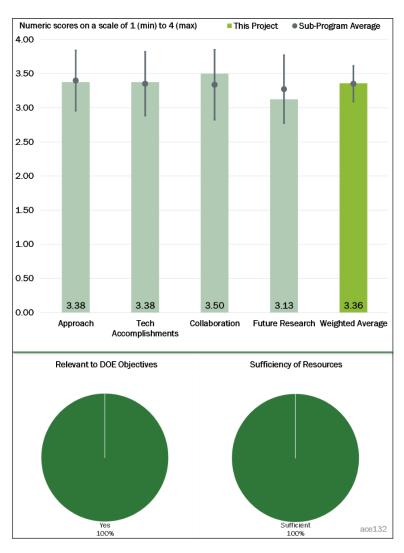


Figure 1-35 – Presentation Number: ace132 Presentation Title: Heavy-Duty Gasoline Compression Ignition Principal Investigator: Chris Kolodziej (Argonne National Laboratory)

#### Reviewer 2:

The reviewer remarked that the approach is a sound combination of single-cylinder engine testing, X-ray tomography, spray simulations, and fast sampling of the in-cylinder gas composition. The aim is utilization of gasoline-like fuels in a diesel engine for enhanced efficiency and reduced emissions. Theory predicts a simultaneous reduction of soot and  $NO_x$  while utilizing a fuel with lower overall demand than diesel. Multiple combustion modes are planned with an additional focus on cold start (the industry sponsor is interested in cold start as well).

# Reviewer 3:

This project approach looked tractable to the reviewer and it can be seen how there is a path to achieving the project objectives. It was a little unclear to the reviewer how the fast-gas sampling system contributes toward achieving the goals. The engine-hardware support from the OEM helps to increase the likelihood of meeting objectives since engine design modification is difficult without support.

# Reviewer 4:

The reviewer found the approach to be generally sound. Reducing heat loss is mentioned several times; indeed, it appears at the top of the list in this presentation in terms of challenges to be overcome. Companies are also targeting this as a key means of increasing diesel efficiency. Yet, the reviewer saw little in the approach in terms of how this goal will be achieved; there was no mention of instrumentation available or being added to even look at this. One would think for something so obviously mentioned as a challenge that the approach described would at least address how it will be studied and perhaps addressed. Either that or it should be moved lower down in the list of challenges so the disconnect is not so obvious.

Ouestion 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that the dynamometer and fuel system are ready. The cylinder head has been modified to provide access for the endoscope and spark plug. The port fuel injection (PFI) SI mode with ethanol and gasoline has been tested. Preliminary engine dynamometer data have been presented. The reviewer stated that NO<sub>x</sub> and soot emissions of GCI were measured and compared with conventional diesel combustion. Better NO<sub>x</sub>-soot tradeoff was observed. Particularly, TEM results show no evident difference between gasoline soot and diesel soot with different EGR level in terms of particulate size and size distribution.

#### Reviewer 2:

The reviewer observed that the project team had gathered initial PFI data from a far-from-ideal scenario (spark plug recessed and above the squish, for example). Slow flame propagation due to the large bore and relatively quiescent chamber resulted in running the engine rich (location of the highest laminar flame speed of the fuels utilized). The engine and test cell modification are well underway. Early work indicated to the reviewer that the soot behavior from gasoline and diesel was very similar in operating parameters.

#### Reviewer 3:

According to the reviewer, the completed milestones for this project show good progress. There is a substantial amount of test hardware, engine modification, and test cell upgrades. This is a substantial amount of good progress. The reviewer said that the non-optimal, initial SI testing on the single-cylinder oil test engine (SCOTE) is fine for initial scoping. The reviewer was unsure why the scoping was done at rich conditions unless this was done to just show that if flame speeds are increased, then there is operable space. The reviewer's first thought would be to not waste any more effort on SI testing with the old cylinder head and bad spark-plug location. The reviewer suggested that the project team consider coordinating the TEM and fast-gas sampling system with the other areas of GCI better as the project continues, as right now this seems a little disconnected.

#### Reviewer 4:

This reviewer commented that a lot of year 1 effort has gone into getting engine hardware squared away certainly a necessary effort, but one that generally creates potential for achieving progress in overcoming the technical barriers rather than progress itself. Finding that gasoline produces less soot than diesel is not exactly a revelation. Switching from diesel to gasoline would presumably require modifications to the baseline engine's "combustion recipe" in terms of bowl shape, injection characteristics, etc. The reviewer asked if any work is being planned on doing some re-optimization studies with CFD and procuring hardware to match the recommendations that result. The reviewer said that progress on that might be interesting to see.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer found strong connections with industry. Collaborations with other teams at ANL generated valuable results for this project. The HD off-road industry workshop provides a platform for discussion and connection with industry.

# Reviewer 2:

The reviewer indicated that this project approach is generally very good. There seems to be strong industry collaboration and the reviewer expected that there will be increased publications and communications of project results as the project really starts to produce deliverables.

#### Reviewer 3:

According to the reviewer, the collaboration with Caterpillar has be specifically active during the engine modification stage. Other collaborative efforts are active but have yet to be implemented (fast sampling valve, endoscopy, etc.) or to bear fruit.

# Reviewer 4:

According to the reviewer, switching an injector from diesel to gasoline can have some unexpected negative impacts on the injection system and the reviewer expressed surprise that no injector manufacturer is in the collaborator list. Aramco is seen as a collaborator on GCI, which makes sense because it has been working on that recently. However, John Dec at SNL has been working in this area for as long, if not longer, and the reviewer was surprised that SNL is not listed as a collaborator. Surely, there should be some coordination between DOE labs who are, or have been, engaged in the same basic research beyond just looking at each other's presentations at Advanced Engine Crosscut (AEC) meetings.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

# Reviewer 1:

According to the reviewer, the current gaps and barriers have been well addressed in the research plan, especially the heat loss and noise at high load, wall impingement at low load, and cold start. The reviewer indicated that including CFD analysis should be a plus for better understanding of the whole process and better productivity.

# Reviewer 2:

The proposed future work looked sound to the reviewer and should guide the team during pursuit of their objectives. Attainment of diesel-like efficiency while defeating the soot-NO<sub>x</sub> tradeoff is commendable, but the reviewer wanted to know whether the goal should not be higher for an advanced combustion modes.

#### Reviewer 3:

The reviewer remarked that there looks to be a clear future direction, but the project is just starting and will quickly learn more to refine the direction as needed. The reviewer encouraged the project team to please continue to frequently evaluate results with collaborators.

# Reviewer 4:

Knowledge led the reviewer to suspect that coming up with a combustion system that will be optimized (and thus achieve maximum efficiency and minimum emissions across the load map) for both LTC and mixing-controlled compression ignition (MCCI) operation will be difficult. It was not clear whether the challenge is being addressed or is being dismissed as trivial. It was also unclear to the reviewer how or if simulation is being brought in as a tool to assist in achieving project goals, how controlling heat loss will be addressed, or even how heat loss will be measured.

Question 5: Relevance—Does this project support the overall DOE objectives?

# Reviewer 1:

The reviewer noted that the program promises to address increasing efficiency while minimizing emissions, which matches DOE's objectives, as does looking at what, for CI engines at least, is an alternative fuel.

# Reviewer 2:

The reviewer indicated that the technology will enable using cheaper gasoline for heavy-duty applications, with very low emissions. Success of this technology will significantly reduce the fuel cost for consumer, lower emission, and lower costs for manufacturers.

#### Reviewer 3:

The reviewer said that the project aims to defeat the NO<sub>x</sub>-soot tradeoff, very much in line with overall DOE objectives.

# Reviewer 4:

The reviewer found that this project is extremely relevant for achieving the DOE's objectives, particularly toward energy security and utilization of different fuels in the heavy-duty sector.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

# Reviewer 1:

The reviewer said that the project team is well positioned from a resource perspective.

#### Reviewer 2:

For the plan as described, the resources appeared to the reviewer to be adequate.

#### Reviewer 3:

According to the reviewer, present resources are sufficient for this project.

#### Reviewer 4:

These seemed fine to the reviewer for the given scope and tasks.

Presentation Number: ace133
Presentation Title: Next-Generation
Heavy-Duty Powertrains
Principal Investigator: Scott Curran
(Oak Ridge National Laboratory)

Presenter Scott Curran, Oak Ridge National Laboratory

Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer praised the work as fantastic, with good potential. The approach used in performing the nextgeneration, heavy-duty powertrain work consists of four projects addressing R&D challenges in achieving enginesystem efficiency goals. The reviewer suggested that the investigators should quantify or outline targets for the engine-system efficiency gains and improvements that will be achievable with each of the critical technologies being investigated in these projects. Advanced diagnostics, neutron imaging, low-temperature combustion, and coldstart and restart are valuable building blocks with reasonable feasibility.

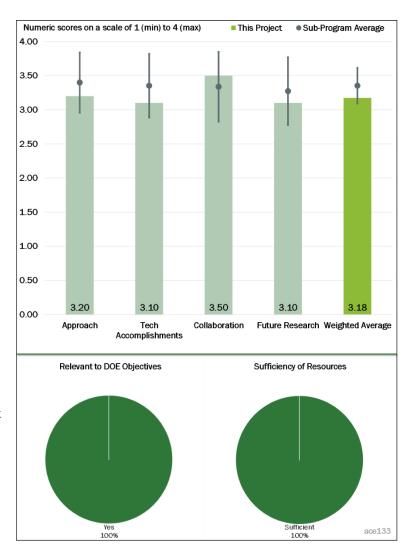


Figure 1-36 – Presentation Number: ace133 Presentation Title: Next-Generation Heavy-Duty Powertrains Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

#### Reviewer 2:

The reviewer stated that the four projects reviewed in this presentation are systematic investigations and development of new diagnostic capabilities and engine-operating scenarios for cold start and clean combustion. The projects are motivated and informed by collaboration with relevant stakeholders.

#### Reviewer 3:

There are four different tasks within this review, which made it a little difficult for the reviewer to assess approach quality. The general approach to using many different methods to attack critical areas of foundational barriers made sense to the reviewer, who thought that the challenge will be to integrate these four separate tasks, or consider whether they even should be lumped together. This may be an area that needs some further consideration.

# Reviewer 4:

The reviewer noted that the approach does focus on barriers to understanding combustion physics better and improving engine efficiency and emissions. However, those four tasks did not seem to be synergistic to the reviewer. Perhaps it is due to the administrative arrangement.

#### Reviewer 5:

According to the reviewer, the program approach includes four different subtasks focused on widely different subject areas. The reviewer commented that there was a somewhat limited discussion of what technical barriers are being addressed and why specifically the different approaches are being utilized. It is generally a good mixture of tasks aligned with future heavy-duty powertrain development, including both hybrid focus, engines, and diagnostic techniques.

For the Task 1 focus on new diagnostics, several different instruments are discussed, but it was not clear to the reviewer how these specific measurements are connected to key overall technical barriers and why they were chosen as key measurements to focus on. For Task 2, the science application of neutron imaging was quite interesting to the reviewer, but it is not very clear how development of high-fidelity models of injection hardware contributes to improved understanding of the combustion processes and improved efficiency for MD and HD engines.

For Task 3, the reviewer said that the focus is exploring medium- and high-load operation with different LTC strategies. However, the discussion of which LTC strategies will be applied was not very clear to the reviewer, who stated that the range of concepts that could be employed is quite broad. It was difficult for the reviewer to understand which combustion concepts the work will focus on or what strategies are planned to investigate and extend high-load operation. The reviewer suggested connecting work on LTC load limits with the hybrid focus in Task 4 since, depending on the type and scale of hybridization employed, the required engine loads may decrease with increased electrification. This may put tighter bounds on the maximum load required from an LTC concept. Additionally, due to the overall vehicle advancements in the SuperTruck programs, key operating loads may differ from historic norms and should be reflected in this work. The reviewer indicated that the vehicle modeling parameters for the work in Task 4 should be more clearly defined and should be reflective of future truck configurations aligned with the advancements seen in the SuperTrucks.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer commented that most of the planned activities on these projects are underway, with the exception of the advanced diagnostics project (Task 1) in which substantial CFD work has been completed and the focus is turning toward the collection of measurements to validate and improve CFD.

# Reviewer 2:

The reviewer indicated that the projects are new and progress is on track. To date, actual data and results are preliminary.

#### Reviewer 3:

The reviewer said that the project is a new start, but progress in several areas is quite limited.

# Reviewer 4:

The reviewer remarked that each of the four tasks has made strong accomplishments, especially in utilizing and improving the unique neutron-imaging capability that will certainly lead to better understanding combustion processes in injector-nozzle flows.

# Reviewer 5:

Regarding Task 1, the Advanced Diagnostics CRADA with Cummins, the reviewer asserted that the  $H_2O$  absorption thermometry probe work looked to have made very good progress with measurements in a hot stoichiometric engine. The reviewer asked if publications of probe performance and capability will be coming out of this work. The next steps on a real-time engine surface temperature probe looked very interesting to the reviewer, but it was unclear exactly where this effort is currently. This is a very difficult topic and the reviewer was concerned that there is a low likelihood of success given challenges like thermal boundary layers, turbulence near the wall, signal trapping from optically thick combustion gases and PM, and surface deposits.

With respect to Task 2, Neutron Imaging, the reviewer indicated that progress looks to be very good with this unique capability. The reviewer encouraged the project team to please continue to work on improving resolution and understanding what quantities can be measured that provide the greatest value for physics understanding and simulation validation.

For Task 3, Next Generation LTC Engines for MD and HD, the reviewer suggested not worrying about  $NO_x$  emissions as much as understanding how to burn gasoline-like fuels in a HD engine. The reviewer encouraged the project team to please coordinate with that of ACE132 on this Task 3. Comparisons to where engine indicated and brake efficiencies can be improved will be very useful. The benchmark diesel efficiencies are very good today so identifying if there is or is not a real opportunity first would be paramount. Lean  $NO_x$  aftertreatment is here and reductions of  $NO_x$  less than 3 g/kWh are not necessarily beneficial. The reviewer warned the project team against continuing efforts to push LTC to full-load operation; industry knows this is not desirable and does not want this.

Regarding Task 4, Cold-Start and Restart for Electrification of MD and HD Powertrains, the reviewer said that the end goal of providing combustion and emissions data during restarts with electrified powertrains is likely very sensitive to the base-engine calibration and restart-operation strategy. The reviewer wanted to know how the project team will proceed to provide a clear understanding of the calibration impacts and will provide a complete engine-side understanding along with the hybrid side.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer applauded the collaboration and coordination with a broad base of industry partners as fantastic and well done.

# Reviewer 2:

According to the reviewer, these project teams are motivated and informed by collaborators who desire to gain more fundamental understanding of different phenomena they must deal with in real engines in the quest to make them cleaner and more efficient.

#### Reviewer 3:

The reviewer remarked that each subtask has a good variety of collaborations and it was good to see a strong set of collaborations with heavy-duty engine manufacturers.

# Reviewer 4:

It seemed to the reviewer like there is good collaboration in each of the four tasks but not necessarily collaboration across the tasks. The reviewer did not know if this is a problem, but suggested that the project team consider if this matters.

#### Reviewer 5:

The reviewer stated that all the tasks have good collaboration across universities, industry and National Laboratories. It looked like the coordination might be a little complicated among the four tasks. The reviewer asked if it would be better to split the tasks and assign collaborators to a project.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that the research is just starting so limited data are available to inform precise future research plans. The current future plans are logical progressions of the current understanding of the challenges that need to be addressed.

#### Reviewer 2:

The reviewer asserted that the general direction for these four tasks looks reasonable and wanted to see how things progress and what challenges arise.

#### Reviewer 3:

The reviewer found that high-level, proposed future work for advancing each of the four tasks is documented. According to the reviewer, more granularity and critical decision points will be helpful in the future.

#### Reviewer 4:

The reviewer noted that there is a logical set of proposed future work plans. For Task 3, the reviewer questioned the likelihood of a new injector and piston bowl combination successfully addressing barriers and also whether that is an appropriate focus.

#### Reviewer 5:

While the proposed work looks fine, it was not very clear to the reviewer if it is going to make actual breakthrough. For example, the third task about the LTC investigation is about acquiring test data, which has been done from various entities. Some uniqueness needs to be presented.

# Ouestion 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer asserted that the projects being investigated include enabling technologies that could potentially form the building blocks as well as help to advance the foundational knowledge base of engine systems to increase engine efficiency and reduce engine-out emissions.

# Reviewer 2:

According to the reviewer, the active engagement of the collaborators is a testimony to the relevance.

# Reviewer 3:

The reviewer commented that this project is extremely relevant for achieving the DOE's objectives in multiple areas of understanding and addressing barriers.

# Reviewer 4:

The reviewer remarked that the program is aligned with DOE objectives for clean and efficient transportation technologies.

#### Reviewer 5:

The reviewer said that the project is very relevant to the DOE objectives in advancing understanding of the combustion process in IC engines.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

According to the reviewer, the funding level is sufficient since most of the engine experiments are underway.

# Reviewer 2:

The reviewer noted that the projects are just starting and assumed that the project scope and resources are well matched at this time.

#### Reviewer 3:

The reviewer said that the program resources are sufficient for the scope.

# Reviewer 4:

These seemed fine to the reviewer, given the initial scope and tasks. However, each of these four tasks could need substantial increases depending on arising challenges.

# Reviewer 5:

The funding and resource seemed to the reviewer to be sufficient. The reviewer suggested that perhaps splitting the tasks into projects may help reduce administrative work, but one can argue that combining those small tasks may actually save administrative overhead.

Presentation Number: ace134
Presentation Title: Multi-Mode
Combustion in Light-Duty SparkIgnition Engines
Principal Investigator: Toby Rockstroh
(Argonne National Laboratory)

#### Presenter

Toby Rockstroh, Argonne National Laboratory

# **Reviewer Sample Size**

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

# Reviewer 1:

The reviewer asserted that the approach taken to develop a pre-chamber ignitor and understand how this type of ignitor can be used in advanced engine concepts is excellent. The PIs did a thorough literature search to understand what has been done and what dependencies have already been established. The prototype design incorporated what had been learned, as did the initial test design. The reviewer observed that stepping through the passive ignitor behavior before starting the active ignitor provides a great baseline and adds layers of complexity

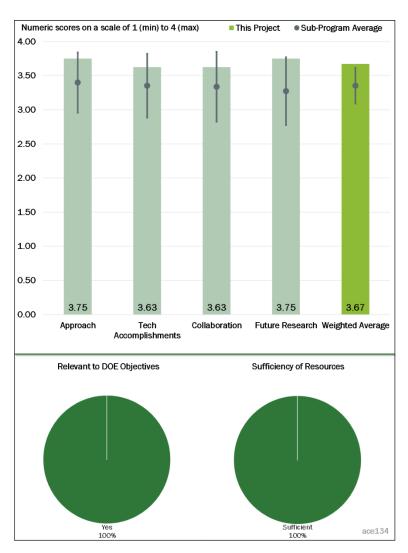


Figure 1-37 – Presentation Number: ace134 Presentation Title: Multi-Mode Combustion in Light-Duty Spark-Ignition Engines Principal Investigator: Toby Rockstroh (Argonne National Laboratory)

that will allow the PI to better understand the important physics. Collaborations are used strategically, such that they help make critical decisions and keep the experimental work productive and focused. Overall, the reviewer remarked that the project organization was great.

#### Reviewer 2:

The reviewer commented that the PI uses state-of-the-art experimental and numerical approaches to improve the understanding of low- temperature combustion strategies for multi-mode engines. According to the reviewer, the plan to overcome technical barriers is sound.

# Reviewer 3:

The reviewer commented that the approach is well defined and relies on a hierarchical approach to isolate the design landscape to formulate a verified pre-chamber design. The investigator presented with clarity the major factors that will lead to an optimized design option that will achieve the goal.

#### Reviewer 4:

The reviewer found that Slide 6 is very clear and the approach is very good.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

According to the reviewer, technical accomplishments have been significant and are on track. Results of the initial collaboration with rapid compression machine work provided an important baseline for understanding the behavior in the engine. These results have been well integrated into the engine study and design of the ignitor. The reviewer found that initial testing of the passive operation of the ignitor provides important results for moving forward and offers great confidence that the ignitor will behave as desired when in active mode.

#### Reviewer 2:

This reviewer reported that the project presented major milestones that have been achieved and further accomplishments are on track to be completed. Accomplishments include parametric fuels studies to isolate appropriate octane-rating sensitivity, as well as demonstrating the optimized designs to achieve the prechamber prototype. The reviewer commented that it was very interesting to see the transition to the current state-of-the-art techniques of additive manufacturing being implemented to fabricate prototypes.

#### Reviewer 3:

The reviewer said that there were three different tasks associated with this period and all three produced expected results. The pre-chamber design looked promising to the reviewer

#### Reviewer 4:

The reviewer commented that Slide 5 is very clear and dates are easy to understand. The reviewer asked for the engine speed on Slides 8 and 9. Slide 10 is very good, and Slides 11 and 12 are very good with clear dates. This reviewer stated that it is good to have high cylinder pressure on Slide 14 expressed interest in seeing higher engine speed and load than 1,500 rpm and 3.2 bar indicated mean effective pressure (IMEP). The reviewer added that three pressure analysis (TPA) and GT-POWER model are relevant.

# Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

According to the reviewer, collaborations have been very productive so far and plans for future collaborations are also very good. Strong collaboration with results from the rapid compression machine tests provide critical insight for designing future experiments. Current collaborations with the ignition chamber at Sandia will provide really critical information for understanding the results in the engine. Support from simulation will also be helpful. In discussions at the poster, the reviewer indicated that the PI also discussed potential collaborations with the Advanced Manufacturing Office (AMO) group to consider the use of additive manufacturing for enhancing the design of this ignitor, which would be really excellent.

# Reviewer 2:

The reviewer found that there was a very good choice of collaborators (Ford, USCAR, and Sandia).

#### Reviewer 3:

The reviewer commented that the project requires good coordination with the various partners for both experiments and simulations. The results showed that the collaboration during this funding period was very good.

#### Reviewer 4:

The reviewer stated that efforts to collaborate with industry, academia, and other National Laboratories are evident. All efforts are complimentary to one another and facilitate the collective efforts to advance prechamber technologies for commercialization.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer asserted that the plan for the proposed future research is sound. The reviewer looked forward to seeing the results next year from an active pre-chamber.

#### Reviewer 2:

The reviewer described proposed future work on Slide 19 as excellent; shows a good choice for effort with three-level factorial experimental design. Additionally, passive and active pre-chambers are very relevant for industry.

#### Reviewer 3:

The reviewer said that the future research plan is well organized and clearly outlines a path toward rapidly developing this ignitor technology. The collaborations are well leveraged in the plan to help achieve project goals.

#### Reviewer 4:

The reviewer commented that the project has proposed a natural extension to its current scope of research and has established realistic milestones schedules.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer noted that the project will improve the current understanding of the ACI combustion mode and the hardware needed to make it possible, which is extremely important for DOE objective of designing the next generation of highly efficient and zero-pollution vehicles.

#### Reviewer 2:

According to the reviewer, gasoline compression ignition is key to improved fuel economy and pre-chambers should be investigated to achieve GCI in on-road engines.

# Reviewer 3:

The reviewer indicated that this program directly supports the objectives of the Vehicle Technology Office and helps in the development of an exciting ignition technology. The work leverages work from other groups to develop and translate a new technology, and the pathway is clearly defined in order to make this a high-impact technology.

#### Reviewer 4:

The reviewer said that the project looks to meet DOE targets by improving ignition, which can enable a 25% increase in engine efficiency, lower pollutant emissions, and more reliable cold start.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer stated that funding supports the objectives for current and next fiscal year.

#### Reviewer 2:

The project appeared to the reviewer to be on track with sufficient resources. It would be very good to see it reach completion.

# Reviewer 3:

The reviewer indicated that all experimental equipment and personnel are at the disposal of the PI to carry out the tasks established.

# Reviewer 4:

According to the reviewer, resources for the project this year are sufficient. The presentation does not include information on funding for future years so it was hard to judge if the resources will be sufficient going forward.

Presentation Number: ace135
Presentation Title: Development of
Simulations Tools for Compression
Ignition Engines
Principal Investigator: Sibendu Som
(Argonne National Laboratory)

# Presenter

Sibendu Som, Argonne National Laboratory

# Reviewer Sample Size A total of four reviewers evaluated this

A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer asserted that the high-fidelity approach is very well suited to Argonne's competence with HPC resources and the Advanced Photon Source.

# Reviewer 2:

The reviewer stated that that three PIs use state-of-the-art numerical approaches to improve the understanding of the flow inside an injector nozzle and to design the next generation of more efficient combustion simulations. The plan to overcome technical barriers is sound.

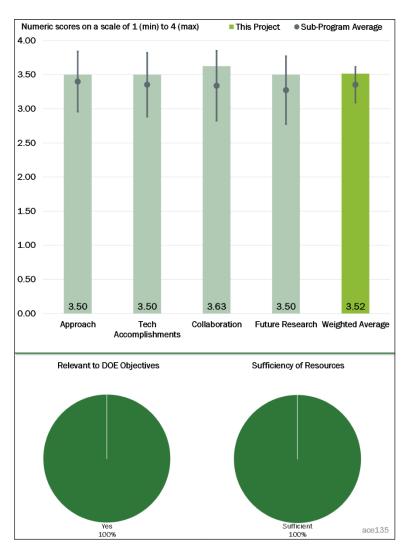


Figure 1-38 – Presentation Number: ace135 Presentation Title: Development of Simulations Tools for Compression Ignition Engines Principal Investigator: Sibendu Som (Argonne National Laboratory)

#### Reviewer 3:

The reviewer found the approach to this work to be very thorough and logical. The PIs have identified problems of great significance through collaborations with experiments and interactions with industry, and their approach to modeling these issues (cavitation in particular) is quite good. In particular, the combination of cavitation modeling with the modeling of the injector surface has made significant strides in our understanding of injector degradation. The reviewer said that the approach for modeling the surface degradation is well reasoned and the increasing level of complexity charts a pathway to better modeling and understanding.

The reviewer suggested that the PI should continue with the focus on uncertainty quantification (UQ) for all aspects of the project to enhance collaboration with experiments.

# Reviewer 4:

This reviewer remarked that the project takes aim at understanding the stochastic of fuel injection, and improving spray and combustion model predictivity. The approach combines several cutting-edge modeling techniques into an all-encompassing predictive model.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer said that the progress is clear and the topics are well chosen. The reviewer understood that there have been some delays with the code release from Converge but the reviewer stated that it is good to push Converge about this as it will benefit industry.

#### Reviewer 2:

The reviewer observed that there were three different tasks associated with this period. Two of them produced the expected results; one was delayed but not the fault of the PI.

#### Reviewer 3:

The reviewer noted that a fully coupled nozzle flow and spray simulation model has been developed. This includes an in-nozzle cavitation model. RANS and LES runs with a diesel surrogate have been performed on the combustion modeling front.

The reviewer remarked that a novel flamelet tabulation model has accurately captured ignition delays and flame liftoff lengths. This has been extended to a novel in-situ flamelet tabulation concept. The modeling is coupled to detailed soot modeling validated with Spray A.

# Reviewer 4:

The reviewer commented that the technical accomplishments of the last year were significant and made good progress toward more accurate prediction of important processes in piston engines. In the case of the cavitation work, the most significant progress was made on accurate prediction of erosion from cavitation. The model improves upon the standard method and uses physics-based understanding to better capture trends from experiments. In the case of the hybrid tabulation flamelet concept, the reviewer noted that progress in this area has shown better agreement between simulation and experiments in cases with multiple injections. The reviewer suggested that the PIs should continue to expand this work for consideration of more than two injections, potentially generalizing it for any number of injections, given the complex injection schedules used in modern engines.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer described the choice of collaborators as excellent. Converge is important for industry to have practical applications. Cummins is a top OEM for diesels; so, that is a very good choice from this reviewer's perspective. Sandia and LLNL are also excellent, and The University of Perugia is important. Additionally, this reviewer inquired about Artificial Neural Network (ANN).

# Reviewer 2:

According to the reviewer, one of the strongest aspects of this project is the collaboration with a number of partners. Collaborations across National Laboratories has helped on both experiments and high-performance computing. The PI is collaborating with a good range of experimentalists to continually benchmark progress in the simulations in a range of different experimental conditions. The PI is also collaborating well with high-performance computing across DOE to ensure the most impact of this work. The reviewer remarked that the PI is also collaborating strongly with industry, both in terms of the equipment manufacturers as well as people who develop simulation software. In particular, the work with Converge is particularly impactful as improved

models are being directly tested and implemented into tools used by industry. Finally, the PI also works well with academia and has a good track record of training students and post-docs.

#### Reviewer 3:

The reviewer indicated that the project requires good coordination with academia, National Laboratories, and industry. The results showed that the collaboration during this funding period was very good.

#### Reviewer 4:

The reviewer noted that the project utilizes a host of participating collaborators.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer observed that the proposed future research is a great extension of the accomplishments from this year. In particular, the work on cavitation and erosion will make a significant impact in collaboration with Cummins and Convergent Science Inc. (CSI) to ensure efficient transfer of information from research to application.

# Reviewer 2:

The reviewer commented that the plan for the proposed future research is sound. It continues the outstanding work that PIs did in the past on advancing the combustion simulations.

#### Reviewer 3:

The reviewer remarked that additional fidelity has been added to the erosion model through the inclusion of material properties and identification of fuel-property effects on needle motion will be a fantastic achievement. Additionally, this reviewer reported expansion to turbulent combustion modeling.

#### Reviewer 4:

The reviewer stated that the future work is logical. However, decision points and alternate development pathways were not clear to the reviewer.

Ouestion 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer praised this project as meeting both technical and information dissemination goals of the Vehicle Technologies Office. The PI is working on problems of great significance to industry and doing a nice job spanning between fundamental research and applications. Additionally, the PIs have very strong collaborations with important partners in government, industry, and academia, disseminating the research effectively.

# Reviewer 2:

The reviewer indicated that the project will improve engine simulations, which are extremely important for DOE objective of designing the next generation of highly efficient and zero-pollution vehicles.

#### Reviewer 3:

The reviewer said that improved predictivity of fuel spray and combustion modeling is a necessity for further advancements toward DOE objectives,

# Reviewer 4:

The reviewer commented that the project is relevant to the DOE objective to do high-fidelity simulations of compression ignition engines. Slide 19 shows this.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

# Reviewer 1:

The reviewer stated that the resources are sufficient for the stated objectives. In particular, the use of the DOE high-performance computing resources is excellent.

# Reviewer 2:

According to the reviewer, funding supports the objectives for the current and next fiscal year.

# Reviewer 3:

The team appeared to the reviewer to have the resources necessary to complete the stated objectives.

# Reviewer 4:

Resources seemed okay, but the reviewer could not find information in the slides that would allow the reviewer to judge this.

Presentation Number: ace136
Presentation Title: Medium-Duty
Diesel Combustion
Principal Investigator: Steven Busch
(Sandia National Laboratories)

Presenter Steven Busch, Sandia National Laboratories

Reviewer Sample Size
A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer praised the approach for this work as excellent; it marries experiment, simulation, and a deep understanding of physics to drive the direction of the research. The experiments are well designed and providing great insight as a result. The experiments are highly supported by great simulation work as well.

# Reviewer 2:

According to the reviewer, the project addresses a pressing need in the combustion and emissions community—there is a lack of fundamental understanding regarding

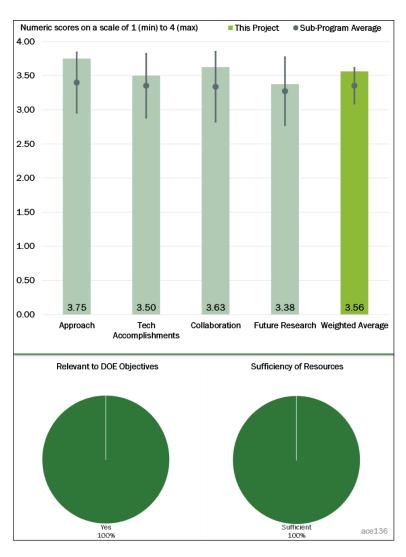


Figure 1-39 – Presentation Number: ace136 Presentation Title: Medium-Duty Diesel Combustion Principal Investigator: Steven Busch (Sandia National Laboratories)

the production of particulates and, more specifically, the impact of spray-wall interactions pertaining to soot production. The overall plan (metal engine studies combined with CFD and optical results) is solid and should ensure result quality and overall dissemination to the scientific community. Initial studies testing hypotheses of injection and bowl-design impacts on particulate production appeared logical to the reviewer.

# Reviewer 3:

The reviewer observed that the PI uses state-of-the-art experimental and numerical approaches to improve the understanding of how spray-wall interactions will promote rapid fuel-air mixing for enhanced efficiency and lower emissions. The plan to overcome technical barriers is sound.

#### Reviewer 4:

The reviewer said that the approach is clearly stated on Slides 5 and 6.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer commented that the technical accomplishments this past year have been very significant. The work in the light-duty engine on both injection-scheduling and catalyst heating and coupled injection and bowl-design has provided significant understanding of these two important problems. According to the reviewer, the hypothesis-driven approach helps to ensure that the research is directed and targeted at making significant progress.

In the case of the injection- scheduling and catalyst-heating study, the reviewer indicated that the test matrix design really helps to address this complicated design space. The current results suggest that the dependencies of catalyst performance on fuel-injection schedule and further analysis of data will hopefully continue to answer these questions. The reviewer stated that coupling with simulation may help identify sources of residual hydrocarbons.

In the injection and bowl-design work, the reviewer praised the results as excellent. In particular, the highly coupled experiment and simulation have led to not just physical understanding, but an entirely new bowl design that will allow for better hypothesis testing. These results not only provide deep insight into the role of in-cylinder flows on combustion efficiency, but also directly impact design methods for future engine configurations.

Finally, the reviewer noted that development of the new engine is continuing and efforts should be made to ensure that this comes online and the same high-quality research approach is used on this new testbed as was applied to the light-duty effort.

#### Reviewer 2:

The reviewer observed that a CFD analysis has revealed insights regarding the impact of a stepped-lip piston on fuel-air mixing. Insights generated reveal the necessity of full CFD simulation rather than relying on sector or axisymmetric mesh assumptions. This finding has archival importance.

The reviewer indicated that post-injection studies revealed unanticipated impacts on particulate production, namely, the addition of post-injection, initially reduced particulates. Particulates only increased when the post injection was retarded. Clearly, this finding reinforces a community-wide lack of insight to the soot formation process, which reinforces the need for the current project. This work found that late injection targeting cannot create sustained vortices near top dead center (TDC). This logical hypothesis was found to be inadequate, again pointing toward a community need for further insights according to the reviewer.

The reviewer noted that a dimpled step-lipped (DSL) piston geometry was designed and studied in simulation. The increased space provided by the DSL design was found to promote vortex formation near TDC. The reviewer said that engine system build-out appears on pace for the FY 2019 timeframe.

#### Reviewer 3

The reviewer noted that there were three different tasks associated with this period and all three produced the expected results.

# Reviewer 4:

The reviewer thought that the slides did not show the progress made.

# Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer remarked that the project requires good coordination with academia (for simulations) and industry (for hardware and experiments). The results showed that the collaboration during this funding period was very good.

#### Reviewer 2:

The reviewer asserted that there is a great choice of partners (Ford, and Wisconsin Engine Research Consultants [WERC]).

#### Reviewer 3:

The reviewer commented that Ford has been intricately involved in building the new engine platform and designing a test matrix. The WERC collaboration for CFD is actively integrated within project results.

#### Reviewer 4:

The collaborations with industry and the simulation partners are very strong and the reviewer suggested that they should be continued. According to the reviewer, it would be good to see future connections with the other work at Sandia and in the Engine Combustion Network (ECN) looking at spray-wall interactions to pass on the deep learning seen in this project to other experiments.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said that future research is clearly stated with milestones.

#### Reviewer 2:

The reviewer found that the plan for the proposed future research is sound. It continues the outstanding work that PI did in the past on optical diagnostics and advanced combustion strategies. The only risk the reviewer saw relates to delays in commissioning the new medium-duty diesel engine, but the PI's record shows that he delivers on his projects.

# Reviewer 3:

The reviewer remarked that the future work plan is reasonable and the PI is interested in addressing important questions. The reviewer suggested that the PI should consider linking simulation in the post-injection study as well to help answer some questions about combustion efficiency.

#### Reviewer 4:

The reviewer stated that the study aims to determine the link between in-cylinder turbulence and vortices on heat-release rates, thermal efficiency, and the NO<sub>x</sub>-soot tradeoff. Then, the study proposes to elucidate what piston-geometry aspects influence vortex formation. Finally, the mechanisms behind post-injection ignition will be studied. However, the reviewer observed that not many specifics or details are provided on how these goals will be systematically investigated.

# Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that the project will improve current understanding of fuel injection, air motion, and combustion-chamber geometry effects on combustion and pollutant formation, which is extremely important for the DOE objective of designing the next generation of highly efficient and zero-pollution vehicles.

# Reviewer 2:

The reviewer stated that the project is relevant to the DOE objective to improve MCCI efficiency.

#### Reviewer 3:

The reviewer said that the study addresses an industry-wide lack of fundamental understanding, which inhibits the ability to meet DOE objectives.

#### Reviewer 4:

The reviewer asserted that this work has direct relevance to the goals of the Vehicle Technologies Office as well as the engine industry in general. This work provides significant insight into a range of different combustion and aftertreatment behaviors in light-duty engines. The method by which the work is carried out—using hypothesis-driven investigation in close collaboration with simulation—ensures impact. The work will continue to make a significant impact as the medium-duty engine is brought online, according to the reviewer.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer remarked that funding supports the objectives for the current and next fiscal year.

#### Reviewer 2:

Resources seemed okay to the reviewer.

#### Reviewer 3:

The resources available for engine build-out, simulation, and experimental operation aspects of the project appeared sufficient to the reviewer.

# Reviewer 4:

The reviewer commented that the resources are sufficient for this work. The program should ensure that laboratory facilities' staff and resources continue to support the build-up of the new engine, which includes collaboration between the researcher and the laboratory facilities' staff to ensure that everything stays on schedule.

# **Acronyms and Abbreviations**

(NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub> Ammonium carbamate

°C Degrees Celsius

1-D One-dimensional

21CTP 21st Century Truck Partnership

2M2B 2-methyl-2-butene

3-D Three dimensional

ACE Advanced Combustion Engine

ACEC Advanced Combustion & Emissions Control

ACI Advanced compression ignition

AEC Advanced Engine Combustion

AEC Advanced Engine Crosscut, Advanced Engine Combustion

Al Aluminum

AMFI Additive-mixing fuel injection

AMO Advanced Manufacturing Office

AMR Annual Merit Review

ANL Argonne National Laboratory

APS Advanced Photon Source

Ba Barium

BES Basic Energy Sciences

BEV Battery electric vehicles

BP Budget period

BSFC Brake-specific fuel consumption

BTE Brake thermal efficiency

C<sub>2</sub>H<sub>4</sub> Ethylene

CA50 Crank angle position in which 50% of the heat is released

CARB California Air Resources Board

CCV Closed crankcase ventilation

#### 2019 ANNUAL MERIT REVIEW. VEHICLE TECHNOLOGIES OFFICE

Ce Cerium

CeO<sub>2</sub> Cerium oxide (ceria)

CFD Computational fluid dynamics

CH<sub>4</sub> Methane

CHA Chabazite

CHT Conjugate heat transfer

CI Compression ignition

CLEERS Cross-cut Lean Exhaust Emissions Reduction Simulations

CNG Compressed natural gas

CO Carbon monoxide

CPU Central processing unit

CR Compression ratio

CRADA Cooperative research and development agreement

Crr Coefficient of rolling resistance

CSI Convergent Science Inc.

Cu Copper

CUC Clean-up catalyst

DDI-PFS Double direct-injection – partial fuel stratification

DEER Directions in Engine-Efficiency and Emissions Research

DEF Diesel exhaust fluid

DFI Ducted fuel injection

DFT Density functional theory

DI Direct injection

DISI Direct injection spark ignition

DNS Direct numerical simulations

DOC Diesel oxidation catalyst

DOE U.S. Department of Energy

DOI Duration of injection

DPF Diesel particulate filter

DSL Dimple step-lipped

DTNA Daimler Trucks North America

E10 10% ethanol content gasoline

ECN Engine Combustion Network

ECU Engine control unit

EERE Energy Efficiency and Renewable Energy

EGR Exhaust gas recirculation

EHN 2-ethylhexyl nitrate

EPA U.S. Environmental Protection Agency

FE Fuel economy

FE Fuel efficiency

Fe Iron

FEA Finite element analysis

FTP Federal Test Procedure

FY Fiscal year

g Gram

GBDI Groundless barrier discharge igniter

GCI Gasoline compression ignition

GDBI Groundless dielectric barrier discharge

GDI Gasoline direct injection

GHG Greenhouse gas

GM General Motors

GPF Gasoline particulate filter

GPU Graphics processing unit

GSA Global sensitivity analysis

H<sub>2</sub> Hydrogen

H<sub>2</sub>O Water

#### 2019 ANNUAL MERIT REVIEW, VEHICLE TECHNOLOGIES OFFICE

HATCI Hyundai Kia America Technical Center

HC Hydrocarbon

HCCI Homogeneous charge compression ignition

HCL Hydrochloric acid

HCT Hydrocarbon trap

HD Heavy-duty

HECC High-efficiency clean combustion

HPC High performance computing

HXN Heat exchanger

IC Internal combustion

ICE Internal combustion engine

IMAP Intake manifold absolute pressure

IMEP Indicated mean effective pressure

IP Intellectual property

ISFC Indicated specific fuel consumption

JM Johnson Matthey

K Kelvin

L Liter

LANL Los Alamos National Laboratory

LD Light-duty

LES Large eddy simulation

LEV Low-emission vehicle

LEVIII Low-emission vehicle level III

LLNL Lawrence Livermore National Laboratory

LTAT Low-temperature aftertreatment

LTC Low-temperature combustion

LTGC Low-temperature gasoline combustion

LTP Low-temperature plasma

LTP-ACI Low-temperature plasma advanced compression ignition

MCCI Mixing-controlled compression ignition

mg Milligram

MHDV Medium- and heavy-duty vehicle

mi Mile

Micro-CT Micro-computed tomography

Mn Manganese

MnO<sub>2</sub> Manganese oxide

MnO<sub>x</sub> Oxides of manganese

MOU Memorandum of Understanding

mpg Miles per gallon

N<sub>2</sub>O Nitrous oxide

Na Sodium

NG Natural gas

NH<sub>3</sub> Ammonia

NMOG Non-methane organic gas

NO Nitric oxide (nitrogen monoxide)

NO<sub>2</sub> Nitrogen dioxide

NO<sub>x</sub> Oxides of nitrogen

NREL National Renewable Energy Laboratory

NSC NO<sub>x</sub> storage component

NTC Negative temperature coefficient

O<sub>3</sub> Ozone

OC Oxidation catalyst

OEM Original equipment manufacture

OHC Oxidation half cycle

ORC Organic Rankine cycle

ORNL Oak Ridge National Laboratory

# 2019 ANNUAL MERIT REVIEW, VEHICLE TECHNOLOGIES OFFICE

OSC Oxygen storage capacity

PAC Plasma-assisted combustion

PC-ACI Pre-chamber advanced compression ignition

PCC Phase-change cooling

Pd Palladium

PFI Port fuel injection

PI Principal investigator

PIV Particle image velocimetry

PLV Projected liquid volume

PM Particulate matter

PN Particle number

PNA Passive NO<sub>x</sub> adsorber

PNNL Pacific Northwest National Laboratory

ppm Parts per million

PRF Primary reference fuel

PRF90 Primary reference fuel 90

Pt Platinum

Q Quarter

R&D Research and development

RANS Reynolds-averaged Navier-Stokes

RASIC Responsible – approving – supporting – informed - consulted

RCCI Reactivity-controlled compression ignition

RCM Rapid compression machine

Rh Rhodium

RHC Reduction half cycle

ROI Rate of injection

RON Research octane number

rpm Revolutions per minute

SACI Spark-assisted compression ignition

SAR Silica to alumina ratio

SCO Selective catalytic oxidation

SCOTE Single-cylinder oil test engine

SCR Selective catalytic reduction

SCRF Selective catalytic reduction on filter

Si Silicon

SI Spark ignition

SiO<sub>2</sub> Silicon dioxide (silica)

SNL Sandia National Laboratories

SO<sub>2</sub> Sulfur dioxide

SOC State of charge

SR Steam reforming

ST1 SuperTruck 1

ST2 SuperTruck 2

SUNY State University of New York

SwRI Southwest Research Institute

T Temperature

TBC Thermal barrier coating

TC Thermocouple

TCI Turbulent chemistry interaction

TDC Top dead center

TEM Transmission electron microscopy

TPA Three pressure analysis

TPS Transient Plasma Systems

TRF Toluene reference fuel

TRL Technology readiness level

TWC Three-way catalyst

U.S. DRIVE U.S. Driving Research and Innovation for Vehicle efficiency and Energy

sustainability

U.S. EPA U.S. Environmental Protection Agency

U.S. United States

UH University of Houston

UQ Uncertainty quantification

USCAR United States Council on Automotive Research

UVa University of Virginia

UW University of Wisconsin

V Volt

VTO Vehicle Technologies Office

WERC Wisconsin Engine Research Consultants

WGS Water gas shift

WHR Waste-heat recovery

X Times

YSI Yield sooting index

Zero-RK Zero-order Reaction Kinetics

Zr Zirconium

ZrO<sub>2</sub> Zirconium dioxide (zirconia)

ZSM-5 Zeolite Socony Mobil -5

