### 4. Advanced Combustion Engines

Improving the efficiency of internal combustion engines (ICE) is one of the most promising and cost-effective near- to mid-term approaches to increasing highway vehicles' fuel economy. The Vehicle Technologies Office's (VTO) research and development (R&D) activities address critical barriers to commercializing higher efficiency, very low emissions advanced internal combustion engines for passenger and commercial vehicles. This technology has great potential to reduce U.S. petroleum consumption, resulting in greater economic, environmental, and energy security.

Already offering outstanding drivability and reliability to over 230 million passenger vehicles, ICEs have the potential to become substantially more efficient. Initial results from laboratory engine tests indicate that passenger vehicle fuel economy can be improved by more than up to 50%, and some vehicle simulation models estimate potential improvements of up to 75%. Advanced combustion engines can utilize renewable fuels, and when combined with hybrid electric powertrains could have even further reductions in fuel consumption. As the U.S. Energy Information Administration reference case forecasts that, by 2035, more than 99% of light-duty (LD) and heavy-duty (HD) vehicles sold will still have ICEs, the potential fuel savings is tremendous.

VTO undertakes R&D activities to improve the efficiency of engines for both LD and HD highway vehicles, whether they run on petroleum-based (gasoline and diesel) or alternative fuels. We support every type of research in these areas, from fundamental science to prototype demonstration. VTO's research focuses on improving engine efficiency while meeting future federal and state emissions regulations through three main approaches.

- Developing advanced combustion strategies that maximize engine efficiency and minimize the formation of emissions within the engine cylinders.
- Developing cost-effective aftertreatment technologies that further reduce exhaust emissions.
- Reducing losses and recovering energy from engine waste heat.

The combustion engines subprogram also works with other subprograms in VTO to integrate and test advanced combustion engines in vehicles, such as the SuperTruck project. Commercialization of these advanced combustion engine technologies could allow the United States to cut its transportation fuel use and corresponding greenhouse gas (GHG) emissions by as much as 20%-40%.

The combustion subprogram supports a number of unique user facilities at the national laboratories. In addition to the national laboratories, research and development is done in collaboration with industry, other federal agencies (such as the National Science Foundation) and universities, as well as through government/industry partnerships:

- The United States Driving Research and Innovation for Vehicle efficiency and Energy sustainability (U.S. DRIVE) Partnership focusing on LD vehicles and
- The 21st Century Truck Partnership, focusing on HD vehicles.

To enable further advances in combustion research and development, VTO also supports research on materials that can withstand high operating temperatures and pressures needed to capitalize on these engines' potential benefits, materials for energy recovery systems and controlling exhaust gases, and materials by design to solve specific issues.

The major goals of the Advanced Combustion Engine (ACE) R&D subprogram are:

- By 2020, improve the fuel economy of gasoline vehicles by 35% compared to 2009 model year baseline, and diesel vehicles by 30%.
- By 2020, further improve HD engine efficiency to 55% (a 30% improvement) with demonstrations on commercial vehicle platforms.
- By 2020, improve NO<sub>x</sub> and PM emissions to EPA Tier 3 and California Low Emission Vehicles (LEV) III standards for LD engines and EPA standards for HD engines.

#### Subprogram Feedback

The U.S. Department of Energy (DOE) received feedback on the overall technical subprogram areas presented during the 2016 Annual Merit Review (AMR). Each subprogram technical session was introduced with a presentation that provided an overview of subprogram goals and recent progress, followed by a series of detailed topic area project presentations.

The reviewers for a given subprogram area responded to a series of specific questions regarding the breadth, depth, and appropriateness of that DOE VTO subprogram's activities. The subprogram overview questions are listed below, and it should be noted that no scoring metrics were applied. These questions were used for all VTO subprogram overviews.

Question 1: Was the program area, including overall strategy, adequately covered?

Question 2: Is there an appropriate balance between near- mid- and long-term research and development?

**Question 3: Were important issues and challenges identified?** 

Question 4: Are plans identified for addressing issues and challenges?

Question 5: Was progress clearly benchmarked against the previous year?

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?

Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?

Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?

Question 10: Has the program area engaged appropriate partners?

Question 11: Is the program area collaborating with them effectively?

Question 12: Are there any gaps in the portfolio for this technology area?

Question 13: Are there topics that are not being adequately addressed?

Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

### Question 16: Are there any other suggestions to improve the effectiveness of this program area?

Responses to the subprogram overview questions are summarized in the following pages. Individual reviewer comments for each question are identified under the heading Reviewer 1, Reviewer 2, etc. Note that reviewer comments may be ordered differently; for example, for each specific subprogram overview presentation, the reviewer identified as Reviewer 1 in the first question may not be Reviewer 1 in the second question, etc.

### Overview of the VTO Advanced Combustion Engine R&D Program: Gurpreet Singh (U.S. Department of Energy) - ace000

#### Question 1: Was the program area, including overall strategy, adequately covered?

#### **Reviewer 1:**

The reviewer stated that the strategic goal of reducing petroleum dependence by increasing efficiency of emissionscompliant ICE powertrains is clearly outlined, as are the primary directions for achieving this down to the goals in terms of percentage gains through advanced combustion strategies, aftertreatment technologies, and loss reduction and waste heat recovery (WHR) techniques. The reviewer further stated that the broad range of programs being pursued to support these approaches is also outlined at a reasonable level of detail.

#### **Reviewer 2:**

The reviewer agreed that the overall program was properly covered with many critical aspects of the program discussed. The reviewer noted that this program supports several national laboratories and each laboratory appears to have specific focuses. The reviewer commented that while the strategy and the synergy between the national laboratories are very good, the support to universities does not seem significant.

### Question 2: Is there an appropriate balance between near- mid- and long-term research and development?

#### **Reviewer 1:**

The reviewer commented that there is a good balance between more academic, even basic research in terms of diagnostics, etc., through component technologies to all up engine demonstrations of new technologies.

#### **Reviewer 2:**

The reviewer stated that the balance is appropriate.

#### **Question 3: Were important issues and challenges identified?**

#### **Reviewer 1:**

The reviewer characterized the important issues and challenges as properly identified.

#### **Reviewer 2:**

The reviewer agreed that the challenges in each technology area are briefly outlined but cautioned that it is difficult to get into too much detail given the scope of the overall program. Nevertheless, the reviewer concluded that the individual project presentations cover these details well in any case. This is based on the reviewer having just finished reviewing 15 individual projects and thus having a relatively good idea of what's being done up and down the line of this research topic.

#### **Question 4: Are plans identified for addressing issues and challenges?**

#### **Reviewer 1:**

The reviewer affirmed that the near- and long-term plans are clearly outlined and describe how the program is tackling the various issues being faced to achieve the overall whole program's efficiency and emissions goals.

Reviewer 2:

The reviewer replied yes.

#### Question 5: Was progress clearly benchmarked against the previous year?

**Reviewer 1:** The reviewer replied yes.

#### Reviewer 2:

The reviewer remarked that more could have been done to specifically address this in this presentation.

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?

#### Reviewer 1:

The reviewer agreed that this is detailed very specifically.

#### **Reviewer 2:** The reviewer answered yes.

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?

**Reviewer 1:** The reviewer replied yes to all of these criteria.

#### **Reviewer 2:** The reviewer replied yes.

### Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?

#### Reviewer 1:

The reviewer declared as tremendous strengths the coordination and participation across academia, DOE laboratories, component and tool suppliers (such as computational fluid dynamics [CFD] vendors and others), energy companies, and engine manufacturers. The reviewer also described the Engine Combustion Network (ECN) (part of ACE005) as a standout example of this level of cooperative research to achieve a common goal. The reviewer concluded that no glaring weaknesses come to mind.

#### **Reviewer 2:**

The reviewer stated that the key strength is the experimental study and the fundamental modeling research in all of the national laboratories that are supported by this program. Conversely, the reviewer described the main weakness as the applied modeling research at Argonne National Laboratory (ANL), which uses commercial code (CONVERGE) to perform engine performance simulation. The reviewer offered that such modeling work using commercial codes does not appear to be appropriate for a national laboratory and that such modeling work should be left to the industry or academia. In the meantime, the numerical model development at universities need to be strengthened. The reviewer further commented that Los Alamos National Laboratory (LANL), which has been developing the new engine simulation code for quite a number of years, has never been able to release anything. The reviewer observed that nowadays the industry has its own code and models, and it is highly probably that the code developed at LANL will never get used.

### Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?

#### **Reviewer 1:**

The reviewer agreed that all of the projects incorporate innovative and sometimes even novel approaches to overcoming the barriers.

#### Reviewer 2:

The reviewer replied yes.

#### Question 10: Has the program area engaged appropriate partners?

#### **Reviewer 1**:

The reviewer agreed, noting as in a previous question that a broad range of partners have been engaged, adding that about the only thing lacking perhaps is engaging government laboratories outside of DOE to a larger extent (such as those with the U.S. Department of Defense and others).

**Reviewer 2:** The reviewer encouraged more collaborations with universities.

#### Question 11: Is the program area collaborating with them effectively?

**Reviewer 1:** The reviewer replied yes.

**Reviewer 2:** The reviewer replied yes.

#### Question 12: Are there any gaps in the portfolio for this technology area?

**Reviewer 1:** The reviewer said no.

#### **Reviewer 2:**

The reviewer observed that some reviewers of individual projects in previous years have complained about the balance between diesel and gasoline engine research, but there appears to be a greater emphasize on gasoline engine research in this year's program, which addresses this concern.

#### Question 13: Are there topics that are not being adequately addressed?

#### **Reviewer 1:**

The reviewer stated that while there is great focused research looking at spray combustion chemistry, emissions, etc., the interactions between them (combustion-turbulence, sprays-emissions, etc.) might themselves be topics of more focused research. The reviewer also suggested that some of the CFD research could be better tied into commercialization to make the progress seen in modeling codes KIVA FE and RAPTOR trickle down faster into the commercial tools used by industry.

### Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

**Reviewer 1:** 

The reviewer referenced previous comments made in question 13.

### Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

#### **Reviewer 1:**

The reviewer replied that the approaches being pursued here appear to address the barriers present in this area.

#### **Reviewer 2:**

The reviewer warned that regarding the new KIVA code development at LANL, it is not clear how successful this activity would be. The reviewer observed that many advancements in engine modeling have been made in the industry in the past 10 years, and that the code development does not incorporate the state-of-the-art models. Even if the new KIVA code is released, it is unlikely that industry will spend resources to move all the sub-models into the new KIVA code. Plus, there is no customer support for the new KIVA code, which would defeat the interest of using it by the industry. The reviewer also pointed out that nowadays, the industry does not use a code that does not have customer support, and concluded that this is why many industry players have abandoned their own version of KIVA-3V and use commercial codes.

The reviewer recommended that VTO form an ad-hoc committee to investigate the necessity of developing new KIVA code. Similarly, the reviewer suggested that the CONVERGE modeling work at ANL may need to be evaluated because this work possibly can be done by universities at a lower cost. The reviewer concluded that the numerical modeling at national laboratories should be focused on fundamental aspects rather than using a commercial code to investigate the engine performance optimization.

### Question 16: Are there any other suggestions to improve the effectiveness of this program area?

#### **Reviewer 1:**

The reviewer stated that ECN as a cooperative team approach to looking at problems is such a good concept that perhaps it can be applied to other areas (aftertreatment, simulation, emissions, etc.) as well.

#### **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 4-1 - Project Feedback

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Heavy-Duty Low-Temperature and Diesel Combustion and Heavy-Duty Combustion Modeling	Musculus, Mark (SNL)	4-14	3.50	3.38	3.38	3.25	3.39
Light-Duty Diesel Combustion	Busch, Stephen (SNL)	4-17	3.30	3.00	3.30	3.00	3.11
Low-Temperature Gasoline Combustion (LTGC) Engine Research	Dec, John (SNL)	4-22	2.90	3.10	2.90	2.70	2.98
Spray Combustion Cross-Cut Engine Research	Pickett, Lyle (SNL)	4-26	3.38	3.38	3.25	3.38	3.36
Gasoline Combustion Fundamentals	Ekoto, Isaac (SNL)	4-30	3.00	3.00	2.83	3.17	3.00
Large Eddy Simulation (LES) Applied to Advanced Engine Combustion Research	Oefelein, Joe (SNL)	4-32	3.60	3.50	3.30	3.20	3.46
Fuel Injection and Spray Research Using X-Ray Diagnostics	Powell, Christopher (ANL)	4-36	3.30	3.30	3.30	3.20	3.29

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Advances in High-Efficiency Gasoline Compression Ignition	Ciatti, Steve (ANL)	4-40	2.83	2.67	3.17	2.67	2.77
Model Development and Analysis of Clean and Efficient Engine Combustion	Whitesides, Russell (LLNL)	4-42	3.33	3.17	2.92	2.92	3.15
Chemical Kinetic Models for Advanced Engine Combustion	Pitz, Bill (LLNL)	4-46	3.80	3.60	3.40	3.60	3.63
2016 KIV A-hpFE Development: A Robust and Accurate Engine Modeling Software	Carrington, David (LANL)	4-49	2.50	2.63	2.00	2.38	2.48
Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes	Daw, Stuart (ORNL)	4-52	3.08	3.08	2.58	2.92	3.00
High-Efficiency Clean Combustion in Multi-Cylinder Light-Duty Engines	Curran, Scott (ORNL)	4-57	3.38	3.38	3.13	3.38	3.34
Accelerating Predictive Simulation of Internal Combustion Engines with High Performance Computing	Ewards, Kevin (ORNL)	4-60	2.86	3.07	3.21	3.07	3.04

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Joint Development and Coordination of Emissions Control Data and Models (CLEERS Analysis and Coordination)	Daw, Stuart (ORNL)	4-65	3.88	3.63	3.88	3.63	3.72
CLEERS: Aftertreatment Modeling and Analysis	Wang, Yong (PNNL)	4-69	3.13	3.25	3.38	3.25	3.23
Ash-Durable Catalyzed Filters for Gasoline Direct Injection (GDI) Engines	Seong, Hee Je (ANL)	4-73	3.30	3.00	3.40	3.10	3.14
Enhanced High- and Low- Temperature Performance of NO <sub>x</sub> Reduction Materials	Gao, Feng (PNNL)	4-77	3.38	3.38	3.63	3.13	3.38
Next Generation SCR-Dosing System Investigation	Karkamkar, Abhijeet (PNNL)	4-80	3.17	3.17	3.08	3.00	3.14
Cummins-ORNL/ FEERC Emissions CRADA: NO <sub>x</sub> Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems	Partridge, Bill (ORNL)	4-85	3.10	3.10	3.10	3.10	3.10
Emissions Control for Lean Gasoline Engines	Parks, Jim (ORNL)	4-90	3.33	3.67	3.83	3.50	3.58

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Neutron Imaging of Advanced Transportation Technologies	Toops, Todd (ORNL)	4-93	3.40	3.40	3.10	3.20	3.34
RCM Studies to Enable Gasoline- Relevant Low- Temperature Combustion	Goldsborough, Scott (ANL)	4-96	3.10	3.30	3.20	3.10	3.21
Fuel-Neutral Studies of Particulate Matter Transport Emissions	Stewart, Mark (PNNL)	4-100	3.50	3.38	3.50	3.38	3.42
SuperTruck- Development and Demonstration of a Fuel-Efficient Class 8 Tractor and Trailer, Engine Systems	Zukouski, Russ (Navistar International Corp.)	4-103	3.33	3.08	3.50	3.25	3.22
Volvo SuperTruck - Powertrain Technologies for Efficiency Improvement	Amar, Pascal (Volvo)	4-108	3.64	3.93	3.36	3.71	3.76
Advancements in Fuel Spray and Combustion Modeling with High-Performance Computing Resources	Som, Sibendu (ANL)	4-113	3.00	3.00	2.83	2.67	2.94
Improved Solvers for Advanced Engine Combustion Simulation	McNenly, Matthew (LLNL)	4-116	3.50	3.42	3.42	3.08	3.40

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Cummins/ORNL- FEERC Combustion CRADA: Characterization and Reduction of Combustion Variations	Partridge, Bill (ORNL)	4-120	3.00	3.13	3.25	3.00	3.09
Thermally Stable Ultra Low- Temperature Oxidation Catalysts	Szanyi, Janos (PNNL)	4-123	3.13	3.50	3.38	3.13	3.34
High-Efficiency GDI Engine Research, with Emphasis on Ignition Systems	Wallner, Thomas (ANL)	4-127	2.50	1.50	2.50	2.50	2.00
Low-Temperature Emission Control to Enable Fuel Efficient Engine Commercialization	Toops, Todd (ORNL)	4-129	3.80	3.70	3.60	3.40	3.68
High-Dilution Stoichiometric Gasoline Direct- Injection (SGDI) Combustion Control Development	Kaul, Brian (ORNL)	4-133	2.90	2.70	2.70	2.70	2.75
High-Efficiency VCR Engine with Variable Valve Actuation and New Supercharging Technology	Mendler, Charles (Envera LLC)	4-136	2.25	2.44	2.13	2.25	2.33
Lean Miller Cycle System Development for Light-Duty Vehicles	Sczomak, David (General Motors)	4-142	3.20	2.90	3.00	3.20	3.03

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Ultra-Efficient Light-Duty Powertrain with Gasoline Low- Temperature Combustion	Confer, Keith (Delphi Powertrain)	4-146	3.33	3.50	2.83	3.00	3.31
Metal Oxide Nano- Array Catalysts for Low-Temperature Diesel Oxidation	Gao, Pu-Xian (U. Conn)	4-150	3.00	2.75	3.00	2.88	2.86
Micro-Jet Enhanced Ignition with a Variable Orifice Fuel Injector for High- Efficiency Lean- Burn Combustion	Lee, Chia-Fon (U. of Illinois)	4-154	2.50	2.13	1.88	2.75	2.27
Affordable Rankine Cycle (ARC) Waste Heat Recovery for Heavy-Duty Trucks	Subramanian, Swami (Eaton Corp.)	4-157	3.08	3.08	3.67	3.25	3.18
Cummins 55% BTE Project	Kocher, Lyle (Cummins)	4-161	3.50	3.38	2.63	3.31	3.30
Improved Fuel Efficiency through Adaptive Radio Frequency Controls and Diagnostics for Advanced Catalyst Systems	Sappok, Alexander (Filter Sensing Technologies, Inc.)	4-166	3.43	3.14	3.64	3.36	3.30
Overall Average			3.20	3.14	3.12	3.09	3.15

#### Heavy-Duty Low-Temperature and Diesel Combustion and Heavy-Duty Combustion Modeling: Mark Musculus (Sandia National Laboratories) ace001

**Presenter** Mark Musculus, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated the project has shown a clear path to achieve the long-term objective, and the team has executed key milestones through optical imaging and CFD modeling of low-temperature combustion (LTC) combustion processes.

#### **Reviewer 2:**

The reviewer stated this remains an excellent program that combines state-of-the-art optical diagnostics with multidimensional engine modeling to examine some of the



more challenging issues in engine development today. The innovation seemed very high to this reviewer, who highlighted said it is quite clever to take the beam steering effect, which at first glance appears to be a serious problem, and turning it around to become a diagnostic solution by using beam width as a measure for scalar dissipation. As is employing infrared (IR) thermometry via window coating and soot luminosity coupling with CFD to potentially develop a soot mass quantification technique.

#### **Reviewer 3:**

The reviewer commented that there is an unusually good balance of experimental and computational approaches within the project. It is a nice presentation of experimental imaging challenges and approaches to overcome them. The reviewer said on the other hand, additional bigger-picture materials pointing to the desired progress directions and connections would have helped.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer declared valuable engine in-cylinder spray data on ECN Spray B was obtained. As the project is for HD engine focus, the reviewer recommended using a larger nozzle with one to three holes if possible. The reviewer also commented that the new heat transfer diagnostic method using IR thermometry is very interesting. Additionally, measurement and CFD modeling on at least some engine conditions is highly anticipated in fiscal year (FY) 2016/2017.

#### **Reviewer 2:**

The reviewer said the progress and technical accomplishments are excellent. The Spray B measurements and analysis are very illuminating, and there seems to be a potential breakthrough in understanding ignition delay increase with injection duration as a scalar dissipation effect with the possibility that the beam steering problem could be turned into a diagnostic tool itself. There are challenges to be overcome with the IR thermometry technique owing to the issues of the metal coatings used initially, but the reviewer remains confident in the team's problem solving abilities; the same with the soot luminosity correlation approach for obtaining integrated soot mass estimates.

#### **Reviewer 3:**

The reviewer noted that experimental challenges and investigation of mechanistic questions seem to have limited the progress on two of the three barriers cited on Slide 2 (i.e., LTC aftertreatment integration and impact of future fuels on LTC). The reviewer pointed out that uncertainty analysis discussion focused on the error bars in the experimental data only. This person recommended considering uncertainty quantification (UQ) and sensitivities for the simulation models, including not just the model-form uncertainty inherent in the three models presented, but also the myriad input coefficients to those models.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

There were good collaborations with various partners from industries and universities the reviewer noted. As stated in Critical Assumptions and Issues, the current optical engine testing is limited in engine speed and load for HD applications, especially off-road diesel engines where rated condition is the most important one. The reviewer highly recommends collaboration in this area.

#### Reviewer 2:

The reviewer commented collaboration with ECN is particularly noteworthy, but also with the various universities and industrial concerns. It might be interesting to work with code vendors such as Convergent Science, Inc. (CSI) to do comparative studies with commercial CFD software in addition to KIVA calculations.

#### **Reviewer 3:**

The reviewer stated the Advanced Engine Combustion collaboration is very effective.

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 declared each milestone in 2016 was critically reviewed and future work is suggested. It would be good to see a detailed plan from University of Wisconsin (UW) on in-cylinder heat transfer modeling and validation. Wall boundary-layer resolution and heat transfer model are critical for accurate modeling, but the current approach in KIVA-ERC code is proven to be not very accurate.

#### **Reviewer 2:**

The reviewer stated future plans appear to be well thought out and will continue to provide valuable insights to the engine community.

#### **Reviewer 3:**

The reviewer noted that Slide 27 mentions a "range of ... in-cylinder geometries," but it was unclear how the single ECN engine could or would be modified or augmented to achieve this worthwhile expansion. As another reviewer noted during the live session, concern begins to arise that some details of the findings/conclusions are engine-specific.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer commented that multi-injection is a promising and innovative approach to improve efficiency and reduce emissions.

#### **Reviewer 2:**

The reviewer stated gains in engine efficiency and emissions reductions that the technology developed in this project will aid in developing, and will certainly lead to decreased petroleum usage.

#### **Reviewer 3:**

The reviewer declared this project can provide valuable understanding on LTC.

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

Reviewer 1:

The reviewer declared resources, including budget, seem appropriate.

**Reviewer 2:** 

The reviewer stated resources appear sufficient.

#### Light-Duty Diesel Combustion: Stephen Busch (Sandia National Laboratories) - ace002

#### **Presenter** Stephen Busch, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer declared the project is a great combination of experimental, diagnostic, and simulation work.

#### Reviewer 2:

The reviewer commented the approach is well coordinated with Sandia National Laboratories' (SNL) optical engine experiments at the core and with supporting activities by UW, CSI, and other national laboratories. The team has an opportunity to further the understanding of LD diesel combustion. The reviewer remarked the scope of work focuses on piston



geometry and pilot injections, and injection timing appears to be quite limited. The project team may want to consider the roadmap for a target higher efficiency based on optimized dilution, compression ratio (CR), heat transfer, etc., from predictive tools and then explore the required hardware. It appears the approach is the other way around: testing hardware and examining its effects.

#### **Reviewer 3:**

The reviewer expressed that the project has a good technical approach. There is a good balance between optical, simulation, and soon-to-be-metal engine work. But, the project needs to directly compare to DOE's engine efficiency goals. Indicated efficiency results show progress, but those results do not relate directly to DOE goals. Metal engine work at Oak Ridge National Laboratory (ORNL) is one way to accomplish this, the reviewer suggested. The reviewer is pleased to see a commercial software vendor as part of project; it is a quick and efficient way to take knowledge gained from this project and impact consumer products.

#### **Reviewer 4:**

The reviewer observed a good approach and that the fundamentals of diesel combustion are being attached. The project work is made up of primarily optical engine work and looking at injection, ignition, and combustion processes. The reviewer reported that the work is supported with simulations by UW with their Fast and Reliable Engine Simulation Code (FRESCO) code as well as CFD support from CSI.

#### **Reviewer 5:**

The reviewer stated the project uses a common engine platform (General Motors [GM] 1.9 liter [L] head) to provide data that ostensibly provides what the principal investigator (PI) terms a "fundamental understanding of advanced combustion processes." The data are also being used to improve computational modeling capabilities mainly using the commercial code CONVERGE, which is used in industry, as well as to test UW's RAN's simulation capabilities (FRESCO simulations). The reviewer also declared that SNL provides data from their optical engine related to measurements of flow patterns and emissions in their optical engine, and three-dimensional (3D) CFD simulations are being carried out using FRESCO. The SNL data are also being used to improve the simulations.

The reviewer remarked the project has been pursued for over 20 years; the most recent emphasis is on piston bowl geometry and the impact of pilot injections. The combination of detailed numerical modeling and experimental in-cylinder measurements is good and is providing information that should improve the predictions. The reviewer remarked some discussions should be included that show comparisons with modeling efforts and what about the model should be changed.

The reviewer asked how important knowing combustion chemistry is in FRESCO, and how sensitive the simulations are to alterations in specific reaction mechanisms. This question relates to surrogates and their chemistries and to using FRESCO in the potential validation of combustion chemistry.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer commented there was great progress despite much time spent rebuilding the metal engine.

#### **Reviewer 2:**

The reviewer said the benefits of stepped-lip piston shown as up to 3% in thermal efficiency while simultaneously reducing smoke and oxides of nitrogen  $(NO_x)$ . This is a good result. In addition to this, the reviewer would like to have seen more direct comparisons between the optical engine and the two software platforms (UW and CSI). The reviewer remarked it would be even better to include spray results from ANL.

#### **Reviewer 3:**

The reviewer said that it is very encouraging to see that squish flow behavior is being understood by exercising the model. This will help understand to interpret engine data when injection timings are swept. The reviewer stated the role of pilot injections in modifying the radial squish flow will be important. However, it may be that heat transfer is primarily being reduced.

#### **Reviewer 4:**

The reviewer stated the experimental work appears to have had a significant setback with the need to rebuild the engine following a piston failure in June. There are, however, interesting data presented as from the stepped piston bowl. Nevertheless, the reviewer noted, the data give little insight to viability or success with respect to LD diesel requirements from the VTO program (Slide 1). Delphi is mentioned as providing advanced injection systems. The reviewer asked if the report could include what the supplier contributed to the program.

#### Reviewer 5:

The reviewer said that a range of results were presented, including scoping studies to assess performance of a stepped-lip piston design. The PI provided no substantive discussion why this design was worthy of investigation; the design appeared to be just fabricated and tested. The reviewer stated that UW's CFD FRESCO code was shown to be able to simulate some of the piston bowl flow patterns. The PI reported on the development of a velocimetry technique to provide temporally and spatially resolved measurements in the piston bowl. The reviewer commented that this technique seems quite interesting and should be further developed and placed in the context of existing measurement capabilities.

The reviewer said that in response to an apparent request for a closer coupling of this project with thermomechanical material stress issues, the PI noted that folding in such an aspect was not within the scope of their efforts. This perspective should be revisited. The reviewer commented that it will certainly be an issue if an engine ultimately flies apart from material failures if operating at peak efficiencies for long periods of time. That is the project team's choice not to consider it. The reviewer suggested that perhaps as part of a more research oriented investigation, the PIs can afford to omit this consideration from their project. However, the reviewer noted, original equipment manufacturers (OEM) are part of this effort (GM/Ford) and they would most certainly need to consider the compatibility of achieving high engine efficiencies with material stresses. If the OEMs do not care about this problem, certainly the PIs need not as well; ultimately though, the consumer could pay the price.

The reviewer remarked that because piston bowl development is included in this project, the PIs should consider employing solid free-form fabrication techniques to cost-effectively fabricate a range of designs. This technology is also capable of fabricating parts in metal. The reviewer said the PIs may consider contacting DOE's Advanced Manufacturing Office, which has a vested interest in this technology, for insights on the optimal rapid prototyping (RP) technology for this application. Even in an acrylonitrile butadiene styrene plastic, much can be learned about flow patterns with rapid fabrication of different designs. The reviewer noted that RP piston bowl geometries will facilitate identifying an optimal bowl design, which apparently is not currently a part of the research plan. It is something the PIs should look into. Again, fabrication in metal is possible, and at the least can be accomplished in a plastic that could facilitate fluid flow patterns which the particle image velocimetry (PIV) capability could use for comparing with computations.

The reviewer noted that the codes considered, UW developed their own code (FRESCO). The reviewer asked if the code, as well as SNL's RAPTOR, is or will become open source. This person also commented that more evidence should be provided about precisely how the data reported in this study are informing the modeling. The reviewer asked where the discrepancies are and what the strategy is for closing the gap with modeling. The reviewer recommended to not just present comparisons, and to provide insights on what need to be changed in the modeling.

The reviewer noted the reference list included articles from earlier reporting periods; this is fine. However, it is more typical that references refer to articles/publications/presentations referenced only in the reporting period.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer expressed that excellent collaboration exists with GM, Ford, UW, and CSI, and the parties are playing their roles well. Additionally, new collaborations for spray measurements with ANL are a very good move.

#### Reviewer 2:

The reviewer stated the project has all the elements required from a collaboration perspective. It would be good to show more evidence of the degree to which the collaboration is occurring. For example, the

#### reviewer asked what technical input the OEMs have offered.

#### **Reviewer 3:**

The reviewer remarked the project would merit a great deal with active participation from OEM that is committed to the LD diesel product in the United States. A committed OEM may be able to provide a more focused approach to the current work.

#### **Reviewer 4:**

The reviewer commented that the collaborations include close coupling with GM/Ford. The PI noted that the project team is interacting with all parties to provide technical input. The reviewer stated the PI should be more specific about the GM/Ford input and how it informs the work that evidences a substantive impact. As presented, it is vague.

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 it was good to see that the Advanced Combustion and Emissions Control Technical Team (ACEC) noise guidelines will be followed. The reviewer also commented that a First Law analysis should be conducted accounting for the combustion, work conversion, heat transfer, and internal energy portions of indicated efficiency for the re-entrant and stepped-lip piston bowls to get additional insight regarding from exactly where the efficiency benefit is coming.

#### Reviewer 2:

The reviewer remarked future work will include continuing study of bowl geometry and pilot injection effects. As noted previously, consideration should be considered to using capabilities of RP to fabricate piston bowl configurations. The reviewer asked if FRESCO has the capability to deal with multicomponent liquid effects, which will be important for surrogate fuels beyond simple single component surrogates and if not, how the PIs will handle this problem. The reviewer noted soot oxidation is mentioned and asked if the FRESCO model will be used in the CFD. If so, the reviewer inquired about what diagnostics will be employed in the experiments and what strategies are proposed if the model does not match the data.

#### **Reviewer 3:**

The reviewer commented the program does little to address the technical targets of 40% fuel economy improvements or Tier 2 Bin 2 emission targets, or cost effective combustion-emission solutions.

#### **Reviewer 4:**

The reviewer asked how the current piston geometry was determined and how the geometry can be improved. Additionally, the reviewer questioned whether the models are now of sufficient fidelity to start to explore an optimized geometry (e.g., applying a generic algorithm). The reviewer stated this has to be on the list of future work at some point. Additionally, this person would also like to see a direct comparison between the two software codes and the optical experiments.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1**:

The reviewer affirmed, yes, from a broad perspective. The project has been in development for a long time. The reviewer asked what timeline the PIs envision before work will be completed.

#### **Reviewer 2:**

The reviewer said, yes, it is relevant. However, the project team can do a better job showing this by comparing back directly to the DOE goals (i.e., a projected brake thermal efficiency [BTE]), and showing how it improves every year.

#### **Reviewer 3:**

The reviewer stated the project scope is relevant. The work underway, however, is far from making any real impact on the merits of LD diesels in the United States. A question the team may ask themselves, the reviewer remarked, is whether the work the team is doing would invite manufacturers towards the introduction of LD diesels to the United States in the next 20 years.

### 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 seem adequate although ultimate judgement would have to come from a cost/benefit analysis based on DOE's investment relative to the commercialization potential.

#### Low-Temperature Gasoline Combustion (LTGC) Engine Research: John Dec (Sandia National Laboratories) ace004

**Presenter** John Dec, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated the project had a good approach and liked that the project team has both an optical and metal engine. The reviewer was pleased to see the focus shift from chasing efficiency to demonstrating control robustness and minimizing boost demand. The reviewer would like to see a more thorough 3D simulation effort to show how well the current tools can predict the team's results.

#### **Reviewer 2:**

The reviewer remarked that as the project team moves the concept forward, it will need to begin to



Yes (100%) Sufficient (100%) acc00 Figure 4-3 - Low-Temperature Gasoline Combustion (LTGC) Engine Research: John Dec (Sandia National Laboratories) -Advanced Combustion Engines

address, at least conceptually, how Tier 3 emissions levels would be achieved. This reviewer pointed out that the presenter commented on ultra-low  $NO_x$  and soot, which implies minimal aftertreatment for these constituents, or at least minimal impact on fuel economy to regenerate such aftertreatment. The reviewer stated that hydrocarbons (HC) remains an issue, especially for cold starting of the engine. The reviewer questioned if there are any means to address how the project team's engine concept would be cold started and does it present an issue for Tier 3 Bin 30 emissions targets. OEM partners could help identify targets for this. The reviewer also asked how does the efficiency of the team's concept compare to a conventional hybrid electric vehicle (HEV) optimized stoichiometric engine concept using an Atkinson or Miller cycle approach.

#### **Reviewer 3:**

The reviewer remarked that understanding the potential of assisted auto-ignition (i.e., spark in this case) could be an important enabler for LTC approaches.

#### Reviewer 4:

The reviewer stated that  $NO_x$  and soot emissions below 2010 HD requirements are not likely to satisfy future regulations because regulated emissions requirements will invariably decrease in the future. Engine-out  $NO_x$  and soot should be reported along with exhaust temperature so that aftertreatment feasibility can be assessed in the context of tailpipe emissions requirements. The reviewer also commented that a realistic boosting system will likely erode the indicated efficiency benefits to the point that the brake efficiency is not very attractive.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer remarked that cylinder head comparison between the two different heads is very interesting. The reviewer asked, given that there was such a large difference in low-temperature gasoline combustion (LTGC) with cylinder heads that were designed for diesel engines, what characteristics would be desirable for a cylinder head designed for LTGC. Additionally, the reviewer questioned what does 5 MW/m<sup>2</sup> ringing intensity sound like. It would be useful for the audience to bring an audio recording of the engine running at this condition so that the audience can hear it. In order to implement this combustion approach in the marketplace, phi sensitive fuel will be required. The reviewer asked how could it be determined if all available gasoline in the market is phi sensitive. The reviewer also questioned what the impact on NO<sub>x</sub> is when spark ignition is introduced into the LTGC combustion approach.

#### **Reviewer 2:**

The reviewer expressed that the results are encouraging and that fuel timing and spark provide some level of combustion phasing control. It was unclear to this reviewer how much control authority is actually needed. The project team should engage their industrial partners and develop a method to quantify combustion robustness to control factors, including both slow-path (air, exhaust gas recirculation [EGR]) and fast-path (fuel timing, s/a) actuators. The reviewer stated this should then be compared to a goal and/or a relevant benchmark. It was disappointing to see the new head perform worse than the new one. The reviewer asked what level of analysis was performed before making the head. Additionally, the reviewer questioned whether the tools are incapable or was the work simply poorly executed. No exhaust gas temperatures were shown. The reviewer requested that they be included in the analysis next time.

#### **Reviewer 3:**

The reviewer commented that some of the project team's colleagues have employed an uncertainty analysis into the project. Given the control challenges of this combustion mode, an uncertainty analysis could help sort/rank control and noise factors and could be very valuable given the transition to Co-Optimization of Fuels and Engines Initiative (Co-Optima) and the inclusion of fuel properties.

#### **Reviewer 4:**

The reviewer stated that careful base-lining of the new head and its comparison to the previous head will be important in understanding the results that will be forthcoming.

#### **Question 3: Collaboration and coordination with other institutions.**

#### Reviewer 1:

The reviewer stated there appears to be strong interaction with relevant stakeholders.

#### Reviewer 2:

The reviewer saw very little proof of collaboration. Yes, there was a fuel specification developed with

GM and a head provided by Cummins, but there were no results from ANL/Lawrence Livermore National Laboratory (LLNL) shown. The reviewer stated that if GM is performing the 3D CFD analyses, please include a sample of the results. If the project team is unable to do so, please find a partner that can support the team's 3D CFD needs in an open way.

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 integrating this work with the Co-Optima fuels program should involve efforts to quantify the range of relevant thermodynamic, in-cylinder time histories present relative to the physical and kinetic characteristics of the fuel being used. For example, to achieve the successful operation over the speed and load range being studied, certain temperature, pressures, and composition time histories are required. The reviewer stated these histories are needed because they match well with the physical characteristics and auto-ignition chemistry of the fuel being used. The interdependence of the in-cylinder thermodynamic time histories and the physical and kinetic characteristics of the fuel is the important fundamental understanding that is needed. The reviewer remarked there is debate as to whether K, the empirical parameter proposed as an attempt to connect the engine operating characteristics with research octane number (RON) and motor octane number (MON) via the Octane Index, is an appropriate metric. Whether it is or is not the relevant metric is an important question that may deserve directed attention. The reviewer said it seems that this is an important issue for the Co-Optima program and to achieve optimization of fuels and engines for minimal GHG and emission impact it will be important to identify the range of in-cylinder conditions present in the current portfolio of combustion approaches and connect those conditions into the physical characteristics and autoignition chemistry of viable fuel mixtures. The reviewer said that this research could be a rich source for that database.

#### **Reviewer 2:**

The reviewer remarked future work should include a complete survey of market available gasoline to ensure that all gasoline is phi sensitive. If any gasoline is found that is not phi sensitive, then this combustion approach will never be more than a laboratory novelty.

#### **Reviewer 3:**

The reviewer expressed there needs to be more work performed to understand control robustness as previously mentioned—both experimentally and 3D (with results that can be shared).

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer affirmed the work is relevant, but the project team should be doing more to show this. Indicated thermal efficiency and indicated mean effective pressure (IMEP) are good indicators, but they do not relate directly back to DOE goals, which are described in fuel economy or BTE terms. The reviewer stated there should be at least a directional one-dimensional (1D) model created to show what boosting system is required. The project team can also work with Cummins on a friction assumption. With this, the reviewer can estimate a BTE. The reviewer further noted all researchers should be doing this and comparing themselves to one another to show who is the most relevant. There should also be a forum to vet the assumptions that go into the model. Maybe this becomes an activity for the advanced combustion engine working group, the reviewer suggested.

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

#### Reviewer 1:

The reviewer would encourage the project team to find a way to work within their available budget to perform the 1D and 3D work in a way that the results can be openly shared.

#### **Spray Combustion Cross-Cut Engine Research: Lyle Pickett (Sandia National** Laboratories) - ace005

Presenter Lyle Pickett, 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, feasible, and integrated with other efforts.

#### **Reviewer 1**:

The reviewer said that the approach here is outstanding. SNL focuses on the advanced spray optical diagnostics where it has the facilities and expertise and then combines this with a large external pool of CFD and experimental collaborators to leverage its results with theirs. The reviewer commented that there appears to be a better balance this year between diesel and gasoline work.

#### **Reviewer 2:**

The reviewer stated that a highquality resolved measurement dataset is an invaluable aid to the





Lyle Pickett (Sandia National Laboratories) - Advanced **Combustion Engines** 

engine and CFD community in industrial practice.

#### **Reviewer 3:**

The reviewer noted the approach involves engaging multiple research organizations for experimental and computational spray research for diesel and gasoline engines.

#### **Reviewer 4:**

The reviewer remarked that this project is motivated by the need to develop a better understanding of sprays (gasoline/diesel) and to provide data for the ECN. The constant-volume chamber (CVC) with spray injection is being used to develop spray data. The CVC ostensibly provides well-defined conditions, allows assessing performance of several injectors, and provides better control of conditions than found in an engine. The reviewer stated that the presentation noted that the CVC is thought to provide data under engine-relevant spray conditions. However, the environment of a CVC is static (constant volume) while that of an engine is dynamic with time-dependent conditions. The reviewer

noted that, in fact, there seems to be a lot in the CVC geometry that is not closely aligned with an engine, which is not necessarily an impediment. The reviewer stated that the situation is of no more concern than claims that a rapid compression machine (RCM) or shock tube provides engine-relevant condition (it does not). Rather, the CVC provides a means to provide fundamental information about spray processes, and that is what should be advertised rather than trying to claim relevancy to the environment of an engine. The reviewer recommended that some clarification of this view is needed. Interest in understanding flash boiling was noted from the presentation by the reviewer, who asked what is being done in this area by this project. This person explained that it is an interesting subject, but information about it was scarce.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said that the increased focus on gasoline fuel Spray G this year has been outstanding. The work with the new PIV diagnostic to understand collapse is excellent work and has thrown new light on the entrainment and velocity inside the spray cone as a function of time.

#### **Reviewer 2:**

The reviewer stated the PIV technique demonstrated this year looks very promising and there are significant findings in many areas, such as the ambient temperature and nozzle inlet passage effects on spray characteristics. The broader collaborative work with the various ECN members also shows quite a bit of progress and useful accomplishments in a wide range of areas: soot, mixing, dribble, etc.

#### **Reviewer 3:**

The reviewer said the development of the high-speed PIV diagnostic is impressive. The project demonstrated operation of this capability by scoping out its operation with iso-octane as the fuel. The reviewer noted that for PIV to work, the seed particles need to faithfully follow the flow and asked if this is the case here with the zirconium (Zr) particles. For example, the reviewer asked, could the droplets be a sort of seed, or even the soot produced. The reviewer said that the project has shown a lot of results of the experiments. However, a better demonstration of how the CVC data are used in CFD development should be established. This reviewer reported that a lot of results were shown: demonstration of the high-speed PIV diagnostic; time evolution between plumes; axial temperature variations at different gas temperatures and its influence on droplet vaporization; nozzle shape effects on spray development; structure of the spray for different fuels; and influence of ambient temperature on ignition delay. The reviewer commented that because the data are ostensibly supposed to be coupled with CFD, it would be appropriate to show more clearly how the spray data and diagnostic capabilities for velocity are being used in the CFD simulations. Many CFD collaborators are listed; however, precisely how they are being incorporated in the project is unclear.

#### **Reviewer 4:**

The reviewer said it is understood that this type of fundamental understanding requires a sustained methodical approach and the fruition in terms of engine design may be slow to develop.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer commented that the ECN must be one of the best examples of collaborative engine research around. The broad inclusiveness of national laboratories, academia, engine makers, component suppliers, CFD vendors, etc., defines outstanding.

#### **Reviewer 2:**

The reviewer commented that the breadth and scope of the ECN collaboration are impressive, but what seemed to be missing (at least in this brief presentation) is a sense of coordination. The reviewer questioned who is working on which sub-topics/questions and why. Notwithstanding the "very tight coordination" touted on Slide 20, the reviewer asked whether the ECN performers are free to define their own niches, and if not, how they are being steered in ways that will create a synergistic whole. The reviewer noted that this is an important aspect to summarize in the AMR.

#### **Reviewer 3:**

The reviewer noted that there is an extensive array of collaborators. In fact, the list is very extensive. However, the precise roles of the collaborators were not evident. The reviewer commented a stronger demonstration for how the CVC data are being used in the CFD modeling should be demonstrated. The reviewer asked what the project is providing to the ECN and what an example is for how the data developed here are being used.

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 the project appears to be focused on the topics of greatest interest and shows a continued responsiveness to the needs of the engine manufacturing community.

#### **Reviewer 2:**

The reviewer observed that the proposed work on gasoline particulate formation at the tip of the injectors is very relevant and timely.

#### **Reviewer 3:**

The reviewer commented that the anticipated speed-up with a heated chamber is suitably ambitious.

#### **Reviewer 4:**

The reviewer stated that future work notes improving model capabilities for the Spray G, with several codes being listed (CONVERGE, OpenFoam, etc.). The reviewer commented that better specificity of precisely what data will be developed that the codes will predict should be provided. For example, soot formation is noted to quantify its formation with Spray C, which is apparently a cavitating spray. The soot diagnostics should be specified and discussed.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said the learning from this project will continue to facilitate building cleaner and more efficient engines, thus reducing petroleum usage.

#### **Reviewer 2:**

The reviewer noted that the overall importance of diagnostics to evaluate engine performance is high and in that regard the project is very relevant. It may be beneficial for the PI, and indeed all the national laboratories, to consider developing a diagnostic consortium of sorts to advertise experimental capabilities across the national laboratories.

#### **Reviewer 3:**

The reviewer stated that the project is indirectly relevant because better spray understanding is essential to better petroleum-combustion efficiency and emissions reduction.

### 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 the resources appear adequate, especially considering the scope of outside collaborators contributing to the project.

#### **Reviewer 2:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/benefit analysis based on DOE's investment relative to the commercialization potential.

#### Gasoline Combustion Fundamentals: Isaac Ekoto (Sandia National Laboratories) - ace006

**Presenter** Isaac Ekoto, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer remarked that spark and plasma ignition is more important than the negative valve overlap (NVO) work. The calorimeter is a good addition, and it might also be important to develop a bench test to investigate ignition system behavior in a flow field.

#### **Reviewer 2:**

The reviewer noted that the work is transitioning to focus on advanced ignition concepts for various combustion concepts.

#### **Reviewer 3:**

The reviewer stated that the purpose of the ignition work is not clear and asked if it is to establish conditions for auto-ignition or to actually initiate combustion.



Relevant to DOE Objectives

### Sufficiency of Resources



Figure 4-5 - Gasoline Combustion Fundamentals: Isaac Ekoto (Sandia National Laboratories) - Advanced Combustion Engines

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer commented that the analysis was an insightful method to explain results from NVO reformate behavior. Furthermore, the calorimeter results were also good, and the reviewer expects more interesting results to come.

#### **Reviewer 2:**

The reviewer stated that there was a good explanation of observed effects of reformate addition. While the explanations offered are noted, project progress continues to be slow.

#### **Question 3: Collaboration and coordination with other institutions.**

#### Reviewer 1:

The reviewer stated the response to industry needs is good.

#### Reviewer 2:

The reviewer commented that more collaboration with OEMs regarding the ignition system testing would be helpful to provide guidance for the project and feedback to industry.

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:

No comments were received in response to this question.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1**:

The reviewer noted that improved understanding of ignition systems and processes in gasoline engines is critical to improving engine efficiency.

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

Reviewer 1:

No comments were received in response to this question.

#### Large Eddy Simulation (LES) Applied to Advanced Engine Combustion Research: Joe Oefelein (Sandia National Laboratories) - ace007

**Presenter** Joe Oefelein, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated that this project provides invaluable information on combusting spray, which can be used for model development. However, it is not clear how complex engine geometry with moving valves and a piston can be handled in the framework of RAPTOR. The reviewer also noted that it is not clear if the end goal is to provide reference simulation data for model development or to provide a software tool for engine development. When considering computing time and a high-performance computing (HPC) resource for engineering purposes, the project should focus on the former.

#### Reviewer 2:

The reviewer commented that this is a well-focused synthesis and presentation of the root-cause challenges faced by engine combustion simulation. The near-DNS approach is a worthy attack on the problem of too many uncertain input tuning coefficients in multiphase reacting CFD.

#### **Reviewer 3:**

The reviewer noted that this project is motivated by the need to develop a better understanding of spray combustion dynamics as related to gasoline direct injection (GDI) and diesel engines. The PI has made a convincing case that the current art on engine simulations is lacking for their abilities to provide high accuracy simulations of in-cylinder processes. The reviewer said the approach advanced in this project is to use large eddy simulation (LES) through the code RAPTOR, which is a first-principles solver optimized for LES. RAPTOR has significant potential for a high impact on engine design when completed, and the PI seems to be making a lot of progress. The reviewer expressed that one can only wish that the pace of development could be increased because the potential for RAPTOR is significant. The reviewer said that the presentation was clear and well developed.



#### **Reviewer 4:**

The reviewer stated that the approach of applying detailed first principles models for the wide range of complex incylinder processes is excellent. However, progress to combine these into an all-up simulation of a diesel or gasoline direct-injected (GDI) engine has yet to be achieved (although progress is measurable and continuing towards that goal). The reviewer noted that the key to the ultimate success of this program will be how the knowledge gained can be transferred to commercial code vendors and ultimately used in a practical way by engine developers. It will be a challenge.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer commented that the project is a good systematic use of UQ to help optimize accuracy per unit computational cost. Additionally, the interphase filtering and new combustion LES closure are highly innovative.

#### **Reviewer 2:**

The reviewer stated that project progress remains good and steady; much is being learned about turbulence, sprays, and combustion and the interactions between them. However, some of this is more along the lines of confirming the known limitations of current methodologies that have to also meet the constraint of speed. The real progress will be in finding ways to take these advanced approaches and producing better engineering tools combustion system designers can use on a daily basis to develop better engines.

#### **Reviewer 3:**

The reviewer stated that the accomplishments included an array of simulations on several combustion and nonreacting configurations. Calibration of the results through comparisons with the configurations selected is an essential part of proving the efficacy of RAPTOR to provide high accuracy results. The reviewer noted that the code appears to incorporate detailed transport and chemical kinetic mechanisms along with multiphase effects from sprays folded into the capabilities so it seems to be quite robust. The reviewer commented that configurations used to provide data for testing RAPTOR include the CVC, non-reacting fuel jet injection, auto-ignition of reacting diesel jets, and ignition delay time predictions from RCM and shock tubes. The work on GDI sprays is perhaps closer to the reality of spray injection in engines and seems to be in progress. The reviewer asked whether, in this simulation, the flame exists only in the region where the droplets have fully vaporized. The reviewer also questioned the conditions where liquid is present in the flaming region and liquid vaporization effects are present and how are they treated.

The reviewer said that in regards to combustion chemistry, a number of chemical mechanisms were used. If RAPTOR is a first-principles solver, the project team should comment on its ability to provide a stringent test of the combustion chemistry. The reviewer asked what strategies would be used to adjust the chemistry to bring measurement and theory into better alignment. The reviewer realized that the chemistry is provided by others and presumably they have strategies for adjusting reactions to improve predictions. To facilitate this effort, the PI might consider a simpler multiphase configuration to test RAPTOR's ability to deal with the complexities of liquid/ combustion/vaporization/transport that might better provide a platform to adjust the inputs to RAPTOR (chemistry, property database, etc.).

#### **Reviewer 4:**

The reviewer noted that although milestones and achievements in FY 2016 are not clearly described, several valuable tasks have been well performed (e.g., combusting spray on ECN Spray A with good agreement with experiment and optimization of chemical models using UQ).

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer indicated that collaboration with other institutions looks very well done. This person recommended that the PI also talk to industry to determine current and future needs in engine combustion modeling.

#### **Reviewer 2:**

The reviewer commented that collaboration perhaps along the lines of a combustion CFD equivalent to the ECN, which is more focused on spray diagnostics and some simulation but not at the high end for the most part, might be a way forward for the project. Engaging CFD practitioners in the engine industry with commercial code vendors as well as research code and model developers in academia and national laboratories might provide more of a dialog to transfer learning from the detailed simulations to the development and application of engineering tools to design and understand in-cylinder combustion systems.

#### **Reviewer 3:**

The reviewer noted that a range of collaborators are included in the project and some appear to be contributing actual data, which the PI is using to assess the efficacy of RAPTOR's capabilities (several examples were given in the presentation). Regarding the radiation modeling, the reviewer asked whether RAPTOR currently has this capability. Concerning wall impingement effects, the reviewer queried whether RAPTOR can simulate the impingement and spreading dynamics of a single droplet, or an aggregate of droplets, at a wall.

#### **Reviewer 4:**

The reviewer observed that the last summary sub-bullet mentions "working closer with industry" on simulation software development, and, on Slide 31, the second comment response cites an attempt to do that. It would have been helpful to hear the project team's specific ideas and plans. The reviewer noted there is zero industry participation evident in Slide 32. Deliberate avoidance of reinventing the wheel of commercial Reynolds-Averaged Navier-Stokes (RANS)/LES-centric CFD was applauded by the reviewer. However, this person recommended the earliest possible coordination with code developers supporting today's design community, and with products that do scale well to O(10,000) processor so that RAPTOR can have the maximum long-term impact.

# 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 it is good to see that actual engine simulations are in the project plan for the coming couple of years. Hopefully, these will prove the concept of detailed modeling that has been followed in this program.

#### **Reviewer 2:**

The reviewer opined that there is a good forward look at milestones and several slides provided helpful historical context. However, a formal timeline is missing. The reviewer noted that the information in that section of the quad chart (Slide 2) is completely off topic and the reviewer was left with no idea of the project duration, past or future.

#### **Reviewer 3:**

The reviewer commented that because RAPTOR is so potentially robust, consideration should be given to using it as a tool to assess kinetic and property inputs required for simulation. For example, combustion chemistry can be uncertain. The project team should consider applying RAPTOR to a simplified multiphase configuration where transport is well defined to assess performance of the combustion chemistry. The reviewer stated this could also provide significant benefit to other projects using commercial codes where the combustion chemistry is needed but validation of it is limited. The reviewer also noted that future work should comment upon the specific computer platform used as well as the computational times involved when presenting results.

#### **Reviewer 4:**

The reviewer stated that it is directionally right to move toward realistic (optical) engine geometries, but the current codes cannot handle as is mentioned in Slide 34. The project team should develop a plan to address this situation.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer stated that the project can provide important simulation data for engineering model development.

#### **Reviewer 2:**

The reviewer stated this project is certainly relevant. Indeed, it seems to be the only simulation effort that is incorporating a first-principles approach to solving the multiphase dynamics associated with fuel spray injection and combustion. The reviewer said that when completed, RAPTOR should be the most advanced tool for simulating the complex multiphase processes found in engines and, thus, provide the means for high accuracy simulations for facilitating engine design.

#### Reviewer 3:

The reviewer noted that in the long run, better simulation tools lead to better, more efficient engines that will lead to reduced petroleum use.

### 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 budget or manpower seems too low for progressing faster and producing more outcomes.

#### Reviewer 2:

The reviewer commented that hopefully the funding can be stabilized at the current level. In comparing all the different avenues of research being pursued by DOE, with a limited funding resources, sometimes cuts have to be made. The reviewer stated this project probably cannot make adequate progress if further cuts are imposed.

#### **Reviewer 3:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

#### Fuel Injection and Spray Research Using X-Ray Diagnostics: Christopher Powell (Argonne National Laboratory) - ace010

**Presenter** Christopher Powell, Argonne 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer said that the application of ANL's unique X-ray source for spray and injector internal flow diagnostics and studies is brilliant and an excellent example of repurposing DOE's technology to aid the engine industry. With this tool, the team has already performed many useful studies and continues to develop techniques and capabilities to extend their research to other important areas.

#### **Reviewer 2:**

The reviewer said that the ANL team has put together a very impressive visualization tool for spray

This Project Numeric scores on a scale of 1 (min) to 4 (max) Sub-Program Average 4.00 3.50 3.00 2.50 2.00 150 1.00 0.50 3.30 3.30 3.30 3.20 3.29 0.00 Approach Tech Collaboration Future Weighted Accomplishments Research Average **Relevant to DOE Objectives** Sufficiency of Resources



Figure 4-7 - Fuel Injection and Spray Research Using X-Ray Diagnostics: Christopher Powell (Argonne National Laboratory) - Advanced Combustion Engines

diagnostics and that it has been well-documented over the last years. The reviewer said that it would be useful to understand if this tool is considered to be mature or it needs to be improved for successful integration to the modeling and predictive tools (e.g., whether the spatial or temporal resolutions are sufficient or whether the room temperature limitations are a significant impediment). The reviewer found that, overall, the impression given is that there is little integration of this work with actual modeling.

#### **Reviewer 3:**

The reviewer said that this project is motivated by a lack of an understanding of fuel injection processes. To fill this gap, the project is rather narrowly focused on using the ANL X-ray source to provide unique measurements related to fuel injection with an emphasis on or near the nozzle. The reviewer commented that data are taken that are indicated as being important for improved spray models. The X-ray source provides unique abilities to image both inside and outside an injector. In this way, it is possible to view inside the nozzle to assess optimal flow paths for atomization including droplet size and their trajectories
#### downstream of injection.

The reviewer detailed that, thus far, the project has demonstrated considerably improved photographic resolution that show significant details nozzle geometry. The multi-hole (Spray G) nozzle images have been shared with the ECN, and industrial partners are showing interest. The approach of using a beryllium nozzle is good because of its ability to facilitate better imaging.

Comparisons with simulations at the University of Massachusetts were shown. More details should be provided. The reviewer asked if the simulation is from a commercial code or was it written in-house. The reviewer noted that the approach provides information under relevant conditions, and asked if this includes high-temperature gas environments.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer praised the improvement to the beam line and the resulting improvement in resolution as staggering. The reviewer suggested that the team continue to pursue correlations between observed features or anomalies in the injector design and a measurable engine or combustion system-level attribute.

#### **Reviewer 2:**

The reviewer said that the effects of cavitation, needle motion, etc. have been observed with extremely high resolution in plastic and metal injector hardware. The results include qualitative and quantitative data, both of great import to the engine community. The reviewer noted that improvements in hardware and techniques are continuously sought to improve the quality and extend the domain of these measurements.

#### **Reviewer 3:**

The reviewer said that the presentation provides little update of technical work for this calendar year. It appears limited to submerged cavitation, and measurements of cavitation on a GDI injector. The reviewer noted that many of the slides touch on collaboration, but there is no content reported.

#### **Reviewer 4:**

The reviewer cited that listed accomplishments include working with the ECN to provide information on injector geometry, internal needle motion, near-nozzle spray density, and mean droplet diameter measurements. Regarding diameter measurements, the reviewer said that more information should be provided. The reviewer asked if such measurements are through the cylinder and what the time resolution is. The reviewer asked how the diameter measurements are made. Some examples should be provided. The reviewer inquired how the measurements compare with more conventional diagnostics (a Phase Doppler Particle Analyzer, etc.).

The reviewer commented that much of the presentation seemed more like an advertisement of the virtue of X-ray diagnostics than a demonstration of new results over the past year and that more results should be provided. The reviewer asked if there is a jumping off point when the diagnostic will be mature and a mainstream instrument or will it always be tied to ANL's facility. If the latter, the reviewer found that would be a limitation to its wider use in industry.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer said that the team has clearly worked closely with many groups and freely provided data

to many. The coordination with the neutron imaging team at ORNL is particularly noteworthy as these two facilities are very complementary, but could also be competitive. The reviewer was glad to see the former appears to be winning.

#### **Reviewer 2:**

The reviewer said that many collaborations are reported, but there was no clear assessment as to the significance of these collaborations. The reviewer noted that there are extensive presentations given, 15 in total, including 7 international conferences. The reviewer asked if this is necessary or seen as distracting from the actual work.

#### **Reviewer 3:**

The reviewer commented that a range of collaborators was indicated that included groups from industry, academia, and national laboratories. However, the importance/necessity of the listed collaborators to the overall success of the project was unclear. Few results were included from these groups. The reviewer also noted that partners from industry were included, such as Delphi Diesel, which perhaps has an intense interest in the X-ray diagnostic. Nonetheless, the collaborators should be expanded to include the major manufactures of atomizers. The reviewer said that the X-ray diagnostic can be used as a design tool and nozzle designers should be part of the team as they stand to gain significantly from the success of this project.

The reviewer noted that the collaboration with ORNL is interesting because Oak Ridge Associated Universities (ORAU) is pursuing virtual injector design. Precisely what ORAU and ANL are sharing in this partnership is not clear. The reviewer said that this concern further indicates that the necessity of the listed partners, and what they brought to this project should be clearly evident.

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 moving into more of a combustion environment will provide even greater benefits to the engine community.

#### **Reviewer 2:**

The reviewer said that there is a good list of tasks listed, citing Slide 18. The authors may explain how these will be incorporated into the main path towards helping the predictive modeling efforts. One suggestion the reviewer offered may be participating in a specific simulation program where the information from the X-ray images proves to be the enabler to overcome a specific barrier, thus resulting in a significant breakthrough in the modeling capability.

#### **Reviewer 3:**

The reviewer commented that future work seems to be developed around measurements for the ECN, cavitation studies, measurement of fuel/air mixing inside a duct, nozzle geometry measurements, etc. The reviewer noted barriers included windows, broadband X-ray capabilities, and high-temperature conditions. While it was not evident from the list of the proposed future work, e.g., and measurements of GDI nozzle geometry, cavitation studies, spark and laser ignition studies and nozzle geometry measurements would contribute to the listed barriers. The reviewer said that more thought should be given to a more-focused effort with clear connections between articulated needs and tasks that will specifically address those needs.

The reviewer noted a study of flash boiling. The reviewer said that this is interesting, but it was not

evident precisely how the X-ray diagnostic would be used on this problem, what data it would provide, and how they it will be used.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer commented that improved spray and combustion diagnostics aid the development of more efficient engines that will use less petroleum.

#### **Reviewer 2:**

The reviewer remarked that the project is relevant. The nature of the diagnostics needs to grow towards providing more useful, close to real-life conditions, and data to the research and engine manufacturers.

#### **Reviewer 3:**

The reviewer said that the project is relevant from a broad perspective. Greater relevance could be realized with a stronger connection with the atomizer/nozzle design industry.

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

#### **Reviewer 1:**

The reviewer was sure that more money could be usefully spent here, but the resources seem to be adequate for the program presented.

#### **Reviewer 2:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/benefit analysis based on DOE's investment relative to the commercialization potential. All that said, the cost/benefit ratio at a level of \$700,000 per year seems high.

#### Advances in High-Efficiency Gasoline Compression Ignition: Steve Ciatti (Argonne National Laboratory) - ace011

**Presenter** Steve Ciatti, Argonne 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer was glad to see some uncertainty analysis brought into the project. The reviewer would like to see a ranking of the most-important control and noise variables, which could help focus the project on leading barriers to control of this combustion mode.

#### **Reviewer 2:**

The reviewer said that the approach does not seem to be systematic and connected from one year to another and referenced comments in the next section.

#### Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which



Compression Ignition: Steve Ciatti (Argonne National Laboratory) - Advanced Combustion Engines

progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said that it would be helpful to see a speed or load map showing efficiencies and highlighting your control approaches in differing areas and also the chief barriers.

The reviewer asked if the exhaust temperatures the team reported are pre- or post-turbo and noted that post-turbo is most relevant to aftertreatment performance. The reviewer said that reporting brake specific fuel consumption (BSFC) with supercharger parasitics included, when the ultimate concept will not include a supercharger, is not helpful. The reviewer asked if maybe indicated specific fuel consumption and BSFC are reported together.

#### **Reviewer 2:**

The reviewer said that it is difficult to relate the technical accomplishments presented this year with the progress made in the past. The benefits of gasoline compression ignition (GCI) are high efficiency, ultra-low  $NO_x$  and low

particulate matter (PM), but its shortcomings are high carbon monoxide (CO) and HC emissions. The reviewer wondered can each of these key metrics be tracked from year to year to facilitate gauging progress, or if there is a better way to gauge progress.

The reviewer noted that experiments with a supercharger reported for several loads of interest. However, only BSFC results (which naturally are not competitive) are shown. The reviewer asked what the indicated or net efficiency was, how it compares to the efficiency results shown in earlier years, and how it compares to a conventional diesel engine.

The reviewer said that good experiments were conducted this year on minimum injection quantity and start of injection (SOI) effects with E10. Experiments have also been conducted at higher engine speed, at constant boost, and at constant lambda. The reviewer asked how the learnings from this are going to be applied to moving the overall concept forward. The reviewer asked can these learnings be made profitably in the context of high-efficiency, low-NO<sub>x</sub> and low PM. If so, the reviewer wondered if the reviewer and reader can be made aware of how these experiments and learnings enable moving the GCI concept forward. For example, if low-pressure (LP)-EGR along with late injection appears to have the leverage to increase exhaust temperature at low load, the reviewer asked how did those these two changes affect efficiency, NO<sub>x</sub>, and PM.

#### **Question 3: Collaboration and coordination with other institutions.**

No comments were received in response to this question.

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 it is proposed that indicated as well as BTE,  $NO_x$ , and PM always be presented so as to be able to relate any new fuel, operating strategy, experiment, or learnings back to the original benefits of the concept. The reviewer also said that progress in reducing CO and HC emission should be systematically tracked.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

**Reviewer 2:** 

No comments were received in response to this question.

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

#### **Reviewer 2:**

No comments were received in response to this question.

#### Model Development and Analysis of Clean and Efficient Engine Combustion: Russell Whitesides (Lawrence Livermore National Laboratory) - ace012

**Presenter** Russell Whitesides, Lawrence Livermore National Laboratory

**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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer applauded the uncertainty analysis and said that too many simulations use nominal values. The reviewer commented that real-world application of advanced combustion regimes, both design and control, will need to deal with these noisy variables.

#### **Reviewer 2:**

The reviewer said that as a counterbalance to a 2015 reviewer's comment, it is refreshing to see a recognition that smaller, pragmatic kinetic mechanisms will continue to be the norm in industrial practice for some time to come and are deserving of careful study

and emphasis in the quest to democratize engine simulation.

#### **Reviewer 3:**

The reviewer commented that the development of fast chemistry solver technologies and the application of them to new architectures that promise significant performance versus cost gains, such as a graphics processing unit (GPU), is of great import to combustion system designers striving to increase simulation accuracy while also reducing computational time. The reviewer said that getting this technology into the hands of commercial code vendors to make these gains of practical utility to the design community is, of course, just as important.

#### **Reviewer 4:**

The reviewer said that the PIs identify the time to perform simulations of in-cylinder simulations of combustion engines as a limitation for achieving detailed simulations of performance of combustion engines. The reviewer explained that GPU refers to NVIDIA's hardware specification for its general purpose GPU. GPU technology is not new and it is widely used in biomolecular simulations. The reviewer remarked that, here, the PIs are developing



its capability for integrating complex chemistry in combustion engine simulations so that such simulations can be performed in a more time-efficient manner.

The reviewer stated that it is not clear why cetane chemistry is of interest, especially given the current emphasis on surrogates, beyond single component fuels, for real fuels and biofuels. The reviewer remarked that this project should move away from cetane and emphasize chemical mechanisms for multicomponent surrogates for gasoline or diesel.

The reviewer commented that the homogeneous charge compression ignition (HCCI) concept is rather mature, and the problems with it well-known. The reviewer questioned what this work brings to the HCCI problem and how will it alleviate the issues with HCCI. The reviewer asked if this project addresses the concerns that have limited wider use of HCCI. Similarly, high-efficiency clean combustion has been known for some time. The reviewer wondered how this project will strengthen its development and how long will it take. The reviewer also asked what the roadmap is for solving the problems with this engine technology and if the yearly work here is more incremental than transformative.

The reviewer commented that a lot of the work seems to be to run a code and evaluate the results, which seems a bit pedestrian. The project repeatedly refers to CFD simulations, but the actual code being used was unclear from the presentation. The reviewer requested that this be specified.

#### **Reviewer 5:**

The reviewer said that this project is to develop a fast interface method for engine simulation where a detailed mechanism is needed. The method is integrated with engine combustion solvers and detailed mechanisms being developed by other LLNL project teams (i.e., ACE076, Matt McNenly of LLNL; ACE013, Bill Pitz of LLNL). The reviewer remarked that the approach seems reasonable, but the project title seems too general and misleading. The reviewer wondered if the model includes physical models like spray and combustion, and commented that, if so, the focus seems incorrect and it should be done by other ACE teams. The reviewer said that if it is simply using a commercial code (e.g., CONVERGE), the project title should not use the term "model development."

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said the accomplishments reported for the past year included an uncertainty analysis of SNL HCCI experiments (for example, data for engine speed, crank angle, CR, temperatures, and engine speed). The reviewer questioned what code was used to predict these things. The reviewer also asked if the SNL fuel used cetane. The reviewer said the presenter should clarify the uncertainty analysis. The reviewer commented that the presenter showed a flowchart that indicates how measured quantities related to derived quantities. The reviewer asked how this was used and what effort was involved with this activity. The reviewer also asked if it is just a flowchart of expected links.

The reviewer said that what the presenter reported was apparently the first engine simulations using all central processing units (CPUs) and GPUs on a computer cluster code. The reviewer asked what the base code was. The reviewer said that the PIs demonstrated results that showed GPUs producing the same results as CPUs but in much less time. The PI showed that they can handle big engine combustion problems.

#### **Reviewer 2:**

The reviewer said the milestone of this project in FY 2016 is to evaluate different load-balancing schemes for chemical kinetics and implement the most promising technique, and that collaboration work is going on with the ACE projects. The reviewer observed that development of the GPU accelerated chemistry solution was demonstrated on a gasoline spark ignited engine case on a workstation class computer. The reviewer remarked that it seems impractical to develop a method on a small-scale computer when a detailed mechanism is considered. It would not be that simple to port the method into a HPC environment. The reviewer said the GPU-enabled zero-order reaction kinetics (Zero-RK) chemistry solver through ACE076 seems like a great achievement.

#### **Reviewer 3:**

The reviewer said the smart-batching of reactions for GPU is innovative. The UQ work seems particularly important. It would be reassuring to see the simulation (kinetics and CFD parts) studied with the same UQ framework as another source of uncertainties alongside the measurement uncertainties, not only the myriad coefficients and grid-dependencies but also the more subtle and basic model-form uncertainty.

#### **Reviewer 4:**

The reviewer said that while the approach sounds good, test problems have shown that the performance gains have not been as good as anticipated. The reviewer commented that work has begun on smart batching, load balancing, and more in an effort to optimize performance. The reviewer said that preliminary tests look good. A lot of test work so far has focused on HCCI, and while there are some benefits of doing so, testing the capability for conventional diesel is also important and should be given more priority.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer noted Science and NVIDIA, and said the link with some of these groups was a bit vague. The SNL connection seemed clear (e.g., presumably data), but the link with the academic institutions and what they specifically bring to this project was not evident. The reviewer commented that a better connection needs to be established with the academic institutions listed to show the need for what they can provide. The reviewer wondered if the project could proceed without any of the academic partners and asked if they provide data or perform simulations.

As previously noted, the reviewer said the actual code used was unclear and wondered if it was the framework of CONVERGE. If so, then the CONVERGE PIs in other presentations at the AMR would presumably reference the combustion chemistry emphasized here and the efficient integration of GPU technology. The reviewer concluded that if that is being done, the researcher should note it in this project.

#### **Reviewer 2:**

The reviewer questioned how the methods developed through the project can be used for other software vendors than Convergent Science, Inc., and universities or industries using other software. The reviewer commented that the project team should consider this and make the methods available to others when needed.

#### **Reviewer 3:**

The reviewer suggested that the research team could adopt a deliberate multi-code approach in areas where R&D conclusions or even software design decisions are historically proven to be shaped to varying degrees by the peculiar limitations, methods, or assumptions of an individual simulation tool. The reviewer said that in these situations, to robustly achieve the verbally stated goal of "bringing fast chemistry to CFD," code-redundancy can add value by not only avoiding such distortions but also exposing otherwise hidden lessons and uncertainty sources. The reviewer commented that this collaboration is too important to be left downstream to the Technology Licensing Office.

#### **Reviewer 4:**

The reviewer observed that some collaboration with other national laboratories, a software vendor, a hardware vendor, and an engine company are noted, but the researchers should seek and support broader 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 said that the future work should move away from a single component fuel (cetane) and begin to incorporate combustion chemistries of multicomponent surrogate fuels. The reviewer stated that the results of this effort were disseminated through a range of presentations at various meetings and conferences. However, to have wider visibility, the PI should emphasize archival publications such as the articles in Proceedings of the

Combustion Institute, Society of Automotive Engineers (SAE), and International Journal of Engines. The reviewer commented that the project could benefit from more publications in such journals.

#### **Reviewer 2:**

The reviewer expressed that it is not clear how the UW work helps this project. The reviewer recommended solving multiple engine cycles, or RANS, to avoid ambiguity on setting up the intake valve closing (IVC) conditions.

#### **Reviewer 3:**

The reviewer said that in addition to the two very worthy topics presented, see comments above under question number three.

#### **Reviewer 4:**

The reviewer said that a one-slide summary of future work planned is somewhat sketchy. The reviewer agreed that greater speed-up is needed if the effort put into this work is to truly pay off in faster, better engine designs. The reviewer commented that uncertainty work could possibly take lower priority to improving computational speed. The reviewer added that increased collaboration is definitely needed.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

**Reviewer 1:** 

The reviewer said yes, from a broad perspective.

#### **Reviewer 2:**

The reviewer said this project can support faster simulation time for engine development CFD analysis using detailed mechanism.

#### **Reviewer 3:**

The reviewer said that faster and more accurate simulations will lead to better engine designs with greater efficiency, hence reduced petroleum use.

### 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 FY 2016 budget seems reasonable.

#### **Reviewer 2:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

#### **Reviewer 3:**

The reviewer commented that leveraging more collaborators inside and outside of DOE would be beneficial to effectively increase the project resources at no additional cost to the program.

#### Chemical Kinetic Models for Advanced Engine Combustion: Bill Pitz (Lawrence Livermore National Laboratory) - ace013

Presenter

Bill Pitz, Lawrence Livermore 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated that it is encouraging to see a recognition that pragmatic surrogate and reduced kinetic mechanisms will continue to be the norm in industrial practice for some time to come. The mechanisms are deserving of careful study and emphasis to support engine simulation. The reviewer encouraged the team to balance its methodical, one-componentat-a-time approach with holistic validation and calibration, to the extent practical, helping ensure that the largest error and uncertainty sources, such as high pressure effects, EGR, and realcycle effects, receive commensurate attention.



#### **Reviewer 2:**

The reviewer said that understanding and developing kinetic models for combustion chemistry is vital but difficult work. The reviewer commented that the LLNL team has demonstrated over the years that their methodology works. The researchers have produced some very accurate, detailed mechanisms that explain what is observed experimentally in laboratory devices and engines. The reviewer said that the researchers' approach works, adding that it may not be as fast as might be desirable, but experience shows the LLNL team's results are much better than faster, more automated methods.

#### **Reviewer 3:**

The reviewer commented that this is very important work to improve combustion simulation accuracy.

#### **Reviewer 4:**

The reviewer said that the approach is outstanding and has been used for many years. The reviewer expressed that it has proven successful in the development of accurate chemical reaction kinetics.

#### Reviewer 5:

The reviewer commented that the approach is sound in that fundamental chemical kinetic models are generated for surrogate fuels for gasoline and diesel. The reviewer added that these models are validated by comparison to fundamental experimental data. The reviewer said such models have become more important in recent years with the growing interest in LTC.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said that the researchers continue to improve and refine their mechanisms for widely used fuels, such as gasoline and diesel, to better match data and extend to new operating regimes. The reviewer said the researchers also continue to expand their palette to new fuel species, adding that the team's process is relatively slow but methodical and deliberate. The reviewer concluded that the researchers' contributions are vital to the community.

#### **Reviewer 2:**

The reviewer commented that the researchers made great progress on improving reactions and developing new reactions.

#### **Reviewer 3:**

The reviewer said that the researchers' presented several worthy accomplishments on Slides 6 through 15. The reviewer said that work on gasoline should continue to be accelerated, including the effect of EGR and more equivalence ratios, pressures, and temperatures. The reviewer commented that the development of improved surrogate mechanisms for high-octane gasoline fuels and gasoline fuels with ethanol is a very critical need.

#### **Reviewer 4:**

The reviewer expressed that the researchers' progress is up to expectation. However, the reviewer requested that the researchers elaborate on the availability of the reaction mechanisms to the broader engine modeling community.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer applauded the direct exposure of results through the LLNL website as an effective, frictionless mode of dissemination that encourages open collaboration. The reviewer said that coordination with Co-Optima, mentioned and discussed in this year's slides, will be very valuable.

#### **Reviewer 2:**

The reviewer said that the team has a large number of partners and clients in industry, academia, and government institutions. The reviewer added that the team's results are the foundation of much of the engine modeling work done today.

#### **Reviewer 3:**

The reviewer said that while the PI has close interactions with other institutions, it would be really nice to show results of such collaborations. The reviewer noted that examples include how the reaction mechanisms are utilized for practical engine combustion simulations and the results as well as how the mechanisms are reduced and the final outcomes.

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 this is one of the best, most cogent summaries of reviewer comments and future plans seen at this year's review.

#### **Reviewer 2:**

The reviewer said that the researchers' entry into improved soot modeling is welcomed as existing models fail to match engine behavior under various conditions. The reviewer also welcomed the continued diesel and gasoline surrogate development in conjunction with better RCM data from various collaborators.

#### **Reviewer 3:**

The reviewer said that improved gasoline surrogates are very important, and it is good to see that they are part of the plan.

#### **Reviewer 4:**

The reviewer stated that it is natural to keep developing reaction mechanisms for higher-order HCs and keep refining the mechanisms. However, there may be a limit above which the usefulness diminishes. The reviewer commented that engine spray combustion is complex and there are other determining factors in the modeling accuracy. The reviewer said that it is good to see that the PI plans to develop soot models, which are extremely important.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said that in order to develop better, more efficient engines, developers need accurate kinetics to aid the design process.

#### **Reviewer 2:**

The reviewer expressed that this is crucial work to improve simulations of combustion chemistry that can be used by industry to improve engine efficiency.

#### **Reviewer 3:**

The reviewer noted that the work also includes the chemical kinetics of certain biofuels.

#### **Reviewer 4:**

The reviewer expressed that very important chemical kinetic mechanisms needed for LTC development result from this project.

### 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 more money could be spent here, but the funding appears adequate for the program proposed.

#### **Reviewer 2:**

The reviewer expressed that more resources should be applied to accelerate progress.

#### Reviewer 3:

The reviewer stated that the PI appears to be able to utilize related resources.

#### 2016 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software: David Carrington (Los Alamos National Laboratory) - ace014

**Presenter** David Carrington, Los Alamos 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer said that it is not clear if this project can achieve the goal of software development for advanced ICE modeling satisfying industries. The reviewer said that mesh generation seems like old technology, and key physical and chemical models such as spray, combustion, and engine-out emissions, are not clearly directed.

#### **Reviewer 2:**

The reviewer said that turning to hp-adaptive finite element method technology is an innovative approach to attack the critical barriers. The reviewer commented that the new code appears likely to become an effective





Figure 4-11 - 2016 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software: David Carrington (Los Alamos National Laboratory) - Advanced Combustion Engines

open-source tool for the research community studying combustion fundamentals. However, the reviewer said that to meet the more ambitious stated goal of "user-friendly (or industry-friendly) software" for engine design, much more investment will be required in the end-user environment, workflow aids, and integration with commercial computer-aided engineering (CAE). The reviewer added that success will require more integration and advanced planning than is presently evident.

#### **Reviewer 3:**

The reviewer said that the mathematical approach seems to be the right direction to improve accuracy. However, it is not clear what the plan is for including chemistry. The reviewer would like to see a comparison to engine simulations.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1**:

The reviewer commented that the researchers demonstrated an impressive rate of progress given the lean development team.

#### **Reviewer 2:**

The reviewer said that key milestones and progress in 2016 are not clearly mentioned or compared with those in 2015. The reviewer noted that the two grid generation methods were tried for a very simple port and valve geometry. The reviewer remarked that the researchers should have demonstrated on real engine geometries, such as a light-duty diesel engine from SNL that was used for CFD analysis by UW-Madison.

#### **Reviewer 3:**

The reviewer would prefer to see more progress and results regarding moving parts for engine simulations and noted that the researcher presented no results for engine-relevant air flow or chemistry.

#### **Reviewer 4:**

The reviewer said that comments below have been made in previous reviews and are still relevant. The reviewer said that it is encouraging to see efforts through the radio frequency interference (RFI) and ANSYS to commercialize the code and make it competitive with other codes so that industry can get interested in using it. It will be healthy to have more competitive CFD codes in the marketplace. The reviewer said that KIVA-3 and KIVA-4 are seeing less and less use within industry. KIVA has become more of a free resource to universities that want an open source-type format so they can do physical modeling, but even there, other competitors like OpenFOAM are taking over the market share.

The reviewer expressed that presenters need to seriously evaluate the business model. The reviewer said it would really be healthy to continue to have KIVA as a competitor to other commercial codes. The reviewer questioned what can be done to hasten the development and deployment of KIVA within industry. The reviewer stated that plenty of work has been done and numerous test cases are shown. However, overall technical progress over the last few years on KIVA-hpFE has been very slow. The reviewer said the key issue now is whether industry is really interested in KIVA-hpFE or not, and observed that it is a free code, yet industry prefers to use other commercial codes. The reviewer said there something wrong with this picture and questioned what can be done to make the usefulness and deployment of KIVA-hpFE within industry faster.

The reviewer stated that perhaps a new business model that increases the chances of KIVA not fading away in the next few years would demand different types of collaborations. The reviewer said that, overall, there needs to be faster progress on getting the remaining work done.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer said that it is hard to see any collaboration with other ACE project leaders but with the current project team members. The reviewer suggested the researchers should talk to ACE project teams on LES at SNL, chemistry solver (Zero-RK), and multi-point injection (MPI).

#### **Reviewer 2:**

The reviewer said that to broaden collaboration and increase its ultimate impact, this project might consider (in parallel with the present RFI, or as an alternative if that proves unsuccessful) the CAE for batteries software approach being pursued by the VTO for CFD-based battery simulation tools. The reviewer commented that it will reduce risk and improve odds for ultimate success to collaborate earlier and more strongly with the engine design, and, more broadly, with CAE software leaders, even if only as a hedge relative to a small or startup business attempting to commercialize the software through monolithic licensing. The reviewer said that if KIVA-hpFE is highly modular as advertised, then this approach might involve licensing novel individual nuggets while leveraging established and well-supported commercial software frameworks, infrastructures, and user communities.

#### **Reviewer 3:**

The reviewer said that some collaborations were mentioned, but it is not clear how they contributed to the success

of the project. The reviewer questioned if there are any collaborative efforts to commercialize the code to promote usage in industry.

#### **Reviewer 4:**

The reviewer stated that there could be more direct collaboration and interaction with industry.

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 further improvements in accuracy are good, but questioned who the customer for the software is. The reviewer asked what efforts are being made to commercialize the code and when engine simulation comparisons will be made to engine measurements.

#### **Reviewer 2:**

The reviewer said that incorporating CHEMKIN into the software seems a wrong direction unless user CHEMKIN license cost is resolved, and the same for mesh generation code and other solvers. The reviewer said the current software should not require additional user cost for third party licenses but be a standalone code like previous versions of KIVA code.

#### **Reviewer 3:**

The reviewer commented that many pragmatic software development, integration, deployment, and sustainment challenges lie ahead that were not explicitly acknowledged in this AMR briefing.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said that the project outcome, if successful, will help industries and academia with developing fuelefficient ICEs.

### 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 \$700,000 is not a small amount of budget to perform this project.

#### **Reviewer 2:**

The reviewer remarked that the presentation provides zero forward-looking milestones, only a long list of efforts, some of which are inherently rather open-ended. The reviewer said that achieving the stated goals of the overall project will require many tens of additional person-years. Slide 2 only presented the budget in terms of "funding to date," but the concern from the 2018 end date is that the planned future funding may be insufficient to fully meet the objectives.

#### **Reviewer 3:**

The reviewer wondered if more resources should be provided to make the code more attractive to industry.

#### Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes: Stuart Daw (Oak Ridge National Laboratory) - ace015

Presenter

Jim Szybist, Oak Ridge National Laboratory

**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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer appreciated that there are novel approaches under investigation. The reviewer stated that this high risk project is exactly what DOE should be supporting because it is something unlikely for industry to investigate due to the perceived risk.

#### **Reviewer 2:**

The reviewer stated that it was a very good approach and applauded the search for the high-reward solutions.

#### **Reviewer 3:**

The reviewer said the project focuses on the high EGR dilution and





National Laboratory) - Advanced Combustion Engines

thermochemical recuperation as a form of waste heat recovery. It has focused on critical issues such as hydrogen  $(H_2)$  generation and catalyst formulations, with detailed experiments documenting the challenges experienced. The reviewer said the approach may be extended to consider (at least with some estimations) the impact of the various approaches (for example, dedicated cylinders for reformation) on load capabilities, or the impact of more sophisticated exhaust flow routes on back pressure and efficiency. The reviewer stated that the schematics seem to omit necessary details such as valves and required probes.

#### **Reviewer 4:**

The reviewer said that steam reforming seems to be the thermodynamic pathway of choice, but it seems that having the requisite exhaust enthalpy will be a challenge.

#### **Reviewer 5:**

The reviewer questioned if the researchers, if successful, are at a point where they can estimate the ultimate benefit. The reviewer also wondered if the researchers could leverage some of the EGR loop-reforming techniques to improve the catalyst light-off during cold start.

#### Reviewer 6:

The reviewer observed that this project is a continuation of an effort to reform gasoline into syngas during operation of an ICE. The reviewer said that the PI's approach is to essentially sacrifice a cylinder, for example, in a four-cylinder engine, and carry out the reforming within the cylinder, or using EGR loop-reforming in which the gases are passed through a catalytic device where the reforming would be carried out. The reviewer said the reporting period appears to be the last year of this project beyond its potential continuation through the combustion laboratory call.

The reviewer stated that the overall approach of reforming gasoline seems interesting, and there are a number of issues with the concept that the work of this project has investigated. The reviewer said that reformed fuel seems to be hydrogen and syngas production. The reviewer wondered if syngas is better than gasoline to warrant converting gasoline to it or hydrogen. The reviewer also asked if the engine would need to be retrofitted in any way with hardware to accommodate the reformed fuel.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer observed that in the reporting period, the researchers approached three strategies: higher CR, partial oxidation, and exhaust manifold. A bench flow reactor was used to study catalyst reforming. The reviewer said that the PI states that the flow reactor replicates engine conditions. This seems highly unlikely because a flow reactor is largely a steady-state device and in-cylinder processes are highly transient.

The reviewer said the overall results pointed to EGR reforming as preferred over in-cylinder reforming where a range of conclusions were noted such as that CR seems to have no substantial benefit. The reviewer stated that a number of issues were addressed, such as the effect of endothermic reactions on catalyst temperature, which cause the temperature to decrease until reforming is not effective, and the effect of fuel addition, which was shown to not significantly increase  $H_2$  production.

The reviewer remarked that a rhodium (Rh) catalyst was used though few details of the catalyst were provided. Future presentations should discuss more the catalyst properties that yield the highest  $H_2$  production as this will determine the efficacy of EGR loop-reforming. The reviewer also said that the researchers noted that "gasoline speciated as a mixture of iso-octane and toluene... results in lower energy balance than iso-octane;" however, this was unclear. The reviewer questioned if the PIs are stating that iso-octane and toluene mixtures are a surrogate for gasoline and asked the researchers to clarify.

The reviewer said that partial oxidation studies showed that  $H_2$  production is significantly increased compared to in-cylinder reforming (using iso-octane as the fuel) and yielded the best overall engine efficiency. The review stated that steam reforming of iso-octane provides the route for thermochemical recuperation. The reviewer commented that accomplishments also showed that the optimal reforming conditions were highly dependent on engine response. Results for ethanol reforming were presented that showed significant amounts of acetaldehyde and methane formation that were dependent on temperature and fuel flow rate. The reviewer said that though it may not fall under technical accomplishments, for the proposed EGR loop-reforming concept to be commercially viable, there should be some interest among OEMs to pursue the idea. The reviewer concluded that without such interest, the concept will remain only as a laboratory demonstration.

#### **Reviewer 2:**

The reviewer said that work has not yielded significant nor expected results. The level of reformate generated in the partial oxidation approach appears to be insufficient to change and enhance the combustion. The reviewer commented that the EGR loop-reforming approach did not provide the sought  $H_2$  concentrations except at extremely high temperatures. However, the iso-octane appears to be more promising. The reviewer said there is some discussion and justification to the work, such as the impact of EGR and combustion phasing on combustion duration, which is indicative of efficiency. Nevertheless, the data do not indicate the impact of  $H_2$  on extended EGR operation.

#### **Reviewer 3:**

The reviewer said the work is technically sound; however, the reviewer would liked to have seen a more explicit roadmap of how the researchers plan to improve the efficiency of the engine via thermochemical exhaust heat recuperation. The reviewer questioned if the options included: increased energy, as shown in the energy balance and implied in the comments made on WHR during the presentation; the capability to run more dilute and pick up efficiency that way; or a combination of these two or others. The reviewer thought the researchers should be able to frame these potential improvements through their modeling capability.

#### **Reviewer 4:**

The reviewer said sometimes a negative result is a good result as it is in this case. The reviewer also commented that it is good that the researchers identified the issues with the in-cylinder reforming so that the approach can be abandoned to focus on the catalytic reforming, which might provide better results.

#### **Reviewer 5:**

The reviewer stated that though the in-cylinder reforming did not perform as desired, researchers performed a very thorough test and analysis campaign. The reviewer said the technology was given a fair chance; it just did not work.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer was pleased to see the addition of a 3D CFD collaborator.

#### **Reviewer 2:**

The reviewer said that collaborations were noted between ORNL and industry (Umicore, Aramco), academia (University of Michigan, University of Minnesota), and other laboratories (SNL). However, the reviewer said some of the indicated collaborations were a bit unclear; for example, a 2015 SAE paper is indicated as being in manuscript form. The reviewer wondered if it has been finalized yet. The reviewer said researchers refer to a 2014 SAE paper as evidence of collaborations with SNL, which seems dated. Regarding "kinetic simulations," it was not clear how this information was used in the project. The reviewer commented that a clearer need for the partnerships listed with the overall project goals should be established in future presentations. For example, the reviewer questioned what the collaborator brings to the project that the PI is unable to provide from within the PI's own organization.

The reviewer also said the collaborators do not appear to include an engine OEM and questioned if that was correct. The reviewer remarked that to establish commercial viability, at least of the concept, an OEM should be included as part of the team with a commitment to pursue this concept if the EGR loop-reforming concept is attractive.

#### **Reviewer 3**:

The reviewer remarked that the project should look for active participation from OEMs that are supportive of these advanced concepts.

#### **Reviewer 4:**

The reviewer stated that the activity would benefit from collaboration with an automotive OEM and that there are many practical issues that the researcher needs to keep in mind. The reviewer was particularly concerned about the comment that ethanol was used because it did not show the coking problem of other fuels.

#### **Reviewer 5:**

The reviewer said the project needs an OEM to be involved to provide feedback regarding an implementation pathway.

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 this is an interesting and fun thermodynamic exercise. The reviewer was concerned that there may not be enough enthalpy in the exhaust gas to achieved steam reforming, which appears to show the highest potential for efficiency improvement.

#### **Reviewer 2:**

The reviewer said that the future work will focus on catalytic reforming, which is appropriate given that incylinder reforming was found have some issues. The reviewer added that that the researcher plans on doing engine experiments using several catalysts with the assistance of Umicore's pre-commercial Rh-based catalyst. The reviewer observed that additionally, bench flow reactor studies will be performed to evaluate catalyst durability, and that these activities seem reasonable. The reviewer commented that missing among them seems to be linking with an OEM to provide more credibility to the approach; namely, that the OEMs can envision EGR loopreforming as a viable technology. The reviewer said that this project has been pursued for six years now, and it seems reasonable that a jumping-off point be developed where an OEM will pursue commercialization of the idea.

#### **Reviewer 3:**

The reviewer said the researchers need to expand the study with the catalyst reforming beyond a single speed load.

#### **Reviewer 4:**

The reviewer said that the work may want to step back and assess the potential of their present approach of high dilution and thermochemical recuperation in light of other approaches pursued commercially, such as Rankine cycle and turbocompounding, both from an efficiency and cost-effectiveness standpoint.

#### **Reviewer 5:**

The reviewer stated that catalyst performance will be the key to success for the EGR loop reforming. Catalyst deactivation mechanisms need to be thoroughly identified and explored. The reviewer commented that for the 3D CFD work, the reviewer would like to see how well the H<sub>2</sub> production, and its impact on combustion, can be modeled. The reviewer remarked that it would also be good to do a quantitative comparison between the best found on EGR loop-reforming and Southwest Research Institute's dedicated EGR concept, ideally on the same engine.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1**:

The reviewer stated that considering the modest budget of \$300,000, a lot has been done. The reviewer commented that this is the kind of stretch efficiency combustion work DOE should be sponsoring.

#### **Reviewer 2:**

The reviewer said that if the catalyzed reforming approach works, the system can be leveraged to improve dilution tolerance and increase engine efficiency.

#### **Reviewer 3**:

The reviewer said that this project is relevant from a broad perspective, but greater relevance would be established if an engine OEM were part of the team, along with the interest toward commercialization of the proposed concept that such a partner would bring to the project.

#### **Reviewer 4:**

The reviewer said that this work has the potential to quantify the opportunities and challenges of optimizing the thermochemical processes of fuel energy conversion with practical engine-imposed constraints.

#### **Reviewer 5:**

The reviewer said there must be active research in the high-risk and high-reward space. The reviewer also said that the benefits are being assessed in a proper and relevant way.

### 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 seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

#### High-Efficiency Clean Combustion in Multi-Cylinder Light-Duty Engines: Scott Curran (Oak Ridge National Laboratory) - ace016

#### Presenter

Scott Curran, 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer said the project took an excellent experimental approach, combining 1D and 3D, multi-cylinder, and transient dyno hardware-inthe-loop capability. The reviewer commented that this is a very good and practical approach to measuring virtual in-vehicle fuel economy of advanced combustion concepts.

#### **Reviewer 2:**

The reviewer said that it would be good to show the results of the simulation on top of the experimental results that were shown. The reviewer questioned if the simulation is being used for suggesting optimal operating conditions with the many variables they must control, and if



Yes (100%) (100%) acc016 Figure 4-13 – High-Efficiency Clean Combustion in Multi-Cylinder Light-Duty Engines: Scott Curran (Oak Ridge National Laboratory) - Advanced Combustion Engines

not, it should be. The reviewer said this could be helpful in developing transient control strategies.

#### **Reviewer 3:**

The reviewer said the approach is overall sound in that emissions aftertreatment is included in the overall scope of ORNL projects. However, more than one organization has investigated reactivity-controlled compression ignition (RCCI) combustion for several years. The reviewer observed that its benefits are high efficiency, low engine-out  $NO_x$  and PM. Its challenges are high engine-out HC and CO emissions. The reviewer suggested that rather than continue to push the efficiency benefits higher, it is time to focus on minimizing HC and CO emissions while retaining efficiency. The reviewer said the researcher should attack key barriers first.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said the project showed good, solid work and that understanding transients will be a key to the researchers' success. The reviewer stated that knowing the transient behavior of the entire engine system, including air handling, EGR, and boosting system, and matching those conditions with the optimal RCCI control algorithm will be a large technical challenge.

#### **Reviewer 2:**

The reviewer commented that the project did a very thorough job showing the benefit, the combustion phasing control, and how it compares to other combustion approaches. However, the reviewer said the project needs to show more on combustion noise with increasing load as the engine switches between the combustion modes.

#### **Reviewer 3:**

The reviewer questioned what benefit a combustion system development and mapping guideline is when the combustion system, especially with regards to CO and HC emissions, is not meeting engine-out requirements. The reviewer said that conducting a fundamental investigation of the discrepancies between measured and modeled efficiencies to look for areas of efficiency loss is a sound scientific approach. The reviewer commented that contributions at this level will be more valuable to industry than optimizing a given set of hardware. The reviewer added that the project needs to look at five-cycle comparisons. Also, the researchers should make fuel economy comparisons to a relevant downsized, boosted baseline. The reviewer concluded that the fact that the RCCI engine does not meet CO and HC emissions standards must somehow be taken into account.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer stated that collaboration with multiple stakeholders is very good and that, as pointed out during the questions and answers, close collaboration with industry will be critical in moving this project forward. The reviewer added that the fundamental issues they are exploring are closely coupled with what will be practical constraints to actually getting this concept out of the laboratory.

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 team has a good understanding of what the issues are.

#### **Reviewer 2:**

The reviewer remarked that quantifying the benefit of the approach over a transient cycle will be key. Also, the researchers need to look at more heavily-loaded cycles (e.g., US06), to see if the aftertreatment system cost and complexity can really be reduced. If conventional diesel combustion is still used at higher loads, the lower light load engine-out  $NO_x$  may have no impact on the aftertreatment system. The reviewer said the researchers also need to make improving combustion efficiency a priority. The reviewer commented that getting the rest of the fuel to burn would be a huge win, and that maybe this is an area to focus the 3D CFD efforts.

#### **Reviewer 3:**

The reviewer remarked that the focus should be on addressing high HC and CO emissions during both steady-state and transient operation.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said that anything that has the potential to reduce emissions and improve efficiency is relevant.

#### **Reviewer 2:**

The reviewer said that RCCI has the advantage of having a very powerful additional control lever (i.e., a second

fuel) for controlling LTC processes. It still has many challenges that need to be understood and overcome if it is to successfully make it from the laboratory to the market. The reviewer expressed that this effort addresses these issues.

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

#### **Reviewer 1:**

The reviewer would like to see this work expedited. The reviewer questioned if within the next year the team can assess the benefit and address the barriers. The sooner this can be done, the sooner it will move to market or the team can refocus on a different technology.

#### Accelerating Predictive Simulation of IC Engines with High Performance Computing: Kevin Edwards (Oak Ridge National Laboratory) - ace017

#### Presenter

Kevin Edwards, Oak Ridge National Laboratory

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

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer said that the project appears to be well-designed, with the overall goal to provide innovative simulation tools for improved predictive modeling. The work is compartmentalized in several projects with strong teams represented. The reviewer commented that the project may need to clarify the need or appropriateness of extending the work to on-board diagnostics (OBD). The reviewer added that OBD flags major faults on emission-related equipment; while intricate in many instances, the approach applied here seems to be rather distant from the detailed modeling here.



#### **Reviewer 2:**

The reviewer noted that the approach is to utilize the HPC capabilities available at ORNL to examine various approaches to speed up, expand, or otherwise promote large-scale computing for engine design purposes. In this, the team is doing well.

#### **Reviewer 3:**

The reviewer commented that the project was a good use of the national laboratories' supercomputing resources.

#### **Reviewer 4:**

The reviewer said that leveraging large computational resources to solve complex engine problems is very important, but questioned how to know if all the simulations that are being run are correct.

#### **Reviewer 5:**

The reviewer said that this project is developed to enable virtual design of an engine, which is a worthwhile venture. The reviewer added that it includes tasks such as virtual engine design through GPU solvers and detailed

kinetics, refining a metamodel approach with LES turbulence modeling, and simulating a GM GDI engine, among other things.

The reviewer stated that the relevance and approach were presented at such a high level as to make it difficult to evaluate technical details of the project. This approach did not support effective communication of the results obtained and their rationale. The reviewer commented that under technical accomplishments, the PI notes that "virtual design has potential to significantly accelerate and expand exploration of the design space." However, the reviewer said that this statement does not belong as a technical accomplishment. Rather, it is an observation that belongs in an introductory slide. The reviewer commented that the code used was unclear, and questioned if it was CONVERGE running on Titan. The reviewer said that if so, this should be clearly stated.

The reviewer remarked that the approach of this project may be logical; however, what the presenter provided did not permit a deeper dive into the methodology to allow an evaluation of it. The reviewer said that the PI should not assume that the audience is familiar with all aspects of the project.

#### **Reviewer 6:**

The reviewer commented that Slide 7 recognizes that fast and accurate predictions are two "among the many barriers." The emphasized vision of virtual engine design will not be fulfilled in industry without a commensurate investment in expert, knowledge-based systems that drastically reduce the expertise required by non-specialist engineers to select, assemble, and verify simulation models. The reviewer added that analogous comments apply to reduced models for OBD-based control. Both areas are good candidates for being downstream and outside of this project. The reviewer referred to prior comments under Question three. The reviewer said that pursuing those aggressively now would appear somewhat premature before large discrepancies such as flash boiling and CO are better resolved. The reviewer said that, as another reviewer commented live during the session, "solve accuracy first, and then speed."

#### **Reviewer 7:**

The reviewer commented that goals should be to produce a ranked list of control factors. The reviewer asked which factors can be used to control variability and which to move the mean.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer stated that accomplishments noted were associated with simulating an atomizer configuration that revealed flash boiling conditions, which was interesting. The reviewer observed that the presenter did not specify the code used in the simulation or the criteria for flash boiling and that also listed in this category was a process for virtual design. However, this is not an accomplishment; it is an observation of a process that belongs elsewhere in the presentation. The reviewer added that the presenter noted that GPU scalability has a significant benefit over CPU. Various results using CONVERGE were shown using heptane. However, the reviewer said that a multicomponent surrogate should be used in the simulations with its associated chemistry, which appears to be a task for future work.

The reviewer observed that there was no discussion of the rational for the 74 reaction kinetics for heptane. The reviewer stated that some simulations of LES realizations were shown. The Oefelein group is developing an LES capability for engine performance. The connection with this effort and the Oefelein group should be noted.

The reviewer said that some of the accomplishments were presented in a rather cryptic form with reference to conference papers where apparently more details would be found. However, this is not conventional. The reviewer said, for example, that the study of the RANS simulation that examines the effect of boundary conditions was hard to follow. The reviewer remarked that the presenter showed a series of figures showing comparisons between measured and predicted crank angles for a kinetic scheme for heptane of 80 species and 450 reactions. However, there was no discussion of the kinetics, model, code, or geometry. The reviewer said, presumably, that this information is found in the SAE publication; however, the presentation should do more than list tasks and include a

figure and citation or two about them. The reviewer suggested that, otherwise, the presenters could just send papers to the reviewers and ask them to evaluate the work; however, that is not the intent of the AMR.

#### **Reviewer 2:**

The reviewer said the project was well-balanced in execution and in the AMR summary presentation. The reviewer commented that it would be helpful to present more clearly what specific code and model enhancements or calibrations and tunings came directly out of this work.

#### **Reviewer 3:**

The reviewer said the report documents very well the efforts on five separate projects. Work on the injector design is illustrated by detail mapping of flash transition across a wide range of boundary conditions. The reviewer said the two-fluid model is a good improvement from last year. The reviewer commented that in the second project, the work on engine design and calibration highlights some anomalies, such as the CO composition history. The reviewer added that this is of interest, but the presenter did not demonstrate the overall work on effective improved calibration approaches. The work highlights emissions versus computation. The reviewer asked if this should be augmented to performance benchmarks.

The reviewer said the cyclic variability in dilute combustion focused on pressure, temperature, and fuel. The report may explain the justification for the ranges chosen, particularly the large fuel variations that reasonably overshadow the variability. The reviewer asked if other issues would be at play and of interest, such as heat transfer and soot deposits.

#### **Reviewer 4:**

The reviewer said that the presenter reports progress on a variety of joint projects such as virtual injector and engine design and cyclic variability. The reviewer commented that approaches all utilize the computing capacity available at ORNL to extend what groups engaged in CFD-based design do already.

#### **Reviewer 5:**

The reviewer said it looks like injector spray simulations need some improvements and asked what the approach to improve it is. The reviewer said there was good progress on accelerating CONVERGE solution time. The reviewer expressed that cycle-to-cycle variability using LES is interesting, but needs to be sped up to be useful to industry. It is not clear how these tools and approaches can be rolled out to industry.

#### **Reviewer 6:**

The reviewer said the researchers need to continue to pursue accuracy and experimental confirmation of the model.

#### **Reviewer 7:**

The reviewer said that researchers have made reasonable progress with regards to simulating flash boiling gasoline sprays. However, researchers need to make more progress in predicting CO and HC emissions. The reviewer said the sensitivity of the code to the random number generator is concerning.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer commented that this was an excellent team. The reviewer asked if the authors could elaborate on how they contribute to the projects.

#### **Reviewer 2:**

The reviewer commented that the correct partners are involved to enable success.

#### **Reviewer 3:**

The reviewer said that the team works with a wide range of industrial partners and other government laboratories.

#### **Reviewer 4:**

The reviewer said that although collaboration is robust, the project appears to extend into some areas that are mature or routine enough to hand off to others such as: simulation-based workflows for virtual engine design; demonstration of CFD scalability to O(100) cores; generic GPU enablement of a CFD solver; more generally,

adaption of software to the characteristics of HPC environments; and sparse-grid sampling to generate design-of-experiments metamodels.

The reviewer said that VTO should consider an industry-led competitive funding opportunity announcement as an alternative mechanism for those parts of the work in order to do the following: conserve expert DOE resources for the core R&D challenges; ensure more sustainable software commercialization; and help promote a healthy competition and ultimately greater diversity among industrial software tools than the sole CFD partner and platform utilized in this research.

The reviewer suggested that as another alternative to the above suggestion, and following on from last year's review comments and the presented responses on this issue, the research team could adopt a deliberate multi-code approach in a few of the areas where conclusions or calibrations are historically proven to be influenced, to varying degrees, by the peculiar limitations, methods, or assumptions of an individual simulation tool. The reviewer commented that in these situations, notwithstanding the OEM partner's choice of a CFD platform and despite the added cost, code-redundancy can add value by not only avoiding such distortions, but also exposing otherwise-hidden lessons and uncertainty sources.

#### **Reviewer 5:**

The reviewer observed that collaborators include GM, General Electric, Ford, LLNL, Cummins, and others; however, it was not clear precisely what these collaborators provided to the project. For example, the reviewer said that under injector design, somewhat curiously, the Powell group at ANL is not listed, yet their project seeks to develop an X-ray capability for improving nozzle design. This person also noted that all collaborators are listed under injector design.

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 efforts to understand cycle-variation is particularly important, valuable, and appropriate for continuing work.

#### **Reviewer 2:**

The reviewer said that the authors may want to tie the upcoming work closer to demonstrable targets that translate to improved engine and hardware design. For example, the reviewer suggested applying the flash boiling modeling predictions to optimize the combustion system on engine with resulting improvements on efficiency, emissions, or overall control. The reviewer commented that, to this effect, collaborating with OEMs on specific designs or engine programs may prove to be useful.

#### **Reviewer 3:**

The reviewer remarked that work with larger chemistry mechanisms using LLNL's sparse chemistry solver technology and additional cyclic variability studies, including some LES utilization, is projected. The reviewer said these are incremental steps in the right direction of exercising the capabilities possible with large-scale computing.

#### **Reviewer 4:**

The reviewer said that proposed work on gaining insights into the SNL's partial fuel stratification combustion concept will be interesting.

#### **Reviewer 5:**

The reviewer stated that future work is to include more simulations that include larger chemistry mechanisms, but questioned if it was for heptane or a surrogate. The future work will also include efforts to assess grid size, assess computational time for CONVERGE, and LES simulations on Titan that will investigate nozzle wobble. The reviewer asked if the Oefelein group will be involved with the LES simulations on Titan, and asked for confirmation that assessment of computational time was for CONVERGE. The reviewer said that the researcher listed tasks but they were a bit vague and the rationale for them was not evident. For example, a future task such

as "assess potential of our approach to improve accuracy and reduce wall-time for virtual engine calibration" does not offer much about precisely how this assessment is to be carried out and what engine calibration means. Finally, the reviewer said that the project lists a lot of presentations. The reviewer encouraged the PI to transition the conference presentations into archival journal articles.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said the project scope is relevant.

#### **Reviewer 2:**

The reviewer stated that speeding up the design process and expanding the design space via HPC will lead to better, more efficient engines that burn less petroleum.

#### **Reviewer 3:**

The reviewer commented that if the tools are developed and provided to industry, then they can potentially be used to improve engine efficiency in the future.

#### **Reviewer 4:**

The reviewer said, yes, from a broad perspective, but the presentation was presented at such a high level that it was difficult to understand how the various tasks combined to meet broad project objectives. The reviewer commented that the PI might consider in future presentations to focus on just one element and provide in-depth information about that. The PI can list all tasks as well, but focus on one. The reviewer said that doing so will allow a capability to assess the quality of the work pursued and its relevance to overall project goals.

### 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 seem adequate for the program plan described.

#### **Reviewer 2:**

The reviewer expressed that the project was a good leverage of advanced scientific computing research (ASCR) resources for HPC.

#### **Reviewer 3:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

Joint Development and Coordination of Emissions Control Data and Models (CLEERS Analysis and Coordination): Stuart Daw (Oak Ridge National Laboratory) - ace022

**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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer said that the combination of approaches used by ORNL and Pacific Northwest National Laboratory (PNNL) are very useful in knowing how new work may contribute. The reviewer said that the priority survey results are very interesting and unique for seeing how technologies mature and grow to ask for more work.

#### **Reviewer 2:**

The reviewer said that the approach to address needed research is wellgrounded in Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) surveys conducted with



OEMs and the catalyst community. The reviewer stated that the shift in research emphasis to passive  $NO_x$  adsorber (PNAs) is consistent with the needs of aftertreatment groups to final solutions for low-temperature operating conditions. Also, continuing to characterize selective catalytic reduction (SCR) ammonia (NH<sub>3</sub>) inventory and other utilization metrics is very desirable for optimizing the use of reductants in lean exhaust aftertreatment systems. However, the reviewer said that real-world aging conditions should be considered in more detail to provide accurate models.

#### **Reviewer 3:**

The reviewer stated that CLEERS audios and workshops are invaluable opportunities for sharing technical work in the aftertreatment community. The reviewer said that CLEERS priority surveys are also extremely helpful and useful to understand industry trends and where research money is being spent.

#### **Reviewer 4:**

The reviewer said there was a good blend of experimental work and modeling. The reviewer said the annual

CLEERS workshop/meeting should definitely be continued, with perhaps a move to the late summer or fall so it does not occur right after SAE, especially if the DEER conferences are not going to continue. The reviewer said the monthly audios also should be continued as well as the annual priorities survey, as these provide guidance on what technologies need to be developed.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said that the measurement of steady-state isotherms and their analysis for the  $NH_3$  adsorption on SCR catalysts and shows the necessity for two different sites to explain the  $NH_3$  inventory results. The reviewer said this excellent work is very useful in modeling along with showing some impact of water and aging on one or both of the sites.

#### **Reviewer 2:**

The reviewer commented that the SCR  $NH_3$  inventory and catalyst characterization protocol development are critical activities for ensuring that appropriate catalyst technologies are optimally utilized and advanced to meet current and future low temperature aftertreatment (LTAT) solutions. The reviewer stated that developing models to predict the  $NH_3$  storage capacity of SCR catalysts and the storage sites is critical to understanding how best to react  $NO_x$  under lean conditions. The reviewer commented that this type of research effort, which is also supported by CLEERS, is best provided by a national laboratory. However, the reviewer said that shifting focus to include the study of PNAs brings into question the availability to conduct the necessary research given the available resources.

#### **Reviewer 3:**

The reviewer said the project showed nice work on fundamental  $NH_3$  adsorption behavior on relevant SCR catalysts. The reviewer said the models are probably more detailed than can be used on a vehicle, but they do shed light on catalyst behavior that could be useful for understanding their operation.

#### **Reviewer 4:**

The reviewer said good work on the  $NH_3$  storage modeling. The project needs to start working more intently on PNAs for cold-start  $NO_x$  control, which is the highest rated in the most recent CLEERS survey; HC traps; and low-temperature catalysts, which are needed for the 150°C challenge and to provide emission control on the more fuel-efficient engines of the future for both gasoline and diesel.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer noted that there was good collaboration with PNNL on the NH<sub>3</sub> storage modeling. The reviewer commented that the researchers did a great job in running the CLEERS conference and the CLEERS audios, which promote pre-competitive collaboration among OEMs, suppliers, universities, and national laboratories. The reviewer added that the CLEERS website is a good place to store the catalyst testing protocols, pre-competitive data, models, and reaction mechanisms so that others can have access to them.

#### **Reviewer 2:**

The reviewer suggested that, with respect to the SCR, more interaction with OEMs and catalyst suppliers in identifying and addressing the emissions and OBD needs of the industry. The reviewer stated that with respect to the protocol development, there is very good interaction and communication with the OEMs to address their needs and those of the catalyst community to provide useful information and technologies.

#### **Reviewer 3:**

The reviewer stated that there was an inherently collaborative set of supporters of this project. The reviewer said that the survey requires a lot of interest in developing a consensus, and the conference calls usually provide an early view of topics of broad general interest.

#### **Reviewer 4:**

The reviewer remarked that the project included numerous collaborations with industry, national laboratories, and universities. That is how CLEERS operates.

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 shifting focus to include PNAs is very appropriate for low-temperature catalyst solutions. The reviewer added that continuing to define aging effects on the performance of SCR catalysts is also of value for the industry.

#### **Reviewer 2:**

The reviewer said that although the future work was not strongly emphasized in the presentation, continuing the work of CLEERS and related efforts is very important.

#### **Reviewer 3:**

The reviewer said there were quick response to CLEERS survey priorities. The reviewer said that focus on low-temperature catalysis and cold adsorbers for HC and  $NO_x$  is very relevant going forward. A more detailed look on copper (Cu) and chazabite (CHA) materials with Raj Gounder sounds interesting, but it will not be enough to simply identify  $NH_3$  storage sites. The reviewer said the project also needs to know how the sites change over catalyst aging and poisoning and how to eliminate sites that do not contribute to  $NO_x$  conversion to give faster response. The reviewer added that the large buffer of  $NH_3$  storage at low temperatures is undesirable from a controls standpoint.

#### **Reviewer 4:**

The reviewer commented that the project needs to start emphasizing PNAs, HC traps, and low-temperature catalysts. The reviewer added that work can, and should, continue on catalysts for lean applications, but there should be some simultaneous research on stoichiometric catalysts as well. The reviewer stated that due to the challenges of providing 99.5% NO<sub>x</sub> conversion over the Federal Test Procedure (FTP) cycle as well as other test cycles, stoichiometric engines are probably going to be here for a long time. The reviewer said that, in addition, even lean gasoline engines will run at stoichiometry at high loads, where the exhaust temperatures are too high for lean NO<sub>x</sub> catalysts to provide the high NO<sub>x</sub> conversions necessary to satisfy stringent emission standards.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said the project directly addresses the need of the automotive OEMs to meet future emissions standards by utilizing lean and LTAT technologies in a timely manner.

#### **Reviewer 2:**

The reviewer said this work allows the use of efficient engines that lead to effective aftertreatment in low-temperature exhaust.

#### **Reviewer 3:**

The reviewer commented that low-temperature catalysis and cold adsorbers will allow for more fuel-efficient powertrains.

#### **Reviewer 4:**

The reviewer remarked that the good experimental data being generated and the resulting models will help engineers design efficient and cost-effective emission control systems for the more fuel-efficient engines of the future. The reviewer said that this will reduce national fuel consumption as well as satisfy the clean air requirements.

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

#### **Reviewer 1:**

The reviewer is slightly cautious with regard to resources. The reviewer said that given the funding levels and the increasing breadth of apparent projects, resources may be somewhat strained.

#### Reviewer 2:

The reviewer commented that resources may not be sufficient to continue the NH<sub>3</sub> storage modeling work on several new SCR catalysts while adding in a lot of new work on PNAs, HC traps, and low-temperature catalysts.

#### **Reviewer 3:**

The reviewer said that resources seem sufficient to support the current level of effort.

#### CLEERS: Aftertreatment Modeling and Analysis: Yong Wang (Pacific Northwest National Laboratory) - ace023

#### 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer remarked that there is a wide range of active projects that appear to address very different areas of catalysis and catalyst development. The reviewer said this leads to the concern that there is not an overriding focus of the research to address a central topic, but rather unrelated areas of catalyst development. The reviewer remarked that, having said that, the quality of work and the researchers is high and the information is useful to the industry.

#### **Reviewer 2:**

The reviewer commented that the projects dovetail very nicely with CLEERS modeling efforts and that the coordination is very effective. The



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reviewer said that the industrial input is key to working on changing needs. However, the reviewer was critical of the large amount of work done on older problems. The reviewer said that, for example, contemporary direction is on Cu zeolites, not iron (Fe) zeolites, and on gasoline particulate filter (GPF) and SCR filters, not diesel particulate filters (DPF). However, the shift to adsorbers is ahead of the game. The reviewer remarked that, having stated this, the use of modern tools and analyses is exceptional. Identifying the active Fe sites and using this cutting edge information to explain and improve performance is very impressive. The reviewer added that the approaches to developing test protocols for adsorbers and catalysts was also well thought-out and coordinated. Differences appear to be as high as 30°C, which can be significant.

#### **Reviewer 3:**

The reviewer said that the PNNL has many nice instruments to analyze and characterize catalyst materials and behavior. The knowledge of how to make active Cu and Fe/CHA is extremely useful. The reviewer stated that there seems to be a disparate number of technologies included in the program and that there is not much modeling

included, although the project is associated with CLEERS. The reviewer could not give more than a good rating due to the mismatch between the content and the title.

#### **Reviewer 4:**

The reviewer commented that the project was excellent and there were copious amounts of experimental data. However, the reviewer did not see much modeling and said that the last letter in CLEERS stands for Simulations. The reviewer said that other than helping ORNL model the NH<sub>3</sub> storage capacity of the SCR catalyst, there is not a lot of modeling here. This project seems to be several different catalyst projects—PNA, DPF, SCR, and lowtemperature catalysis—under one umbrella project, with an emphasis on gathering experimental data rather than modeling or simulations. The reviewer asked if the presenter planned to start modeling the data generated at some point.

## Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer said that the results are impressive and contributing to the advancement of the field; the Cu-SSZ13 contribution is a good example. However, the results on Fe zeolites, although thorough and new, are perhaps of little interest. The reviewer said that emphasis today is on Cu zeolites and that perhaps the learnings on structure versus performance can be transferred into more meaningful systems. The reviewer added that the DPF results are a little confusing. Wafers were used with one surface being as-received and the other surface being machined, changing the surface porosity. The reviewer asked if the wafer was representative of actual DPF walls. The reviewer expressed that perhaps the presenter needs to run the wafer experiments with two machined surfaces rather than one. Finally, the reviewer said that the PNA work is impressive, but that not much new from what was reported by Ford in August 2014. Nonetheless, the methods and results seem transferrable to other materials.

#### **Reviewer 2:**

The reviewer said that the SCR characterization and optimization activities are well regarded and appropriate for providing LTAT solutions for the automotive industry. The reviewer commented that this activity coupled with the engagement of PNNL with catalyst protocol development to advance useful catalyst technologies is critical to meeting future exhaust emissions standards. The reviewer remarked that this work should continue; however, when developing catalyst technologies such as SCR, the presenter should address aging conditions and give consideration to poisoning and deactivation mechanisms at an earlier stage.

#### **Reviewer 3:**

The reviewer said that there was a good understanding of the deactivation of the Cu/SSZ13 SCR catalyst. Also, the reviewer said good job on identifying Fe monomers as primarily responsible for the low-temperature  $NO_x$  conversion of Fe/SSZ catalysts, while Fe dimers are primarily responsible for the  $NO_x$  conversion at high temperatures. The reviewer commented that the presentation demonstrated great efforts on the oxidation protocol and adsorber protocol development. The reviewer said kudos to Ken Rappe and also said good work on the DPF investigations. The reviewer commented that the researchers need to accelerate efforts on PNA development, which ended up as the highest priority item on the annual CLEERS survey, with an emphasis on the sulfur (S) tolerance and thermal durability of the PNA. The reviewer stated that the response to last year's comment that more emphasis needs to be placed on the S tolerance of catalysts was not very satisfying; in other words, this work is occurring in a cooperative R&D agreement (CRADA) with Cummins because data generated in a CRADA are typically only available to the participants of that CRADA and not available to the general community.

#### **Reviewer 4:**

The reviewer could not tell what the transportable emissions measurement system image on Slide 8 was supposed to show. The reviewer commented that there was a nice explanation of Fe/CHA aging results. There is not much chance to use a three-site NH<sub>3</sub> storage model on a vehicle because it is too complicated. The reviewer added that it may be useful to explain catalyst behavior in the lab. The reviewer commented that there was nice insight into other devices (i.e., Ce PNA, SCR-coated DPF [SDPF]).

#### **Question 3: Collaboration and coordination with other institutions.**

#### Reviewer 1:

The reviewer said that the projects related to protocol development and the work to characterize and optimize catalyst solutions for lean applications is well supported with interaction with either OEMs and/or catalyst suppliers.

#### Reviewer 2:

The reviewer remarked that it is good to validate reactors through ACEC protocols with the round robin catalyst. The reviewer noted several collaborations with ORNL, universities, and industry.

#### Reviewer 3:

The reviewer said that there was good collaboration with ORNL on the  $NH_3$  storage modeling and with the ACEC Technical Team of U.S. DRIVE.

#### **Reviewer 4:**

The reviewer said the researcher has a broad team with much depth and that perhaps it is okay to have a few partners doing the work with others to provide guidance. The reviewer said that the exception is the round robin work on LTAT protocol. The reviewer added that the researcher ought to consider more collaboration with zeolite and/or catalyst companies, at least from an advisory point of view.

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 inclusion of PNA development into the research portfolio is very appropriate as is the continuing development of protocols for down-selecting advanced catalyst technologies for LTAT. The reviewer said, however, that the resources available to support the wide range of projects does not appear to match funding and manpower.

#### Reviewer 2:

The reviewer was very comfortable with future direction. The reviewer said that using the zeolite structure data for SCR improvement is clearly the next step. The reviewer was very optimistic the team will make significant progress and said that no changes are recommended in this portion of the program.

The reviewer said that on LTAT, certainly methane (CH<sub>4</sub>) oxidation is important for natural gas engines. However, the reviewer did not see much market penetration of natural gas (NG) vehicles (greater than 10%), even if oil prices increase. The reviewer said that, further, recent work reported satisfactory CH<sub>4</sub> light-off of around 240° Celsius (C) (A.I. Osman et al./Applied Catalysis B: Environmental 187 (2016) 408–418). The reviewer suggested focusing on HCs from LTC of diesel and/or gasoline-based systems.

The reviewer suggested that the presenter proceed with SCR filter work. The reviewer said that the tools are phenomenal and recommended looking at different SCR coatings such as membrane on inlet and outlet walls or in-wall coatings. Also, the reviewer suggested that the presenter should consider looking at GPF.

#### **Reviewer 3:**

The reviewer said that a move away from cerium (Ce) and towards zeolitic low-temperature nitric oxide (NO) traps is a good one. The reviewer would like to see more modeling in the program per the title. The reviewer commented that other topics of high interest would be nitrous oxide (N<sub>2</sub>O) minimization and formaldehyde trapping and oxidation. The reviewer added that PNNL would seem well-suited to tackle those topics.

#### **Reviewer 4:**

The reviewer said that the presenter needed to emphasize low-temperature catalysts for both diesel (lean) and gasoline (stoichiometric) applications. The reviewer commented that the focus should be on the low-temperature reduction of  $NO_x$  in addition to the oxidation of  $CH_4$  and other hydrocarbons because the future emission standards

will require very high conversions of both species. The reviewer said that, again, the assessment of S tolerance and desulfation capability needs to be investigated for any catalyst that is developed.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer said that all catalyst projects support the current and future catalyst knowledge base desired by the automotive OEMs.

#### **Reviewer 2:**

The reviewer said that knowledge of lean, LTAT devices promotes more widespread use of fuel-efficient powertrains and development of new, improved fuel-efficient powertrains.

#### **Reviewer 3:**

The reviewer stated that all of the technologies being developed will be needed to allow more fuel-efficient engines to satisfy stringent emission 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 said that there appears to be a wide range of different projects underway. The reviewer added that known funding restraints and the scope do not seem to align as well as they should.

#### **Reviewer 2:**

The reviewer commented that it seems like a lot of money to cover the approaches. The reviewer added that most money seems to be spent on SCR activity and PNA seems to be just starting. The reviewer added that low-temperature oxidation was limited to round robin as presented and that SDPF work was limited in scope.

#### **Reviewer 3:**

The reviewer stated that resources seem sufficient for the current level of effort.
# Ash-Durable Catalyzed Filters for Gasoline Direct Injection (GDI) Engines: Hee Je Seong (Argonne National Laboratory) - ace024

## Presenter

Hee Je Seong, 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, feasible, and integrated with other efforts.

## **Reviewer 1:**

The reviewer said that the approach for studying a three-way catalyst (TWC) plus GPF systems appears well-designed.

# **Reviewer 2:**

The reviewer stated that there was a clear goal description as well as approach.

# **Reviewer 3:**

The reviewer said that this activity supports the need for research in the area of filter technology to meet future emissions and PM/particle number (PN) requirements globally. The reviewer commented that focusing research on the combination of the





Figure 4-17 - Ash-Durable Catalyzed Filters for Gasoline Direct Injection (GDI) Engines: Hee Je Seong (Argonne National Laboratory) - Advanced Combustion Engines

TWC plus GPFs is also very appropriate from an OEM's point of view for performance and packaging. The reviewer added that understanding the mechanisms of TWC plus GPF catalysts is important R&D for OEMs trying to adapt to future PM standards and diagnosing catalyst functionality and health.

# **Reviewer 4:**

The reviewer commented that the described approach to investigating ash-durable catalyzed filters is focused on integral studies using a bench-scale flow reactor. Use of the Advanced Photon Source (APS) and other substrate characterization techniques really only tells you about the physical effects on the substrate or blocking of channels due to ash. The reviewer said that you might be able to see where the ash is, but you are not measuring chemical changes in the washcoat or even the substrate. The reviewer added that the focus on engine scale or bench scale devices complicates the understanding of the effective phenomena seen. The reviewer noted the incredible integrity of the presenter, Dr. Song, who was very honest about how his laboratory results differed from results seen previously in the literature (Slide 15). The reviewer said that Dr. Song may not yet be able to explain why he sees differences, but he is continuing to investigate.

# **Reviewer 5:**

The reviewer said that the presenter needs to emphasize field-aged GPFs. The reviewer suspected that the ash developed from injecting oil into the fuel and rapidly aging the GPF is not the same as normal ash from a gasoline engine driven over tens of thousands of miles. The reviewer said that researchers are exposing the GPF to much less fuel and therefore much less S with this procedure, which might account for the lack of calcium sulfate  $(CaSO_4)$  in the ash. The reviewer said that some of the test conditions were not apparent in the presentation, like how many miles the field-aged GPF had been driven and under what conditions like time, temperature, and flow rates. Also, the conditions used during the rapid aging were not apparent, such as the exhaust temperature, flow rate, and the duration of aging. The reviewer did not know why the presenter did not observe ash deposits along the walls with the laboratory-aged filters, when published literature indicates that there is ash along the wall with field-aged GPFs. The reviewer said it is not primarily in the end plugs as the presenter suggests.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer said that the project shows interesting results, especially on ash, although it seems there could be more data considering the effort level.

# **Reviewer 2:**

The reviewer observed that there was a systematic approach and very thorough analysis. The reviewer added that the presenter needs to correlate more to real-life conditions and filter exposure as well as different oil type exposure.

# **Reviewer 3:**

The reviewer said that determining the effects of ash and ash components on the performance of TWC and GPF catalysts is very important to understanding how to diagnose the state of the catalyst as well as what to expect from an activity point of view. The reviewer said that establishing where the ash components are located within the GPF helps predict how the catalyst will perform. Similarly, understanding the impact of the calcium (Ca) and phosphorous (P) on reactions is also critical for predicting the performance for the required 150,000-mile life of the aftertreatment system. The reviewer said, however, that correlation with field-aged catalysts is needed to better predict aging mechanisms and performance of in-use catalysts. The reviewer said that artificial means of loading ash-loading catalysts may be significantly different. Also, identifying where the ash components reside in the GPF and why that distribution occurs would be important information for OEMs. The reviewer said, finally, understanding how washcoat load effects light-off must be understood better. The reviewer added that why higher washcoat load increases the light-off temperature requires more understanding.

# **Reviewer 4:**

The reviewer said that technical achievements are appropriate to a new project. This project only started in October 2015 so results to date are mostly preliminary, which may explain the deviation from what is shown in the literature. The reviewer said that it would be nice to see experiments done to isolate the independent phenomena instead of convoluting the mass transport and kinetic limitations.

# **Reviewer 5:**

The reviewer expressed a desire to understand why the results are not consistent with published literature in regards to ash layer deposition and the presence of  $CaSO_4$  in the ash. The reviewer said that if the presenter's comments are based on the rapid aging results, the presenter might need to rethink the procedure. The reviewer said that if the presenters' comments are based on field-aged GPFs, the presenter needs to reveal how many miles the vehicles were driven and the conditions during the mileage accumulation. The reviewer said that it was not apparent on Slide 17 what the designations LL, LH, HL, and HH mean. Also, the test conditions are missing, such as temperature and oxygen ( $O_2$ ) level.

# **Question 3: Collaboration and coordination with other institutions.**

# Reviewer 1:

The reviewer observed contributions from academia and industry.

# Reviewer 2:

The reviewer said that the inclusion of an automotive OEM that has direct injection (DI) engines in the marketplace along with substrates and catalyst suppliers and facilities that provide analytical characterization services enhances the value of the information and work.

# Reviewer 3:

The reviewer noted that there was good collaboration with Hyundai and Corning.

# Reviewer 4:

The reviewer commented that there was an excellent set of collaborators; however, where they are having impact is not conveyed for all of them.

# **Reviewer 5:**

The reviewer said that additional laboratory or university partners for chemical characterization studies would be useful. The reviewer added that more focus on the fundamentals would help the overall 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 further establishing the effects of oil derived poisons on the performance of the washcoat and filter is important. However, the presenter must give consideration to the interaction with the upstream catalyst that will also be present in these aftertreatment systems.

## Reviewer 2:

The reviewer said that there are many choices to consider for focused efforts.

## **Reviewer 3:**

The reviewer suggested that the presenter consider real-life conditions for field performance of filters and oil samples as would be seen in the real world.

## **Reviewer 4:**

The reviewer said that proposed future work is appropriate and that there was strong interest in the kinetic studies and ash chemistry.

## **Reviewer 5:**

The reviewer said that the presenter needed to emphasize field-aged filters instead of laboratory-aged filters.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer said that global emissions requirements will include PM/PN management to meet standards. The combination of catalyst technologies to achieve these standards while minimizing the effect on engine performance and packaging is critical to designing acceptable aftertreatment solutions.

## **Reviewer 2:**

The reviewer said it was key for proper engine performance.

## **Reviewer 3:**

The reviewer suggested that the presenter could enable the use of more lean gasoline engine systems, meeting DOE's goals.

#### **Reviewer 4:**

The reviewer said that this is definitely relevant to DOE interests. The reviewer added that ash can be a very strong, negative influence on the life of aftertreatment catalysts.

# **Reviewer 5:**

The reviewer said the GPFs will be necessary to allow more fuel-efficient gasoline turbocharged DI engines to meet future particulate standards.

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

Reviewer 1:

The reviewer said this project is appropriately funded and staffed.

**Reviewer 2:** 

The reviewer said the resources seem sufficient at the time.

# Enhanced High- and Low-Temperature Performance of $NO_x$ Reduction Materials: Feng Gao (Pacific Northwest National Laboratory) - ace026

# Presenter

Feng Gao, 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, feasible, and integrated with other efforts.

## **Reviewer 1:**

The reviewer said the focus of this work to improve both the low- and high-temperature performance of SCR catalysts is very consistent with the needs of the automotive OEMs. The reviewer added that both ends of the operating window must be addressed to have a viable solution for  $NO_x$ control in lean systems. The reviewer commented that using fully formulated catalysts that incorporate alkali earth co-cations into the formulation to achieve better performance on the low-temperature operating end of the window is somewhat novel and unexpected due to the poisoning nature of sodium (Na) in vehicle applications. The reviewer said that explaining why this is the case would also be of interest.

## **Reviewer 2:**

The reviewer commented that characterizing real-world materials in various aging states using the most advanced techniques is delivering exceptional results. Getting guidance on direction from an OEM keeps the direction pertinent. The reviewer added that the method of isolating Cu sites to determine which are significant is impressive. The reviewer commented that emphasis on low-temperature performance is also critical.

## **Reviewer 3:**

The reviewer said that SCR catalysts are relevant for use in lean, fuel-efficient powertrains. The reviewer remarked that there were model catalysts used to represent proprietary catalysts that could not be discussed in public. The reviewer expressed that there is no interest to use beta zeolite in SCR catalysts and that the HC adsorption is catastrophic. The reviewer said that the presenter did not show any work on adding Fe to Cu/CHA. This would have been interesting.



#### **Reviewer 4:**

The reviewer said the presenter needed to include S poisoning assessments of the catalysts being developed. The reviewer added that S can be particularly detrimental to the low-temperature activity of SCR catalysts.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer commented that the presenters did great work in probing the Cu sites that give good activity and selectivity at both low and high temperatures. Again, the reviewer said, the project needed to assess S poisoning.

#### **Reviewer 2:**

The reviewer said that the results on the two different Cu sites are very impressive and valuable. It is this kind of fundamental understanding that drives catalyst compositional work. The reviewer added that the recommendations on zeolite formulation is valuable and impressive. The reviewer commented that it was interesting work on Fe-Cu beta zeolite and with Na. The reviewer suggested that it would be valuable to see recommendations and then verifying.

#### **Reviewer 3:**

The reviewer said that the technical approach to lower the light-off temperature for  $NO_x$  reduction by using alkali metals is novel. The reviewer commented that a significant amount of characterization work has been done to substantiate the activity of the catalyst and the mechanism that is driving the observed behavior; this is very appropriate work for PNNL to perform. The reviewer commented that, going forward, more attention has to be directed at understanding aging mechanism that include HCs and S poisoning. The reviewer remarked that optimizing catalyst formulations for either standard or fast  $NO_x$  reactions is also appropriate. Because different lean applications will produce different ratios of NO/nitrogen dioxide ( $NO_2$ ), catalyst formulations should be optimized to take advantage of the available species. The reviewer added that with regard to combining Cu and Fe catalysts, some of this work has been performed by others and should not be emphasized in this project.

#### **Reviewer 4:**

The reviewer commented that the fundamental attribute study of Cu/SSZ 13 seems contradictory to patent literature on desirable silicon (Si)/ aluminum (Al) ratio. The reviewer said that the use of Na+ to neutralize Bronsted sites seems novel, and improved, high-temperature NO<sub>x</sub> conversion was an unexpected result. The reviewer said that it would be good if it could be shown that adding Na also improves the SCR activity response with NH<sub>3</sub> load on the catalyst.

# **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer said that the inclusion of Cummins and Johnson Matthey Catalysts (JM) in this work should help achieve results that are meaningful and applicable to lean  $NO_x$  aftertreatment solutions.

#### **Reviewer 2:**

The reviewer commented that the team is very strong with key players. The reviewer added that state-of-the-art equipment with industry samples and guidance made results pertinent and will likely lead to faster implementation.

#### **Reviewer 3:**

The reviewer remarked that there was good collaboration with Cummins and JM.

#### **Reviewer 4:**

The reviewer noted that partners were Cummins and JM.

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 should be primarily focused on extending the operating range of the SCR formulations to low temperatures and secondarily toward extending the upper temperature limit. The reviewer added that preserving activity after appropriate aging is performed will be critical to determining if the technologies under development will survive in vehicle aftertreatment systems.

## **Reviewer 2:**

The reviewer said that realizing the project is closed, the reviewer is still craving recommendations for future work for other research groups.

# **Reviewer 3:**

The reviewer noted that the project was completed. The reviewer said that the presenter mentioned transferring remaining work under CLEERS, but the reviewer said that it was not clear exactly what this means.

## Reviewer 4:

The reviewer noted that the project is completed.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# **Reviewer 1:**

The reviewer commented that there was very relevant R&D and it was consistent with the call for LTAT solutions for highly efficient lean combustion engines. The reviewer said that the United States Council for Automotive Research (USCAR) has stated this area of research is needed going forward and would strongly support this work.

## **Reviewer 2:**

The reviewer said that high lean  $NO_x$  conversion across a wide temperature window is an enabler for more fuelefficient powertrains.

## **Reviewer 3:**

The reviewer commented that we will need SCR catalysts with better  $NO_x$  conversion at both low temperatures and high temperatures as well as better thermal durability for future emission standards and future fuel economy standards. The reviewer said, of course, that the low-temperature activity will depend on whether  $NH_3$  is available at those low temperatures.

# 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 there was no issue with resources or funding.

Reviewer 2:

The reviewer noted that it was a co-funded CRADA.

**Reviewer 3:** 

The reviewer noted that the project is completed.

# Next Generation SCR-Dosing System Investigation: Abhijeet Karkamkar (Pacific Northwest National Laboratory) - ace027

Presenter

Abhijeet Karkamkar, Pacific Northwest National Laboratory

**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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer remarked that the approach to most of the work is very good and has even focused on making new materials, such as the double salts. The reviewer said there are still other materials that can provide  $NH_3$  upon decomposition, especially some liquids, which have not been included for evaluation based on the literature. The reviewer commented that a number of these have been looked at by the Paul Scherer Institute.

## **Reviewer 2:**

The reviewer remarked that the investigator seemed to understand the technical gaps well and the real need for the project. The reviewer was curious to know how the SCRs make



the engine more efficient. The reviewer said that was listed on the slide, but the reviewer was not clear how that is accomplished. Also, it was not clear how the system would work to drive the  $NH_3$  into the SCR. The reviewer said the project description says that it is about a system, but the data seem like the project is more of a study on  $NH_3$  storage.

## **Reviewer 3:**

The reviewer said that the project goal is to develop alternative  $NH_3$  carriers for  $NH_3$  dosing in low-temperature exhaust. The reviewer observed that several materials were studied for specific properties, including volumetric expansion,  $NH_3$  storage capacity,  $NH_3$  decomposition temperature, material stability, and safety.

## **Reviewer 4:**

The reviewer said that the researchers should investigate urea alternatives to determine if they are more appropriate for the low-temperature exhaust conditions that will exist in global driving cycles and with the emergence of everincreasing engine efficiency leaving less energy in the exhaust for catalysis. The reviewer said that this activity supports an important function of establishing OEM specifications and targets for urea alternatives. Additionally, the reviewer commented that higher density  $NH_3$  storage materials that release  $NH_3$  at the appropriate temperature will be needed to obtain the level of  $NO_x$  control required for both LD and HD applications while minimizing the need for replacing the  $NH_3$  source.

# **Reviewer 5:**

The reviewer said that the research follows clear direction from USCAR CRADA to focus on material selection and development for vapor  $NH_3$  delivery for SCR systems. The reviewer commented that technical barriers identified by the research plan, such as improved  $NH_3$  storage and low-temperature delivery, as well as reviewers' concerns from the prior year, namely, mitigating hydrochloric acid (HCl) are being addressed methodically through base material and structural material considerations. The reviewer said that although it was not in the scope of the project, it would improve the score to present any available system-level requirements and status for a vapor  $NH_3$ delivery system. The reviewer said the researchers claimed that no injector would be needed to deliver vapor  $NH_3$ for SCR; however, precise amounts of  $NH_3$  would be required for a proper SCR reaction, and it is not clear how this would be achieved. The reviewer added that additional system considerations include the packaging of solid  $NH_3$  delivery systems.

# **Reviewer 6:**

The reviewer said that it is good that the presenter recognized the big issue with HCl production and worked to minimize it. The reviewer remarked that a steady dose of 600 parts per million HCl that was observed with magnesium chloride would not be good for the exhaust system, the paint around the exhaust pipe, or the environment.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer said there was very good progress towards stated goals with the synthesis and study of eutectics. The reviewer suggested quantifying and minimizing volume expansion and said that the project took an innovative look at micro-encapsulation with porous supports.

## **Reviewer 2:**

The reviewer expressed that there was a very good review of the materials and the researcher used those studies to determine next steps with new materials. The reviewer would like to see a system-level demonstration of the dosing system and how it works effectively on the vehicle.

## **Reviewer 3:**

The reviewer said that excellent technical progress has been made in the areas chosen for study. While statements from USCAR members state that the deposits from carbamate make it a poor choice, such deposits can form in any system that has carbon dioxide ( $CO_2$ ) and  $NH_3$  together in the gas phase. The reviewer said this issue could be explored and taken as a challenge because many patents and some papers have been written to address keeping important areas of a system above 70°C.

## **Reviewer 4:**

The reviewer commented that the presenter did a good job on minimizing the HCl production with the composites and on minimizing the volume expansion. The reviewer added that it was a clever method to evaluate volume expansions with the syringes.

## **Reviewer 5:**

The reviewer said that technical accomplishments for this year are solid, though the reviewer would have liked to see more progress on the HCl as this is a potentially very serious issue that needs to be addressed. The reviewer said, additionally, that the impact of  $CO_2$ /water (H<sub>2</sub>O) on material performance seems like a show-stopping issue. The reviewer asked if there are risk mitigation plans for either of these.

# Reviewer 6:

The reviewer said the exclusion of potentially viable alternatives to urea, such as carbamate, has not been adequately explained. The reviewer said the decomposition products are essentially  $CO_2$  and  $NH_3$ . With respect to project goals, a better definition of target release temperatures and maximum recovery of  $NH_3$  is needed. The reviewer said that volumetric increases under  $NH_3$  loading is important, but not necessary for the primary metric. The reviewer added that as a national laboratory project, the researcher must present more understanding of the kinetics involved.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer questioned how many meetings with USCAR are occurring because the presenters have increased the communications. The reviewer asked if those meetings have aided in the relevance of the project by getting feedback. The reviewer also asked if there are USCAR participants who are willing to partner on a demonstration. The reviewer said that is a good opportunity to work those details and next steps.

## **Reviewer 2:**

The reviewer said the inclusion of the USCAR OEM members in this work is essential because the OEMs will use this information to write specifications for dosing systems. However, the use of a consultant chemist in this field, with thorough knowledge of reactions involving these NH<sub>3</sub> compounds, would provide good feedback on the metrics used in this work. The reviewer added that frequent group meetings to discuss the project progress keep this project focused.

# **Reviewer 3:**

The reviewer said that while USCAR is certainly a broadly-based group of relevant collaborators, this group could be expanded to include other OEMs interested in SCR.

# **Reviewer 4:**

The reviewer said that there was good communications with the USCAR SCR team.

## **Reviewer 5:**

The reviewer noted that there was good collaboration within tightly defined CRADA. The reviewer added that possible improvement would be interactive dialogue for system-level requirements and possibilities as they relate to this subsystem work.

## **Reviewer 6:**

The reviewer said that the partnership with USCAR is good, but asked if a university or laboratory that could help with analysis. The reviewer commented that there are material evaluation and characterization studies and mechanistic studies that would help this project considerably, much more so than the volumetric expansion study.

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 these are good next steps on the project. The reviewer would like to see a system demonstration if it can be accomplished. The reviewer did not understand how the use of SCR makes engines more efficient and said that it would be helpful to quantify how the use of  $NH_3$  will help the process directly and improve efficiency.

## **Reviewer 2:**

The reviewer observed that there was a good focus on eutectics and double salts, but commented that the researchers could throw an even wider net. The reviewer suggested that a look at materials, with a greater focus on how they would actually be used in a system, would also be useful.

# **Reviewer 3:**

The reviewer expressed that it was a good follow-on for composites and eutectic double salts to continue to improve potential applicability with additives to improve form retention.

# **Reviewer 4:**

The reviewer was not clear how to mitigate chloride (Cl) ion effects in the exhaust. The reviewer said that as this work progresses, the researchers should develop more appropriate targets and goals.

# Reviewer 5:

The reviewer noted that there were concerns raised by another reviewer on the stability of the air conditioning (AC) materials if they are exposed to air or the exhaust gas, which would be likely in an on-vehicle system. The reviewer said that future work should include additional analysis on how delivery conditions in a vehicle system would impact the material stability. The reviewer said that this is currently not included in the future plans and that the future work plan is vague.

# **Reviewer 6:**

The reviewer said the researcher needs to develop materials that will release large amounts of NH<sub>3</sub> at temperatures between 150°C and 180°C in order to show an advantage over the aqueous urea system. The reviewer added that it looks like some of the double salts do not release all of the NH<sub>3</sub> until about 300°C, although some is released at lower temperatures. The reviewer said that the presenter might propose how the NH<sub>3</sub> storage materials would be recharged, for example, during oil changes. The reviewer asked how long it would take.

Also, the reviewer asked how the gaseous  $NH_3$  that is released from the solid source would be stored. The reviewer questioned if there would be a ballast that could store the  $NH_3$  because the presenter cannot count on the rate of  $NH_3$  release from the solid source to match the  $NO_x$  flux emitted from the engine. Finally, the reviewer asked how much energy would be needed to heat the solid source in order to release the  $NH_3$ .

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer commented that the development of a solid source of  $NH_3$  that releases  $NH_3$  below  $180^{\circ}C$  will allow the use of SCR catalysts that can reduce  $NO_x$  at lower temperatures. The reviewer said that this allows the minimization of the fuel used to pre-heat the exhaust during the cold start, which will save fuel. The reviewer added that it will also allow effective emission control on more fuel-efficient diesel engines that produce lower exhaust temperatures.

## **Reviewer 2:**

The reviewer said that the urea alternatives that provide high density  $NH_3$  storage are required by OEMs in lean aftertreatment systems to meet more stringent emissions standards and the need for LTAT. The reviewer commented that minimizing the need for reductant refills is important from a customer satisfaction perspective and for packing in vehicles.

## **Reviewer 3:**

The reviewer suggested enabling lower temperature aftertreatment, especially for NO<sub>x</sub>.

# **Reviewer 4:**

The reviewer commented that low-temperature delivery of  $NH_3$  can enable efficient engine operation through a wider ambient and engine operating map by providing an aftertreatment solution that operates more broadly and requires less energy penalty, in other words, heating DPF or heating exhaust for DPF to be functional. The reviewer said that solid delivery methods of  $NH_3$ , furthermore, offer potential for longer service intervals and simplify transportation.

# **Reviewer 5:**

The reviewer did not understand how the use of SCR makes engines more efficient. The reviewer said that it would be helpful to quantify how the use of  $NH_3$  will help the process directly and improve efficiency.

## **Reviewer 6:**

The reviewer remarked that the need for new materials is significant, but this project seems to be moving further from its true mission and into materials that are unlikely to be relevant for DOE petroleum displacement 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 stated that the resources were sufficient for component-level effort. The reviewer added that if USCAR sees a value proposition for vapor-based  $NH_3$  delivery, additional system-level considerations should be included, and this would require additional resources.

#### **Reviewer 2:**

The reviewer commented that it would be good to have or see a system demonstration with this equipment. The reviewer did not see this as part of the project, but it would be good to add this on the project for some kind of either engine demonstration or vehicle demonstration to show how it will work.

**Reviewer 3:** 

The reviewer said that there was no issue with funding or staffing.

**Reviewer 4:** 

The reviewer said that the resources seem sufficient.

Cummins-ORNL\FEERC Emissions CRADA: NO<sub>x</sub> Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing Smart Catalyst Systems: Bill Partridge (Oak Ridge National Laboratory) - aceO32

# **Presenter** Bill Partridge, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer found the work to be an excellent approach that utilizes a fundamental understanding of NH<sub>3</sub> adsorption, analyses using spatially resolved capillary inlet, testing methods, and acquisition and analyses of field-aged samples on an applesto-apples basis. The approach has a high probability of achieving desired results. The only improvement may be in expanding into more contemporary zeolite systems, just to check if results are transferable. Non-transferability could be a major risk to the program.

# **Reviewer 2:**

The reviewer thought the project had a very good approach, especially to use field-aged samples to help develop and verify the model. However, the reviewer found the units and type of field-aging process needed to be explained. The reviewer wanted to know if the process was expressed in miles, cycle, or fuel; whether everything was prepared the same way; and whether the two samples were repeated or intended to be different to provide some range to the model. The reviewer also questioned whether the use of actual field fuel and good quality fuel were part of the model and how much S was in the fuel.

# **Reviewer 3:**

The reviewer found the project to be tightly focused, and it was targeting key challenges in a stepwise manner.



# **Reviewer 4:**

The reviewer commented that the ultimate goal needs to be clearly defined. The reviewer also wanted the objectives of the project to be correlated with the title of the CRADA.

# **Reviewer 5:**

The reviewer noted that general VTO barriers (cost-effective emission control, modeling for emission control, emission control durability) translated well into specific project objectives, which follow: enable and improve predictive catalyst-performance models, based on controlling physics and chemistry and independent of specific application platform (truck, bus, boat, power); characterize spatiotemporally distributed catalyst performance; investigate aging impacts (performance at different catalyst states); validate and improve models, and mine data and insights for OBD and control methodologies; and develop methods for real-time catalyst-state assessment.

The reviewer commented that the implemented approach could be improved by considering a larger sample of field-aged catalysts for characterization and direct mapping of field-aged samples to physical phenomena (temperature aging, flow-based aging, reaction-based [i.e., oxidation] aging, and poisoning). By correlating/ modeling catalyst aging and performance assessment techniques with a very limited set of field- aged samples, which were reported to have been subjected to a typical but uncharacterized duty cycle, the reviewer noted that current research and subsequent models have a high risk of being application/platform dependent and of less general usefulness.

The reviewer proposed that an improved approach would employ a multi-application, field characterization study using advanced spatiotemporal characterization and assessments to properly characterize failure mechanisms across applications with known field-aging schedules to insure that the catalyst-capacity measure is the appropriate model.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

## **Reviewer 1:**

The reviewer commented that this project seemed to provide some significant technical accomplishments with the catalyst modeling. The reviewer said that it will be interesting to actually perform a trial of the model versus the actual performance to determine the model performance and find out if the trial is truly self-diagnosing and able to predict within some X% of efficiency.

## **Reviewer 2:**

The reviewer found good progress in extending the confidence in the measurements, modeling, and real-world behavior through additional catalyst measurements. The reviewer also stated that the interpretation of the operando data to confirm how the sites are degrading in real catalysts is very useful in understanding bench- versus field-aging.

## **Reviewer 3:**

The reviewer found the evaluation led to some very promising diagnosis methods. The use of unused  $NH_3$  capacity (UC) is novel, and the correlation of pulsed response to UC is valuable. Models are not perfect, and more work is needed to improve them, but they are impressive. However, the reviewer questioned why the first field-aged sample (FA-1) is different from the FA-2 (e.g., poisoned, thermal, etc.). Deterioration can be caused by many things, and the reviewer advised knowing what effect the project team is modeling.

## **Reviewer 4:**

The reviewer noted that the work was a good systematic approach using field-aged catalysts, but in order to have better correlation, the reviewer needed to understand what those catalysts were exposed to.

## **Reviewer 5:**

The reviewer proposed that a reasonable laboratory approach to assess capacity, once additional field samples are confirmed, may offer possibilities for diagnostics if control steps can be effectively integrated into the SCR control system as active control and not intrusive control. The reviewer stated that the claim that the project has

"demonstrated a practical method for catalyst state assessment" is premature without relating the aging impacts/ echanism to the state assessment, considering a larger sample of catalyst applications, and understanding the mechanisms involved.

In 2015 the reviewers indicated that more thorough characterization methods for field-aged parts were necessary, and this continues to be an unaddressed issue in 2016. The budget may be constraining the performance of catalyst field aging along with data acquisition; however, the reviewer stated that a larger sample of field-aged samples could potentially be correlated to rapid aging test (RAT) results and the controlled RAT tests used to characterize the physics.

# Question 3: Collaboration and coordination with other institutions.

# **Reviewer 1:**

The reviewer praised the collaboration with Cummins as clearly excellent. Even though this is a CRADA, the reviewer would like to see more direct paths to distributing the results to other industry members beyond the coordination with the CLEERS organization. The reviewer wondered if this could evolve into a memorandum of understanding.

# Reviewer 2:

The reviewer stated that the collaboration seemed sufficient.

# **Reviewer 3:**

The reviewer noted a good variety of collaborators in industry and academia and suggested that it may make sense to include a catalyst supplier for additional input into the project.

## **Reviewer 4:**

The reviewer stated that the close collaboration with the CRADA is obvious and obviously working well. The reviewer noted, however, that it is not clear how the others have helped.

## **Reviewer 5:**

The reviewer found that the CRADA somewhat constrains participants and limits the sharing of detailed results.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer stated that future plans are well-focused on practical OBD-type developments. On the other hand, the reviewer would like to see some additional work/focus on how to integrate the work with sensor developments—it is mentioned, but could be more definitive.

# **Reviewer 2:**

The reviewer commented that future work seems logical and noted that it will be interesting to actually perform a trial of the model versus the actual performance to determine the model performance. The reviewer asked if the model is truly self-diagnosing and predicting within some X% of efficiency. Also, the reviewer wondered about any impact of fuel and fuel impurities on SCR performance that would need to be incorporated into the aging conditions, or whether that would be an issue for SCRs.

## **Reviewer 3:**

The reviewer would like the project to focus on transient behavior and OBD work for real-life comparison/ applicability.

## **Reviewer 4:**

The reviewer noticed one gap in the future approaches that relates to determining the cause of deterioration. The reviewer believed that the model might only be related to thermal or poisoning deterioration and suggested that the project determine the nature of the deterioration being modeled. The reviewer found another gap dealing with

transferring these models to other zeolite systems and suggested that the model only need to get a peak in the box. The reviewer commented that the project team would not want to be here in two years with a working model that is only pertinent to a catalyst that is two generations old.

## **Reviewer 5:**

The reviewer commented that future work was generally described but could provide more detail. The reviewer cautioned not to expect a robust solution for a catalyst aging model, which has been developed and fit by data from only two field-aged catalysts with little known about aging history.

The reviewer suggested that the researchers' approach in the future work plan, "Evaluation of alternate aging conditions, sample locations and catalyst types," could provide a bit more detail on the next priority for aging conditions and catalyst types. An improved approach would be to confirm the catalyst state assessment model across a range of field-aged and RAT-aged catalysts with some association to mechanisms of performance change.

Another suggestion from the reviewer was to possibly investigate productive control schemes that are approaching the duty cycle—the intrusive  $NH_3$  step method—but which actually are part of SCR dosing control to make a more robust onboard solution. (The reviewer pointed out that the Air Resources Board generally does not accept intrusive OBD tests.) Providing data to quantify tailpipe criteria emissions during the  $NH_3$  step and  $NH_3$  slip in the analysis would also improve the future work.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer commented that the development of practical OBD methods for lean aftertreatment is critical for continuing to develop lean combustion systems.

## **Reviewer 2:**

The reviewer commented that proper aftertreatment technology allows best optimization of engine thermodynamics.

## **Reviewer 3:**

The reviewer stated that modeling of catalyst aging is relevant to minimize safety factors (overdesign) in applied catalysts and controls by saving money and reducing fuel consumption in SCR systems.

## **Reviewer 4:**

The reviewer stated that SCR can improve fuel economy, but it is not clear how the modeling process could assist in the improvement of fuel economy, except for modeling when the SCR has reached a low-efficiency point and would need to be regenerated or replaced.

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

#### **Reviewer 1:**

To properly perform catalyst aging characterization, modeling, and controls development, the reviewer believed there needs to be significantly more funding than has been allocated for this project. Additional funding or funding of a similar project could enable improvements in the field-aging component as well as a more appropriate assessment of the modeling effort for catalyst state and possibly more highly vetted suggestions for control and OBD algorithms.

#### **Reviewer 2:**

The reviewer commented that it seems like there is a lot being accomplished for the project budget. While the reviewer was not sure about the specific headcount and hardware, the outcome could be significant for the HD and LD markets with a catalyst modeling approach.

**Reviewer 3:** The reviewer stated that progress appears to be at a good pace for the size of the project.

Reviewer 4:

The reviewer found no indication that resources were not sufficient nor was there any negative impact on the work.

# Emissions Control for Lean Gasoline Engines: Jim Parks (Oak Ridge National Laboratory) - ace033

**Presenter** Jim Parks, Oak Ridge 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer stated that the approach is excellent, particularly the iterative experiments using modeling, bench, and vehicle work. Running rich/lean to generate  $NH_3$  for a downstream SCR, and quantifying the fuel penalty, seems feasible. Ford (Theis) substantiated the approach, favoring a TWC or a lean  $NO_x$  trap due to S poisoning.

The reviewer expressed concerns about this being an older lean burn engine approach. More recent concepts are more diluted, either with air or EGR, to give lower  $NO_x$  and temperatures, perhaps more like diesel. The reviewer suggested that the project team look at GCI work, or a Toyota paper (SAE 2015-01-1896). Given



the FC advantages, even versus stoichiometric high-EGR approaches (2% versus EGR to 15% versus traditional stoichiometry), there is money to play with (e.g., \$200-\$250 in the 2020-2025 timeframe at 2% benefit). This might pay for a urea system (\$250) if the cost of platinum group metals (PGM) can come down. The reviewer suggested that the project team explore lower NO<sub>x</sub>, lower temperature, and urea-SCR supplementation.

# **Reviewer 2:**

The reviewer found this project to be a nice blend of lab work and engine work. The reviewer commented about the investigation of the effect of the TWC formulation on the light-off performance on Slide 18. The reviewer asked whether the project team had assessed the different formulations for  $NH_3$  selectivity and HC conversion during rich operation. It is critical that the TWC provide essentially 100% steam reforming capability during the rich periods to satisfy the very stringent HC standards. This means there has to be some ceria in the TWC because it is needed for steam reforming, but the resulting  $O_2$  storage capacity will delay the production of  $NH_3$  after a lean/rich transition. So the amount of ceria needs to be optimized to maximize the  $NH_3$  generation while still providing 100% steam reforming capability. The reviewer recommended that the project team initiate some controls

development and investigate multi-step purges in order to reduce the CO slip and fuel economy penalty associated with the rich periods.

# **Reviewer 3:**

The reviewer commented that the focus of this presentation is on technical aspect of the technology. The reviewer believed the project needs to also address the commercial aspect of the approach, benefits versus cost/complexity, and impact on fuel economy of running rich/lean versus SCR costs.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# Reviewer 1:

The technical results are excellent to outstanding. The reviewer commented that the project team had quantified most or all major characteristics of the system under steady-state conditions, and the reviewer thinks that the approach looks feasible. Light-off seems good enough. The NH<sub>3</sub> and N<sub>2</sub>O trade-off in rich-lean and light-off is quantified and reasonable. Cycle time, NH<sub>3</sub>:NO<sub>x</sub>, and SCR loading on engine are impressive and seem reasonable. Poisoning and aging impacts are not stoppers, although desulfation can be a problem at 650°C if advanced low-temperature lean burn concepts are used. Although not shown here, the reviewer presumed that the PI has evaluated the above as a function of temperature; if not, this will be needed.

# **Reviewer 2:**

The reviewer found the project to be an interesting investigation into PGM sintering versus aging time. The reviewer noted the good work in evaluating the effects of S on NH<sub>3</sub> production, HC conversion during rich operation, and the ability to recover the performance with a rich desulfation. Because the NH<sub>3</sub> production and HC conversion of the TWC both decreased significantly after S poisoning, it will be important to keep the TWC purged of S by periodically exposing it to high temperatures and slightly rich operation. In the close-coupled location, this should happen passively. But, a desulfation procedure will need to be available for the case of extended low-temperature operation.

HC slip will be the biggest challenge during rich operation. It will require that the TWC operates at a minimum of 400°C and preferably 500°C to promote steam reforming of the different types of HC in the exhaust. The higher temperatures will allow for running less rich and still generating more  $NH_3$  and less  $N_2O$ . The less rich operation will in turn help minimize the CO slip and fuel economy impacts during rich operation. Two-step purges should still need to be investigated (extra-rich initially to reduce the catalyst, then less rich to generate  $NH_3$  during the rest of the purge).

## **Reviewer 3:**

The reviewer believed there was good consideration of reviewers' comments, but suggested that the project team consider different SCR formulations to address  $N_2O$  emissions.

# Question 3: Collaboration and coordination with other institutions.

## **Reviewer 1:**

The reviewer commented that the project team has all the key parts to the system—OEMs, catalyzer, and aging support. The reviewer really liked the project team's additional collaborators and noted that the project team was well connected with key players.

## Reviewer 2:

The reviewer praised the great combination of academia and industry.

## Reviewer 3:

The reviewer liked the good collaboration with GM and discussions with other groups such as Ford and Fiat Chrysler Automobiles (FCA).

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The future plans appear to address the challenges and barriers, and the reviewer offered several suggestions. As mentioned above in the approaches, the project team needs to look at emerging lean gasoline concepts with lower engine-out  $NO_x$  levels and lower temperatures from Toyota, Delphi, and ANL. Another suggestion was that transient work will be critical to feasibility. The reviewer suggested that the project team consider supplementing the approach with a urea system. Urea consumption could be very low, and perhaps the reduced rich time and/ or PGM can help pay for much of it. Lastly, the reviewer proposed considering SCR filters. A peak in the box is needed, as GPFs are gaining a foothold in the European Union (EU) and China, and may be needed/desired in the United States. This is not as critical as the above considerations.

# **Reviewer 2:**

The reviewer believed there was a need to really emphasize HC slip during the purges because HC slip will be one of the biggest challenges for any system requiring periodic rich operation. Aging of the SCR catalyst will be interesting as SCR catalysts can be deactivated by high-temperature rich conditions.

# **Reviewer 3:**

The reviewer suggested considering the possible influences of H<sub>2</sub>.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# **Reviewer 1:**

The reviewer commented that less gasoline operation will reduce fuel consumption and satisfy DOE objectives of reduced petroleum use. However, it will require extremely high performing emission control systems to satisfy stringent emission standards such as the Tier 3 standards.

# **Reviewer 2:**

The reviewer noted that dedicated EGR can be very competitive to lean-burn gasoline. However, CI gasoline is emerging with potential further advantages.

# **Reviewer 3:**

The reviewer stated that lean burning engines are key for best performance.

# 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 \$400,000 is not enough. This ought to be 1.5-2 times higher, given the emerging interest in lean-burn and the challenges and options that need to be evaluated.

## **Reviewer 2:**

The reviewer encouraged the PI to consider applying more resources to the calibration, including the multi-step purges. Calibration and controls will also be needed to maximize the feed gas  $NO_x$  during rich operation (to generate high levels of  $NH_3$  quickly for the SCR catalyst and allow short rich periods) while minimizing the feed gas  $NO_x$  during lean operation (to reduce the consumption of the stored  $NH_3$  and allow longer lean periods for improved fuel economy).

# Neutron Imaging of Advanced Transportation Technologies: Todd Toops (Oak Ridge National Laboratory) - ace052

# Presenter

Todd Toops, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer complimented the project as a very nice effort to develop an advanced spray/injector diagnostic tool. The information gained and models developed could be very useful for industry and academic researchers.

# **Reviewer 2:**

The reviewer remarked that this is a good approach to complement other injector diagnostic techniques, such as X-rays and visible light spray testing.

# **Reviewer 3:**

The reviewer stated that the approach develops and uses a novel tool (neutron imaging) available only at

the national laboratories to diagnose engine-related problems.

# **Reviewer 4:**

The reviewer noted that this project is another successful re-tasking of unique DOE resources to aid the engine industry. While some explanation of the differences between this work and the ANL APS work is made here, some more extensive joint report on how the two facilities actually complement each other is needed. Of course, seeing more actual collaboration with complementary results would be even better.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer commented that fuel injector and particulate filter measurements are reported. Some collaborative, complementary results with the ANL team are included in the injector work, which is noteworthy.



# **Reviewer 2:**

The reviewer noted that engaging with the ECN is a very good thing. The reviewer questioned whether it would be possible using other diagnostics, like high-speed movies, to make some sort of assessment of the cycle-by-cycle variability of the injector being studied. This would give some indication of the amount of smoothing contained in the composite images obtained from the neutron imaging.

# **Reviewer 3:**

The reviewer found very good progress has been made in providing some new insights for gasoline fuel injector behavior using this tool. More results have been provided on flash boiling, sac volume, and dribble on gasoline spray characteristics. Good progress has also been made with GPFs.

# **Reviewer 4:**

The reviewer commented that resolution of injector and spray measurements so far do not seem to be good enough to be able to draw strong conclusions. GPF measurements are very insightful and provide information that is not available any other way.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer noted collaboration with a number of academic and industrial partners and remarked that more is always better though.

# **Reviewer 2:**

The reviewer suggested that as the tool becomes more developed, it would be advisable to engage OEMs and other injection equipment suppliers.

# **Reviewer 3:**

The reviewer stated that it sounds like the amount of beam time available is limiting the amount of collaboration with fuel injector suppliers and preventing looking at more conditions and more injectors. Still, collaboration should be sought with more fuel injector suppliers like Bosch or Delphi as they know the issues needing to be solved in detail and stand to benefit the most, indirectly impacting the OEMs.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer commented that a fouling study will be interesting. Improved image processing and understanding occlusion effects from heavy hydrocarbons (HHC) are also important for improving diagnostics results to aid modelers, as is improving the geometry description for spray gasoline.

## **Reviewer 2:**

The reviewer noted that the project had a well laid-out path for further development of the tool.

## **Reviewer 3:**

The reviewer suggested higher resolution is the correct thing to work on to improve the measurements and make them useful.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer remarked that a better understanding of the injection process provided by the diagnostics here will aid in designing more efficient engines that use less petroleum.

# **Reviewer 2:**

The reviewer asserted that this is a good example of DOE being able to develop and provide advanced tools and diagnostic capability that could be helpful to industry but which industry could not afford to undertake itself.

# **Reviewer 3:**

The reviewer noted that the technique could be developed that will provide insight into injector behavior. This is important to understand how injectors interact with the engine combustion system.

#### **Reviewer 4:**

The reviewer stated that neutron imaging has the potential of becoming a useful tool in developing fuel injectors and particulate filters, for example, which are key enablers of high efficiency engines that meet emissions 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 noted that the project needs more resources to accelerate progress.

Reviewer 2:

The reviewer found that resources seem adequate for the proposed work

# RCM Studies to Enable Gasoline-Relevant Low-Temperature Combustion: Scott Goldsborough (Argonne National Laboratory) - ace054

**Presenter** Scott Goldsborough, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer remarked that the project is rather narrowly focused on using the RCM to provide combustion properties for developing and evaluating the kinetic chemistries of transportation fuels at a range of pressures and temperatures. A twin piston RMC is used to measure ignition delay time (IDT), which is the main property that is used to compare predicted and measured values using a model of the RCM.

The reviewer noted that the project team refers to the RCM as providing IDT properties under engine relevant conditions and poses the question to



the team about how researchers can infer performance under engine, e.g., HCCI, conditions. The reviewer asserted that it is not at all clear that IDT data from an RCM provide such relevant conditions, nor is it evident that there is much in the RCM environment besides temperature and pressure that could be construed as engine relevant conditions. For example, the RCM has no turbulence, swirl, or any liquid within the RCM such as would be present within an engine from sprays and droplets injection, which sets the initial conditions for in-cylinder processes. The condensed phase fuel of an RCM is pre-vaporized so the environment of an RCM may in fact and in reality not be faithful to that of engine. The reviewer recommended that the project team pull back from characterizing the RCM environment as being engine relevant because it is not.

The reviewer noted the mention that engine data are shared with the project; however, the utility of such data is unclear. Currently, in-cylinder conditions cannot be simulated from a first-principles approach with the same high fidelity modeling that the RCM is amenable to, with its single phase and 1D transport environment. As a result, the reviewer stated that it is not clear how engine data will be folded into this project. Some discussion of how engine data are related to the RCM would be relevant.

# **Reviewer 2:**

The reviewer stated that the project is very instrumental towards acquiring RCM data to support the improvements in chemical kinetic modeling for relevant fuels for the transportation industry. The work employs a RCM facility with good range capability and is developing novel analysis techniques using UQ and global sensitivity analysis (GSA). The current efforts to improve the RCM machine operational issues should be addressed right away by possibly engaging outside help to eliminate the 2-3 ms delay in the synchronous motion.

# **Reviewer 3:**

The reviewer noted that fundamental ignition delay data have been collected extensively for gasoline fuel surrogate components and gasoline/ethanol blends in ANL's RCM facility and compared to models yielding reasonable matches with the test data. However, the gasoline surrogate model needs to be improved to capture the low-temperature, high-pressure region. In order to perform engine high load simulation work, data at higher ambient pressure might be needed.

## **Reviewer 4:**

The reviewer commented that RCM experiments for ignition delay measurements are very standard, and this project does not go beyond the standard utilization of RCM. The introductory slides indicate the development of new diagnostics, but such results were not shown. While the ignition delay data are important for model validation, it seems that this project merely cranks out more ignition delay data. Thus, it seems to lack novelty in the project approach.

## **Reviewer 5:**

The reviewer asked how this work compares to, complements, and/or dovetails with kinetic work by Bill Pitz at LLNL.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

## **Reviewer 1:**

The reviewer praised the presentation as documenting very well the efforts undertaken in the gasoline surrogate work, with special emphasis on the LTC behavior. For clarity, the reviewer wondered if the project team could include the dilution ratios on the figures related to the five-member ring naphthenes.

The reviewer commented that ignition delay studies of Fuels for Advanced Combustion Engine-F (FACE-F) with Ethanol blends appear to be well correlated with modeling work. The work seems to attempt to correlate the studies with the HCCI engine work from University of California at Berkeley. The reviewer noted that the data presented appears to be unclear and asked if the project team could help by labeling the figures with more informative information and help the readers distinguish the RCM and engine data.

## **Reviewer 2:**

The reviewer remarked that most of the proposed milestones have been accomplished with others in progress. Results are solid and promising with the collaboration with other institutions, and the first part of this project is well accomplished.

## **Reviewer 3:**

The reviewer observed that the outcome of this project, ignition delay of various gasoline surrogates, is well within expectation. There are no additional insights into the chemical kinetics of the ignition delay. There have been many similar studies using RCM for gasoline-type fuel chemistry study. The reviewer suggested that it needs to be clear that this project does not repeat what has been done in the literature.

# **Reviewer 4:**

The reviewer said that a lot of data were obtained in the reporting period, including for gasoline/ethanol blends (E10), principally being IDT with reasonable agreement shown. The reviewer highly recommended that the project team present some information about the sort of modeling of the RCM that is at the heart of comparing IDT data with simulations.

The reviewer commented about the "New approaches developed in 2016 to demonstrate correlation between RCM measurements and observed engine trends...." by stating that, again, the RCM environment does not appear to be entirely relevant to engine conditions where sprays set the initial conditions for combustion because it pre-vaporizes the fuel. There are certain engines/conditions where ignition can occur within the multiphase domain of the injected spray. Data for this situation are also relevant to developing combustion chemistries. The reviewer stated that the point is researchers do not know how combustion chemistries developed from purely gas phase combustion configurations such as an RCM would compare with chemistries developed from multiphase configurations where the flame/ignition process would occur with the multiphase domain.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer commented that there were very good collaborations with LLNL, University of California at Berkeley, Northeastern University, and international institutions.

# **Reviewer 2:**

The reviewer said the project team was a very good team. The reviewer suggested that the project team possibly incorporate more engine representation to help validate the findings and provide a way for further migration of models and chemistry to applications.

# **Reviewer 3:**

The reviewer stated that the collaboration seems to be reasonable. It seems to include the exchange of information only, but not closely working together to interpret the data at a deeper level. The team seems to be focused on RCM experiments. The reviewer said that the presentation indicates that there is collaboration with Northeastern University on UQ, but it is not clear how the interaction would be. The reviewer encourages two-way interaction and more details.

## **Reviewer 4:**

The reviewer found the collaborations to be well-developed, but it would be useful to provide more discussions of the models used to validate the RCM data as the project has collaborators who provide engine data. Some discussion for precisely how these data are used to develop combustion chemistries and how the RCM fits in with them would be useful.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

## **Reviewer 1:**

The reviewer said that the work provides significant information on ignition delays. The reviewer queried whether the current work is looking at other metrics to help improve or validate today's mechanisms (e.g., select speciation). The reviewer also wanted to know how the present work is considering the uncertainties associated with the LTC mechanisms. On the uncertainty front, the reviewer asked what role the absence of chemical intermediaries plays and whether there are any effects present in the measurements due to local perturbations.

## **Reviewer 2:**

The reviewer stated that, basically, the proposed future work showed a good extension of present work and offered that study at higher ambient pressure might be needed for the future engine (diesel or gasoline) case study.

# **Reviewer 3:**

The reviewer noted that future work will include more testing of surrogates and collaborations with groups at SNL to further quantify autoignition behavior. The project team mentioned that tests will be conducted on multicomponent surrogates. The reviewer suggested that some discussion of how blending ratios would be selected is appropriate, and an E10 surrogate (RD-587) will be examined. The reviewer remarked that a simple experiment would be to also measure the IDT with the certification fuel and compare results with E10 and asked how this will be done. The plan to collaborate with LLNL to reduce uncertainty in rate controlling reactions and improve model

predictions was not clear to the reviewer, who asked about how the collaboration will be done. The reviewer also wanted to know the specific role in the RCM in this process as it was vague.

# **Reviewer 4:**

The reviewer encouraged proposed future work to use gas chromatography (GC) to obtain gas speciation. The project needs to go beyond the standard ignition delay measurements.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer commented that understanding combustion chemistry is important in the design of new, more efficient engines that will reduce petroleum usage.

# **Reviewer 2:**

The reviewer found that this project is relevant from a broad perspective. However, as noted previously, the RCM does not in general provide engine relevant conditions for reasons mentioned previously. It provides but one of a number of combustion properties useful for validating combustion chemistry.

#### **Reviewer 3:**

The reviewer noted that this project is mostly on fossil fuel (gasoline). Although there are results for ethanol/gasoline blends, ethanol chemistry is very well established. Thus, it is not clear how this project will help improve the understanding of ethanol chemistry to promote the displacement of petroleum 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 stated that funding appears to be adequate for proposed plan.

**Reviewer 2:** 

The reviewer noted that resources seem to be reasonable.

# **Reviewer 3:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

# Fuel-Neutral Studies of Particulate Matter Transport Emissions: Mark Stewart (Pacific Northwest National Laboratory) - ace056

# Presenter

Mark Stewart, 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, feasible, and integrated with other efforts.

## **Reviewer 1:**

The reviewer expressed that the approach of characterizing PM with a very wide range of tools is excellent.

#### **Reviewer 2:**

The reviewer commented that this is a very important research project as OEMs are looking for data to help support development and implementation of GPFs for vehicles. The reviewer liked the fact that the project team is also trying to determine the particle size for filtration efficiency and regeneration. The reviewer observed that it is very important to understand the fuel properties of both splash and matchblended fuels, so it would be helpful to



list that in the data for the project. It would also be helpful to list the tools and methods used to collect the data on the slides.

# **Reviewer 3:**

The reviewer said that the approach appropriately leverages project team core competencies and facilities, with UW running advanced engine testing with candidate next-generation gasoline engine technologies and PNNL conducting highly detailed PM characterization.

## **Reviewer 4:**

The reviewer stated that there was an excellent use of advanced tools on a wide range of filters. Wafers are a good idea, and also looking at early loadings is very important. The reviewer noted that particulate characterization is important at this stage of program, but ash is more important than soot for GPF. Both were evaluated.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### Reviewer 1:

The reviewer found the overall research accomplishments to be fantastic and very relevant. Again, further clarifying the fuel properties to the particle size and number is important for a complete understanding of the soot loading and GPF efficiency. It would also be helpful to list the tools and methods used to collect the data on the slides. It is hard to make sense of the data on Slide 7 as the reviewer is not sure if this is splash or match-blended fuels. The reviewer asked which tools were used on Slide 8.

#### **Reviewer 2:**

The reviewer observed that technical accomplishments include advances in particulate characterization, device scale modeling, significant amount of new filtration data, and detailed Lattice Boltzmann simulations.

#### **Reviewer 3:**

The reviewer remarked that the data and understanding that have been achieved are impressive, especially the impact of different fuels. Their application into modeling, where appropriate, would be great to see more of. Including ash into the data analysis and modeling would be good also.

#### **Reviewer 4:**

The reviewer found characterization of the soot as a function of fuel and operating conditions to be quite interesting. The operating conditions seem a little broad as well as the fuels, but it is good to see the whole spectrum. The filtration efficiency work versus filter and PM size is also important and valuable. Such data are new for GPF. The Lattice Boltzmann simulations are quite interesting and explain much of the porosity impact on back pressure and filtration efficiency.

# **Question 3: Collaboration and coordination with other institutions.**

## Reviewer 1:

The reviewer remarked that there was good collaboration with GM and UW on this project. Other collaborators are listed on Slide 21, a very nice list.

# **Reviewer 2:**

The reviewer commented that this project has a strong project team with good collaboration and partners leveraging their core competencies: GM is the main industry partner providing part of funding, hardware, and expertise; the Engine Research Center (ERC) at UW conducts experiments and assist with analysis and modeling; and four filter and three analysis subcontractors are involved.

#### **Reviewer 3**:

The reviewer asserted that interaction with UW and GM has been very productive.

#### **Reviewer 4:**

The reviewer observed that ERC, GM, and filter suppliers are the key partners, but a catalyzer is missing as the project moves into a TWC plus GPF.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer commented that this is an excellent list of needed future work on this project. The reviewer highly recommended asking for additional funds to overcome any technical challenges or barriers in accomplishing the project (as listed on Slide 22) and to accomplish the goals of Future Work on Slide 23.

# **Reviewer 2:**

The reviewer indicated that future research seems appropriate as it involves further expanding the set of tested filter samples, including catalyzed filter substrates to improve filtration models.

# **Reviewer 3:**

The reviewer remarked that the future work plan is primarily aimed at further refining the models and methods on a wider range of uncoated GPF samples. Although some of the first generation GPFs will be uncoated, the majority of these and all future systems will be catalyzed. The reviewer encouraged the project team to generate future base data to primarily focus on catalyzed samples and recommended shifting to characterizing cordierite only. In gasoline application, high thermal mass materials like AT and silicon carbide (SiC) have little use. They are valuable for characterizing porosity, as the project team has shown.

Also, a key risk and a general unknown is whether polycyclic aromatic hydrocarbon (PAH) emissions are higher from a GDI engine than an MPI engine. The hypothesis is that PAHs are integrated into immature soot, and this passes through the TWC. Given the toxicity of PAHs on small solid particles, this understanding is perhaps the most critical at this time. This might be beyond the scope of this project, but the project team could take the GDI results and easily slap on a TWC and vary the filter temperature to see PAH response for maybe 10% ethanol blend with gasoline (E10) to 20% ethanol blend with gasoline (E20). It might be easy to get similar results on MPI PM characterization. This reviewer noted that China is seriously looking at MPI GPFs, as well as the EU OEMs.)

# **Reviewer 4:**

The reviewer commented that much is still left to do.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

## **Reviewer 1:**

The reviewer commented that understanding how to manage the filtration efficiency and regeneration of a GPF will help to minimize the back pressure on the engine and thus allow it to operate at the maximum efficiency.

## **Reviewer 2:**

The reviewer stated that the project allows for use of new combustion technologies.

## **Reviewer 3:**

The reviewer noted that this project addressed the barriers for enabling high-efficiency engine technology that would result in direct petroleum savings. Specifically, the following are addressed from the VTO multi-year program plan: lack of cost-effective emission control, lack of modeling capability for combustion and emission control, and lack of actual emissions data on pre-commercial and future combustion engines

## **Reviewer 4:**

The reviewer said that although U.S regulations, even in California (1 mg/mi), will not require a GPF, some of the emerging high-efficiency concepts may have high PM/particle number (PN) emissions. OEMs are also interested in utilizing GPFs to minimize public relations risk.

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

## **Reviewer 1:**

The reviewer asserted that it seems that, based on the list of the challenges and barriers listed on Slide 22, the project might need additional funding to complete. The data for a closed coupled GPF and catalyzed filters are a significant hurdle for the industry so these kinds of data are very relevant for the coming years. It would be helpful to support the project with additional funds if the project team deems it necessary to overcome the challenges and barriers in accomplishing the goals and future work.

## **Reviewer 2:**

The reviewer commented that funding has been \$200,000 and \$250,000 for the past two fiscal years, respectively, which appears adequate for the scope of this project.

# SuperTruck - Development and Demonstration of a Fuel-Efficient Class 8 Tractor and Trailer, Engine Systems: Russ Zukouski (Navistar International Corporation) - ace059

## Presenter

Russ Zukouski, Navistar International Corporation

**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, feasible, and integrated with other efforts.

## Reviewer 1:

The reviewer remarked that the approach is comprehensive and balanced. It hits the major opportunities for efficiency downspeeding, pumping, combustion, and parasitics. The reviewer liked that Navistar is using many of the technologies it had to develop to get low engine-out NO<sub>x</sub> and that WHR is not needed to demonstrate 50% BTE. The reviewer commented that it seems that all these 50% BTE strategies are incremental or practical and can be readily employed, delivering immediate societal benefit.



# Reviewer 2:

The reviewer stated that a good set of technologies has been developed and demonstrated. The reviewer found a 50% BTE to be an impressive demonstration. The approach is systematic and produced good results, and the 55% path is somewhat more tenuous but not bad.

# **Reviewer 3:**

The reviewer found an excellent approach with selected technologies, which included a focus on combustion heat retention, friction reduction, alternative fuels, two types of waste heat recovery, and a very good effort at rational electrification of parasitics by considering multi-voltage (12 Volt [V], 24 V, and 48 V) architecture to achieve goals. The reviewer commented that it was outstanding to find bandwidth to consider alternative fuels to achieve stretch goals and facilitate parallel work in this area. The plan to leverage industry partner knowledge is excellent.

# **Reviewer 4:**

The reviewer noted that it is good to see that Navistar finally brought back WHR with Rankine cycle technology,

which had been criticized last year. There is no way to achieve 50% BTE goal without WHR. The reviewer said that a lack of technical planning and technical vision in the early stage caused the program to miss the timing and the goal.

#### **Reviewer 5:**

The reviewer commented that this team was caught in an unfortunate situation that was outside their control. Under these difficult situations, the team did the best that they could, and the reviewer commended the team for their perseverance and hard work. The reviewer said that the fundamentals of their approach were sound, the project team just did not get to pursue them to the extent necessary to leave the reviewer with confidence that the end results in September will be very inspiring. Nor did the team have the opportunity to really push on the most challenging longer term technical approaches for improving engine or transport efficiency.

## **Reviewer 6:**

The reviewer commented that the project objectives were clearly identified, but the path to achieve them is somewhat muddled. While the main path to achieve a 50% BTE engine is a combination of improved combustion, downspeeding, improved air breathing, and parasitic loss reduction, a number of other technologies appear to have been tried that yielded no promising results. eTurbo and thermal barrier coatings are some, to name a few. The technical pathway identified towards a 55% BTE engine constitutes use of diesel plus natural gas (NG) or diesel plus ethanol, which are far removed from practical use. The reviewer commented that though the technology mix towards an integrated truck with a 50% freight efficiency improvement was identified through CFD simulations, the reviewer doubts that it will ever be demonstrated.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer mentioned balanced contributions from downspeeding, pumping, combustion, and parasitics to get 50% BTE. The variable valve actuation (VVA) work is unique and valuable as is the rocker stop device to eliminate idling. This is especially critical and unique for the vocational vehicle segment. The work on late combustion enhancement is also unique and important to minimize emissions. It appears to have delivered unexpected efficiencies.

Regarding 55% BTE, the reviewer believed that Navistar appears to be the only holdout now that may pursue the dual fuel strategy, and the company has generated impressive results. Of the four participants, Navistar seems best poised to actually employ NG-diesel LTC in the market, given their vocational vehicle business and proximity to NG fueling stations (local or fleet). In the reviewer's opinion, this is a key consideration in the next step to sponsoring 55% BTE work. It would be nice to get LTC more developed to see if it is real.

Navistar also contributed by discovering WHR using eTurbo is not the way to go, and this is a mixed blessing. The reviewer commented that the company is late on ORC, but this forced the company to not rely on WHR for 50% BTE, the only participant to do this, possibly unique worldwide. (Iveco was first to state it was possible.)

## **Reviewer 2:**

The reviewer found that the descriptions of Navistar's activities were very generic in comparing this presentation with the results/accomplishments presented by the other SuperTruck team at this year's AMR. Navistar has accomplished a 49.6% BTE with the final target of 50% to be demonstrated in the next several months so despite their handicap, the team made progress.

In looking at the results presented, the reviewer expressed concern with the disparity between Navistar's system model and the actual dynamometer results shown in the graphs on Slide 13 of the presentation. Likewise, the data for dual fuel testing on Slide 14 and the current performance of the organic Rankine cycle (ORC) system do lend confidence to the viability of achieving the improvement projected for the dual fuel, downsized, and ORC II engine given in the bar chart on Slide 15. The reviewer commented that coupling the above remarks to brief statements made in the presentation indicating that Navistar is still working on aftertreatment performance and combustion modeling (kinetics) gave the reviewer concern as to the level of success the company will be able to claim at the

end of the program in September 2016. Lack of technical backup slides for the reviewer to probe further into their accomplishments only enhances this feeling. These comments are made strictly based on demonstrated accomplishments. The reviewer said that they have not been weighted with a consideration of the handicap the researchers were handed after the project started.

## **Reviewer 3:**

Regarding the 50% BTE engine, the reviewer noted good progress with the technology mix identified. With the development of WHR system, Navistar is optimistic that the current 49.6% efficiency can be improved beyond 50%. As for the 55% freight efficiency vehicle demonstration, CFD simulations were performed to identify the technology mix. The reviewer said that it appears unlikely that this milestone will be met before the end of the project. Concerning the 55% BTE engine, the reviewer commented that details provided are somewhat sketchy and heavily reliant on combustion system improvement and the WHR system.

The reviewer concluded that though the overall performance does not measure up with that of other awardees like Cummins or Volvo, the path taken to achieve the 50% BTE is more practical. Navistar has relied on a strategy that is a combination of improved gas exchange, improved combustion system, and WHR, which is commendable.

# **Reviewer 4:**

The reviewer remarked that it was very good work.

## **Reviewer 5:**

The reviewer said that even without the pause in the middle of program, Navistar should have been able to achieve 50% BTE goal if the company had WHR in the early stage.

# **Reviewer 6:**

The reviewer noted the Navistar has achieved the 50% BTE goal with technologies that have a high potential for production, such as a variable geometry turbo, friction reduction through base engine redesign, and mild electrification. Efficiency is further enabled by closely coupled and integrated high efficiency aftertreatment.

The reviewer commented that the novel packaging for WHR on the rail is an interesting approach for R&D simplicity and relatively low-risk potential for early adopters to confirm the technology in their fleets. The reviewer remarked that it was great to share data on approaches that did not make the downselect and the logic for future technology improvement/application consideration. The reviewer said that the three voltage architecture for mild electrification for efficiency is outstanding.

# Question 3: Collaboration and coordination with other institutions.

## **Reviewer 1:**

The reviewer said that Navistar leveraged key players in major aspects of this project. It appears the company delivered unique results in several of these, like VVA (Jacobs), dual fuel (ANL), and friction using crank and cam shafts (Mahle, ANL).

## **Reviewer 2:**

The reviewer noted that it was an outstanding effort to leverage a large industry partner/supplier knowledge base to achieve successful results. The extensive list of suppliers and national laboratories supporting modeling work and product development facilitates knowledge transfer and accelerates technology to production through the supply chain.

# **Reviewer 3:**

The reviewer noted that Navistar had many collaborators.

## **Reviewer 4:**

The reviewer commented that Navistar has worked with various Tier 1 suppliers and two national laboratories in this effort to evaluate various technologies, and the work seems to be well coordinated.

## **Reviewer 5:**

The reviewer remarked that there was a large number of active partners contributing to the program.

## **Reviewer 6:**

The reviewer suggested that working with so many partners, considering the lack of resource internally, would be the best way to go at this stage.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer commented that the program is coming to an end and Navistar had a good plan to finish this program.

#### **Reviewer 2:**

The reviewer wanted to see at least future DOE 55% BTE participants pursue a dual fuel LTC approach. In the reviewer's opinion, Navistar seems best poised and most serious to do this. Achieving 55% BTE is very difficult so the reviewer had expected a winnowing by any participants to common approaches. The reviewer asserted that it is best to spend public money for this on diversification so reviewers can get a peek at a range of technologies.

#### **Reviewer 3:**

The reviewer said that the project is successfully completed and with an excellent result to meet the 50% BTE goal and modeled the 55% BTE target with a rational plan to move forward. Success factors, as a result of SuperTruck, are intensely integrated modeling design approaches across the supply chain, an industry improved focus, and a highly upgraded capability to analyze, design, and apply critical efficiency technologies to commercial truck engines.

#### **Reviewer 4:**

The reviewer had no comment, saying comments were not applicable for this project as it is ending.

#### **Reviewer 5:**

The reviewer noted that the pathway to 55% BTE engine appears to rely on dual-fuel technology, a prospect that is less desirable to most customers.

#### **Reviewer 6:**

The reviewer noted that it is not clear how Navistar can achieve the 55% BTE goal, even with analytical solution.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer commented that if this project results in improved high efficiency truck engines, the achievement could severely reduce our nation's overall fuel consumption. This in turn could lead to reduced  $CO_2$  emissions and environmental impact.

#### **Reviewer 2:**

The reviewer noted that there were large petroleum savings.

#### **Reviewer 3:**

The reviewer remarked that 50% BTE technologies on the path to production will definitely improve petroleum displacement in the high fuel consumption Class 8 HD truck sector. The 55% pathway modeled provides a road map for industry and DOE to eliminate barriers for production engines to perform at superefficient levels.

## **Reviewer 4:**

The reviewer said 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 noted that the resources seem to have been appropriate to the effort required.

# **Reviewer 2:**

The reviewer commented that obviously Navistar lacked resources to keep the project going, but the reviewer thought the company recovered splendidly.

# **Reviewer 3:**

The reviewer observed that the very large budget coupled with substantial industry commitment has resulted in outstanding results for this project and the entire SuperTruck effort. The momentum is a great start for further acceleration of efficiency and smart, rational electrification going forward.

# **Reviewer 4:**

The reviewer noted that, with the time running down and lack of internal resources, the project team had to rely more on suppliers. The reviewer thought that with their help, the project team should be able to achieve the goal. However, time is not on the team's side because it is way behind other competitors.

# **Reviewer 5:**

The reviewer stated that even after accounting for the fact that Navistar has suffered financial difficulties, which seem to seep into the technical progress of this effort, the progress made seems less than that of other companies. Unless Navistar comes through with final outstanding results, the \$40 million investment from DOE needs to be considered excessive compared to the returns.

# Volvo SuperTruck - Powertrain Technologies for Efficiency Improvement: Pascal Amar (Volvo Trucks) - ace060

**Presenter** John Gibble, Volvo Trucks

**Reviewer Sample Size** A total of seven reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer commented that the approach used in the project was outstanding. The team took aggressive approaches including novel combustion strategies to achieve the fuel efficiency gains. Furthermore, the project team used a systems-level approach to maximize efficiency from several components, which also was the key to the team's success.

# **Reviewer 2:**

The reviewer stated that this was an interesting program. Volvo has developed a unique approach to achieving 55% BTE. It will be very interesting to see if the company is successful. Personally, the reviewer expressed concern about the increased losses associated with the additional gas exchange processes Volvo is introducing.





# Reviewer 3:

The reviewer commented that Volvo is unique in elucidating its approach: first, evaluate the best technologies for hitting the end point, 55% BTE, and then apply the best to meeting the immediate goal of 50% BTE. The expenditures up front might have appeared to not be an efficient engineering approach to meeting the short-term objective, but it appears to have been quite successful.

## **Reviewer 4:**

The reviewer found the project to be well designed and thought over: the design targets for the 55% BTE engine were first scoped through simulations, which in turn determined the scope and technology mix for the 50% BTE engine. The 50% BTE engine's performance was validated through dynamometer tests. Finally, the 50% BTE engine along with a mix of vehicle technologies was integrated into a final demonstration vehicle exhibiting 88%
improvement in vehicle efficiency. Yet, the reviewer stated that the only reason for concern is the high CR concept that uses two cylinders: one for compression and the second one for combustion. Similar concepts are being proposed elsewhere and appear to offer promise. However, considering the fact that the real estate under the hood is limited, the proposed concept might not be viable for transportation purposes.

# **Reviewer 5:**

The reviewer remarked that Volvo used an excellent modeling approach to achieve 55% engine BTE using an integrated computational approach (CFD, GT POWER, probability density function [PDF], and chemical kinetics) with confirmation peer review of assumptions and experimental testing where possible, such as in an optical engine.

# **Reviewer 6:**

The reviewer commented that Volvo had an interesting, alternate approach to achieving the 55% BTE goal of SuperTruck I. Some clarification as to the real world feasibility of this approach would have been helpful to differentiate this from an academic paper study using 55:1 CR strategy.

# Reviewer 7:

Regarding the 55% BTE goal, the reviewer was not convinced that a new novel engine concept would be the way to go mainly because of the modeling fidelity. Because this concept has not been tested in a multi-cylinder dynamometer cell, the combustion models cannot be validated. If the 3D and kinetic combustion models are used to calibrate the GT-POWER model, the fidelity of the model would be in question. The 300-bar peak cylinder pressure (PCP) is way too high, which can change the chemistry of the modeling base that we have not dealt with in a conventional engine As a result, the heat release in the GT-POWER model may run too fast, thus predicting unrealistic performance. Furthermore, the temperature can be very high, which can have a big impact on  $NO_x$  emissions. In addition, the pumping loss would be huge, and how the team models the flow loss through valves is unknown. The reviewer is not sure if this engine is 2010 emission compliant.

Regarding 50% BTE, the reviewer said that it is not clear whether turbocompounding and WHR with Rankine cycle technologies would be used together. If so, there is little or no chance that this type of technology would be accepted by the customer. The reviewer asked for clarification and stated that it would not be a good idea to put all technologies into one presentation, unless it is really used together to demonstrate a 50% goal.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer noted that the piston bowl design achieved remarkable results, and it was great to see the amount of SuperTruck developed technology that is making its way into product.

# **Reviewer 2:**

The reviewer complimented the project team on a very nice job completing the work and was particularly impressed with the team's plans for a 2017 commercial introduction of technologies developed in this program. That is the sign of a very successful program.

# **Reviewer 3:**

The reviewer commented that the team made excellent gains in fuel efficiency. It was very encouraging to hear the volume of fuel already saved using the introduction of SuperTruck technologies into Volvo trucks.

# **Reviewer 4:**

The reviewer remarked that reaching the 50% goal is amazing with one year shorter than their competitors, considering that the project team was two years behind at the beginning and then made up one year. The reviewer enthused well done.

# **Reviewer 5:**

The reviewer praised the outstanding results overall for 50% BTE engine demonstration with multiple technologies

graduating as technology to the customer on production engines (injection system, wave piston, turbocompounding unit, and aftertreatment system). The reviewer noted that results on modeling with a pathway to achieve 56% engine BTE were published in an SAE paper.

# **Reviewer 6:**

The reviewer commented that like the others, Volvo developed technologies in the 50% BTE stage that will make it to market. However, as the company elucidated these technologies more than the others, it appears that more technologies and higher efficiencies will be delivered. The wave bowl design combined with 3,000 bar pressure is valuable, unique (at least at 3,000 bar), and impressive. Turbocompounding has been used a number of years by Volvo and Daimler, and the box design of aftertreatment is coming over from Europe. Nonetheless, the DOE work seems to have helped move these to the next stage. The five-stage WHR steam turbine also is impressive.

The results on 55% BTE at this stage are very advanced compared to others. This is a direct result of Volvo's longterm approach. If the company can pull off the new combustion strategy that delivers a 55:1 CR, Volvo is uniquely estimating that only a 1% BTE point is needed from WHR to attain 55% BTE. If so, the company is a short shot away from eliminating WHR. That is a unique concept.

# **Reviewer 7:**

The reviewer noted that all the program targets were met or exceeded. However, the outstanding contribution of this effort are the technologies—wave piston, high-pressure fuel injection system, improved aftertreatment system, turbocompounding, etc.—that are likely to make it into the 2017 model year (MY) Volvo vehicles. Very rarely do technologies developed in an R&D effort make it to a final product. This effort appears to be an exception.

# Question 3: Collaboration and coordination with other institutions.

#### **Reviewer 1:**

The reviewer asserted that there was a good interface with universities.

#### **Reviewer 2:**

Per the slide deck that was provided for developing the 55% BTE engine, the reviewer noted that CFD simulations were performed in collaboration with Pennsylvania State University (Penn State). Also, single- cylinder engine tests and GT-POWER simulations were carried out at University of Michigan (UM) and Lund University.

#### **Reviewer 3:**

The reviewer effused about the impressive use of advanced modeling methods to derive the 55% BTE approach. The reviewer suggested that the Lund collaboration in particular likely resulted in the unique 55% BTE combustion approach.

# **Reviewer 4:**

The reviewer remarked that this project had a good combination of industrial and academic collaborators, which helped contribute to successfully meeting the program goals.

#### **Reviewer 5:**

The reviewer noted that it was difficult to improve collaboration. Strong universities were well represented and tasked for modeling expertise (i.e., UM, Penn State, and Lund University). The reviewer noted that critical engineering and Tier 1 partners were also incorporated for testing and improving the innovation to market path (Delphi and Ricardo) and consulting for lubricants from the petroleum industry (Mobil).

#### **Reviewer 6:**

The reviewer commented that it is good to see the team work with so many partners.

# **Reviewer 7:**

The reviewer found that the team had collaborations and a good working relationship among the team members, but collaborations could be improved by broadening the team beyond the suppliers who were the major collaboration partners.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer noted that this project is over, but hopes that work on Volvo's proposed 55% BTE concept will continue and be reported in public forums in the future.

# **Reviewer 2:**

The reviewer stated that Volvo appears to be offering a high-risk, unique approach to meet the 55% BTE goal. Many have proposed these unique compression cylinder engines. The high CRs, sometimes more than 100:1, offer high efficiency. However, no one has been able to make a practical engine. The reviewer said that this is well-worth DOE funds and a good expenditure of public money. Volvo appears uniquely poised to deliver a 55% BTE engine with minimal Rankine cycle WHR.

#### **Reviewer 3:**

The reviewer commented that the project has come to an end. Future incorporation of technologies developed in this program into product in the marketplace speak highly of the approach taken by this SuperTruck I team.

#### **Reviewer 4:**

The reviewer remarked that the project is an outstanding success and complete. The lessons learned are DOE funding has enabled parallel engineering efforts in complete engine systems design and vehicle design that facilitated step improvements with an integrated approach. Modeling capabilities to accelerate development and engineering have been significantly improved and more intensely integrated and operationalized into the design process to improve product development going forward. The stretch 55% BTE goals are a real roadmap for future designs.

#### **Reviewer 5:**

The reviewer said that the project is near its end so there is not much to report on regarding future research.

# **Reviewer 6:**

The reviewer stated that because the project has ended, this criterion does not apply.

#### Reviewer 7:

The reviewer asserted that working with universities on a new engine concept is good. However, the reviewer was not convinced that the new engine concept would be needed, which can diversify the funding source, which may not be a good investment in terms of the future of the product.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1**:

The reviewer commented that the planned commercial introduction of many of the technologies developed in this program is a testimony to its relevance.

# **Reviewer 2:**

The reviewer stated that the SuperTruck I goals were exceeded, directly supporting DOE objectives.

#### Reviewer 3:

The reviewer noted that per Volvo's projections, the 50% BTE engine concepts to be introduced into its engines are likely to save 120 million gallons of (diesel) fuel consumption spread over the next 5 years.

#### Reviewer 4:

The reviewer found the success factor to be clear: multiple engine-efficiency technologies graduate to market at an accelerated pace through the SuperTruck program.

# **Reviewer 5:**

The reviewer remarked that the project is highly relevant to DOE objectives for petroleum displacement because truck fuel-efficiency gains are central to the project's goals and deliverables. The project has already realized petroleum displacement.

Reviewer 6: The reviewer said 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 stated that this was a good use of DOE funds, investing in technology development that is making its way into consumers' hands.

# **Reviewer 2:**

The reviewer noted that the project team had a large budget and accomplished large results for a well-managed and delivered project.

**Reviewer 3:** 

The reviewer commented that Volvo had already achieved the program goal.

# Advancements in Fuel Spray and Combustion Modeling with High-Performance Computing Resources: Sibendu Som (Argonne National Laboratory) - ace075

**Presenter** Sibendu Som, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer said that the work provides a good approach seeking to minimize excessive tuning of models to experimental data and promoting improved predictive simulations with higher fidelity models. The work focuses on detailed chemistry combustion models, finer mesh for grid-convergence, high-fidelity LES turbulence models, and two-phase physics-based fuel spray and nozzleflow models. This is combined with high-performance computing facilities.

# **Reviewer 2:**

The reviewer commented that the work is moving towards predictive simulation



of the ICE with more high fidelity codes by finding ways to make them faster. Now the project team is working on capacity computing, where some fidelity is sacrificed for speed and quantity of cases simulated.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer noted that the speedup achieved with the tabulated equivalent strain flamelet (TESF) model is good progress in an important direction. The project team seemed to assert that all of the significant observed variation in individual nozzle flow rates is due to upstream flow conditions in the injector. The reviewer is skeptical of this claim and recommends a careful review and/or experimental and/or UQ consideration of other sources of variation, including orifice geometry, etc.

# **Reviewer 2:**

The reviewer remarked that the work is technically sound. It covers several distinct areas of work. The gasolineinjector modeling features an overall assessment leading to more effective simulations, consideration of flash boiling, and spray work including useful discussions on phase change and effects of backflow. The reviewer asked whether the project team could clarify if this work is being benchmarked with experimental studies and whether the team could explain the novelty of their cavitation work and compare it with the current state-of-the-art.

The reviewer stated that the LES modeling continues to be of great interest, in particular the plume-merging studies. The reviewer questioned if the authors would be able to apply these to selective engine cases to assess and provide what significant improvements may be attained in the context of emissions and fuel economy.

The reviewer would have liked to have seen how the earlier work on wobble, optimized reduced mechanisms for a diesel surrogate, and dribble mass predictions are being utilized. Some of these were indicated as future work in 2015.

# **Reviewer 3:**

The reviewer stated that progress has been good. The TESF model has been developed that can simulate the turbulent chemistry cost effectively. Collapsing phenomena have been observed for flash boiling conditions as well as high back-pressure conditions. The reviewer remarked that collapsing of sprays at both these conditions is now being predicted, especially with LES. In addition, the details of the entrainment flow measured by SNL are also being predicted.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer found the team to be very good.

# **Reviewer 2:**

The reviewer complimented the very good collaboration existing among other national laboratories, universities, Convergent Science, and industry.

# **Reviewer 3:**

The reviewer noted that leveraging ASCR resources for HPC using industrially relevant software and enginedesign use cases by means of collaboration were all good. However, in this mode the reviewer pointed out that it is crucial to avoid (in reality or perception) unfair subsidies for product development for a single chosen partner. The reviewer commented that DOE should ensure this project does not result in unfair subsidies for any specific commercial partner and does not create such an appearance now, or in the future. Source code access for spray and HPC could lead to post-competitive product development if DOE is not careful.

The reviewer stated that mitigation of these issues should be considered in one or both of two ways: removing those activities from the project scope and/or a deliberate multi-code strategy. Because conclusions or calibrations are historically proven to be artificially shaped (to varying degrees) by the peculiar limitations, methods, or assumptions of an individual simulation tool, the latter redundancy approach can add value by not only avoiding such distortions but (frequently, from past experience) also by exposing otherwise-hidden lessons and uncertainty sources.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer noted that future research is clearly indicated. The authors could establish targeting selective engine cases to assess improvements in the context of emissions and fuel economy. This may be done in closer collaboration and allocating some of the resources with engine OEMs.

# **Reviewer 2:**

The reviewer suggested that the model, with its new developments and capacity computing, should be exercised on a small subset of engine design, for example, just spray geometry variables that affect spray characteristics. The following spray variables can be swept over relevant ranges of interest: L/D; number of plumes; spray angle; nozzle entrance effects; nozzle surface roughness; pre-hole diameter; fuel temperature; and pitch circle.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

No comments were received in response to this question.

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

No comments were received in response to this question.

# Improved Solvers for Advanced Engine Combustion Simulation: Matthew McNenly (Lawrence Livermore National Laboratory) - ace076

# Presenter

Matthew McNenly, Lawrence Livermore National Laboratory

# **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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer commented that the project team gave a good, clear presentation of its approach, which was tied meaningfully to others' efforts.

# **Reviewer 2:**

The reviewer remarked that the approach has been reasonably proven and has yielded excellent results.

# **Reviewer 3:**

The reviewer commented that the broad approach is similar to that used in past years. The project team is creating reactor Jacobians for LLNL's chemistry algorithms. This effort is anticipated to reduce computational time significantly.



Some simulation results were shown for a homogeneous reactor. The reviewer asked the project team to please provide a rationale for the relevance of this configuration to an engine. The chemistry solver is incorporated with CONVERGE, and results are shown for HCCI simulation. The reviewer commented that the approach of verification/validation of the chemistry solver with a 1D counterflow flame should be further discussed. This configuration is a bit removed from an engine environment and does not include any multiphase effects such as multicomponent vaporization which is intrinsic to both certain engine conditions and most certainly multicomponent surrogates of the type this project is investigating. The reviewer would like an explanation.

# **Reviewer 4:**

The reviewer noted that the project team is developing an advanced mathematical method to solve full mechanisms of multicomponent fuels, which has the potential to improve the design tool for industrial engine design and optimization. The demonstrated computational efficiency for multicomponent fuels (more than 2,000 species)

makes it feasible for full 3D CFD simulations with full mechanisms for chemistry in an affordable time although it has to demonstrate its scalability within the 3D CFD solver on an HPC/GPU.

# **Reviewer 5:**

The reviewer commented about the impressive portfolio of modeling tools and improvements to those tools but found it hard to determine the accuracy of the simulations (i.e., compared to experimental data) from the presentation content. The reviewer suggested that perhaps the project team should include some detail on how the simulations results are confirmed in future reviews.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer remarked that being able to significantly reduce the computer time while obtaining the same solution is outstanding.

# **Reviewer 2:**

The reviewer commented that better treatments to support soot prediction are a welcome and valuable direction of progress. The research on heuristic logic for automated mechanism debugging and timestep improvement is innovative and broadly valuable. The reviewer enthusiastically looked forward to seeing the planned report and user guide.

# **Reviewer 3:**

The reviewer congratulated the project team for earning a 2015 R&D 100 award. The solver has demonstrated good speed-up on a homogenous reactor. The reviewer found some issues that needed improvement or clarification. For example, the reviewer observed that the accuracy of the faster solver was not well validated. The reviewer questioned how the solver would perform in a heterogeneous reactor, e.g., in-cylinder combustion. Lastly, the reviewer asked whether this solver/algorithm is robust/effective for different multicomponent fuels other than the demonstrated fuels.

# **Reviewer 4:**

The reviewer noted that  $C_{20}H_{42}$  is listed as a biodiesel component, and that this needs some further elaboration. As a general rule, it will not be a biodiesel component. The reviewer remarked that it depends highly on the biofeedstock. For example, algae will yield different dominant species from rapeseed, which in turn will be very different from a fatty acid methyl ethers (FAME) fuel.

The reviewer commented that there is confusion about the fuel systems being investigated. The project team notes a 9-component surrogate last year, then a 12-component surrogate this year, and yet further a 13- component surrogate this year. The reviewer noted that an improved cetane mechanism is being incorporated into the model development and stated that this is confusing. The reviewer asked that the project team please try to bring some clarity and rationale to the choice of surrogate components.

The reviewer noted that some IDT data for methyl decanoate (MD) are included, but asked about the relevance of MD and whether it covered the performance for a FAME (biodiesel) fuel. The reviewer wanted further discussion of this issue. For the surrogates investigated, the reviewer questioned why they have to contain tens of thousands of reactions as it seemed a bit of overkill. LLNL has capabilities for mechanism reduction so this concern needs greater clarity.

The reviewer commented that the Zero-RK award is impressive and offered congratulations. Among the things that are listed as important to add to the Zero-RK model are a pressure-dependent reaction rate table and large molecules. The reviewer asked if Zero-RK could be incorporated into CFD code that addresses multiphase spray-injection effects.

The reviewer asked about how the soot is handled. Presumably gaseous precursors can be computed (e.g., polycyclic aromatic hydrocarbons [PAHs], acetylene, etc.). It would be instructive to compute a flow configuration

and predict the distribution of soot precursors, which presumably can be done right now. Then, when a soot model is incorporated, it would be useful to see how the distribution of soot aggregates track with the predictions of the precursors.

# Question 3: Collaboration and coordination with other institutions.

# **Reviewer 1:**

The reviewer noted that the project has collaborations with academia, industry, and national laboratories to have solver development/validation, make the solver accessible to industry, and closely work with industry on the applications of the solver.

#### **Reviewer 2:**

The reviewer stated that the collaborators on this project are adequate and span the range from academia, industry, and national laboratories. The project includes several industries that market or use computer codes (Convergent Sciences, Cummins, GM, and NVIDIA). The reviewer would like an explanation as to why King Abdullah University of Science and Technology is not listed among the academic collaborators, while the university is providing some data.

# **Reviewer 3:**

The reviewer observed that Co-Optima has clearly increased the depth of collaboration.

# **Reviewer 4:**

The reviewer said that the team has collaborated with other institutions, including academics and industry.

#### **Reviewer 5:**

The reviewer noted that GM is evaluating tools in CONVERGE and said to continue to pursue collaborations with OEMs.

# 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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer commented that a range of challenges for future work is listed, one of which is soot. The project team may be able to get some insights about soot with the team's current capabilities by simply tracking predicted soot precursor distributions and use this information to compare with measured PM emissions from a suitable combustion configuration. The reviewer suggested that an engine may be too complex to use as an experimental configuration for this purpose, but a combustion fluid (CF) flame might work. The reviewer noticed that spray dynamics are listed as remaining challenges and asked whether this include multicomponent evaporation processes. The reviewer wanted to know the meaning of nonlinear fuel component interactions.

# **Reviewer 2:**

The reviewer remarked that turbulence/chemistry interaction closure is an appropriate focus and may change some of the present conclusions relative to mechanism optimization and computational approaches. This future work may necessitate closer collaboration with the CFD solvers that utilize Zero-RK, and the reviewer recommended a deliberate multi-code strategy to ensure the greatest impact on the industry.

# **Reviewer 3:**

The reviewer commented that the proposed research will extend the solver with new soot model algorithms and chemistry-turbulence interaction, which would potentially improve soot prediction and solution of chemistry in a turbulent flow using considering transport effects. However, it does not provide feasible approaches and potential barriers/alternatives.

# **Reviewer 4:**

The reviewer encouraged future work in simulating practical engine combustion using CFD. Soot modeling is also necessary at the next step. However, the reviewer did not encourage tackling the problem of spray dynamics

because the spray model uses a parcel approach and does not truly represent the fuel drops and spray dynamics are heavily influenced by turbulence. The reviewer noted that this project is mainly focused on the chemistry solver; thus, it does not seem logical to tackle the problem of turbulence. Nonetheless, the reviewer encouraged the project team to pursue the problem of turbulence-chemistry interactions.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

**Reviewer 1:** 

The reviewer commented that better, faster chemistry will aid in the development of better, more efficient engines that burn less petroleum.

Reviewer 2:

The reviewer noted that this work can be applicable to biofuel combustion simulation.

**Reviewer 3**:

The reviewer responded, yes, from a broad perspective.

# 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 resources to be adequate for the planned activity.

**Reviewer 2:** The reviewer said that the resources are appropriate.

**Reviewer 3:** 

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

# Cummins-ORNL\FEERC Combustion CRADA: Characterization and Reduction of Combustion Variations: Bill Partridge (Oak Ridge National Laboratory) - ace077

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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer stated that the project seeks to assess fluctuations in cylinder charge and to apply remedies in hardware and control strategies. The results will be improved combustion uniformity and implementation of advanced combustion strategies.

# **Reviewer 2:**

The reviewer commented that the project team used a good approach relative to developing the new diagnostic capabilities. The reviewer understood that this is a CRADA, but stated it would be good to see what insights are learned given the capability of modern CFD tools.



The reviewer asked if tools are able to accurately match (i.e., predict) the measurement. If required, the reviewer suggested that maybe this can be done independently of the CRADA partner, if that is what is required to make the information public.

# **Reviewer 3:**

The reviewer noted that this project addresses the need for accurate and efficient diagnostics for in-cylinder processes in engines. The project team has developed a range of diagnostics for engines, including the development of an EGR probe that has proven to be quite effective that the team continues to improve, a wavelength modulation spectroscopy method that improves the signal-to-noise ratio (SNR), a method to measure cycle-to-cycle variations in oxygen concentration, and a diagnostic to measure exhaust transients.

The reviewer observed that the overall importance of diagnostics to evaluate engine performance cannot be overstated. In that regard, the project is relevant. In developing the project team's approach, the reviewer remarked that it may be beneficial for the team, and indeed all the national laboratories, to consider developing some sort

of a diagnostics center spread across the laboratories that catalogues capabilities. This effort could begin with making a list of all laboratory capabilities, who does what, identifying what needs to be measured that cannot now be measured, and then coordinating activities. In this project, as an example, the EGR probe is interesting, and the reviewer asked whether other laboratories have a need for it. The reviewer presumed the answer to be yes.

In the development and application of the diagnostics mentioned, the reviewer commented that it would be relevant to compare capabilities against competing technologies. Though this may have been done in prior presentations, the reviewer stated that it would be useful to make the comparison part of the presentation of experimental results.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# Reviewer 1:

The reviewer thought it was impressive that ORNL was able to improve the signal and reduce the noise for the new probe design. The reviewer commented that it would have been good to have the on-engine results performed sooner so they could have been included in the presentation.

# **Reviewer 2:**

The reviewer found the work presented to be practical and valuable and an example of a well-run CRADA. The work studied back-flow measurements using a multi-color EGR probe. The probe is effective in estimating the exhaust gases moving upstream of the intake port during the engine valve overlap. This year's work has focused on analysis of the cylinder charge. The probe has been reworked to improve the data quality and ability to capture fast transients. Some questions arise regarding the uncertainty evaluation of the measurements. There is no formal treatment of uncertainty (e.g., benchmarking the optical technique with gas analyzers).

# **Reviewer 3:**

The project team reported EGR probe measurements of  $CO_2$  and  $H_2O$  in-cylinder measurements, developed a new probe design with improved SNR, and developed a new diagnostic for measurement of exhaust  $O_2$ ,  $H_2O$ , temperature, and pressure. The effectiveness of these diagnostics was demonstrated with some experimental results. The reviewer thought it would be useful for the project team to consider ways to make the EGR more robust such that it could be used in the sooting region of engines.

# Question 3: Collaboration and coordination with other institutions.

# **Reviewer 1:**

The reviewer remarked that it was a very impressive team, which has been very successful in providing good performance results.

# **Reviewer 2:**

he reviewer said that there was good collaboration with the CRADA partner.

# **Reviewer 3:**

The reviewer pointed out that the project team has a CRADA with Cummins that has provided valuable input to the project. Academic partners are also included that have facilitated improved performance of the EGR probe. The reviewer wanted to have better clarity on what each of the partners—from academia and industry—provides to the project and their relevance as doing so would establish the need for the partnership. The reviewer also stated that it would be useful to provide some data from the partners to show how they are folded into 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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer commented that future work is indicated as it would be important to develop approaches on how to

use the information provided to limit the variability on flow. It will be important to understand how this variability influences engine efficiency or causes it to deteriorate.

# **Reviewer 2:**

The reviewer thought it would be good to see this new diagnostic evaluated on other projects and to see how well current simulation tools are able to predict.

# **Reviewer 3:**

The reviewer observed that future work will include improving the EGR probe with a new design for collimated fiber output, measuring high temperature exhaust, adding a CO-measurement capability, and developing new measurements for parameters. The reviewer stated that these tasks are relevant though are a bit vague. More specificity would be advantageous to the understanding of the research going forward. Presumably, at some point the probe development effort will be completed. The reviewer asked when the EGR probe design is expected to become a mature diagnostic.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# **Reviewer 1:**

The reviewer agreed that reducing variations is a good thing and asked if the CRADA partner can quantify the potential benefit. It would help to gauge the relevance (and budget) of this as compared to other projects.

# **Reviewer 2:**

From a broad perspective, the reviewer remarked that this project is relevant by its ability to provide new and more accurate measurements of engine performance, though it is somewhat narrowly focused. As noted above, it would be beneficial to combine the efforts here with those from other national laboratories to develop a national consortium of engine diagnostics (e.g., a catalog of engine measurement capabilities). Such an effort could both alert the community at large of diagnostic capabilities and thereby draw attention to the unique capabilities and perhaps also better focus the development and instrument efforts of existing diagnostics (e.g., such as is included as part of this project).

# 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 are sufficient, but again it would be good to see this new diagnostic evaluated on other projects.

# **Reviewer 2:**

The reviewer stated that resources seem adequate although ultimate judgement would have to come from a cost/ benefit analysis based on DOE's investment relative to the commercialization potential.

# Thermally Stable Ultra-Low Temperature Oxidation Catalysts: Janos Szanyi (Pacific Northwest National Laboratory) - ace078

# 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer found a good blend of experimental work and characterization data. The reviewer commented that there was a nice balanced division of effort between GM and PNNL that harnessed the strengths of both organizations (GM for reactor testing and PNNL for catalyst characterization).

# **Reviewer 2:**

The reviewer noted that the approach with various characterization tools was strong. The reviewer commented that not knowing the compositions of the excellent catalysts GM brought to the project is a deficiency. The temperature of hydrothermal aging was only 750°C.



Figure 4-30 - Thermally Stable Ultra-Low Temperature Oxidation Catalysts: Janos Szanyi (Pacific Northwest National Laboratory) - Advanced Combustion Engines

Higher temperatures are important to mimic real aging conditions, in the reviewer's opinion.

# **Reviewer 3:**

The reviewer stated that this work supports the need for LTAT requested by USCAR and the automotive OEMs. Additionally, this activity also supports the OEM's need for reduced PGM usage and cost by using Cu-based catalysts in place of both platinum (Pt) and palladium (Pd) for CO oxidation. In the past, the use of Cu-based catalysts did not hold up well after hydrothermal aging. In contrast, as this work shows, the reviewer acknowledged that selecting the correct praseodymium (Pr) and Zr support material can greatly enhance the survivability of the catalyst after hydrothermal aging. A second challenge that was addressed in this work was the resistance to S poisoning of the CO oxidation reaction or the ability to regain that function after regeneration. The reviewer noted that using these challenges as part of a benchmarking process for various Cu formulations easily discriminated the CO activity of the catalysts tested.

Yes

(100%)

Sufficient

(100%)

# **Reviewer 4:**

The reviewer stated that the focus on  $C_3$  hydrocarbons is a good start, and moving to longer chains and aromatics would be beneficial. The reviewer remarked that including S studies in base-metal catalysts is critical, as well as hydrothermal aging. The use of theoretical density functional theory (DFT) in addition to experiments is very nice. PNNL has many instruments to fully analyze and characterize catalyst materials and their behavior. The reviewer commented that the project team should have included  $CO_2$  in feedgas. Another reviewer comment was that it would have been nice to look at HC and  $NO_x$  interactions and the potential to reduce  $N_2O$  formation versus Pt/Pd diesel oxidation catalysts (DOCs).

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer commented that the results presented used appropriate gas feeds, fuel poisons, and aging and showed that Cu formulations incorporating Pr and Zr can act as effective CO oxidation catalysts at low temperatures. Although not resistant to S poisoning, the catalyst does show the ability to be regenerated at higher temperatures. The characterization work was able to directly link the deactivation of other Cu formulations to either the loss of surface area or the formation of surface carbonates. The reviewer commented that what was not explained well was why the hydrothermally aged Cu/Pr/Zr (Cu/GMR6) formulation showed a lower light-off temperature than the fresh. This is not expected because the fresh catalyst should have high surface area and should be relatively free of carbonates. With respect to S, requiring 750°C for effective regeneration may have a detrimental effect on the long-term activity of the catalyst and limit where in the aftertreatment system the catalyst can be located. Finally, the reviewer commented that formation of N<sub>2</sub>O under the reaction conditions presented in this study must be investigated due to GHG accounting.

# **Reviewer 2:**

The reviewer commented that the GMR5 and GMR6 catalysts are good, and the GMR6 catalyst even gets better because it shows that lanthanum (La) is a structural stabilizer and Pr increases oxygen mobility. The reviewer noted the interesting result where carbonate formation in the absence of S leads to loss of activity at 175°C as well as the interesting isotopic results shown related to oxygen mobility. This reviewer also reported the following: HC and NO light-off impact; S does not make Cu sulfate; and just the support. In conclusion, the reviewer observed very interesting results.

# **Reviewer 3:**

The reviewer said that the work on catalyst fundamentals was excellent, but the reviewer had just some issues with the approach as noted above.

# **Reviewer 4:**

The reviewer stated that the project team needed to include  $CO_2$  during the activity measurements. It will always be present in the exhaust as long as hydrocarbons are combusted, and if carbonate formation caused the deactivation at 175° C without  $CO_2$  in the feedgas (as shown on Slide 12), the presence of  $CO_2$  will only make it worse. The thermal aging assessments (72 hours of high-temperature hydrothermal aging [HTA] at 750°C) is much more realistic than what was used for the NO oxidation work last year (1 hour at 700°C).

The S poisoning work on Slide 15 demonstrates the well-known S sensitivity of base-metal catalysts as they have to operate at 600°C or more to keep them purged of S and to maintain high activity (see SAE 922251). The project team indicated that it assessed S regenerations at 500°C and 750°C, but the reviewer does not recall seeing the performance after the 750°C desulfation. The reviewer asked if it was more effective than the 500°C desulfation.

The reviewer was not sure what the project team meant in the summary when it said "modest  $C_3$  hydrocarbon oxidation activities (...but not  $Co_2O_3$  and  $Mn_2O_3$ )." The reviewer wanted to know what exhibited more  $C_3$  activity than the Cu/CeO<sub>2</sub> catalyst.

# Question 3: Collaboration and coordination with other institutions.

# Reviewer 1:

The reviewer observed that combining the synthesis and characterization capability of PNNL with GM formulation and testing is a good match for this work. Perhaps including a catalyst supplier to supply additional preparation expertise would benefit the formulation aspect.

# Reviewer 2:

The reviewer pronounced the collaboration between the groups involved to be good.

# Reviewer 3:

The reviewer commented that the GM partner directed the work.

# Reviewer 4:

The reviewer liked the good collaboration with GM and mentioned the commendable division of labor.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer suggested that future work to address any remaining characterization using long chain HCs is appropriate for the intended application.

# Reviewer 2:

The reviewer said that the project ends this year, but it has raised a number of questions that will hopefully be more fully explored.

# Reviewer 3:

The reviewer stated that the project was completed, and final reports and publications will be completed but no new research. The reviewer picked a middle rating here because "not applicable" was not a choice.

# **Reviewer 4:**

The reviewer remarked that the project is complete and there are no future plans.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# **Reviewer 1:**

The reviewer stated that this project supports USCAR - U.S. DRIVE initiatives to address the need for effective lean aftertreatment systems and technologies at low temperatures.

# Reviewer 2:

The reviewer commented that catalysts like this are enablers of using more efficient combustion methods that give lower exhaust temperatures.

# **Reviewer 3:**

The reviewer mentioned that low-temperature DOCs are important to improve fuel efficiency of lean powertrains.

# **Reviewer 4:**

The reviewer said that low-temperature catalysts will be a requirement for future engines with improved fuel economy that reduce our dependence on foreign oil, as the higher efficiency engines will generate lower exhaust temperatures.

# 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 no issue with funding or resources in general.

# Reviewer 2:

The reviewer stated that a good amount of funding from GM shows industry interest.

# Reviewer 3:

The reviewer said that the project is complete.

# High-Efficiency GDI Engine Research, with Emphasis on Ignition Systems: Thomas Wallner (Argonne National Laboratory) - ace084

# Presenter

Riccardo Scarcelli, Argonne National Laboratory

# **Reviewer Sample Size**

A total of one reviewer evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer stated that this project addresses a near-term technology of increasing dilution tolerance with advanced ignition systems. While the improvement in efficiency in a given engine will be small, it has the potential of impacting the whole LD fleet and therefore having a large impact on petroleum reduction.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# Numeric scores on a scale of 1 (min) to 4 (max) This Proiect Sub-Program Average 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 1.50 2.00 2.50 0.00 Approach Collaboration Weighted Tech Future Accomplishments Research Average **Relevant to DOE Objectives** Sufficiency of Resources Yes Sufficient (100%)(100%)

Figure 4-31 – High-Efficiency GDI Engine Research, with Emphasis on Ignition Systems: Thomas Wallner (Argonne National Laboratory) - Advanced Combustion Engines

# **Reviewer 1:**

In the reviewer's opinion, progress has been poor this year. The modeling progress is good but adds minimally to the knowledge base. The modeling work supports the main experimental evaluation but cannot justify the project itself.

The stretch goal of 20% over a stoichiometric GDI engine with production spark was adopted in June of 2015. The reviewer questioned where this goal is coming from and stated that this is an incorrect goal as the baseline should be a stoichiometric GDI engine with production spark and EGR. Thus, the reviewer would anticipate increases of the order of 1%-5% with advanced ignition systems. According to the reviewer, the data in Slide 15 show this point very clearly.

The reviewer suggested that the focus should be largely on an experimental evaluation of various advanced ignition concepts like transient plasmas, corona ignition, and laser ignition. Over the past three years much of this

experimental work has been done and reported. Small gains in engine efficiency and combustion stability have been reported. Thus, the reviewed noted that the big picture conclusion and information of the worth and current state-of-the-art of advanced ignition systems have been accomplished. The reviewer questioned what more the project could hope to contribute.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer remarked that better guidance from OEMs is needed to keep this project focused on the main thing. Collaboration should not occur for the sake of collaboration.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer commented that the focus should be on understanding the mechanism of ignition with Transient Plasma Systems, Inc. (TPS), Corona, or laser ignition, and improving the process to gain dilution tolerance. More optical engine experiments should be conducted.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

No comments were received in response to this question.

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

No comments were received in response to this question.

# Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization: Todd Toops (Oak Ridge National Laboratory) - ace085

**Presenter** Todd Toops, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer praised the range of methods used in analyzing the catalytic materials in the project as excellent. Also, the reviewer commented that the goals of the characterization include mimicking realistic conditions as well as exploring the impact of S.

# **Reviewer 2:**

The reviewer stated that the evaluation techniques were great. Regarding proposing to compare the low-temperature combustion diesel (LTC-D) fuel to real-life fuels, the reviewer suggested considering the worst case fuel, which contains HC chains and aromatics.

# **Reviewer 3:**

The reviewer found a clear approach, developed with strong relevance to the CLEERS priorities, the U.S. DRIVE workshop report, and the U.S. DRIVE ACEC Technical Team Roadmap. ORNL is developing and employing the protocols to evaluate novel catalysts. In addition, the laboratory is leading round-robin testing and identifying new materials through collaborations.

# **Reviewer 4:**

The reviewer stated that the project was a nice detailed look at several different types of catalysts (oxidation catalysts, PNAs, and HC traps). The reviewer commented that Slide 6 (comparing  $SnO_2$ -MnO<sub>x</sub>-CeO<sub>2</sub> with simple conditions and full protocol) shows that it is very important to use the protocols recommended by the ACEC Technical Team. For some reason, the NO curve is missing from the graph on the right side.





Figure 4-32 - Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization: Todd Toops (Oak Ridge National Laboratory) - Advanced Combustion Engines

# **Reviewer 5:**

The reviewer commented that the breadth of work occurring at ORNL under the central theme of carbon monoxide/ hydrocarbon (CO/HC) oxidation and remediation appears well coordinated and very appropriate. Exploring catalyst solutions for low-temperature oxidation of CO and HC species is strongly supported by USCAR engine and aftertreatment objectives. The inception stage exploration of multiple pathways to achieve high CO and HC oxidation performance is critical to finding viable solutions employing different catalyst technologies in a timely manner. However, the reviewer commented that a better understanding of how poisons, such as S, alter the activity of the catalysts under development is needed to provide a thorough characterization of the technologies.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer commented that the findings of this project are very interesting and potentially useful. The work on zirconia as the shell of a catalyst was very interesting and should be continued. Also, the silver (Ag)-zeolite system for HC storage is very interesting.

# **Reviewer 2:**

The reviewer said that the evaluation techniques were great. There is a need to fully understand observed phenomena, such as why PGM inclusion improves S tolerance and removal. The reviewer also asked why  $CuO_x$ - $CoO_y$ - $CeO_2$  (CCC) shows the ability to store and release  $NO_x$  with peaks at certain temps and whether that that peak can be influenced.

# **Reviewer 3:**

The reviewer stated that there were several strong technical accomplishments achieved this year: identified mixed metal oxides that improve HC conversion (need for additional catalyst for low-temperature activity); measured S tolerance of CCC (showed need for PGM, specifically Pt); explored S mitigation strategies for PGM with CCC, which improves S tolerance; developed a new core/shell technique that improved zirconium dioxide (ZrO<sub>2</sub>) surface area, which led to improved HC conversion; implemented nano Pd dispersion on Ce-Zr nanoparticle dispersed on aluminate and approaching target activities; determined that the key attribute of a Ag/Al HC trap is deep ion exchange and low Si:Al ratio; and demonstrated the NO adsorption on the ZSM-5 zeolite and the impact of the pretreatment temperature.

# **Reviewer 4:**

The review commended the project team for considering both thermal aging and S poisoning effects. Slide 13 shows the harsh impact of SO<sub>2</sub> on the CCC catalyst (with and without Pt), although having a front zone of Pt/ $Al_2O_3$  appeared to mitigate the effect of S on the CCC catalyst. Unfortunately, the reviewer noted that the  $C_3H_6$  performance on Slide 12 was better with CCC in front of the Pt/ $Al_2O_3$  catalyst, presumably by oxidizing the CO before the Pt/ $Al_2O_3$  catalyst and removing the CO inhibition. The reviewer asked if the project team had tried a PA+CCC split-bed system during the light-off tests.

The reviewer also wanted to know why the Pt/CCC catalyst looks so much worse than the CCC catalyst after poisoning on Slide 14 and whether the Pt catalyzes the oxidation of  $SO_2$  to  $SO_3$ . The reviewer complimented the nice work on the Zr-on-Si core-shell catalyst and the very nice micrographs. The reviewer noted that  $CO_2$  needed to be included in the feedgas (Slide 12) as it can promote carbonate formation. If the project team wants to see  $CO_2$  formation, maybe the team could run tests with and without the feedgas  $CO_2$ .

The reviewer remarked that the researchers involved in this work have developed novel approaches to achieve higher CO and HC oxidation activity at low temperatures. The use of these techniques of dispersing the precious metal and/or combining PGMs with non- PGM catalysts to enhance oxidation activity is of significant interest in the catalyst community and applicable to aftertreatment systems in use today. Both the formulation and characterization assets of the national laboratory are well suited for this work. However, the reviewer pointed out that understanding the S poisoning mechanism for the Pt plus carbon composite catalyst (Pt+CCC) and using HCs other than propylene would benefit the research and provide a clearer picture of the performance of the catalysts. In

addition, work at Ford has shown that Rh, without Pd, can perform as a more effective CO light-off catalyst on the right support. This work should including Rh-based catalysts as a comparison of activities. The HC trap work also supports the need for HC remediation, but requires additional testing that includes aged samples and appropriate feed conditions.

# **Question 3: Collaboration and coordination with other institutions.**

# Reviewer 1:

The reviewer commented that interaction with the automotive OEMs through USCAR and catalyst formulators increases the value of the research performed here. Also, this work takes advantage of the many assets at ORNL.

# **Reviewer 2:**

The reviewer remarked that there is a broad group of collaborators, both commercial and university-based.

#### **Reviewer 3:**

The reviewer stated that there was a good combination of industry and academia.

#### **Reviewer 4:**

The reviewer found the addition of more partners, especially catalyst suppliers, to be excellent.

#### **Reviewer 5:**

The reviewer indicated that it was good to have a catalyst supplier as a partner, and an OEM would also be a helpful partner.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer noted that given the breath of research and the limited funding available, it is not certain that all the work can be addressed satisfactorily. Given that, the future work discussed is appropriate and has the potential to significantly add to the activity of the catalysts and their characterization.

# **Reviewer 2:**

The reviewer found the future work proposed to be very appropriate. The areas of trapping and enhanced activity by maintaining dispersion are very important. It is hard to tell if the trapping will receive the effort it deserves because of the importance of preventing emissions at low temperatures.

#### **Reviewer 3:**

The reviewer stated that performance analysis under laboratory conditions was okay, and there is a need to consider real-life conditions as well.

# **Reviewer 4:**

The reviewer noted strong future directions to investigate S interactions and support modifications but plans for trapping materials could be better described.

# Reviewer 5:

The reviewer suggested that the project team should plan to include other hydrocarbons in its PNA and HC trap work, such as  $C_2H_4$  as it is more abundant in diesel exhaust than  $C_3H_6$ .

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# **Reviewer 1:**

The reviewer stated that this is highly relevant inception stage research and consistent with the call for LTAT by USCAR and the needs of the OEMs in general.

# **Reviewer 2:**

The reviewer noted that, as for most projects in this category, by enabling the use of more efficient combustion, these systems support the move to improving overall fuel economy.

# **Reviewer 3:**

The reviewer stated that aftertreatment performance is the key for best efficiency of engine.

#### **Reviewer 4:**

The reviewer stressed that low-temperature catalysis is the key barrier to high efficiency combustion strategies.

#### **Reviewer 5:**

The reviewer said that low-temperature catalysts will be required for emission control on future engines with higher fuel efficiency and therefore lower exhaust temperatures.

# 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 these experiments involving synthesis and bench studies are costly as more resources are necessary to meet project and program goals, especially for the NH<sub>3</sub> SCR.

#### **Reviewer 2:**

The reviewer found funding and resources to be borderline sufficient.

# **Reviewer 3:**

Despite comments about insufficient resources last year, the reviewer noted that the goals of the project have been modified slightly to move forward.

# **Reviewer 4:**

The reviewer said that resources seem sufficient.

# High-Dilution Stoichiometric Gasoline Direct-Injection (SGDI) Combustion Control Development: Brian Kaul (Oak Ridge National Laboratory) - ace090

**Presenter** Brian Kaul, 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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer stated that the research team is good and has previously demonstrated high competence in identifying deterministic coupling of causes and effects. It has leveraged the Cummins-ORNL CRADA, which is pursuing this question from a diagnostic development approach. The team is moving toward developing models of the phenomena of interest, and its approach to the problem appears technically sound.

# **Reviewer 2:**

The reviewer noted that this project uses a fast EGR probe to measure the external EGR cycle-by-cycle variation



Figure 4-33 - High-Dilution Stoichiometric Gasoline Direct-Injection (SGDI) Combustion Control Development: Brian Kaul (Oak Ridge National Laboratory) - Advanced Combustion Engines

in order to understand the physics behind the effect of EGR on high dilution gasoline combustion. The results shown are encouraging and with good repeatability. Based on the feedback from the EGR measurement, engine cycle-to-cycle and next- cycle control strategies have been developed. However, further improvement is needed for implementation in engines. HPC modeling has also been used to assist the development of the control strategy.

# **Reviewer 3:**

The reviewer suggested that it might be worth developing a P-diagram for combustion stability and identifying real world sources of noise. Some could have significant impact and would need to be addressed (i.e., injector deposits). OEM input could be very helpful here.

# **Reviewer 4:**

The reviewer commented that engine control development to reduce cycle-to-cycle variability is an important topic, but it is not clear how simulation is going to impact the project.

# **Reviewer 5:**

The reviewer stated that this project is not focused on key barriers related to improving engine efficiency in a significant way to reduce petroleum usage. An attempt should be made to quantify benefits of reducing cyclic variability to permit operation at the edge of stability to determine if it is worthwhile, especially in light of the fact that OEMs already have model-based controls to control a variety of engines, each with its own idiosyncratic long-loop EGR dynamic composition behavior. Much of this work falls in the domain of OEM controls engineering, and given their vast resources and knowledge of real-world, hardware-specific behavior, this project will not have much, if any, impact on future controls direction.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer commented that good progress has been made against the objectives of the program. The techniques used lead this program to the right direction. However, more work is needed to develop better control models. CFD modeling will definitely help in finding the way to improve the control models by providing more insight of what is happening inside the cylinder.

# **Reviewer 2:**

The reviewer remarked that this is a very challenging problem. It is still not clear the exact extent to which overcoming this problem will benefit engine performance. However, from the perspective that every little bit helps, it is important to understand. It would be helpful to quantify the potential benefit. The reviewer thought that a prediction of the potential benefits could be made.

# **Reviewer 3:**

The reviewer commented that the use of a fast EGR sensor is an interesting technique to diagnose engine operation. Only minor progress has been demonstrated with the controls development. It is not relevant to reduce the coefficient of variation (COV) by 2% when the starting point is near 20% COV.

# **Reviewer 4:**

The reviewer stated that it is absolutely worthwhile to go after 1% efficiency gains by reducing cyclic variations, but given the vast number of engineers working at the OEMs on reducing cyclic variations due to a variety of causes, the reviewer asked how this project will make an impact. None of the results presented this year are any closer to showing to this reviewer that all of this is going to be worthwhile at the big picture level and that there is a pathway for industry to capture the findings of this study.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer remarked that there is very good collaborations with Cummins, National Instruments, ANL, and Bosch. Broader collaboration could be sought.

# **Reviewer 2:**

The reviewer suggested that if the project team could engage with OEM control engineers, it might be constructive. The reviewer also wanted to know how the approach the team is taking melds with what industry is doing.

# **Reviewer 3:**

The reviewer stated that the project team needs to include an OEM controls team to understand how techniques in this project might be implemented in a production controls environment.

# **Reviewer 4:**

The reviewer stated that it is imperative that the project should be guided by a controls team at an OEM. Otherwise, there is a risk that this project can end up doing a lot of good work, but be largely irrelevant or a duplication.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# Reviewer 1:

The reviewer noted that, basically, the proposed future work showed a good extension of present work.

# Reviewer 2:

The reviewer suggested that the team should make an estimate of the potential benefit.

# **Reviewer 3:**

The reviewer found that it is not clear what model-based control means for this project. Future work needs to include a practical assessment of the potential engine efficiency improvement that is available based on this work.

# **Reviewer 4:**

The reviewer commented that it is risky to apply learnings from a lean combustion project. In that case, engine torque (or indicated mean effective pressure [IMEP]) is largely proportional to fueling level alone. Hence, using fueling to control the next cycle heat release to reduce COV is appropriate. Using such a fueling scheme to control a stoichiometric combustion engine, where torque is proportional to fuel plus air, may have some unforeseen challenges.

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

# Reviewer 1:

The reviewer indicated that better controls can lead to more efficient engines that reduce fuel consumption.

# **Reviewer 2:**

The reviewer asserted that further understanding the causes of cyclic variations, and their relative weights, will be useful information.

# Reviewer 3:

The reviewer remarked that improved controls to allow increased dilution tolerance can be leveraged to increase engine efficiency.

# **Reviewer 4:**

The reviewer commented that the chances of having a significant impact on petroleum displacement are minimal.

# 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 seem sufficient for the proposed work.

# High-Efficiency VCR Engine with Variable Valve Actuation and New Supercharging Technology: Charles Mendler (Envera LLC) - ace092

**Presenter** Charles Mendler, Enerva LLC

**Reviewer Sample Size** A total of eight reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer suspected poor combustion performance with the high CR because typical pent roof combustion chamber geometries are not conducive to CRs much beyond 12.5-13:1. The reviewer suggested that some CFD or fixed CR experiments would be valuable prior to completing the build of the variable CR (VCR) engine to define the correct maximum CR.

Internal EGR is necessary for good combustion stability at low loads, but at a high CR, there will be no provision for the required valve overlap to generate the internal EGR.

The reviewer noted that the project team claims improved time to torque



due to low CR operation. There is a need for at least GT-POWER modeling to demonstrate that this is feasible with the turbo required for the brake mean effective pressure (BMEP) needed for the application.

The claimed CR increase over several seconds means that VCR will not be useful on typical vehicle transients, which are quite fast relative to a several second switching time. Fast switching is needed for high-to-low CR transients, and slow switching is acceptable for low-to-high transients.

# **Reviewer 2:**

The reviewer thought that friction (the work associated with changing the CR) will be a big challenge and that there may not be a way to ameliorate this if it turns out to be the problem the reviewer thought it will be. To achieve such a significant improvement in engine efficiency, no potential improvement should be left on the table. In light of the likelihood of higher friction, the reviewer asked why not try to recoup some of that loss by pursuing lean combustion.

# Reviewer 3:

The reviewer stated that the project appears to be addressing the issues of VCR basic function, but is not yet addressing some of the logistical issues that have been created. For example, power requirement for moving the cylinder liners should be estimated/calculated and accounted for. Because this is targeted for light duty, operation during a realistic drive cycle needs to be considered to fully quantify the potential benefits of this system. The comparison to Chrysler and Ford BSFC and power is not clear, and the reviewer questioned whether this is really an apples-to-apples comparison.

#### **Reviewer 4:**

The reviewer remarked that the approach to performing the work has strengths of generally following industry accepted approach (establish baselines and metrics [example: V8 pickup/40% fuel economy improvement, similar power], modeling of potential benefits [GT-POWER modeling], hardware development, dyno testing, and controls). The reviewer was concerned that the overhead valve (OHV) V8 baseline powertrain selected for comparison may need reconsideration and that single-cylinder work to confirm GT-POWER results and optimize injector system/combustion chamber is not in scope. The reviewer noted that an unoptimized combustion system may not perform well when moving directly to a multi-cylinder engine.

# **Reviewer 5:**

The reviewer acknowledged that the appeal of a VCR engine is not new and many approaches have been suggested and studied over the years. The approach taken here is perhaps more complicated and risky than some previous avenues pursued so the question (yet to be answered) is can it be made to work effectively.

# **Reviewer 6:**

The reviewer stated that the technical solution proposed (i.e., VCR, Atkinson, and valve lift profile switching) is quite reasonable, but the approach to execute the project is quite poor. At a minimum, there should have been some level of engine testing (e.g., single cylinder) to confirm the combustion performance and to inform the GT-POWER model. To simply say "it is lambda = 1" does not allow the project team to avoid the requisite analyses.

#### **Reviewer 7:**

The reviewer commented that it seems there should have been much more thermodynamic analysis done up front. For the two years of review, there has only been one point from GT-POWER simulation discussed that shows a good BSFC, not great, but just good. Beyond that, it seems a single-cylinder version of this mechanism and cylinder arrangement should be the first logical step. Going from one point on GT-POWER to a full four-cylinder engine seems a big investment and big step without much validation.

#### **Reviewer 8:**

The reviewer stated that the VCR 2.0 is an improvement from the previous iterations from a design standpoint. Using GT-POWER to do the efficiency calculations does not consider the changes to the actual combustion event. So, this project would benefit from CFD modeling to provide insight into the effect of changes to the combustion chamber as CR changes. This will feed into changes in the heat release rate. If the heat release rate is not correct from a trend-wise standpoint, then the estimates of friction, heat release, and ultimately friction will be erroneous. This project would also benefit from additional focus on engine thermodynamic tradeoffs (i.e., higher indicated efficiency versus higher friction losses with a higher CR).

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1**:

The reviewer found reasonable progress with the main focus on developing hardware prototypes for a multicylinder engine.

# **Reviewer 2:**

The reviewer commented that the project team has made good progress in moving towards a testable configuration. That is where the fun and challenges will start.

# **Reviewer 3:**

The reviewer stated that the progress on building a working prototype of VCR 2.0 is looking good.

# **Reviewer 4:**

The reviewer said that progress on hardware development is at a good pace, and the evolution from the 1.0 to 2.0 VCR mechanism is good. But, there was significant reference to GT-POWER results but none were shown so it is impossible to evaluate the technical progress from a combustion/performance/efficiency process. The reviewer said that before making hardware, a detailed modeling study should show the expected full-map performance and efficiency to determine if the VCR system is appropriate.

# **Reviewer 5:**

The reviewer stated that the engine design is progressing nicely. However, the amount of learning associated with this project could be increased by presenting tradeoffs with different valve strategies, different CRs, etc.

# **Reviewer 6:**

The reviewer asserted that there are no data available yet or shown on efficiency improvement and performance. Testing with new hardware is planned. It will be good to have some numerical analysis prior to engine testing to make estimates of performance and provide guidance.

# **Reviewer 7:**

The reviewer remarked that the project has a design and parts are being procured, but there is little confidence that the goal of 40% FE improvement will be achieved. No analysis was shown to show how the engine is predicted to compare to 40%. There was no comprehension on the part of the project team how quickly changing CR (during a drive cycle) directly relates to fuel economy; CR being increased over seconds shows a lack of understanding. The reviewer said that, similarly, saying gas loads will be used to lower CR as a way to keep friction low to minimize losses is flawed. Using gas pressure to move the structure is a loss. The statement that no valve pockets are needed because no valve overlap is needed at high CR is also flawed. The reviewer asked about internal EGR at light- to mid-loads. The reviewer contended that by not doing the upfront combustion development on a single-cylinder engine, the project runs the risk of condemning a good idea.

# **Reviewer 8:**

The reviewer observed that the project lacks added work on the simulation of the mechanical systems to consider parasitic losses.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer remarked that collaboration with Eaton on valve train technology is good, but there is a substantial lack of combustion researchers, OEM's who can give input on the design, or other support on the various aspects of the engine that need to be considered.

# **Reviewer 2:**

The reviewer commented that Eaton is a good partner. The reviewer would like to see more active engagement of OEMs other than sighing the activity.

# **Reviewer 3:**

The reviewer said that compared to the other 15 projects being reviewed by this reviewer, this has the fewest collaborators although the coordination is good with the ones the project team has.

# **Reviewer 4:**

The reviewer stated that Eaton and Envera are working well together. For the VCR device, collaboration would be greatly improved if an OEM or Tier 1 were co-developing. The reviewer noted that the production pathway will require a significant base engine design change with high level commercialization issues that must be resolved relating to combustion design for DI potential durability risks (base engine block and head change) and existing manufacturing considerations (new engine line tooling may be needed).

# **Reviewer 5:**

The reviewer noted that Envera is the lead and Eaton is a subcontractor, but the roles seem to be separate and not collaborative. This project could really benefit from university solid modeling and CFD modeling to provide additional understanding of the structure of the engine architecture, vibration dynamics, and the effect on the combustion process. The reviewer said that it will help to identify where and when losses occur and provide insight to paths forward after the completion of the project.

# Reviewer 6:

The reviewer noted that there is still a need for an engine testing partner.

# Reviewer 7:

The reviewer offered that for this project to be successful and generate any useful information, it needs to engage an OEM or an experienced engineering service provider.

# **Reviewer 8:**

The reviewer commented that a small fraction of the funding going to a university to build a full map GT-POWER model would have been money well spent and would have lent validity to 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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# Reviewer 1:

The reviewer found the test plans to be good. It seems that modeling could play a much bigger role in this project. The reviewer suggested that the project team may need an outside partner to help with this and should consider this in the team's future plans.

# Reviewer 2:

The reviewer said that the plan to run the multi-cylinder engine and obtain results is part of the base plan. It is critical to measure power, performance, and engine-out emissions and relate them clearly to the baseline. Additional OEM or Tier 1 collaboration for confirmation of modeling, combustion system, and value proposition would improve the future research plan.

# **Reviewer 3:**

The reviewer remarked that there is not much to see other than a schedule in the presentation. More details of work to be performed would be needed to properly assess the engine test plan, etc.

# **Reviewer 4:**

The reviewer commented that the actual answer to the question about future research needs will be determined once testing has started and problems need to be addressed.

# **Reviewer 5:**

The reviewer stated that the project team gave far too little discussion of how the engine performance will be validated. The reviewer continued that not only steady-state points, but transient demonstrations, simulated Federal Test Procedure/New European Driving Cycle/US06/World Harmonized Test Cycle (FTP/NEDC/US06/WHTC) operation, and so on are required to evaluate the systems. Other reviewers noted significant work was needed to validate the hardware design of the VCR system.

# **Reviewer 6:**

The reviewer commented that steady-state results will show the benefit of the combustion approach. Given the chosen VCR approach, steady-state results are almost meaningless for quantifying the benefit of VCR. The future work must show the transient response capability of the hardware (i.e., how fast from the CR change).

# **Reviewer 7:**

The reviewer said that the experiments that are proposed appear to be a demonstration. It is not clear that the amount of data collected and analysis associated with the project will provide insight into the thermodynamic

tradeoffs. For instance, if the BTE does not increase as expected, the reviewer questioned whether the data will provide insight into whether this is a friction problem, a heat transfer problem, or a combustion chamber design problem. These learnings are ultimately how DOE and the community benefit from the project.

# **Reviewer 8:**

The reviewer stated that the approach lacks a fundamental plan to demonstrate the thermodynamic and mechanical measures (like a friction measurement).

# Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer noted that a successful VCR engine will contribute to additional efficiency gains beyond business as usual and support DOE objectives.

#### **Reviewer 2:**

The reviewer said this was an interesting idea, and important information could be generated.

# **Reviewer 3:**

The reviewer found VCR to be a very intriguing technology. It has the potential to increase engine efficiency, but also has the potential to make engines a lot more compatible with a wider range of fuel composition in the marketplace. It is a worthwhile technology to pursue in the DOE portfolio. The value of the project will be maximized by focusing on the thermodynamic tradeoffs associated with changing CR.

#### **Reviewer 4:**

The reviewer remarked that if a production-viable VCR system could be developed, it has been shown that useful efficiency improvements could be realized.

#### **Reviewer 5:**

The reviewer stated that the approach would appear to be a possible path to higher efficiency engines that will reduce petroleum usage.

# **Reviewer 6:**

The reviewer suggested that if the approach were successful, it has potential. The barriers should include cost versus competitive technologies.

#### **Reviewer 7:**

The reviewer remarked that VCR technology and variable valve train technology have been clearly identified as enablers to support DOE petroleum reduction objectives. The value proposition and pathway to production for a VCR device could be clearer to insure potential is achieved the marketplace in the near term.

# **Reviewer 8:**

The reviewer commented that the technologies being explored are relevant, but they are not being explored in a robust and relevant way.

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

#### **Reviewer 1:**

The reviewed stated that the resources look okay.

#### **Reviewer 2:**

The reviewer said that the resources are sufficient for the project as scoped. Additional support for more advanced GT-POWER modeling and single cylinder work could improve the score.

# **Reviewer 3:**

The reviewer remarked that it seems as there is a lack of thermodynamic analysis and expertise in this project.

# Reviewer 4:

The reviewer commented that there is a very high project amount for making hardware that may or may not achieve the necessary performance.

# **Reviewer 5:**

The reviewer commented that there are some key elements missing from the project (e.g., 1D and 3D simulations and understanding the impact of friction and control) and the project team does not seem willing to address them. Without these, the project can easily come to the wrong conclusion. As such, the funding is excessive given that the reviewer will not have confidence in the result.

# **Reviewer 6:**

The reviewer would like to see a higher contractor share for work of this magnitude.

# Lean Miller Cycle System Development for Light-Duty Vehicles: David Sczomak (General Motors) - ace093

**Presenter** David Sczomak, General Motors

**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, feasible, and integrated with other efforts.

# **Reviewer 1:**

The reviewer remarked that an integrated, comprehensive strategy was presented in very nice detail. This appears to be a well thought-out plan. The use of the modeling tools is contributing to the fuel spray and combustion chamber geometry design.

# **Reviewer 2:**

The reviewer stated that the authors addressed the technical barriers in a systematic and organized way, at least in terms of concepts, by adopting 1D and 3D CFD analysis for engine and for aftertreatment design. If successful, the project is relevant to DOE objectives. Regarding the 35% targeted efficiency improvement, perhaps a more detailed explanation should be provided of how exactly



such a high portion of 18% efficiency gain is expected to come just from lean combustion strategies and from Miller cycle implementation. It is known that the Miller cycle early intake valve closing (EIVC) strategy has  $NO_x$  reduction benefits while the late intake valve closing (LIVC) shows thermal efficiency improvement if carefully tuned. The project team does not mention which one (of the two) Miller cycle strategies it has chosen.

# **Reviewer 3:**

The reviewer stated that the lean Miller cycle approach is an excellent approach to achieve fuel efficiency gains. Included as well in the approach is a systems-level approach including downsizing to achieve the fuel efficiency gains. Both approaches are needed to meet the aggressive targets. It was good to see challenging approaches being pursued (DOE funding is well suited for pushing the boundaries).

# **Reviewer 4:**

The reviewer commented that the approach on this five-year project includes annual go/no-go milestones for DOE review with a projected completion in December 2019 with a final vehicle demonstration. The technical

approach includes integration of all key engine components and systems (air handling, fuel injection, heat transfer, friction, aftertreatment, and 12 V system hybridization). Most of the targeted 35% efficiency improvements are expected from advanced combustion (18%) followed by advanced integration (10%), downsizing (8%), and lean aftertreatment system (-1%).

# **Reviewer 5:**

The reviewer indicated that the schedule and approach follow a generally accepted R&D plan: modeling, singlecylinder, multi-cylinder dynamometer, and vehicle. Technologies identified have the potential for production implementation.

Efforts to downsize similar to the current approach to downsize a 3.5 L port fuel injection (PFI) to a 2.5 L GDI application for fuel savings are already appearing in the marketplace and may not represent a substantial R&D benefit. U.S. Environmental Protection Agency (EPA) studies have shown that GDI downsizing has not reaped the targeted 8% potential targeted for this project and has been more like 1%-3%. Considering marketplace available GDI applications, the schedule of single-cylinder work could be more aggressive and modeling work more detailed to indicate potential for progress.

Data metrics for go/no-go should be presented (i.e., key 12 FTP/Highway Fuel Economy [HWFE] speed load points modeled to 25% efficiency and peak usable power/torque match 3.5 L PFI baseline engine).

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

# **Reviewer 1:**

The reviewer remarked that the baseline single-cylinder engine testing and CFD spray modeling have been performed, helping in understanding the spray, the mixing, and the combustion behavior, but also revealing aspects that should be avoided, i.e., spray collapsing. Major engine components are being redesigned, while thermal management 3D analysis is being performed to ensure if the flows, temperatures, and stresses in the engine are within acceptable limits. The air handling system is also being analyzed under several boosting options (super-charger, turbocharger and their combinations) along with their advantages and disadvantages. Among the challenges, it is not clear yet if the lean combustion regimes at low temperatures will ensure sufficient exhaust temperatures for aftertreatment light-off and proper operation. If thermal efficiency individual percentage improvement methods prove successful, i.e., lean combustion and Miller cycle, the project will support DOE's goal of reducing petroleum dependence significantly, given its large number of gasoline engines applications.

# **Reviewer 2:**

The reviewer stated that all year one milestones (single-cylinder work) have been met and year two (multi-cylinder effort) are underway.

# **Reviewer 3:**

The reviewer commented that limited results are available after 1.5 years out of 2 years of single-cylinder development, and very limited data were presented on lean Miller cycle results with go/no-go gate approaching in 4 months (October 2016).

With a downsized engine, data for the potential to meet power requirements and actual engine-out emissions should be presented to confirm that the end result will directly relate to DOE metrics. Proof of concept must include the capability to match power performance, capability to meet efficiency targets, and engine-out emissions, which have the potential to be managed with aftertreatment systems potentially available for production in the near term.

# **Reviewer 4:**

The reviewer stated that there is still a lot to do until the decision gate in late 2016, but the progress has been good. The reviewer asserted that the models for the injection process were good.

# **Question 3: Collaboration and coordination with other institutions.**

# **Reviewer 1:**

The reviewer remarked that the collaborators and the technical partners are representative for this research work. AVL single-cylinder testing baseline testing has been completed. It is not mentioned if the transient reactor capability study for aftertreatment development is being performed at an internal GM facility or at a partner/ collaborator's external facility.

# **Reviewer 2:**

The reviewer complimented the very good collaboration with GM as the project lead supported by the following key suppliers—AVL, Bosch, NGK, Delphi, Eaton, and Umicore—all leveraging their core capabilities.

# **Reviewer 3:**

The reviewer pronounced it good that top Tier 1 suppliers have been named to fill in the technology roadmap (Bosch, Delphi, NGK, and Umicore). More details on each supplier's role, work plan, and data would have improved the score. The reviewer listed injection system strategy, ignition strategy, aftertreatment configuration, and noted a very limited indication of progress.

# **Reviewer 4:**

The reviewer commented that the strategic partners were identified; however, it was not clear whether they were strictly supplying what GM asks for or whether their expertise is directly contributing to the project.

# **Reviewer 5:**

The reviewer found the collaborations to be limited to suppliers and one subcontract (AVL). However, the coordination among the team is good. The project would benefit from expanding the collaborations beyond suppliers.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

# **Reviewer 1:**

The reviewer stated that the project milestones appear relevant to meeting objectives: optimizing a stratified charge engine (SCE) using piston, sprays, ports, injection, and dilution strategies; designing a multi-cylinder engine with new boost and new aftertreatment; and incorporating appropriate go/no-go gates in October 2016 followed by procurement of hardware, building a multi-cylinder engine, and demonstrating the fuel efficiency targets.

# **Reviewer 2:**

The reviewer said that future FY 2016 tasks of optimizing single-cylinder engines (piston, sprays, ports, injection, and dilution strategies), optimizing Miller cycle strategies (LIVC, EIVC) and designing a multi-cylinder engine with new boost and aftertreatment seem very appropriate. FY 2017 tasks include hardware procurement for multi-cylinder engine builds, optimization of multi-cylinder engine on a dynamometer, and demonstrating fuel efficiency targets.

# **Reviewer 3**:

The reviewer stated that the plan looks good and comprehensive.

# **Reviewer 4:**

The reviewer stated that the project is on track and the next steps are consistent with the project's goals leading up to the late 2016 gate review. After that gate review, a closer examination of next steps in research will be more relevant.

# **Reviewer 5:**

The reviewer indicated that the future research follows an R&D plan that could have had more aggressive timing. The proof of concept for single-cylinder work (progress demonstrating potential to meet 25% fuel efficiency while matching power to 3.5 L PFI and reasonable engine-out emissions) should be demonstrated before a significant effort is made on a multi-cylinder engine.
### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### Reviewer 1:

The reviewer said that higher efficiency engines such as being developed here will reduce petroleum usage.

#### **Reviewer 2:**

The reviewer remarked that this project entails a very comprehensive approach to reaching the 35% fuel efficiency target compared to the 2010 baseline. Increased engine efficiency directly contributes to petroleum displacement.

#### Reviewer 3:

The reviewer stated there is a 35% improvement in baseline fuel economy, and the stretch goals shown on Slide 3 are directly relevant to DOE's objectives.

#### **Reviewer 4:**

The reviewer noted that this project directly enables petroleum displacement by fuel efficiency improvements in gasoline engines, which dominate the U.S. passenger car and light truck fleet.

#### **Reviewer 5:**

The reviewer commented that, generally, the 25% fuel savings effort support DOE objectives. The value of downsized GDI application development should be revisited.

### 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 good combination of DOE and corporate funds should be adequate to meet goals.

#### **Reviewer 2:**

The reviewer noted that this is a relatively large project at \$20 million (\$8.2 million DOE share) spanning 5 years but very appropriate given the high level goal that is very challenging.

#### **Reviewer 3:**

The reviewer said that DOE and cost share resources combined appear appropriate for this research.

#### Reviewer 4:

The reviewer commented that resources are sufficient. OEM commitment is substantial and indicates commitment to the technology.

#### Ultra-Efficient Light-Duty Powertrain with Gasoline Low-Temperature Combustion: Keith Confer (Delphi Advanced Powertrain) - ace094

Presenter

Keith Confer, Delphi Advanced Powertrain

#### **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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer enthused that this is an excellent approach progressing through a single-cylinder combustion chamber and controls activities, steady-state dynamometer, and onto the FTP with a keen eye on emissions and cost considerations. The project approach calls for an outstanding three generations of engines and a realistic plan for systematic drivability and emissions development. The approach should consider torque/power targets and time to torque.

#### **Reviewer 2:**

The reviewer stated that the project proposes to utilize a unique LTC regime, GDI CI (GDCI), to achieve





the targeted 35% fuel economy improvement. While promising very high engine efficiency, GDCI requires an aftertreatment system approach that works with the low-temperature challenges of a highly efficient engine that is also planned. FY 2015 milestones are complete, and significant progress has already been made towards many FY 2016 milestones.

#### **Reviewer 3:**

The reviewer said that this is a traditional, proven approach to work on single-cylinder, multi-cylinder, then generational improvements on identified problems. The reviewer saw no mention of modeling except for emissions approaches, but assumed it is integral to the engine design and approach. The reviewer believed that simulations had been done on fuel consumption, etc., several years ago.

Question 2: Technical Accomplishments and Progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer found the continuous progress to be impressive as 210-215 g/kWhr over the range of loads is close to world-class for engines in this stage of development. Identification of emissions issues with some early performance data and several possible solutions is a big step. Achieving and characterizing transient operation on a vehicle, with Gen 3 designed, is real progress and reduces one of the larger risk factors. The reviewer had a much better understanding of the potential for this system based on these results.

#### **Reviewer 2:**

The reviewer listed numerous technical accomplishments: engine controls and calibration, evaluation of fuel efficiency on test cycles, test vehicle using Gen 1.0 and Gen 1.8 GDCI hardware, development of Gen 2, and design of Gen 3 engine and aftertreatment for the GDCI multi-cylinder engine.

#### **Reviewer 3:**

The reviewer said excellent progress. Full engine and vehicle FTP results shown for GDCI LTC are on path and producing 32% of the target 35% fuel economy improvement over baseline for a vehicle.

The reviewer noted good progress on the level of data provided to the development community for the Gen 1 engine-out criteria emission and temperatures for aftertreatment considerations. FTP data presented for the Gen 1 engine show engine-out emissions comparable to current spark ignition engines with significantly lower  $NO_x$  and some HC and CO penalty.

Substantially lower exhaust temperatures of 200°C-300°C versus 450°C-700°C have been characterized on the FTP for potential novel LTC aftertreatment. The challenge has been identified for lower temperature exhaust.

The Gen 2 engine has data with about 11% improved BSFC over the Gen 1 engine, indicating a potential to meet the 35% target. A realistic consideration for  $NO_x/BSFC$  tradeoff has been presented.

The reviewer found clear plans and accomplishments for aftertreatment approaches presented for temperature considerations, such as insulated exhaust and high power intake air heater, expanded exhaust re-breathing, close coupled catalyst, HC trap, SCR, and low-temperature catalysts.

It was indicated during the presentation that peak power and torque tests were run successfully on the Gen 1 engine, implying that targets were met. It would improve accomplishments to present data on torque/power targets and time to torque.

The reviewer proposed that characterization of a full range of temperatures/constituents in the exhaust (peak temperatures, temperature histograms, levels of and CO) would be helpful to the aftertreatment development community to develop or apply solutions.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer commented that Delphi is the project lead and is currently in negotiations with an OEM partner. UW, ORNL, and Umicore round out the team, all contributing their key expertise, which is much needed to set up this project for success. The lack of an automotive OEM partner is a big concern as the originally proposed OEM declined to participate in the project and feedback from other OEMs has generally been that they are currently pursuing other technical directions and cannot take another project on.

#### **Reviewer 2:**

The reviewer remarked that this program continues to be mostly a Delphi program, with a significant contribution on emissions by Umicore. Some apparently minor collaboration on injectors is being done at UW and on emissions analyses by ORNL. ANL is doing significant work on GCI combustion fundamentals, and the reviewer wondered why Delphi is not making use of this. This reviewer certainly hoped that their public reports were not being solely relied upon. The reviewer stated that the top priority needs to be on securing an OEM partner. This establishes credibility, and, without this, skepticism will prevail and the project team will lose significant inputs on issues.

#### **Reviewer 3:**

The reviewer found very good collaboration with institutions to resolve critical barriers relating to LTAT (Umicore). There is a good level of data sharing for the development community considering the level of investment in cost share, and a good level of OEM involvement until 2016. The reviewer expressed concern with the apparent dropout of OEM partner Hyundai (Hyundai America Test Center Inc.) as engine technology is highly linked to this OEM. The score can be improved with the addition of an OEM partner and the effort to engage the broader aftertreatment community with high level requirements for this LTC. For example, if exhaust temperatures are consistently low, traditionally underused technologies for light duty such as HC/NO<sub>x</sub> traps may be a potential solution.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer remarked that excellent progress has been made so far. Future work very appropriately includes further refinement of controls and calibration (transient emphasis), Gen 3 GDCI engine design/build/test with next generation hardware including fuel injectors and aftertreatment architecture, and low-temperature exhaust aftertreatment system.

#### **Reviewer 2:**

The reviewer commended the work as outstanding because it has third-generation engine hardware incorporating lessons learned. As a low-temperature exhaust aftertreatment system is one of the highest priority remaining GDCI technical challenges, it is excellent to leverage ORNL expertise in low-temperature catalysts as well as Umicore. If possible, some general requirements for this LTC aftertreatment should be made available to a broader community as it may accelerate solutions.

Transient results planned should include consideration for maximum power/torque, power density (kW/l), time to torque/power relative to baselines (for acceleration considerations), and some indication of capabilities in the real world, such as cold start drivability down to  $-10^{\circ}$ C. With lower temperatures, traditionally underused (due to durability issues) HC/NO<sub>x</sub> traps may be a robust consideration.

#### **Reviewer 3:**

The reviewer commented that the future work is boiler plate: build and test Gen 3 and work on aftertreatment and calibration. The future tasks generally address the barriers, but the details are missing.  $NO_x$  control seems a major gap, with no specific mention. The reviewer noted gasoline oxidation catalyst (GOC), exotherm temperatures, and durability of the catalyst against flaking and damaging the turbo, and asked how the project team will test and address this before the turbo is wrecked.

A major milestone will be benchmarking with alternative approaches. There are several systems at various stages of development that look quite competitive on GHG emissions. An honest assessment is needed. Securing an OEM partner will validate any advantages.

Various versions of 48 V hybridization will be the norm if/when this architecture goes into production. Even a P2 hybrid electric vehicle (HEV) can significantly help on numerous transient trouble spots. The reviewer encouraged the project team to look at opportunities to take advantage of this as a way of maybe relieving emissions issues, delivering incremental fuel consumption benefits, or relieving demanding transient demand, etc. The project team should not be spending many resources on trying to solve these kinds of problems. This belongs in more fundamental work such as at ANL. The project team needs to find engineering solutions like this, and perhaps some simulation time on this would be very valuable in this regard.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer remarked that this project supports the overall DOE objective of petroleum displacement by improving engine efficiency (targeting 35%). Specifically, this project supports VTO's goal to improve the efficiency of LD engines for passenger vehicles through advanced combustion and minimization of thermal and parasitic losses.

#### **Reviewer 2:**

The reviewer commented that a 35% reduction in LD fuel consumption is clearly in line with DOE goals for petroleum displacement.

### 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 this is a relatively large project at \$25 million (nearly \$10 million DOE share) spanning 4 years, but the funding level is very appropriate given the broad scope encompassing optimization of all engine systems to reach the very challenging goal of 35% engine efficiency improvement over the 2010 baseline.

#### **Reviewer 2:**

The reviewer found a generally sufficient level of resources as excellent progress is being achieved. With additional proof of concept demonstration for efficiency, engine-out emissions, and transient performance, more resources could be justified to accelerate LTC aftertreatment solutions to enable production use of the technology.

#### **Reviewer 3:**

The reviewer warned that the project is in serious jeopardy without a contributing OEM partner.

#### Metal Oxide Nano-Array Catalysts for Low-Temperature Diesel Oxidation: Pu-Xian Gao (University of Connecticut) - ace095

**Presenter** Pu-Xian Gao, University of Connecticut

### **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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer commented that one aspect of this project that is very unique is the growth of nano-array catalysts in an existing honeycomb support. This is still a key area that needs to be demonstrated to work under a wide range of conditions, but this remains an interesting concept. With ORNL and Umicore involved, it should be handled in an appropriate way.

#### **Reviewer 2:**

The reviewer stated that the use of rare earth and base metals combined with unique support in place of traditionally supported PGM catalysts is a novel,



inception stage approach for achieving low-temperature CO oxidation. However, the project team continues to employ conditions in much of the characterization work that do not reflect the actual exhaust environment the catalyst will experience. Minor testing under these more realistic conditions showed considerably less performance than with idealized flow conditions. In order to downselect appropriate materials to advance to the next level, realistic test conditions and aging treatments must be employed sooner. Otherwise, considerable time is wasted on catalysts that will not be utilized in aftertreatment systems. Specifically, feed components and aging protocols consistent with USCAR initiatives must be used to lend credibility to results.

#### **Reviewer 3:**

The reviewer noted that the in-situ growth of nano-array catalysts on monoliths is very interesting, although the reviewer wondered how relevant this would be commercially. The reviewer wanted to know, for example, how possible is the scale-up of this coating method, how durable are the nano-arrays, and are they more susceptible to thermal stresses, sintering, and aging.

#### **Reviewer 4:**

The reviewer pointed out the need to have assessed S poisoning effects by now (based on comments from last year). There is no need to present any more data collected under unrealistic conditions (e.g., no  $H_2O$ , no  $CO_2$ , and no  $NO_x$ ). The reviewer only wanted to see data that have been collected with the full catalyst testing protocol specified by the USCAR ACEC Technical Team in the future.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer noted that minor progress had been achieved in the characterization of multiple catalyst formulations using more realistic feed conditions and aging treatments. The HC species used were appropriate and represented challenging molecules to convert at low temperatures. However, poisoning effects were not addressed and comparison to a reference, traditional PGM catalyst was not done as a benchmark. The reviewer noted that from a manufacturing perspective, using a growth technique to deposit an active catalyst material on a substrate may preclude the adoption of this technology. Manufacturability is a critical element to both OEMs and catalyst manufacturers. The reviewer inquired as to whether any progress has been made to reduce this challenge.

#### **Reviewer 2:**

The reviewer commented that progress forward in a project with so many pieces and types of catalysts is very challenging. Interesting results have been obtained, but some aspect of the data is difficult to understand, particularly the very abrupt propane light-offs for some catalyst systems, the doped cobalt oxides, and the Pt-titania  $(TiO_2)$  catalysts. These data, and CO-oxidation, are very interesting; however, in the last year more work needs to have been done using the ACEC protocol compositions with HTA, which they have begun. A truer idea of the merit of these catalysts can then be made.

#### **Reviewer 3:**

The reviewer stated that technical accomplishments in the past year include both PGM-free and Pt nano-arrays grown in-situ. One concern is that the Pt size increased due to HTA, which again brings up the question as to the nano-array stability. Current testing methods do not allow for separation of kinetic and mass transport properties, and this is very important in understanding the mechanism.

The reviewer commented that the to-do list on this project remains very long and it looks like things are a bit behind schedule. Hopefully, the collaborations with ORNL and Umicore will allow for pathways to make some quicker progress and keep the project focused.

#### **Reviewer 4:**

The reviewer noted that transition metal results on Slide 12 are of limited value because they were collected under totally unrealistic conditions. Similar considerations hold for other data, such as the perovskite catalysts on Slide 15 and the  $Pt/TiO_2$  data on Slides 19 and 21. Slide 23 demonstrates the huge difference in catalyst performance between the simple conditions and the full protocol conditions. The CO and  $C_3H_6$  data with the full protocol are encouraging.

The reviewer commended the project team on its thermal aging conditions (50 hours at 800°C HTA aging), but recommended that the team must incorporate realistic evaluation conditions in its work.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer commented that there was good collaboration with ORNL and Umicore.

#### **Reviewer 2:**

The reviewer remarked that this project has improved some since last year with the inclusion of additional universities and hoped that the planned Umicore work will help keep the evaluations realistic and the work focused and on track.

#### **Reviewer 3:**

The reviewer stated that including or consulting with an OEM should be part of this project as this would provide a reality check on the work and helpful suggestions for testing.

#### **Reviewer 4:**

The reviewer asserted that while there are excellent collaborators on this project, their contributions are hard to pull out from the discussion of the results.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer noted that lots of work remains and it may be necessary to focus on the most promising one or maybe two of the catalyst systems to get as complete a set of analyses as possible.

#### **Reviewer 2:**

The reviewer said that there is still a very large to-do list with rather vague plans presented in this presentation. Efforts to mitigate sintering, water, and S are still necessary. The reviewer was not sure that this project will progress to engine testing, even in the final year, but would much rather see the efforts focused and relevant than moving on to engine testing just for the sake of the demonstration. Some effort should be spent on understanding the role of kinetics versus mass transport.

#### **Reviewer 3:**

The reviewer stated that the project team must include S poisoning assessments in the future work. Also, the team must utilize full exhaust mix on all experiments.

#### **Reviewer 4:**

The reviewer stated that the project team indicated last year that more progress would be made testing under realistic conditions and aging methods; that has not materialized as expected. There reviewer expressed concern that this will be appropriately addressed going forward.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer found this project to be consistent with the industry need for low-temperature catalyst solutions to meet future emissions standards while minimizing cost. However, unless the concept catalysts are characterized under more appropriate conditions in a timely manner, the technology and usefulness of the data are questionable.

#### **Reviewer 2:**

The reviewer said that developing low-temperature activity is offered by this project, especially in non-PGM catalysts, so the studies with aging and S are very pertinent to assess these catalysts.

#### **Reviewer 3:**

The reviewer stated that LTAT will be necessary for more efficient engines in the future.

#### **Reviewer 4:**

The reviewer commented that, theoretically, yes, this meets DOE's petroleum displacement objectives. The further this project progresses, the less likely this is becoming, not because it was a bad idea, but just because the research community is learning that there were unforeseen complications with these materials.

### 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 funding and staffing to be appropriate.

#### **Reviewer 2:**

The reviewer remarked that with the development of catalyst studies using more realistic conditions, the resources should be sufficient. The main issue may be based more on focusing on the most effective catalysts.

#### Reviewer 3:

The reviewer noted that the budget on this project is quite high considering the accomplishments to date and the likelihood that it will not get to engine testing.

#### Micro-Jet Enhanced Ignition with a Variable Orifice Fuel Injector for High-Efficiency Lean-burn Combustion: Chia-Fon Lee (University of Illinois) - ace096

**Presenter** Chia-Fon Lee, University of Illinois

#### 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, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer found this project difficult to assess. Because of the constraints on information disclosure associated with an incubator project, the presentation could only talk in generalities. It seems that the approaches being pursued are fundamentally sound and the evaluation being done is comprehensive. The proof will be in the data, which are yet to come.

#### **Reviewer 2:**

The reviewer commented that the barrier to address is stated to be "Lack of cost-effective emissions control," but stratified charge engines are known to produce high NO<sub>x</sub> due to



near stoichiometric combustion and high particulates due to inadequate mixing. The G equation in KIVA is an inadequate and insufficient tool to predict emissions in a stratified charge engine.

#### **Reviewer 3:**

The reviewer stated that the development approach is reasonable with some preliminary simulations followed by single-cylinder evaluation and optical measurements. Not knowing more details about the technology approach, it is hard to say if the preliminary simulations were adequate.

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### Reviewer 1:

The reviewer noted that it seems that a significant technical work has been accomplished. How good it is will not

be known until the data have been obtained. This reviewer also asserted that the PI is very good and his work is credible.

#### Reviewer 2:

The reviewer remarked that progress is impossible to assess because no results were presented.

#### **Reviewer 3:**

The reviewer observed that, again, this is hard to rate given the lack of details. There are several easy criticisms/ questions to offer. There was a focus of not putting fuel on the liner, but nothing was said about the piston. The 150-mm liquid length seems excessive. Depending on the approach, this could produce a noncommercial amount of soot off the piston top.

The reviewer asked for the combustion efficiency (e.g., will the lean regions near the walls burn). The reviewer asked what the approach is to deal with the high  $NO_x$ , and how that impacts engine efficiency. The reviewer would like to know where the spark plug is located and also what happens at high load. The reviewer also inquired about the power density, if still stratified. Finally, if lambda is one, the reviewer asked what the knock limit is given the newly styled piston and combustion chamber.

#### Question 3: Collaboration and coordination with other institutions.

#### Reviewer 1:

The reviewer wished there was a not applicable review category to check. As an incubator project, collaboration does not seem appropriate for this project

**Reviewer 2:** 

The reviewer stated that there is no collaboration.

#### **Reviewer 3:**

The reviewer suggested that this project would benefit from the involvement of someone with combustion system development experience (e.g., an OEM or an engineering service provider). Without this involvement, the reviewer was skeptical that the project will deliver any meaningful results.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer looked forward to results.

#### Reviewer 2:

The reviewer commented that it seems that a viable plan is in place to get data and evaluate the concept.

#### **Reviewer 3:**

The reviewer stated that getting measured results on a running single-cylinder engine is a good next step. This should inform the models and allow them to be correlated. The big unknown is will the technology deliver the expected results on the single-cylinder engine, and if not, can it ever be made to work.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer was not familiar with the details of the incubator program, but it seemed to the reviewer that if this project is successful, it could contribute to improved lean burn engine development.

#### **Reviewer 2:**

The reviewer stated agreement with any technology that addresses emissions and efficiency is relevant, but it is unclear how relevant this project truly will be, given the minimal details shared.

#### **Reviewer 3:**

The reviewer remarked that the concept is unlikely to work.

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

No comments were received in response to this question.

#### Affordable Rankine Cycle (ARC) Waste Heat Recovery for Heavy-Duty Trucks: Swami Subramanian (Eaton Corporation) - ace097

#### **Presenter** Swami Subramanian, Eaton Corporation

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

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated that most of the work is still in progress. The steps presented on the Approach/Strategy slide seem to be in the right direction. Perhaps additional plots and visual representations other than words would help the reader understand the project team's intent faster.

The reviewer remarked that the use of the existing coolant as the working fluid eliminates the driver's burden to buy additional fluids— a feasibility study is in progress. The evaluation of different WHR architectures should include at least a basic schematic/drawing of the main WHR components: pump, boiler, expander, condenser, etc.

#### **Reviewer 2:**

The reviewer noted that very early in the program, the plan looks fair. It would go a long way to have had a first-order analysis that would show what it takes to get a 5% fuel economy (FE) improvement—how much heat is needed, what efficiencies are needed, etc.

#### **Reviewer 3:**

The reviewer stated that, in the literature, the working fluid for WHR is typically ethanol, and the expected fuel economy benefit in real world driving is around 3%-5%. This project chooses to use the engine coolant as the working fluid with a target 5% FE improvement. If successful, it would represent a significant advance in WHR technology.

The project is well-designed and covers all the tasks related to the WHR system development. A major challenge with WHR is the systems integration/optimization. The reviewer commented that this task should start from the



very beginning instead of near the end of the project. The reviewer recommended that increasing the fan power requirement should also be considered along with the charge air cooler design.

#### **Reviewer 4:**

The reviewer noted that this project is at an early stage and the project team is pursuing an interesting strategy. The reviewer had concerns regarding the 5% FE increase with WHR systems. There were no thermodynamic data supporting this number presented in the presentation, and it seems like an aggressive goal. The reviewer said that it would be good to know the assumptions that go into the projected 5% FE benefit from this project.

#### **Reviewer 5:**

The reviewer stated that although it is early in the project, the approach seems appropriate. However, the working fluid composition study is the basis of the viability of the concept. The reviewer had concerns about some boundary conditions that need attention. The first is that the ratio of glycol to water directly impacts the heat capacity of the system. The reviewer asked how the integrity of the working fluid will be maintained and how dissolved gases will be addressed. Second, the reviewer referred the project team to concerns about the fact that the heat transfer into the working fluid may include nucleate boiling. The reviewer wanted to know what steps will be taken to minimize the effects of insulating air bubbles inhibiting heat transfer (i.e., abrasive slurry extrusion through coolant passages to increase smoothness and the addition of surfactant to the working fluid to help disperse vapor bubbles that may form).

#### **Reviewer 6:**

The reviewer commented that using coolant as a working fluid is an excellent idea; however, the performance would be challenging to meet the target due to high-temperature decomposition of the coolant. It is not clear how 5% FE is defined. The reviewer wanted to know if it would be for a single point at 65 mph cruise speed or over the 13 mode composite Supplemental Emission Test point.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1**:

The reviewer noted that this project has just started and good progress has been made in identifying the working fluid.

#### **Reviewer 2:**

The reviewer commented that the project team has been meeting the schedule since the start in February.

#### **Reviewer 3:**

The reviewer remarked that the project is at a very early stage. The work accomplished to date is appropriate for the stage of the project.

#### **Reviewer 4:**

The reviewer observed that the progress is organized, and the results from the Roots expander and its drive design will be critical in establishing the viability of this system.

#### **Reviewer 5:**

The reviewer did not observe much, other than performing the 13-point engine testing baseline. The project team has laid out a plan at least regarding its intentions. The plot in Slide 13 could use additional explanatory notes. Regarding the CFD analysis, no details are provided regarding what the simulation conditions are; how the calibration, if any, will be performed and assessed for accuracy; what will be achieved; and what exactly is to be modeled. At this stage, it is too early to make further comments in the absence of some intermediate results.

#### **Reviewer 6:**

The reviewer found not too much progress that can be evaluated because the program just started not too long ago.

#### **Question 3: Collaboration and coordination with other institutions.**

#### Reviewer 1:

The reviewed found the collaboration and coordination with industry partners, universities, and/or subcontractors to be excellent.

#### **Reviewer 2:**

The reviewer stated that there was a good cross section of academia and industry.

#### Reviewer 3:

The reviewer remarked that this project includes a large number of collaborators with distinct roles. Each brings a unique expertise to the project.

#### **Reviewer 4:**

The reviewer praised working with PACCAR as an excellent starting point, specifically with PACCAR's MX-13 engine. Also, a list of partners seems to be very clearly defined for their roles.

#### **Reviewer 5:**

The reviewer said that the list of collaborators contains appropriate industry leaders. The success of this project is dependent on the integration of the Roots expander with the PACCAR engine/control systems.

#### Reviewer 6:

The reviewer commented that the Collaborations and Coordination information seems to be more explicit, revealing which task each partner should address. The partners seem to be well coordinated by the project team. Perhaps more explanations (i.e., what models or testing facilities and what laboratories each of the collaborators use) would help the reviewer to understand the team's activities better.

# 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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer commented that it will be interesting to see the project moving forward.

#### **Reviewer 2:**

The reviewer commented that all plans are in place to deliver the results. The reviewer looked forward to hearing from the progress next year.

#### Reviewer 3:

The reviewer noted that the project is logical and well planned in general. It seems to lack an alternative in term of working fluid if the current choice fails to meet the target.

#### **Reviewer 4:**

The reviewer commented that the future research includes most of the necessary steps, but has not been performed yet by the project team. The project milestones are relevant to DOE objectives according to this reviewer, who listed the following: multi-component CFD analysis; two-phase heat transfer correlation development; Affordable Rankine Cycle (ARC) analytical model development; and WHR components (expander, working fluid, and heat exchangers) design finalized with a go/no-go review in December 2016.

#### **Reviewer 5:**

The reviewer stated that the Critical Assumptions and Issues slides list a number of risks that have a potentially high impact on the project. As a result, the go/no-go decision at the end of FY 2016 is very important. Given the early stage of the project, this go/no-go decision point may be too early in the project timeline. If these critical assumptions and risks cannot be satisfactorily answered at this time, the go/no-go decision point should be postponed to an appropriate time.

#### **Reviewer 6:**

The reviewer pointed out that, while understanding that the project is in its earliest stages, there are some areas that

need attention. The first is the sensitivity of the WHR system to coolant mixture regarding efficiency and engine heat transfer. The second is the failure mode analyses of the WHR and expander systems to address the effects on the control system when departures from expected Roots expander output occur. The third is the criteria emissions output failure mode effect management (FMEM) when the Roots expander underachieves with power addition.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer noted that effective WHR will increase overall engine efficiency and hence reduce petroleum usage.

#### **Reviewer 2:**

The reviewer mentioned that WHR would be likely seen in the Phase 2 of EPA HD GHG rules. WHR is one of the most effective technologies to achieve high performance in FE.

#### **Reviewer 3:**

The reviewer commented that low-cost WHR is in direct alignment with DOE's objectives and supports petroleum reduction.

#### **Reviewer 4:**

The reviewer commented that, if successful, the project would be relevant to a significant fuel consumption reduction.

#### **Reviewer 5:**

The reviewer remarked that, if successful, the technology would results in fuel savings that would support DOE objectives of petroleum displacement.

#### **Reviewer 6:**

The reviewer stated that so much opportunity exists to have dramatic reductions in transport fuel consumption, given the poor fuel economy exhibited by over-the-road freight and other commercial vehicles. If successful, the objectives have the potential to reduce both the GHG impact of transport and the cost as well.

### 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 project resources of \$4 million may just be sufficient to meet the stated milestones in a timely fashion, given the multitude of collaborations under such a tight schedule.

#### **Reviewer 2:**

The reviewer stated that funding seems to be adequate for the remaining tasks.

#### **Reviewer 3:**

The reviewer remarked that given the early stage of the project, the project resources appear to be sufficient.

#### **Reviewer 4:**

The reviewer commented that, so far, it is still too early to tell, but it seems that the project is on schedule.

#### Cummins 55% BTE Project: Lyle Kocher (Cummins) - ace098

**Presenter** Lyle Kocher, Cummins

**Reviewer Sample Size** A total of eight reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer stated that the Cummins team has laid out an aggressive, yet viable, path to achieving 55% BTE.

#### **Reviewer 2:**

The reviewer stated that the approach looks good and noted the project team's attack on thermal heat losses and heat recovery barriers to enable a 55% BTE demonstration.

#### Reviewer 3:

The reviewer commented that the project is using a traditional, fully comprehensive approach that utilizes Cummins' strengths, particularly in fuel injected engines (FIE), turbocharging, and WHR. Some technologies offer big gains, like WHR (4%-4.5% BTE) and combustion and FIE (1.3% BTE each), while others offer smaller increments.



The integrated approach and estimated BTE improvements of various approaches gets the project team to its goal.

#### **Reviewer 4:**

The reviewer found the approach to be reasonable and systematic to meet a stretch 55% BTE goal by targeting high-pressure injection, multiple EGR loops, and a higher CR. The reviewer mentioned that it was excellent to set interim real goals to have initial 50% BTE on an engine dynamometer running very soon without WHR. Major risks have been identified. It is a very nice approach to manage moisture level in the low-temperature EGR loop with the WHR system.

To improve the approach, the reviewer said that more detail on risk mitigation and contingency plans for known challenges could improve the score. The reviewer wanted to know, for example, what specific plans are in this work to overcome known high risk issues with the planned approach. For thermal coatings, the reviewer referenced the statement, "previous work with insulated combustion systems have been challenged to demonstrate improved efficiencies," and opined that more detail on what novel approach not attempted with thermal coatings or contingency to make up efficiency would improve the approach. Also a risk is that engine-out NO<sub>x</sub> will be

higher due to higher temperature combustion. The reviewer commented that in this case, the upper limit to engineout  $NO_x$  should be reported as a metric as it is likely well understood by aftertreatment system designers and manufacturers.

#### **Reviewer 5:**

The reviewer commented that the project entails a systems-level approach towards the challenging BTE goal. A systems-level approach is required to achieve success for such an aggressive goal. Emissions are included in the approach including impacts on fuel efficiency. WHR is also included.

#### **Reviewer 6:**

The reviewer stated that the approach for this project is very good. There is a recognition that, to push to the maximum efficiency, every component on the engine system needs to be evaluated. There is no single silver bullet.

#### **Reviewer 7:**

Based on other presentations the reviewer had seen on advanced combustion regimes, the key to progress is a robust engine control system and strategy. In this project, fuel and air handling system control define the combustion and effectiveness of the aftertreatment system. The reviewer commented that whether the hardware/ software pairing for 50% BTE (engine only) is sufficient or appropriate for a production vehicle is unknown, but the controls system effectiveness will dictate the overall performance of the whole engine system.

#### **Reviewer 8:**

The reviewer noted that it would be a good R&D project, but was not convinced that the proposed approach has any potential path to become a commercially viable approach. Two noticeable issues are high engine-out  $NO_x$  and condensation issues for the LP EGR system. The reviewer asked if the engine can meet the 2010 emission standards, specifically on the cold FTP cycle with such high engine-out  $NO_x$ . Condensation can bring up a big warranty issue if the LP EGR cooler fails. The reviewer did not see any good solution for that.

Also, it seemed to the reviewer that the Cummins ISX engine would be used for this program. This engine has limitations on peak cylinder pressure. It is not going to be a good engine platform to achieve the program goal because this engine is old and it will be at the end of life when the program is completed.

# Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### **Reviewer 1:**

The reviewer stated that the project has just started, but the accomplishments to date are impressive. The project team has a detailed technical road map that has been developed through verified simulation and laboratory testing. The project team is engaging in the fundamental activities necessary to overcome the barriers it has identified.

#### **Reviewer 2:**

The reviewer commented that there has been an impressive delivery of results in such a short period. Cavitation modeling and piston crown thermal barriers are cutting edge. The decision on SCR filters and dual-loop EGR, which is borrowed from Cummins' and others' light-duty programs, is promising. As a result of this, the reviewer observed 0.4% BTE points from unique aspects of this and noted exhaust manifold design and turbocharging optimization. The reviewer said that the high EGR rates allow much leverage in NO<sub>x</sub> and efficient combustion. The next-generation WHR is significantly adding to the knowledge base in the industry. The reviewer thanked the project team for publicly reporting the amount of data and results

#### **Reviewer 3:**

The reviewer noted that the project has just started, and the accomplishments are appropriate for the short timeframe.

#### **Reviewer 4:**

The reviewer remarked that the results were excellent for a newly started project with leverage from prior SuperTruck engine work. The piston design data indicate that targeted incremental efficiency improvements have

been comfortably exceeded. The reviewer said that injector prototypes, engine friction reduction prototypes, and WHR prototypes have been tested with good results and plans for further confirmation/optimization.

#### **Reviewer 5:**

The reviewer commented that the technical accomplishments being made in this project are outstanding. From an academic standpoint, the reviewer would like to encourage Cummins to make as much information as possible public through technical publications. The reviewer understood that there are issues with proprietary information, but the thermodynamic and structural analyses that were conducted would be very informative.

#### **Reviewer 6:**

The reviewer stated that the project team had advised the reviewer that the engine will be run on certification diesel, but various fuel compositions need to be evaluated. The reviewer had two items of concern: the first is that at some point key parameters of those fuels will affect items related to technical barriers, such as  $NO_x$  performance (cetane and FAME content) and PM emissions (aromatic content). The other is that BTE is also dependent on the catalyst efficiency at the feedgas temperature and equivalence ratio. The additional fuel required to maintain catalyst light off and/or DPF effectiveness will reduce BTE.

#### Reviewer 7:

The reviewer said that this project is just beginning so there is not much to report on at this stage.

#### **Reviewer 8:**

The reviewer remarked that it is too early to tell, with a big question mark.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer stated that the work is basically an internal Cummins program; however, the company is engaging with the national laboratories doing relevant work in CRADAs and spray diagnostic and modeling development.

#### **Reviewer 2:**

The reviewer said that there are no collaborations on this project external to Cummins. The reviewer was not sure any are necessary though. Including a university partner to perform thermodynamic analyses could be useful to add academic depth, and increasing the amount of public information could be useful.

#### **Reviewer 3:**

The reviewer noted that this is all internal work to Cummins. The reviewer would have preferred to see project benefit, and knowledge, spread to numerous parties. However, given the tight timeframe, external collaborations may have been difficult. The reviewer commented that proper project management could have pulled this off though. There is work being done with the supply chain partners.

#### **Reviewer 4:**

The reviewer commented that the project appears to be all internal Cummins, without external collaborators. Although Cummins has excellent capabilities in the fuels systems and turbo areas, the team should consider additional institutions to provide alternate viewpoints on the approaches.

#### **Reviewer 5:**

The reviewer found this work to be a very Cummins specific project with limited need for external collaboration. Work products are well supported by analysis and data are presented that are excellent. The reviewer commented that including an aftertreatment partner, and potentially a third-party engine laboratory for confirmation testing, would improve the score. The expertise of unnamed suppliers is clearly needed to complete development and their recognition/inclusion for major work could improve the score.

#### **Reviewer 6:**

The reviewer remarked that it appears that all of the work is being done at Cummins with no outside partners on the project. Working with different divisions of the same company is not really collaborating. The project needs to improve collaborations by bringing in outside partners to the project.

#### **Reviewer 7:**

The reviewer acknowledged not knowing the entire history of this project, but the only participants appear to be Cummins companies. The reviewer was unsure how to rate this because other projects had outside vendor/ university/government laboratory participation.

#### **Reviewer 8:**

The reviewer was unsure that Cummins Turbo Technologies and Cummins Fuel Systems can be viewed as partners because they all belong to Cummins. The reviewer opined that this would not be the best use of funds to support a single company.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer was looking forward to additional development from this project-excellent work.

#### **Reviewer 2:**

The reviewer stated that Cummins has an excellent plan for this project. The reviewer looked forward to the results to come.

#### **Reviewer 3**:

The reviewer said that the project is just in the beginning stages. The planned research is in good shape for now (as proposed).

#### **Reviewer 4:**

The reviewer stated that it seems that SCR filters are a key technology, and Cummins states higher  $NO_x$  will likely be needed to deliver the goals. However, there are no plans stated here to pursue advance de- $NO_x$ . This would especially be critical to implementation, given the likelihood of a nationwide low- $NO_x$  standard. The reviewer noted that other barriers have been identified, and steps appear in place to chase them down.

#### **Reviewer 5:**

The reviewer noted that a very good plan was presented and the approach is being followed in future plans. As indicated, more information on risk mitigation and contingency (what other pathways are possible if one of the high risk approaches does not achieve targets) would improve the score.

#### **Reviewer 6:**

The reviewer was surprised that some form of port injected water is not under investigation for  $NO_x$  mitigation coincident with efforts to reduce combustion duration for more efficient heat release characteristics. The reviewer noted that, historically, efficiency comes at the expense of higher engine-out  $NO_x$  and lower  $NO_x$  comes at the expense of torque and/or efficiency.

#### **Reviewer 7:**

The reviewer said that the future work seems to be comprehensive, including all pieces that are needed for the demonstration.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer stated that 55% BTE enabling technologies contribute directly to DOE objectives of petroleum displacement through efficiency gains.

#### **Reviewer 2:**

The reviewer noted that work to achieve a 55% BTE target performed by engine manufacturers with a high level of cost share clearly supports DOE objectives for petroleum displacement.

#### **Reviewer 3:**

The reviewer suggested that this project can lead directly to petroleum displacement by improving the fuel efficiency of diesel engines, which dominate the transportation industry in the United States.

#### **Reviewer 4:**

The reviewer found this project to be highly relevant because there is a direct link to reduced petroleum consumption.

#### **Reviewer 5:**

The reviewer commented that development of any efficient technologies can always support overall DOE goal.

#### Reviewer 6:

The reviewer stated that it is assumed that achieving a 55% BTE for a given operating point implies a broad area of in-cycle efficiency gains. Modeling of many more operating points should be performed to ensure there is indeed a reasonable BTE gain translating into real fuel economy gains.

### 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 reaching 55% BTE is a tough goal, and resources for this project look to be on target for the difficulty to achieve this.

#### **Reviewer 2:**

The reviewer remarked that the budget is good considering this is follow-on work from SuperTruck. It is difficult to obtain this level of activity at the project's current funding level without leverage of the prior work. The reviewer noted that if prior SuperTruck work had not been done, then the budget would be very lean.

#### Reviewer 3:

The reviewer commented that it seems that it is okay at this early stage.

#### **Reviewer 4:**

The reviewer noted that Cummins stands to gain quite a bit of expertise (and potentially a competitive advantage) with this research. The reviewer was surprised that there are no other participants to both fund and participate in this project.

#### Improved Fuel Efficiency through Adaptive Radio Frequency Controls and Diagnostics for Advanced Catalyst Systems: Alexander Sappok (Filter Sensing Technologies, Inc.) - ace099

#### Presenter

Alexander Sappok, Filter Sensing Technologies, Inc.

**Reviewer Sample Size** A total of seven reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

#### **Reviewer 1:**

The reviewer applauded the approach to the project as excellent. The research teaming is strong, with partners having well-developed roles (Slide 13 is great). Year 1 is focused on development and refinement of the sensor and screening tests. The reviewer remarked that two quarters into the project (started in October 2015), the project team is on track to meet the goals.

#### **Reviewer 2:**

The reviewer noted that the approach of using live RF sensors to measure catalyst state during vehicle operation



appears to be feasible based on researchers' previous work and, of course, would be highly desirable. The planned research appears to cover the bases in terms of developing and testing the technology.

#### **Reviewer 3:**

The reviewer remarked that a nice approach was laid out.

#### **Reviewer 4:**

The reviewer observed that the project was an excellent extension of the technology. The methodology to sort through the challenges looks solid, and the project team is working with a great cross section of the industry.

#### **Reviewer 5:**

The reviewer noted that the RF sensor project for soot-loading measurement was quite successful. An RF sensor provides more information than the pressure drop across the DPF. This information helps to reduce the frequency of trap regeneration, thus improving fuel economy. It is not obvious, however, that fuel efficiency could be improved when the same technology is being used for SCR and/or a TWC. The feasibility study should include if

additional information obtained by the radio frequency (RF) sensor (i.e.,  $NH_3$  or oxygen storage) could actually improve fuel efficiency. The reviewer said that this task should be performed at an early stage of the project. Other than this missing link, the rest of the project is well-designed.

#### **Reviewer 6:**

The reviewer stated that improved sensing supports OBD requirements and can enable some improvements in closed-loop control. It is not clear from the presented material how much better RF sensing is than other competing technologies

Question 2: Technical accomplishments and progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

#### Reviewer 1:

The reviewer stated that this is a new project so there are no major accomplishments to review.

#### **Reviewer 2:**

The reviewer remarked that this is a new project in its first year so only the first six months' work has been completed. However, the sensors have been developed and testing is underway so progress is good for the limited time the project has been underway.

#### **Reviewer 3:**

The reviewer mostly graded the project high for the prior work, but there is no reason to think the background shown is not considered as great understanding of the technology.

#### **Reviewer 4:**

The reviewer commented that the success of the DPF sensing was good background to have, but it was a little confusing differentiating that work from this project's accomplishments.

#### **Reviewer 5:**

The reviewer commented that there has been good progress in the first two quarters of the project based on solid prior work on DPF sensor project. Already in this new project, there has been significant work on the RF cavity, both in development and simulations. Additionally, work has begun in regard to catalyst selection and a bench reactor has been commissioned to do the testing. The reviewer noted that preliminary results show excellent promise for NH<sub>3</sub> storage.

#### **Reviewer 6:**

The reviewer noted that there has been good progress in term of sensor-related development, testing, and planning. The RF sensor response to  $NH_3$  storage on the SCR catalyst is very promising. The reviewer found the demonstration of fuel savings (the DOE goal) is not very convincing if the project is under the assumption that added information on catalyst state would naturally lead to improvement in fuel efficiency.

#### **Question 3: Collaboration and coordination with other institutions.**

#### **Reviewer 1:**

The reviewer lauded the truly outstanding research team and collaborator list, which has well-defined roles and regular, in-person meetings (which the reviewer thought was excellent).

#### **Reviewer 2:**

The reviewer stated that collaboration and coordination with industry partners, national laboratory, city fleet, and/or subcontractors seems to be in place.

#### **Reviewer 3:**

The reviewer said that there were good partnerships for hardware, testing, and carry-through to implementation.

#### **Reviewer 4:**

The reviewer noted that a very good, comprehensive team has been assembled, which should contribute to a successful project.

#### **Reviewer 5:**

The reviewer found an excellent level of collaboration, with involvement from the national laboratories, OEMs, and Tier 1 suppliers.

#### **Reviewer 6:**

The reviewer praised working with partners that know what is needed for the industry and understand all the application challenges.

#### **Reviewer 7:**

The reviewer stated that a pretty broad team has been assembled including DOE national laboratories, several engine makers, and fleet operators. The reviewer commented that adding a couple of universities would make the project perfect.

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 technology and, when sensible, mitigating risk by providing alternate development pathways.

#### **Reviewer 1:**

The reviewer stated that this program is probably the best planned seen this year and it was again working on relevant issues with a directly applicable solution.

#### **Reviewer 2:**

The reviewer said that the R&D plan looks satisfactory for achieving the project goals.

#### **Reviewer 3:**

This project has an excellent trajectory, and the reviewer looked forward to watching its progress.

#### **Reviewer 4:**

The reviewer said that the plan looks good.

#### **Reviewer 5:**

The reviewer stated that this was a good plan going forward.

#### **Reviewer 6:**

The reviewer commented that the proposed future work is logical and well planned in terms of sensor-related development. Again, a major void in the project is the pathway from the sensor development to the actual vehicle fuel efficiency improvement. The reviewer said that the knowledge of the SCR catalyst state seems to be more useful for diesel emissions fluid dosing control than engine control itself. The reviewer questioned how the engine would operate in a more efficient way given the knowledge of the SCR catalyst state and suggested that this question be addressed as soon as possible and used as a decision point.

### Question 5: Does this project support the overall DOE objectives of petroleum displacement? Why or why not?

#### **Reviewer 1:**

The reviewer stated that maximizing aftertreatment system performance will aid in reducing fuel consumption, thus reducing petroleum usage.

#### **Reviewer 2:**

The reviewer said that reducing the uncertainty in aftertreatment effectiveness/maintenance will lead to improved efficiency, thus supporting the DOE objectives of petroleum displacement.

#### Reviewer 3:

The reviewer stated the project allows the engine to run at more efficient conditions and still control the catalyst to very high effectiveness and be capable for OBD. The project should be a very cost-effective solution towards running such conditions.

#### **Reviewer 4:**

The reviewer commented that use of the sensor and avoidance of unnecessary regeneration events would positively impact fuel economy and the durability of aftertreatment devices.

#### Reviewer 5:

The reviewer stated that, if successful, the technology would results in fuel savings, which would support DOE objectives of petroleum displacement.

#### **Reviewer 6:**

The reviewer remarked that there is some potential to increase vehicle efficiency through improved sensing technology. It is not the strongest knob though.

### 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 budget and spend rate seem to be in line and sufficient for progress.

**Reviewer 2:** 

The reviewer stated the resources look appropriate.

**Reviewer 3:** 

The reviewer remarked that the funding levels seem reasonable for this work.

**Reviewer 4:** 

The reviewer indicated that funding seems to be adequate for the remaining tasks.

**Reviewer 5:** 

The reviewer noted that the resources are sufficient given the scope of project. The reviewer would always like to see contractors match the DOE input, but that can be difficult for small companies.

#### **Acronyms and Abbreviations**

1D	One dimensional
3D	Three dimensional
AC	Air Conditioning
ACE	Advanced combustion engine
ACEC	Advanced Combustion and Emissions Control
Al	Aluminum
AMR	Annual Merit Review
ANL	Argonne National Laboratory
APS	Advanced Photon Source
ARC	Affordable Rankine Cycle
ASCR	Advanced Scientific Computing Research
BMEP	Brake Mean Effective Pressure
BSFC	Brake-specific fuel consumption
BTE	Brake Thermal Efficiency
°C	Degrees Celsius
Ca	Calcium
CaSO <sub>4</sub>	Calcium Sulfate
CAE	Computer-Aided Engineering
CCC	Co-precipitated CuOx, CoOy, and CeO2 catalyst
Ce	Cerium
CF	Combustion Fluid
CFD	Computational Fluid Dynamics
CH <sub>4</sub>	Methane
СНА	Chabazite
CI	Compression Ignition

Cl	Chloride
CLEERS	Cross-Cut Lean Exhaust Emissions Reduction Simulations
СО	Carbon Monoxide
CO <sub>2</sub>	Carbon Dioxide
COV	Coefficient of variance
CPU	Central processing unit
CR	Compression Ratio
CRADA	Cooperative Research and Development Agreement
Cu	Copper
DEF	Diesel Emissions Fluid
DFT	Density Functional Theory
DI	Direct Injection
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DPF	Diesel particulate filter
E10	10% ethanol blend with gasoline
E20	20% ethanol blend with gasoline
ECN	Engine Collaboration Network
EGR	Exhaust Gas Recirculation
EIVC	Early Intake Valve Closing
EPA	U.S. Environmental Protection Agency
ERC	Engine Research Center
EU	European Union
FA	Field Aged
FACE	Fuels for Advanced Combustion Engines
FAME	Fatty Acid Methyl Ethers

FCA	Fiat Chrysler Automobiles
Fe	Iron
FE	Fuel Economy
FEM	Finite Element Model
FIE	Fuel Injected Engines
FRESCO	Fast and Reliable Engine Simulation Code
FTP	Federal Test Procedure
FY	Fiscal year
GC	Gas Chromatography
GDI	Gasoline Direct-injected
GDCI	Gasoline Direct Compression Engine
GHG	Greenhouse gas
GM	General Motors Corporation
GOC	Gasoline Oxidation Catalyst
GPF	Gasoline Particulate Filter
GPU	Graphics Processing Unit
GSA	Global sensitivity analysis
H <sub>2</sub>	Hydrogen
H <sub>2</sub> O	Water
НС	Hydrocarbon
HCCI	Homogeneous Charge Compression Ignition
HCl	Hydrochloric Acid
HD	Heavy-Duty
HEV	Hybrid Electric Vehicle
ННС	Heavy Hydrocarbons
НРС	High Performance Computing

HTA	High-temperature hydrothermal aging
HWFE	Highway Fuel Economy
ICE	Internal Combustion Engine
IDT	Ignition delay time
IMEP	Indicated Mean Effective Pressure
IR	Infrared
ISFC	Indicated Specific Fuel Consumption
IVC	Intake Valve Closing
JM	Johnson Matthey Catalysts
L	Liter
La	lanthanum
LANL	Los Alamos National Laboratory
LD	Light-Duty
LES	Large Eddy Simulation
LIVC	Late Intake Valve Closing
LLNL	Lawrence Livermore National Laboratory
LP	Low-pressure
LTAT	Low temperature Aftertreatment
LTC	Low-Temperature Combustion
LTGC	Low-Temperature Gasoline Combustion
MD	Methyl Decanoate
mm	Millimeter
MON	Motor Octane Number
MPI	Multi-Point Injection
ms	Milliseconds
MY	Model Year

N <sub>2</sub> O	Nitrous Oxide
Na	Sodium
NG	Natural gas
NH <sub>3</sub>	Ammonia
NI	National Instruments
NO	Nitric Oxide
NO <sub>x</sub>	Oxides of Nitrogen
NO <sub>2</sub>	Nitrogen Dioxide
NVO	Negative Valve Overlap
O <sub>2</sub>	Oxygen
OBD	On-Board Diagnostics
OEM	Original Equipment Manufacturer
ORAU	Oak Ridge Associated Universities
ORC	Organic Rankine Cycle
ORNL	Oak Ridge National Laboratory
РАН	Polycyclic aromatic hydrocarbon
РСР	Peak Cylinder Pressure
Pd	Palladium
PDF	Probability Density Function
Penn State	Pennsylvania State University
PFI	Port Fuel Injection
PGM	Platinum group metals
PI	Principal Investigator
PIV	Particle image velocimetry
PM	Particulate matter
PN	Particulate number

PNA	Passive NO <sub>x</sub> adsorber
PNNL	Pacific Northwest National Laboratory
Pr	Praseodymium
PR	Pressure Rise
Pt	Platinum
R&D	Research and development
RANS	Reynolds-Averaged Navier Strokes
RAT	Rapid Aging Test
RCCI	Reactivity Controlled Compression Ignition
RCM	Rapid compression machines
RF	Radio-Frequency
RFI	Radio frequency interference
Rh	Rhodium
RK	Reaction kinetics
RON	Research octane number
S	Sulfur
SAE	Society of Automotive Engineers
SCE	Stratified Charge Engine
SCR	Selective Catalytic Reduction
SDPF	SCR-Coated DPF
Si	Silicon
SiC	Silicon Carbide
SNL	Sandia National Laboratories
SNR	Signal to Noise Ratio
SOI	Start of Ignition
TESF	Tabulated Equivalent Strain Flamelet

TiO <sub>2</sub>	Titanium Dioxide
TWC	Three-Way Catalyst
UC	Unused Capacity
UM	University of Michigan
UQ	Uncertainty quantification
USCAR	U.S. Council for Automotive Research
U.S. DRIVE	U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability
UW	University of Wisconsin
VCR	Variable compression ratio
VTO	Vehicle Technologies Office
VVA	Variable Valve Actuation
WHR	Waste Heat Recovery
Zr	Zirconium
ZrO <sub>2</sub>	Zirconium Dioxide