

2011 CLEERS Industry Priorities Survey Final Report Analysis, Summary, and Recommendations

9/27/2011



INTRODUCTION AND BACKGROUND

Objectives

CLEERS, which stands for Cross-Cut Lean Exhaust Emissions Reduction Simulations, is a collaboration among industry, the Department of Energy (DOE) and universities that began in 2001 under the guidance of the DOE Diesel Crosscut Team. The main objective of this collaboration is to support the exchange of non-proprietary data and information among original equipment manufacturers (OEMs), emission control suppliers, academia, and DOE regarding emission controls and emission controls modeling and simulation. CLEERS provides an informal framework for technical communication among the various partners and also provides a mechanism for industry feedback to the Department of Energy on programmatic and technical issues. The activities are overseen by a CLEERS Planning Committee that implements rules and procedures, updates reports and recommendations to the oversight authority, which is now the DOE Advanced Engine Crosscut Team. The CLEERS Planning Committee is also responsible for coordinating the CLEERS Technical Discussion (Focus) Groups and organizing an annual public workshop.

In late 2010, DOE and the DOE Advanced Engine Crosscut Team requested that the CLEERS Planning Committee conduct another survey of its industry partners concerning their most pressing needs related to research and development for transportation emission controls. In addition, the Crosscut Team requested that the new survey should include opportunities for the industry partners to comment on how effective the CLEERS activity has met its mission. The CLEERS Planning Committee revised the questions from the previous (2008 and 2007) surveys to account for recent developments in engine and emissions control technology, include specific questions regarding CLEERS activities, and clarify ambiguities remaining from the previous surveys. The new survey was then conducted via email during February and March of 2011.

As for previous surveys, the 2011 survey was intended to provide current information about how the research and development resources of DOE and its industry and academic partners can best be leveraged to facilitate the transition of the U.S. transportation sector to a more sustainable, energy efficient, and environmentally friendly condition. Unlike the 2008 survey, the 2011 survey did not focus specifically on identifying ‘technology gaps’ (that is, aftertreatment areas which were perceived as not receiving sufficient research funding and attention). This time the emphasis was instead on highlighting shifts in technology and specific ways in which CLEERS as an activity under the DOE Advanced Engine Crosscut Team could better serve its constituents. Major results from the 2011 survey have been publically discussed at the April 2011 CLEERS Workshop in Dearborn, Michigan and the Annual DOE Merit Review in May 2011. As with many surveys of this type, unconscious biases can be inadvertently built into the survey process. The public discussions provided an opportunity to identify such unintended biases and misunderstandings so that they could be accounted for in the final results. When it is finally approved for release, this report will be posted for public download on the CLEERS website (www.cleers.org).

Modifications to the survey questionnaires in 2011

For 2011, the CLEERS Planning Committee recognized that responding to the survey involves an intrinsic cost to industry participants. Thus the questionnaires were modified significantly from previous versions to reduce responder time and effort. As before, responders were asked to identify if they were

associated with the heavy duty diesel, light duty diesel, or gasoline sectors, and each company was invited to submit responses in each area. Responders were asked to answer on the basis of their individual organization's specific needs and business interests. In a few cases, multiple responses were received from the same company in each area. For purposes of this survey, such responses were individually compiled. However, for future surveys, it is recommended that measures be taken to make it easier for companies to submit a consensus response in each area.

A copy of the 2011 questionnaire and accompanying instructions are included in the Appendix. Briefly, the questionnaire consisted of four separate pages, and responders were asked to rank each selection on the first three pages as having High, Medium, or Low priority. The first page concerned priorities for specific emissions control technology areas; the second page focused on the importance of current CLEERS activities; and the third page attempted to identify directions in which expanding the focus of CLEERS databases would benefit the industry. The last page was reserved for any additional comments responders wished to provide. This last page was important in that it provided an opportunity to identify gaps in the coverage of the survey. There was only minor commentary on the last page from most responders, implying that the basic scope and construction of the survey did not have any major shortcomings. This also appeared to be confirmed by feedback received in the public discussions.

2011 Survey Participants and Analysis

Survey questionnaires were sent to organizations which are either direct members of the DOE Advanced Engine Crosscut Team or which have close working relationships with Crosscut members. The specific organizations receiving questionnaires were: Detroit Diesel, Cummins, Caterpillar, International, Ford, Volvo, Chrysler, GM, EPA, TARDEC, Chevron, Exxon-Mobil, Conoco-Phillips, Shell, BP, Delphi, Umicore, BASF, Johnson Matthey, and Corning. Most of these companies were also included in the 2008 survey. Individuals receiving the questionnaires were typically identified by their respective Crosscut Team representative or CLEERS Focus Group participant.

As in the past, the survey results have been summarized such that connections to specific companies and individuals are not revealed. However, responses have been broken down into 6 categories that include the responder's industry sector (i.e., heavy duty diesel, light duty diesel, and gasoline) and organization type (i.e., OEM, emission control supplier, and fuel company/non-DOE government). Considering the responses in terms of these categories is helpful in identifying distinct interests and trends among these groups. Altogether, 25 completed questionnaires were returned. A contact person at a few organizations could not be identified consequently no response was received. Of the responses received, 10 identified themselves as associated with the heavy duty diesel sector, 11 identified their affiliation as light duty diesel sector, and 4 came from gasoline sector organizations. 16 of the responses were from OEMs, 4 from emission control suppliers, and 5 from fuel supplier companies and non-DOE federal government organizations. Some companies had more than one response for a given industry sector, but all were included in compiling the overall results. It was noted, however, that in some of the cases with multiple responses from a single company, the answers were not in complete agreement. Thus it was recognized that the responses from some companies did not represent a corporate consensus.

An explicit numeric ranking scheme was used for compiling the results to provide a more consistent and less arbitrary basis for making comparisons than in the past. Weighted scores were computed for each question assuming that each 'High' response was assigned a rating of 100, each 'Medium' response was

assigned a rating of 50, and each ‘Low’ response was assigned a rating of 0. Cumulative scores for each question were then evaluated by the formula

$$\text{Cumulative Score} = (\text{NHi} \cdot 100 + \text{NMed} \cdot 50 + \text{NLow} \cdot 0) / (\text{NHi} + \text{NMed} + \text{NLow}) \quad (1)$$

where NHi, NMed, and NLow were the number of High, Medium, and Low responses for each question, respectively. Cumulative scores were determined for each of the responder categories above as well as collectively over all categories. Even though the resulting scores from Eqn.(1) provide explicit quantitative measures of the responses, we found that it was not necessarily appropriate to work strictly with the absolute numbers, since different weighting assumptions and different interpretations by the responders about some of the questions affected the final rankings. We found instead that the most consistent trends were revealed by considering each of the cumulative scores on a relative rather than absolute basis. This was taken into consideration in the discussion that follows.

The specific emissions controls technology areas included in the present survey were selected based on the experience of the CLEERS Planning Committee members and comments received from Crosscut Team members and participants in the CLEERS focus telecom discussions. The first area, diesel particulate filter (DPF) technology, focuses on control of particulate emissions from diesel engines. Most versions of DPF technology include catalytic coatings on the filter surface to promote soot oxidation, and these are sometimes termed catalytic diesel particulate filters (CDPFs). DPFs are being widely implemented and consequently have more direct application interest among Crosscut Team members. Another key technology area, ammonia-based selective catalytic reduction (SCR) of nitrogen oxides (NO_x), is also in the process of commercial implementation and is a key element of multi-functional emissions control systems. Since one of the most common implementations of ammonia-SCR employs urea slurry as an ammonia source, versions of SCR utilizing urea are frequently referred to as urea-SCR. Some more recent versions of ammonia-SCR make use of alternative ammonia sources that do not require urea injection. Lean NO_x trap (LNT) technology is commercially used in a number of diesel and gasoline applications. As a point of clarification, some parts of industry refer to LNT systems as NO_x storage and release (NSR) catalysts. This year’s CLEERS survey used the traditional ‘LNT’ terminology in the questionnaire. Besides DPF, ammonia-SCR, and LNT/NSR technologies, the survey included questions about oxidation catalysts (oxycats). The latter have recently received a heightened industrial focus. Hydrocarbon-based selective catalytic reduction (HC-SCR) of NO_x was included in the present survey, but this technology has been found to be incapable of fully meeting industry’s emission control needs after over two decades of research and development. Thus HC-SCR has typically had less interest among CLEERS participants in the recent past. Because of continued waning interest, it may be appropriate to remove questions about HC-SCR technology from future surveys.

2011 CLEERS Survey: Technical priorities

	<u>Overall</u>	<u>Overall w/o Other</u>	<u>HD Diesel</u>	<u>LD Diesel</u>	<u>Gasoline</u>	<u>OEM</u>	<u>Supplier</u>	<u>Other Orgs.</u>
<u>Particulate Control</u>								
Non-cat characteristics of filter media	46.00	52.50	50.00	54.55	12.50	46.88	75.00	20.00
Filter catalyst chem. & phys. properties	54.00	52.50	60.00	54.55	37.50	59.38	25.00	60.00
Part. & soot cake chem. & phys. properties	50.00	50.00	55.00	45.45	50.00	50.00	50.00	50.00
Coating effects on filtration, soot oxidation	60.00	57.50	60.00	63.64	50.00	65.63	25.00	70.00
Filter measurement, sensing, diagnostics	70.00	77.50	75.00	77.27	37.50	78.13	75.00	40.00
<u>NOx Control-SCR</u>								
Urea SCR cat. properties (incl. poisoning & aging)	76.00	75.00	85.00	81.82	37.50	71.88	87.50	80.00
Urea NOx reduction chemistry & kinetics	72.00	75.00	75.00	81.82	37.50	75.00	75.00	60.00
Urea injection fluid dynamics & controls	38.00	37.50	45.00	40.91	12.50	37.50	37.50	40.00
Urea decomposition chemistry & kinetics	58.00	65.00	70.00	59.09	25.00	59.38	87.50	30.00
Ammonia oxidation, storage, & release	66.00	60.00	60.00	63.64	87.50	65.63	37.50	90.00
Urea SCR cat. measurement, sensing, & diag.	64.00	70.00	70.00	68.18	37.50	68.75	75.00	40.00
HC SCR cat. properties (incl. poisoning & aging)	18.00	10.00	30.00	9.09	12.50	9.38	12.50	50.00
HC SCR NOx reduction chemistry & kinetics	18.00	12.50	30.00	9.09	12.50	12.50	12.50	40.00
HC SCR cat. measurement, sensing, & diagnostics	10.00	7.50	15.00	9.09	0.00	9.38	0.00	20.00
<u>NOx Control-LNT</u>								
LNT cat./storage med. properties & durability	42.00	35.00	45.00	45.45	25.00	34.38	37.50	70.00
LNT chemistry & kinetics (rich & lean)	44.00	42.50	40.00	50.00	37.50	43.75	37.50	50.00
Oxygen storage impact on LNT	46.00	45.00	45.00	50.00	37.50	43.75	50.00	50.00
LNT cat. measurement, sensing, & diagnostics	38.00	37.50	35.00	36.36	50.00	37.50	37.50	40.00
Reduction of PGM content	50.00	52.50	40.00	63.64	37.50	50.00	62.50	40.00
<u>Oxidation, Adsorbing, Reforming Devices</u>								
Oxidation cat. prop. (incl. poisoning & aging)	62.00	65.00	75.00	72.73	0.00	62.50	75.00	50.00
Oxidation cat. chemistry, additives, & kinetics	42.00	50.00	40.00	59.09	0.00	56.25	25.00	10.00
Oxid. cat. measurement, sensing, & diagnostics	38.00	40.00	45.00	45.45	0.00	34.38	62.50	30.00
HC traps	46.00	45.00	50.00	40.91	50.00	46.88	37.50	50.00
Fuel reformers	30.00	17.50	40.00	22.73	25.00	12.50	37.50	80.00
<u>System and Component Interactions</u>								
LNT-SCR	42.00	47.50	35.00	45.45	50.00	46.88	50.00	20.00
LNT-DPF or SCR-DPF	52.00	60.00	55.00	59.09	25.00	56.25	75.00	20.00
Oxycat-LNT or Oxycat-SCR	36.00	42.50	40.00	45.45	0.00	37.50	62.50	10.00
Oxycat-DPF	28.00	30.00	45.00	22.73	0.00	18.75	75.00	20.00
LNT-TWC	14.00	15.00	10.00	4.55	50.00	18.75	0.00	10.00
Full vehicle simulations	36.00	40.00	40.00	36.36	25.00	40.63	37.50	20.00

Table 1. Cumulative rankings for aftertreatment technology priorities (normalized distribution).

2011 CLEERS Survey: CLEERS activities								
	Overall	Overall w/o Other	HD Diesel	LD Diesel	Gasoline	OEM	Supplier	Other Orgs.
Current CLEERS Activities								
Coordinate public workshop	80.00	95.00	75.00	90.91	62.50	93.75	100.00	20.00
Coordinate monthly telecons	52.00	62.50	50.00	54.55	50.00	59.38	75.00	10.00
Maintain website	74.00	80.00	75.00	77.27	62.50	78.13	87.50	50.00
Identify/validate std. lab protocols for catalysts	64.00	75.00	50.00	77.27	62.50	71.88	87.50	20.00
Coordinate national labs	72.00	70.00	70.00	77.27	62.50	62.50	100.00	80.00
Utilize special national lab facilities	76.00	77.50	65.00	86.36	75.00	75.00	87.50	70.00
Develop kinetic/aging models for LNT/SCR/DPF	70.00	70.00	70.00	68.18	75.00	65.63	87.50	70.00
Obtain/share commercially relevant catalysts	60.00	67.50	60.00	68.18	37.50	62.50	87.50	30.00
Transfer models/data to other DOE projects, industry	74.00	75.00	65.00	72.73	100.00	71.88	87.50	70.00
Proposed CLEERS Activities								
Develop public database of engine out measurements	36.00	40.00	35.00	40.91	25.00	31.25	75.00	20.00
Maintain experimental & simulated bench reactor database	50.00	60.00	60.00	50.00	25.00	50.00	100.00	10.00
Maintain engine dyno & vehicle exp. & simulated data	50.00	57.50	50.00	59.09	25.00	50.00	87.50	20.00
Distribute research grade open source aftertreatment models	60.00	55.00	65.00	59.09	50.00	53.13	62.50	80.00
Maintain black box aftertreatment device models	28.00	32.50	35.00	31.82	0.00	31.25	37.50	10.00
Increase utilization of atomistic catalyst modeling	56.00	50.00	65.00	54.55	37.50	40.63	87.50	80.00
Expand protocols to include engine dyno measurements	38.00	42.50	45.00	36.36	25.00	37.50	62.50	20.00

Table 2. Cumulative rankings for current and proposed CLEERS activities (normalized distribution).

2011 CLEERS Survey: Expanded CLEERS databases								
	Overall	Overall w/o Other	HD Diesel	LD Diesel	Gasoline	OEM	Supplier	Other Orgs.
Public Experimental Data								
Std. lab measurements from LNT & SCR protocols	50.00	60.00	55.00	54.55	25.00	50.00	100.00	10.00
Non-std. lab measurements from LNT & SCR protocols	48.00	57.50	50.00	54.55	25.00	46.88	100.00	10.00
Engine out species & temperature	54.00	60.00	55.00	63.64	25.00	50.00	100.00	30.00
Engine dyno measurements with aftertreatment devices	48.00	50.00	50.00	54.55	25.00	43.75	75.00	40.00
Vehicle measurements with aftertreatment devices	44.00	45.00	45.00	50.00	25.00	37.50	75.00	40.00
Public Simulation Results								
I/O files for lab reactor LNT, SCR, or DPF simulations	42.00	50.00	50.00	36.36	37.50	46.88	62.50	10.00
I/O files for engine dyno LNT, SCR, or DPF simulations	40.00	47.50	40.00	45.45	25.00	43.75	62.50	10.00
I/O files for vehicle drive cycles with LNT, SCR, or DPF	42.00	50.00	45.00	45.45	25.00	46.88	62.50	10.00
I/O files for lab reactor with advanced cats/designs	16.00	17.50	25.00	13.64	0.00	21.88	0.00	10.00
I/O files for vehicle drive cycles with advanced cats/designs	20.00	22.50	25.00	22.73	0.00	28.13	0.00	10.00
Public Donated Software								
Black box component models for commercial/public software	36.00	27.50	40.00	36.36	25.00	31.25	12.50	70.00
Open source component models with public user group	60.00	57.50	65.00	59.09	50.00	59.38	50.00	70.00
Restricted Access Data or Software								
Non-public data or results for restricted user groups	24.00	27.50	30.00	27.27	0.00	28.13	25.00	10.00

Table 3. Cumulative rankings for possible expanded CLEERS databases (normalized distribution).

ANALYSIS AND SUMMARY OF SURVEY RESPONSES

We preface this section by noting that the procedure used for identifying survey responders did not provide any mechanism to develop overall consensus perspectives from the organizations involved. Thus, some of the responses are more reflective of the personal opinions of the responders than the overall positions of their companies. On the other hand, in other cases there was an explicit effort by the responder to coordinate answers across his/her organization. Likewise, in our analysis of the results we made no attempt to separate answers from higher level managers who are not regular CLEERS participants from those provided by technical experts who have been intimately involved in CLEERS discussions. As a consequence, the results below include all responses. With this in mind, we recommend that planning for future surveys should include consideration of measures to capture a broader consensus from each responding organization according to industry sector (i.e., heavy duty diesel, light duty diesel, and gasoline). We expect that this would help clarify some of the points of confusion discussed below.

One other important difference between the present survey and previous CLEERS surveys is that hybrid vehicle technologies are now becoming a much more prominent topic of interest. We observed that some of the survey responses reflected emergence of a somewhat distinct class or priorities for those involved with hybrid versus more conventional vehicle technology. It may also be appropriate in future surveys to distinguish the hybrid-related responses as a separate category.

Technical Priorities

In the following section the normalized priority scores concerning emission controls technology (page 1 of the questionnaire) are summarized collectively for all 25 responses combined as well as for the individual responder categories described above. Table 1 lists the cumulative scores computed by Eqn. (1).

Key observations are:

- When separate responder categories are not considered ('Overall' column), it appears that the highest global concerns center on control of particulate and lean NO_x emissions. More specifically, the largest technical challenges are perceived to be associated with measurement, sensing, and diagnostics for particulate filters and the functioning of the urea SCR catalyst for NO_x control. Oxidation catalyst function is also ranked highly.
- The relative interest in LNT technology appears to be reduced compared to previous surveys. The most critical LNT technical issue identified in the overall results appears to be a continuing need to reduce the precious metal content (and thus cost) of the catalyst.
- Regarding aftertreatment component interactions, coupling between SCR or LNT NO_x reduction catalysts and the particulate filter appear to be of greatest concern. This applies to both internal coupling where single devices are designed to have multiple functions (e.g., carry out both filtration and NO_x reduction) and device-to-device coupling where the output of one device influences the operation of another (e.g., where upstream removal of NO_x reduces the ability of a DPF to oxidize soot).

- The technology area receiving the lowest apparent interest among the survey responses was hydrocarbon (HC) SCR. However a reduced level of activity does continue in this area.
- There are shifts in the priority rankings when scores for the organization categories are considered. This is even apparent in the second and last columns of Table 1, where the fuel company and government ('Other') responses have been separated from the rest. In the second column we observe a slight elevation of the scores in many categories, implying that the technical concerns of the companies directly involved in producing and marketing vehicles and associated emission control hardware are significantly different from the fuel companies and government members of the DOE Advanced Engine Crosscut Team. This is confirmed in the last column, where we see clear differences compared to the diesel manufacturers and emission control suppliers. Note for example the high ranking of fuel reforming by the 'Other' responders compared to all the others. This may be an example of how the growth of hybrid vehicle technologies is affecting priorities in the CLEERS community.
- There are significant differences in technical priorities among the other categories. For example, there is much less concern about particulate controls among the gasoline sector members compared to those involved with heavy and light duty diesels. Concerns about LNT activity (both individually and in association with other components) has greater importance to the gasoline community. The most important priorities for suppliers appear to be concentrated on catalyst function and durability in all types of NO_x and particulate control devices.
- There also appears to be some divergence in priorities between OEMs and emission control equipment suppliers (for example in some of the particulate and oxidation catalyst areas). At this point it's difficult to say how important these differences really are because the small sample size for suppliers (4 total) adds significant statistical uncertainty.

Current and Proposed CLEERS Activities

As noted above, one objective of the new survey is to get feedback from the industry partners on how effectively CLEERS has met its mission. The second page of the questionnaire provided respondents the opportunity to provide this feedback. Table 2 summarizes the cumulative scores computed with Eqn. (1) for the overall responses as well as the organization categories.

Notable observations regarding the survey results for current CLEERS activities are:

- The cumulative responses confirm that the annual public workshop has widespread support, especially among OEMs and emission control equipment suppliers. The only responders not indicating strong support for the workshops were those in the 'Other' category (fuel suppliers and non-DOE government organizations). Workshop participation by members of the 'Others' category is typically low.
- The cumulative scores indicate that the CLEERS roles in data and information exchange (via the website), assisting in the coordination among (DOE) national labs, facilitating the utilization of specialized equipment and capabilities at national labs, and utilizing national lab data to support the development and transfer of aftertreatment device models to industry also have broad support

across industry. This is consistent with the results of past surveys and appears to indicate that CLEERS has been successful at meeting most of its original objectives in these areas.

- An unexpected outcome from the cumulative scoring was the somewhat lower ranking of the CLEERS technical telecoms, standard lab protocols, and sharing of commercially relevant catalyst data. The cumulative scores produced by Eqn. (1) contrast rather sharply with subsequent verbal feedback from workshop and Focus Group participants and the high attendance at telecom meetings (typically 20-30 participants, many from international locations in Asia and Europe). Further, it was pointed out that, compared to scores in other survey areas (e.g., Technical Priorities), the cumulative scores for all of the current CLEERS activities are quite high. This is an area where the comments at the workshop and on the focus calls are not fully consistent with the survey responses.

The second part of the second page of the survey questionnaire included a list of proposed new activities which have been suggested to the CLEERS Planning Committee by participants of the CLEERS Focus Groups. Relevant highlights from the resulting cumulative scores for these questions are:

- The area of highest interest appears to be in having CLEERS facilitate the distribution of ‘research grade’ aftertreatment models which can be used to collectively evaluate reference cases (e.g., performance characterization of reference catalysts subjected to the CLEERS protocols) and derive consistent kinetic parameters from shared laboratory data. This was an original CLEERS goal; however, it appears more reachable now in contrast with the status of aftertreatment modeling more than 10 years ago.
- Another area of growing interest revealed in the present survey is in utilization of atomistic-scale modeling of catalysts. Like the distribution of research aftertreatment models, the promotion of atomistic catalyst modeling has been previously considered as a possible role for CLEERS. It is possible that the recent improvements in computational tools and theories for atomistic-scale catalysis modeling has increased optimism among the emissions controls community that practical benefits can now be derived from this type of modeling. Many CLEERS participants in the Workshop and Focus discussions have voiced the opinion that atomistic modeling now has the capacity to realistically describe trends in supported catalyst activity.
- CLEERS has already implemented some very limited sharing of laboratory and engine dynamometer derived aftertreatment measurement data, but the interest shown in Table 2 indicates that more needs to be done to meet this need.
- As with the technical priority areas, there are some divergences in the responses of OEMs and suppliers regarding new directions for CLEERS. The modeling and data needs for these two groups are different, with the suppliers showing more interest in the sharing of catalyst data associated with formulation effects.

Expanded CLEERS Databases

The third page of the survey questionnaire was designed to get additional information about how the industry participants consider that the data exchange role for CLEERS might be enhanced. The questions on this page were again selected based on previous suggestions by individual Focus Group participants.

Some highlights from the cumulative the results are:

- The highest interest in potentially expanded roles for CLEERS in data exchange are in experimental engine-out dynamometer species and temperature measurements, simulation results for transient laboratory reactors, vehicle simulation results for drive cycles involving different types of aftertreatment devices, and open-source aftertreatment component models. Except for the last item (open-source models), CLEERS has already been involved to a limited extent in distributing such data. However, the survey responses seem to imply that the industry partners would like to see an appreciable increase in the level of this activity.
- Regarding open-source aftertreatment component models, the CLEERS Planning Committee has previously noted that such an activity would require careful definition of the software platforms utilized and would potentially require additional funding to account for the costs associated with software documentation, verification, validation, and user support. Sharing open-source models is the most clearly defined new priority arising from this survey..
- Of all the responder categories, those companies identified with Gasoline sector appeared to have the least interest in expanded CLEERS database activities. The one exception was in the distribution of open source component models, where the score was relatively high.
- The expanded database categories receiving the lowest overall scores are the exchange of laboratory and vehicle simulation results for advanced catalysts and reactor designs, non-public data sharing among restricted user groups, and sharing of black-box (i.e., inaccessible and proprietary) component models. Comments from some participants in the CLEERS Workshop indicate that the question about ‘advanced’ catalysts and reactor designs was somewhat unclear, so its low score may reflect uncertainty in interpretation rather than actual lack of interest.

Additional Comments

A very few responders provided written comments on the last page of the questionnaire, which were helpful in resolving some of the uncertainties in the cumulative score data from the first three pages. In some cases, the responders preferred to relay their additional comments verbally rather than in writing. In general, both written and verbal comments centered on suggestions of how to improve the survey process or ways to increase the direct benefits of CLEERS to industry partners. Regarding ways to improve the survey, the main points raised were:

- The more streamlined layout of the new questionnaire (requiring minimal writing on the part of the responders) is an improvement over the previous questionnaires.
- However, some of the questions/topic areas were worded such that their meaning was not necessarily clear, resulting in different interpretations by responders. More precise wording or possibly an accompanying set of explanatory footnotes might be helpful in future surveys.
- In future surveys, it would be good to enlist the help of companies in doing more to coordinate their responses so that the responses are more reflective of a common consensus in their respective industry sectors. Also, regarding questions about specific CLEERS activities, it would

be helpful for companies to include input from those staff members who have the most direct experience or familiarity with those activities.

Other comments received centered on specific concerns about the technology areas included in CLEERS discussions and concerns about how CLEERS can increase the availability of shared data and modeling tools. These can be summarized as follows:

- CLEERS organizers need to consider expanding the scope of technologies that are discussed and evaluated to include more on passive adsorber devices (e.g., for NO_x, hydrocarbons, and CO), which might be employed to supplement more conventional aftertreatment during engine cold start and severe drive cycle transients.
- It would be helpful for there to be more discussion of non-urea sources of NH₃ for NO_x reduction and multi-functional aftertreatment components, especially combined SCR/DPF devices.
- Additional emphasis on models for full vehicle simulations, especially lean exhaust hybrids would be beneficial.

SUMMARY AND HIGHLIGHTS

Technical Priorities

- ▶ Specific aftertreatment technology priorities vary significantly among the heavy duty diesel, light duty diesel, and gasoline industry sectors and between OEMs and emission controls equipment suppliers. This diversity of needs poses special challenges for CLEERS but it also creates unique opportunities for cross-disciplinary stimulation of new technical approaches and concepts.
- ▶ The greatest current concerns for companies in the heavy duty and light duty diesel sectors are related to chemical kinetics, sensing, and diagnostics for particulate filter devices and the chemical kinetics and durability of urea SCR catalysts for lean NO_x control.
- ▶ Gasoline sector companies are less concerned about particulate device operation and more concerned about fundamental characterization of the particulates generated by lean gasoline engines.
- ▶ Reduction of precious metal loading is the most pressing concern regarding lean NO_x trap (NSR) technology.
- ▶ Concern regarding the aging and poisoning of oxidation catalysts has increased apparently due to the impact of upstream NO oxidation on urea SCR catalysts and diesel particulate filters.
- ▶ Device interactions and multi-functional components (especially those involving LNT or SCR catalyst interactions with particulate filters) are a high priority for heavy and light duty diesel companies.
- ▶ Present industry interest in hydrocarbon SCR for lean NO_x control is very low.

Current CLEERS Activities

- ▶ Overall the most highly rated current CLEERS activities are the public workshop, the coordination and facilitation of industry access to national lab capabilities, and the distribution of fundamental, pre-competitive data on aftertreatment components.
- ▶ The CLEERS monthly telecons, standard catalyst characterization protocols, and sharing of commercially relevant catalyst data are ranked almost as high. Subsequent feedback from workshop

and Focus participants indicate that some survey respondents may have had no exposure to the focus group conference calls.

- ▶ Current CLEERS activities are meeting some the original objectives set forth by the Crosscut Team.

Proposed New CLEERS Activities

- ▶ Both the written survey responses and subsequent verbal feedback indicate increasing interest in CLEERS providing explicit assistance in the generation and distribution of open source aftertreatment component models. The focus of such models would be to provide a consistent set of tools that would allow comparisons and sharing of pre-competitive information among CLEERS participants in industry, universities, and national labs.
- ▶ CLEERS public distribution of experimental datasets of reference reactor and engine measurement data and simulation results is viewed as strong value added.
- ▶ Interest in atomistic-scale catalyst modeling is growing. There are indications that this type of modeling can have a practical impact on aftertreatment technology.

Expanded CLEERS Databases

- ▶ Industry interest in expanding CLEERS shared databases is strongest in regard to experimental engine-out species and temperature measurements, laboratory reactor simulation results, simulations of vehicle drive cycles with various aftertreatment technologies, and open-source aftertreatment component models.

RECOMMENDATIONS

Based on the above results, the CLEERS Planning Committee and Focus Group Leaders recommend the following:

Regarding Technical Priorities

- ▶ R&D efforts in diesel exhaust emissions controls should maintain emphasis on experimental data and models for soot and NO_x oxidation kinetics and improved sensing and diagnostics in particulate filter devices.
- ▶ R&D efforts in diesel exhaust NO_x control should emphasize chemical kinetics and durability of urea SCR catalysts.
- ▶ Lean NO_x trap (NSR) modeling and simulation R&D should focus on lean gasoline exhaust.
- ▶ Research on lean gasoline particulates should focus on fundamental particulate characterization.
- ▶ Aftertreatment component interactions and multi-functional component performance are a high priority of the CLEERS participants.

Regarding Current CLEERS Activities

- ▶ In terms of allocating DOE's budget and personnel resources, the highest priority should be given to continuing the CLEERS public workshops, coordinating the various national laboratory R&D activities on lean exhaust emissions controls, and open sharing of pre-proprietary data among the broad CLEERS community.
- ▶ As much as possible, CLEERS monthly telecons, development of standard catalyst characterization protocols, and identification and sharing of reference catalysts be continued as they are currently implemented.

Regarding Proposed New CLEERS Activities and Expanded Databases

- ▶ A panel of experts should be identified from among the CLEERS community (including representation from industry, national labs, and academia) to encourage and solicit sharing of pre-competitive aftertreatment component models.
- ▶ The panel should consider ways in which sharing of experimental and reactor and engine data can be expanded under CLEERS.
- ▶ The panel should also consider and propose directions for more effective utilization of atomistic catalyst modeling.

Appendix- 2011 CLEERS Questionnaire

2011 Survey of CLEERS R&D Priorities and Activities

General Instructions

- Questionnaires for **HD diesel**, **LD diesel**, and **Gasoline** are separate, and each company can submit a separate response for any or all of the 3 areas.
- Answers should be based on the responder's understanding of their organization's specific needs/business interests.
- There are 4 separate pages in each questionnaire. On the first 3 pages, please indicate your level of interest in each option as "High (**H**), Medium (**M**), or Low (**L**)". On the 4th page, please feel free to add any additional comments or concerns you have that are not covered on the first 3 pages.
- Your responses regarding **Technology Priorities** will help us update our identification of the most pressing aftertreatment technology issues where CLEERS can help answer pre-competitive questions. At the top of the page, please identify if you are answering for the **HD diesel**, **LD diesel**, or **Gasoline** market.
- Your input on **CLEERS Activities** will help us determine which CLEERS activities are most important. We also invite you to list up to 3 additional activities/roles not included in the list which you believe would be beneficial.
- Your feedback on **Expanded CLEERS Databases** will help us identify in more detail if/how shared databases might be used more effectively by the CLEERS community. It has been proposed that CLEERS should increase its role in facilitating exchange of pre-competitive results from aftertreatment simulations. This could take the form of experimental data, computational results, and even component software. We would also like you to list up to 2 additional components you would like to see in the database that are not already listed.
- The **Additional Comments** page is provided for any additional input and comments you might have beyond that covered in the previous pages.

Technology Priorities

Market Perspective (choose one)

Heavy duty diesel

Light duty diesel

Gasoline

Please indicate High (**H**), Medium (**M**), or Low (**L**) in importance (choose one).

Particulate Emissions Controls

H **M** **L** -Non-catalytic characteristics of particulate filter media

H **M** **L** -Particulate filter catalyst chemical and physical properties

H **M** **L** -Particulate/soot cake chemical and physical properties

H **M** **L** -Coating effects on filtration and soot cake oxidation

H **M** **L** -Particulate filter measurement, sensing, and diagnostics

NOx Emission Controls- Selective Catalytic Reduction

H **M** **L** -Urea SCR catalyst properties (including poisoning and aging)

H **M** **L** -Urea NOx reduction chemistry and kinetics

H **M** **L** -Urea injection fluid dynamics and controls

H **M** **L** -Urea decomposition chemistry and kinetics

H **M** **L** -Ammonia oxidation, storage, and release

H **M** **L** -Urea SCR catalyst measurement, sensing, and diagnostics

H **M** **L** -HC SCR catalyst properties (including poisoning and aging)

H **M** **L** -HC NOx reduction chemistry and kinetics

H **M** **L** -HC SCR catalyst measurement, sensing, and diagnostics

NOx Emission Controls- Lean NOx Traps/NOx Storage and Reduction Catalysts

H **M** **L** -LNT catalyst/storage medium properties and durability

H **M** **L** -LNT chemistry and kinetics (lean and rich)

H **M** **L** -Oxygen storage impact on LNT kinetics

H **M** **L** -LNT catalyst measurement, sensing, and diagnostics

H **M** **L** -Reduction of precious group metal (PGM) content

Oxidation, Adsorbing, and Reforming Devices

H **M** **L** -Oxidation catalyst properties (including poisoning and aging)

H **M** **L** -Oxidation catalyst chemistry, additives, and kinetics

H **M** **L** -Oxidation catalyst measurement, sensing, and diagnostics

H **M** **L** -HC traps

H **M** **L** -Fuel reformers

System Level and Component-Component Interactions

H **M** **L** -LNT-SCR

H **M** **L** -LNT-DPF or SCR-DPF

H **M** **L** -Oxcat-LNT or Oxcat-SCR

H **M** **L** -Oxcat-DPF

H **M** **L** -LNT/TWC

H **M** **L** -Full vehicle simulations

CLEERS Activities

Please indicate as High (**H**), Medium (**M**), or Low (**L**) in importance (choose one).

Current CLEERS Activities

- H** **M** **L** -Coordinate public workshop on aftertreatment modeling and simulation.
- H** **M** **L** -Coordinate monthly technical telecons.
- H** **M** **L** -Maintain website for announcements, data sharing, member interactions.
- H** **M** **L** -Identify and validate std. lab protocols for catalyst measurements.
- H** **M** **L** -Coordinate aftertreatment R&D at national labs.
- H** **M** **L** -Utilize national lab facilities to measure kinetics & catalyst properties.
- H** **M** **L** -Develop kinetic/aging models for LNT, DPF, urea-SCR devices.
- H** **M** **L** -Obtain, share commercially relevant reference catalysts.
- H** **M** **L** -Transfer CLEERS models and data to other DOE projects and industry.

Proposed CLEERS Activities

- H** **M** **L** -Develop public database of donated engine out emission measurements. **H** **M** **L**
- Maintain a database of experimental and simulated bench reactor measurements of reference catalysts and exhaust particulates.
- H** **M** **L** -Maintain a database of experimental and simulated engine dynamometer and vehicle measurements of aftertreatment catalysts and particulate filters.
- H** **M** **L** -Distribute open source, research-grade aftertreatment models derived from CLEERS data for use with DOE's AUTONOMIE vehicle simulation program.
- H** **M** **L** -Maintain a database of 'black box' aftertreatment device models supplied by national labs, universities, or vendors which can be used interchangeably in commercial and internal vehicle simulation platforms.
- H** **M** **L** -Increase utilization of atomistic-scale computational modeling to guide development of advanced aftertreatment catalysts ('catalysts by design').
- H** **M** **L** -Expand CLEERS protocols to include procedures and measurement standards for engine dynamometer measurements of aftertreatment performance.

Are there additional CLEERS activities not listed above which you would like to see? If so, please list up to 3.

Expanded CLEERS Databases

Please rank each as High (H), Medium (M), or Low (L) priority (choose one).

Public Experimental Data (from national labs, universities, or industry). This might be loosely patterned after the Engine Combustion Network (<http://www.sandia.gov/ecn/>).

H M L -Lab measurements (in a standard format) from CLEERS LNT and SCR protocol experiments with model or commercial catalysts.

H M L -Lab measurements from non-standard characterization experiments (variable user-defined format) with LNT and SCR catalysts or exhaust particulates.

H M L -Engine out species and temperature for a range of combustion technologies.

H M L -Engine dynamometer measurements with one or more aftertreatment components (variable user defined format).

H M L -Experimental vehicle measurements (chassis dynamometer or on road) involving one or more aftertreatment components (variable user defined format).

Publicly Accessible Simulation Results (Note: It is assumed that any software used must be either documented in the open literature or commercially available).

H M L -I/O files for simulations of lab LNT, SCR, or particulate reactor experiments available in the open literature or through the CLEERS website.

H M L -I/O files for simulations of engine dynamometer and aftertreatment experiments available in the open literature or through the CLEERS website.

H M L -I/O files for simulations of vehicle drive cycle aftertreatment performance experiments available in the open literature or through the CLEERS website.

H M L -I/O files for simulations of hypothetical laboratory experiments with advanced catalysts or modified aftertreatment reactors.

H M L -I/O files for simulations of hypothetical engine dynamometer or vehicle experiments with advanced catalysts or modified aftertreatment devices, configurations, or operating strategies.

Publicly Accessible Donated Software Modules

H M L -'Black box' component models (pre-compiled and/or encrypted) with defined I/O file protocols which can be used by anyone with the appropriate simulation platform(s) (public or commercial) to make comparative simulations.

H M L -Open source aftertreatment component models with defined I/O protocols, version updating, verification/validation, and a public user group (similar to the MFIX software platform for multi-phase flow reactor modeling developed and currently supported by DOE, www.mfix.org).

Restricted Access Data or Software

H M L -Non-public data or results from any of the above categories which is restricted to specific user groups (e.g, CRADA or MOU partners or CLEERS subgroups).

Are there additional types of databases not listed above which you would like to see? If so, please list up to 2 more.

Page 4: Additional Comments

Please use the space below to add any additional comments or suggestions you might have regarding any of the topics covered in the previous pages or other specific feedback you might have regarding how CLEERS might be enhanced to make it more directly useful to you. You may also contact Stuart Daw directly at dawcs@ornl.gov , 865-946-1341.