

2013 CLEERS Industry Priorities Survey Final Report

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EXECUTIVE SUMMARY

This report summarizes results from the 2013 survey of the CLEERS industry partners concerning their current needs and priorities in exhaust emissions controls technology for trucks and cars. CLEERS, which stands for **Cross-Cut Lean Exhaust Emissions Reduction Simulation**, is an informal collaboration among industry, the Department of Energy (DOE) and universities that operates under the auspices of DOE Diesel Crosscut Team. CLEERS main objective is to support the exchange of non-proprietary data and information among original equipment manufacturers, emission control suppliers, academia, and DOE regarding emission controls and emission controls modeling and simulation. The CLEERS industry priority survey is conducted approximately every two years to obtain the latest information from industry participants on their perspectives concerning rapidly changing technology issues and the most appropriate ways in which the CLEERS collaboration can facilitate non-proprietary R&D to help resolve those issues.

The results reported here are based on an anonymous random sampling of CLEERS industry partners from among the DOE Diesel Crosscut Team and their direct collaborators. The survey was conducted by means of standard questionnaires sent to: Detroit Diesel/Daimler, Cummins, Caterpillar, Navistar, Ford, Volvo, Chrysler, GM, EPA, TARDEC, Chevron, Exxon-Mobil, Conoco-Phillips, Shell, Delphi, Umicore, BASF, Johnson Matthey, Eaton, and Corning. No national labs or DOE representatives were included in the survey. While the survey process was not rigorously constructed to be statistically representative, we believe that the results represent a useful qualitative reflection of the opinions of a broad cross-section of industry experts from the responding organizations.

Regarding emission controls technologies, the highest overall priorities identified by the responders were:

- On-board diagnostics and multi-functional particulate filters.
- The mechanisms and dynamics of NH₃ storage and release in NH₃ selective catalytic reduction.
- Low-temperature catalysts for nitrogen oxides reduction and oxidation of hydrocarbons and carbon monoxide.
- Passive adsorbers and multi-zone catalysts.
- Lean NO_x trap catalysts with lower precious metal content.

Some high priority technology concerns were associated with specific responder groups:

- Nano-particulates were of greatest concern to those from the gasoline and supplier groups.
- Emission controls suppliers indicated higher priority to LNT mechanisms and kinetics, hydrocarbon selective catalytic reduction of nitrogen oxides, and modeling of hybrid electric vehicles.
- Three-way catalysts were of primary concern to the gasoline sector responders.
- Heavy-duty diesel manufacturers and suppliers indicated the highest level of concern regarding the impact of alternate fuels on emissions and emissions controls.
- Interest in micro-kinetics and atomistic-scale modeling of catalysts was strongest among a subset of heavy-duty diesel responders but low in other groups.
- Vehicle-level system modeling, including drive-cycle interactions between engines and aftertreatment had high priority in all groups except heavy-duty diesel responders.

The lowest responder priorities were generally indicated for the following:

- New filter membranes and particulate oxidation kinetics.
- Generation of NH₃ from non-urea sources.
- Modeling urea-spray/injection dynamics.
- LNT catalyst modeling issues other than supporting lower precious metals.

- Refinement of catalysts for hydrocarbon selective catalytic reduction of nitrogen oxides.

Regarding CLEERS activities, the highest levels of support were for:

- The CLEERS public workshops.
- Coordination of national lab R&D.
- Monthly focus technical telecons.

Some CLEERS activities were indicated by certain responder groups as having higher priority:

- CLEERS development of standardized catalyst characterization protocols was most highly ranked by gasoline responders.
- Light-duty diesel manufacturers and suppliers indicated the highest support for CLEERS to generate benchmark aftertreatment models and data that can be publicly shared.

Other observations concerning CLEERS were:

- The website has been moderately successful in serving the CLEERS community but there is room for improvement.
- Access to unique national lab facilities was not highly ranked, but after the survey it was determined that many responders were confused by the language used in the questionnaire.
- Having CLEERS provide shared reference catalysts received a low ranking from all groups.

Some important issues raised by the survey need additional follow up:

- How to reconcile the indicated low priority for particulate oxidation kinetics, micro-scale kinetics, urea-SCR mechanisms and kinetics, and urea spray dynamics, when these processes are known to be highly important in low-temperature emissions controls.
- How to interpret the apparent lack of priority for hybrid electric vehicle simulation among manufacturers.
- The need to encourage greater participation in the CLEERS technical telecons from suppliers.
- The specific improvements needed in the CLEERS website and shared databases.
- How national labs and universities can best respond to industry concerns about working with commercially relevant catalysts while maintaining their pre-competitive focus.

INTRODUCTION AND BACKGROUND

Objectives

CLEERS stands for **C**ross-**C**ut **L**ean **E**xhaust **E**missions **R**eduction **S**imulation. CLEERS is an informal 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 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 procedural rules and standards, 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 2012, 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 2011) 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 March and April of 2013.

The 2013 survey was organized along the lines of the previous surveys 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. As in 2011, the present survey did not focus on identifying ‘technology gaps’ (that is, aftertreatment areas which were perceived as not receiving sufficient research funding and attention) but instead on highlighting shifts in perceived technology barriers and specific ways in which CLEERS might better serve its broad spectrum of participants. Some results from the present survey were presented at the Annual DOE Merit Review in May 2013, and a more detailed summary was presented to the Advanced Engine Crosscut Team at their July 2013 meeting at USCAR. As much as possible, we have used our experience with previous surveys to reduce unintentional biases and confusion into the survey questionnaires. Discussions with the Crosscut Team and individual responders have helped to identify such biases and misunderstandings in order to improve our interpretation of the results. In this report we have attempted to explicitly note areas where questions still remain. Once this report is approved for release by the Crosscut team, it will be posted for public download on the CLEERS website (www.cleers.org).

Modifications to the survey questionnaires in 2013

In recognition of the time involved in responding to these surveys, we have continued to work toward shortening and simplifying the questionnaires. As in previous surveys, responders were asked to identify

whether they were primarily associated with the heavy duty diesel, light duty diesel, or gasoline sectors, and each company was allowed to submit responses in each area where they had strong interest. 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. In keeping with past practice, such responses were individually compiled. Given the diversity of CLEERS participation among some companies and the time involved, it was determined to be impractical to request each company to review all of their individual responses to develop a single consensus response in each area.

A copy of the 2013 questionnaire and accompanying instructions are included in Appendix A. Briefly, the questionnaire consisted of an introduction and instruction page, two pages of multiple-choice responses, and a final page for unstructured comments and concerns. On the two multiple-choice pages, responders were asked to rank each selection as having High, Medium, or Low priority. The first multiple-choice page concerned priorities for specific emission control technology areas where simulation and modeling are needed; the last multiple-choice page focused on specific CLEERS activities. On the second multiple-choice page responders were asked to list any other potential CLEERS activities or focus areas they would like to see that were not covered in the multiple-choice list. On the final page, responders were asked to provide any other comments or suggestions, either specific to CLEERS or about the general state of emissions control R&D and the role of modeling and simulation.

2013 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 this year were: Detroit Diesel/Daimler, Cummins, Caterpillar, Navistar, Ford, Volvo, Chrysler, GM, EPA, TARDEC, Chevron, Exxon-Mobil, Conoco-Phillips, Shell, Chevron, Delphi, Umicore, BASF, Johnson Matthey, Eaton, and Corning. Most of these companies were also included in the previous two surveys. Individuals receiving the questionnaires were identified by their respective Crosscut Team representative or CLEERS Focus Group participant. No national labs or DOE representatives were included in the survey.

As in the past, the present survey results have been summarized such that connections to specific companies, institutions, or individuals are not revealed. However, response results have been broken down into different categories that include the responder's industry sector (e.g., heavy duty diesel, light duty diesel, or gasoline) and organization type (e.g., OEM, emission control supplier, non-DOE government or fuel supplier). As before, we found it is helpful to consider the responses in terms of these categories to better recognize and understand the distinct interests and concerns among the diverse group of companies participating in CLEERS. Altogether, twenty-four (24) completed questionnaires were returned. Some of our previous survey contacts had left their previous organizations, and, when alternate contacts could not be identified, no response was available. Of the responses received, fifteen (15) were from original equipment manufacturers (OEMs), five (5) from emission control suppliers, two (2) from non-DOE government organizations, and two (2) from fuel suppliers. Seven (7) of the responders identified themselves as associated with the heavy duty diesel sector, seven (7) identified their affiliation as light duty diesel sector, and ten (10) came from gasoline sector organizations. Some companies had more than one response for a given industry sector, but all were included in compiling the overall results. Since we did not ask each organization to generate an overall consensus on each survey question, multiple

answers from some organizations were not in complete agreement. While this complicates the analysis, it also demonstrates the diversity of opinion within single organizations.

Quantitative measures of the responses were generated by assigning numerical values to each response: **High Priority=3; Medium Priority=2; and Low Priority=1**. Average scores were then computed for each topical area considering all the responders together as well as for each of the responder categories individually. This made it possible for us to assess the relative priorities of the different emission control topics and CLEERS activities. In general we found that average scores of **2.0** or above corresponded to topics or activities with widespread interest or support. However, as before, we found that it was not necessarily appropriate to only consider the absolute numbers, since different weighting assumptions and different interpretations by the responders about some of the questions affected the final rankings. So in some cases relative rather than absolute scores were useful for indicating trends. Likewise, we found it useful to evaluate response standard deviations to reveal diversity of opinion within groups.

RESULTS AND DISCUSSION

Table 1 below summarizes the major trends seen in the collective responses from all the participants regarding the emissions control technologies of greatest concern. In this case, the results are divided into two columns, with the highest priority areas (with their average scores in red) on the left and the lowest priority areas (and their average scores in red) on the right. A complete listing of all the scores for Table 1 is given in Appendix B. One clear trend revealed here is that there is a very high level of interest globally among the CLEERS industrial community regarding the development of improved diagnostics and sensors for diesel particulate controls. There is also strong interest in the development of multi-functional filters with NO_x reduction and HC oxidation capability in addition to particulate removal. For NO_x control with NH₃ catalytic reduction, the biggest concerns center on how to account for NH₃ storage on the catalyst and its loss via oxidation. Accurate models for these processes would be key for evaluating the catalyst state as part of on-board diagnostics. The area of highest general concern for catalytic NO_x control with LNTs is in minimizing the level of expensive PGMs in the catalysts. But as can be seen from the average scores, LNT technology in general appears to be of lesser concern than the other technology areas in the table. The scores for low-temperature catalysis, passive adsorbers, and system level simulations (with aftertreatment included) seem to reflect a growing general recognition that optimal use of advanced combustion engines will require simultaneous consideration of both the engine and emissions control components in the context of realistic drive cycle transients.

There are also some significantly lower priority areas revealed in Table 1. The lowest of these appear to be associated with new particulate filter materials, atomistic scale modeling, and NO_x control with LNT or HC SCR catalysts. From a purely technical perspective, the relatively low ranking for particulate oxidation kinetics seems to be inconsistent with the strong interest in particulate filter diagnostics and sensing. Subsequent discussions with responders suggest that this may be a case where the questionnaire wording was confusing and the relationship between diagnostics and the regeneration properties of particulate materials was not clear in the way these choices were presented. On the other hand the low average score for the micro-kinetic modeling area appears to be an example of where there was a high degree of variation among the different groups and responders. This is illustrated later in summaries for the different responder categories.

<u>Technology Area</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
Particulate Controls	<ul style="list-style-type: none"> • Particulate OBD (2.67) • Multi-function filters (2.54) 	<ul style="list-style-type: none"> • New filter membranes (1.67) • PM oxidation kinetics (1.96)
NOx Control/NH3 SCR	<ul style="list-style-type: none"> • NH3 storage & oxidation (2.50) • SCR OBD (2.46) 	<ul style="list-style-type: none"> • Non-urea NH3 (1.88) • Urea injection (2.00)
NOx Control/LNTs	<ul style="list-style-type: none"> • Low PGM catalysts (2.00) 	<ul style="list-style-type: none"> • Mechanisms & kinetics (1.79) • Poisoning & aging (1.83) • Catalyst OBD (1.83) • Low-T catalysts (1.83)
Other Control Issues	<ul style="list-style-type: none"> • Low-T oxidation catalysts (2.30) • Passive HC/NOx adsorbers (2.21) 	<ul style="list-style-type: none"> • New HC SCR catalysts (1.71) • New TWCs (1.75)
Modeling & Simulation	<ul style="list-style-type: none"> • Vehicles with adv. combustion + aftertreatment (2.42) • System level drive cycles (2.21) 	<ul style="list-style-type: none"> • Atomistic cat. modeling (1.75) • Micro-kinetic catalyst modeling (1.96)

Table 1. Summary of priorities for emission control technology areas based on the average scores over all responders, regardless of category.

Table 2 lists the high and low emissions control technology priorities as before, except that now only the heavy-duty diesel responders were included. As above, improved particulate control diagnostics, sensors, and filter multi-functionality were given high priority and new filter materials were of much lesser interest. As might be expected nano-particulates and TWCs, which are typically associated with gasoline engines, were of less concern to the heavy-duty diesel group. Given the recent trend in this sector in favor of NH₃ SCR for NO_x control, the high level of interest in NH₃ SCR diagnostics and mechanisms and the low level of interest in LNTs and HC SCR are also perhaps not surprising. Low-temperature performance of oxidation catalysts was ranked relatively high, consistent with the overall average response. One major change compared to the overall responder averages was an apparently higher interest in the heavy-duty diesel group for utilizing the micro-kinetic and atomistic modeling compared to the other groups. We observed that such group-to-group deviations in priority could frequently be indicated in higher standard deviations among the scores (see for example Appendix B). Also, the heavy-duty group seemed to indicate a greater interest in shared models and data from dynamometer-scale measurements and in the effects of alternate fuels. Conversely, heavy-duty diesel interest in hybrid simulation and system simulation of advanced combustion engines combined with aftertreatment appeared to be relatively low.

Table 3 summarizes the emission control simulation priorities among light-duty diesel responders. As one might expect, there were similar trends compared to the heavy-duty diesel group, but there were also some important differences. The most notable of the latter include: a stronger interest in vehicle systems simulation with advanced combustion engines and aftertreatment linked; a higher interest in NO_x control with LNTs; and less interest in micro-kinetic models. As noted above, it appears that the questionnaire wording may have obscured the connections between modeling particulate oxidation kinetics and filter regeneration diagnostics.

<u>Technology Area</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
Particulate Controls	<ul style="list-style-type: none"> • Particulate OBD (2.43) • Low-T DPF regeneration (2.43) • Multi-function filters (2.29) 	<ul style="list-style-type: none"> • New filter membranes (1.29) • Nano-PM character (1.43)
NOx Control/NH3 SCR	<ul style="list-style-type: none"> • NH3 storage & oxidation (2.71) • Low-T SCR catalysts (2.71) • SCR OBD (2.57) 	<ul style="list-style-type: none"> • Non-urea NH3 (1.71)
NOx Control/LNTs	<ul style="list-style-type: none"> • Low PGM catalysts (1.86) • Cat aging & poisoning (1.71) • Low-T catalysts (1.71) 	<ul style="list-style-type: none"> • Mechanisms & kinetics (1.43) • Catalyst OBD (1.57)
Other Control Issues	<ul style="list-style-type: none"> • Alternate fuel effects (2.43) • Low-T oxid. catalysts (2.29) 	<ul style="list-style-type: none"> • TWC kinetics & mechanisms (1.14) • New HC SCR catalysts (1.86)
Modeling & Simulation	<ul style="list-style-type: none"> • Micro-kinetic catalyst modeling (2.43) • Atomistic cat. modeling (2.00) • Shared models & dyno data (2.00) 	<ul style="list-style-type: none"> • Hybrids + aftertreatment (1.29) • Vehicles with advanced combustion + aftertreatment (1.57)

Table 2. Summary of priorities for emission control technology areas based on average scores from the heavy-duty diesel responders only.

<u>Technology Area</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
Particulate Controls	<ul style="list-style-type: none"> • Particulate OBD (2.85) • Multi-function filters (2.57) 	<ul style="list-style-type: none"> • New filter membranes (1.71) • PM oxidation kinetics (1.85)
NOx Control/NH3 SCR	<ul style="list-style-type: none"> • NH3 storage & oxidation (2.86) • SCR OBD (2.57) 	<ul style="list-style-type: none"> • Non-urea NH3 (2.00) • Urea injection (2.14)
NOx Control/LNTs	<ul style="list-style-type: none"> • Mechanisms & kinetics (2.29) • Catalyst OBD (2.14) • Low PGM catalysts (2.14) 	<ul style="list-style-type: none"> • Poisoning & aging (1.86) • Low-T catalysts (1.86)
Other Control Issues	<ul style="list-style-type: none"> • Low-T oxid. catalysts (2.57) • Passive HC/NOx adsorbers (2.57) • Multi-zone catalysts (2.28) 	<ul style="list-style-type: none"> • New HC SCR catalysts (1.43) • TWC kinetics & mechanisms (1.57)
Modeling & Simulation	<ul style="list-style-type: none"> • Vehicles with adv. combustion + aftertreatment (2.71) • System level drive cycles (2.29) 	<ul style="list-style-type: none"> • Atomistic cat. modeling (1.71) • Micro-kinetic catalyst modeling (2.00) • Shared models & dyno data (2.00)

Table 3. Summary of priorities for emission control technology areas based on average scores from the light-duty diesel responders only.

Technology-based priorities coming from only gasoline responders are summarized in Table 4. Like the two diesel groups, the gasoline responders also gave high priority to improved diagnostics for particulate controls and NH₃ SCR and low priority to new filter materials and HC SCR. Also like the light-duty diesel group, the gasoline responders ranked system simulation with advanced engines and aftertreatment as a high priority and small-scale catalyst modeling (micro-kinetic and atomistic) as a low priority. The distinctive interests of the gasoline responders are revealed their greater interest in NO_x control with LNTs, nano-particulates, and TWCs. It also appears that the priorities of the gasoline responders for linked simulations of advanced engines and aftertreatment and system level simulations of drive cycle performance are similar to those of the light-duty diesel group.

Technology Area	Highest Priority	Lowest Priority
Particulate Controls	<ul style="list-style-type: none"> • Nano-PM characterization (2.90) • Characterization & modeling filter mech. (2.70) • Particulate OBD (2.70) • Multi-function filters (2.70) 	<ul style="list-style-type: none"> • New filter membranes (1.90) • PM oxidation kinetics (2.00)
NO_x Control/NH₃ SCR	<ul style="list-style-type: none"> • SCR OBD (2.30) • NH₃ storage & oxidation (2.10) 	<ul style="list-style-type: none"> • Urea injection (1.60) • Mechanisms & kinetics (1.80)
NO_x Control/LNTs	<ul style="list-style-type: none"> • Low PGM catalysts (2.00) • Low-T catalysts (1.90) 	<ul style="list-style-type: none"> • Mechanisms & kinetics (1.80) • Aging & poisoning (1.80) • Catalyst OBD (1.80)
Other Control Issues	<ul style="list-style-type: none"> • Multi-zone catalysts (2.40) • TWC kinetics & mechanisms (2.30) 	<ul style="list-style-type: none"> • Oxid. mechanisms & kinetics (1.80) • New HC-SCR catalysts (1.80)
Modeling & Simulation	<ul style="list-style-type: none"> • Vehicles with adv. combustion + aftertreatment (2.80) • System level drive cycles (2.40) 	<ul style="list-style-type: none"> • Atomistic catalyst modeling (1.60) • Micro-kinetic catalyst modeling (1.70)

Table 4. Summary of priorities for emission control technology areas based on average scores from the gasoline responders only.

Different priorities between OEM and emission control responders are revealed by Tables 5 and 6. Suppliers appear to have a generally wider range of high priority categories than OEMs, and they also indicate higher concerns for nano-particulates, SCR catalyst poisoning and aging, LNT modeling and diagnostics, HC SCR, novel catalyst structures, and hybrid vehicle simulations. The relatively low priority assigned by suppliers to new filter materials appears to imply that they do not see major needs for modeling and simulation in selecting or designing new filter materials.

Somewhat surprisingly, the suppliers collectively appear to agree with most OEMs in assigning lower priorities to atomistic and micro-kinetic modeling. It is difficult to understand the lack of priority for more fundamental modeling, because it seems at odds with the indicated high concern for low-temperature oxidation catalysts. These concerns appear to parallel the findings of the recent low-temperature exhaust

<u>Technology Area</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
Particulate Controls	<ul style="list-style-type: none"> • Multi-function filters (2.67) • Particulate OBD (2.67) 	<ul style="list-style-type: none"> • New filter membranes (1.73) • PM oxidation kinetics (1.87)
NOx Control/NH3 SCR	<ul style="list-style-type: none"> • NH3 storage & oxidation (2.53) • SCR OBD (2.47) 	<ul style="list-style-type: none"> • Urea injection (2.07) • Non-urea NH3 (2.07)
NOx Control/LNTs	<ul style="list-style-type: none"> • Low PGM catalysts (2.13) • Low-T catalysts (1.80) 	<ul style="list-style-type: none"> • Poisoning & aging (1.47) • Catalyst OBD (1.67)
Other Control Issues	<ul style="list-style-type: none"> • Low-T oxidation catalysts (2.47) • Passive HC/NOx adsorbers (2.33) 	<ul style="list-style-type: none"> • New HC-SCR catalysts (1.60) • Alternate fuel effects (1.80)
Modeling & Simulation	<ul style="list-style-type: none"> • Vehicles with adv. combustion + aftertreatment (2.47) • System level drive cycles (2.13) 	<ul style="list-style-type: none"> • Atomistic catalyst modeling (1.60) • Micro-kinetic catalyst modeling (1.93) • Vehicles with hybrids + aftertreatment (1.93)

Table 5. Summary of priorities for emission control technology areas based on average scores from the OEM responders only.

<u>Technology Area</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
Particulate Controls	<ul style="list-style-type: none"> • Particulate OBD (3.00) • Nano-PM characterization (3.00) • Multi-function filters (2.60) 	<ul style="list-style-type: none"> • New filter membranes (1.80) • PM oxidation kinetics (2.00)
NOx Control/NH3 SCR	<ul style="list-style-type: none"> • NH3 storage & oxidation (2.80) • SCR OBD (2.80) • Poisoning & aging (2.40) 	<ul style="list-style-type: none"> • Non-urea NH3 (1.80)
NOx Control/LNTs	<ul style="list-style-type: none"> • Mechanisms & kinetics (2.20) • Catalyst OBD (2.20) 	<ul style="list-style-type: none"> • Low PGM catalysts (1.80) • Poisoning & aging (2.00) • Low-T catalysts (2.00)
Other Control Issues	<ul style="list-style-type: none"> • New HC-SCR catalysts (2.40) • Multi-zone catalysts (2.40) • Alternate fuel effects (2.40) • Oxid. Mech. & kinetics (2.20) • Low-T oxid. catalysts (2.20) • Passive HC/NOx adsorbers (2.20) 	<ul style="list-style-type: none"> • TWC kinetics & mechanisms (1.80)
Modeling & Simulation	<ul style="list-style-type: none"> • System level drive cycles (2.60) • Vehicles with adv. combustion + aftertreatment (2.60) • Hybrids + aftertreatment (2.40) 	<ul style="list-style-type: none"> • Atomistic catalyst modeling (2.00) • Micro-kinetic cat. modeling (2.00)

Table 6. Summary of priorities for emission control technology areas based on average scores from the emission control supplier responders only.

workshop held at USCAR in November 2012. We suspect that poor wording in the questionnaire may have caused confusion that led to inconsistent answers. The relative priority for including fundamental kinetics modeling in addressing low-temperature catalysis is an important issue to resolve, since this is an area in which the fundamental science activities in DOE could provide direct support to the CLEERS community.

Table 7 summarizes the numerical responder rankings for different CLEERS activities. One area of general agreement across all groups was the high ranking of the annual public CLEERS Workshops. This was further supported by numerous individual comments from the responders. Other CLEERS activities that were generally ranked high by most groups were the coordination of R&D at national labs and the organization of the monthly technical telecoms. There appeared to be some divergence among the groups in terms of their interest in public data and models and experimental protocols generated by CLEERS. Some responders ranked the data, model, and protocol functions of CLEERS very highly, while others considered it less important. This may reflect differences in the in-house capabilities at the different institutions for making experimental measurements or constructing computational models of emissions control component performance. All groups appeared to generally agree on assigning low priority to CLEERS acting as a repository of shared reference catalysts. Our impression here is that the OEM responders generally feel that they have all the access to commercially relevant catalyst samples that they need from the catalyst suppliers.

<u>Activity</u>	<u>Highest Priority</u>	<u>Lowest Priority</u>
All Responders	<ul style="list-style-type: none"> • Public workshops (2.63) • Natl. lab coordination (2.54) 	<ul style="list-style-type: none"> • Shared reference catalysts (1.92) • Access to natl. lab facilities (2.08)
All OEMs	<ul style="list-style-type: none"> • Public workshops (2.60) • Monthly tech. telecoms (2.60) 	<ul style="list-style-type: none"> • Shared reference catalysts (2.00) • Access to natl. lab facilities (2.13)
EC Suppliers	<ul style="list-style-type: none"> • Public workshops (3.00) • Natl. lab coordination (3.00) • Public lab/dyno/model data (3.00) 	<ul style="list-style-type: none"> • Access to natl. lab facilities (1.60) • Shared reference catalysts (1.60) • Monthly technical telecoms (1.80) • Std. catalyst protocols (1.80)
HDD/OEM	<ul style="list-style-type: none"> • Public workshops (2.67) • Monthly tech. telecoms (2.67) • Natl. lab coordination (2.67) 	<ul style="list-style-type: none"> • Std. catalyst protocols (1.67) • Access to natl. lab facilities (1.67) • Shared reference catalysts (1.67) • Public lab/dyno/model data (1.67)
LDD/OEM	<ul style="list-style-type: none"> • Public workshops (2.80) • Monthly tech. telecoms (2.60) • Aftertreatment models & data (2.60) 	<ul style="list-style-type: none"> • Shared reference catalysts (2.00)
Gasoline/OEM	<ul style="list-style-type: none"> • Monthly tech. telecoms (2.57) • Std. catalyst protocols (2.57) • Natl. lab coordination (2.57) 	<ul style="list-style-type: none"> • Shared reference catalysts (2.14)

Table 7. Summary of priorities for CLEERS activities based on average scores from each responder group.

The low numerical ranking for access to national lab facilities was initially puzzling. Subsequent feedback from responders concerning the question of national lab access revealed that they generally interpreted ‘access’ to mean the physical availability of national lab facilities to direct use by outside researchers. Upon reflection, we realized that we had miscommunicated our intent here, which was to get feedback on how much our industry partners felt the results generated by the unique experimental and computational facilities at the labs contributed to CLEERS. Based on follow up discussions, we expect that the numerical responses would have been rather different if we had clarified the wording here to mean what was actually intended.

Additional comments provided by responders in the last section of the questionnaire included the following major points:

- Low-temperature catalytic oxidation of CH₄ emissions is an area of growing concern.
- Control of emissions from lean/dilute low temperature combustion should continue to be a high priority for CLEERS.
- On-board diagnostics and sensors, especially for NH₃ and particulates, continue to be of high importance to both OEMs and suppliers.
- There is continued interest in CLEERS providing vehicle-level simulations and measurements of engine out temperatures, flows, and species.
- CLEERS workshops and telecons are doing a good job of providing technical updates on latest developments.
- CLEERS workshops have done a good job of facilitating exchange of information about aftertreatment model development/improvement but there needs to be a shift toward actual examples of model application/usage.
- There is widespread interest in CLEERS supporting more system level modeling.

SUMMARY AND CONCLUSIONS

As noted above, the results from this survey should not be construed to represent a statistically representative sampling of all the U.S. transportation industry or reflect the official positions of their managers. But we believe the results do include the opinions of a broad cross-section of industry experts who are highly knowledgeable about the emissions control technology needs and concerns of their respective institutions. Most of the responders have also been frequent participants in CLEERS, so they are significantly aware of CLEERS activities. In some cases the responders coordinated with others in their organizations to develop a degree of consensus, but the level of internal coordination varied greatly among organizations and there was no attempt to control that in the survey implementation. Nevertheless, we expect that these findings represent at least a qualitative reflection of the perspectives of the CLEERS industry partner technology priorities and the role that the CLEERS collaboration can play in facilitating the needed non-proprietary R&D.

Concerning emission controls technology priorities, the survey revealed the following:

- All responding groups surveyed place high priority on on-board diagnostics and multi-functional filters for particulate emissions control.

- Characterization of nano-particulates was of greatest concern to those from the gasoline and supplier groups.
- All groups generally ranked new filter membranes and particulate oxidation kinetics as having low priority, even though low-temperature oxidation of particulate emissions is of widespread concern.
- All groups had high concern about understanding the mechanisms and dynamics of NH₃ storage and release in NH₃-SCR and the associated utilization of on-board diagnostics.
- All groups indicated high priority for developing low-temperature catalysts, and the heavy-duty diesel responders expressed the specific concern about low-temperature catalytic oxidation.
- All groups indicated that generation of NH₃ from sources other than urea should have a relatively low priority.
- Most groups indicated that lean NO_x trap technology should have generally lower priority than urea-SCR, and the greatest remaining LNT issue continues to be reducing the precious metal content of the catalyst.
- Suppliers gave higher priority to continuing the study of LNT mechanisms and kinetics and diagnostics compared to OEMs.
- There was broad interest among all groups in low-temperature oxidation catalysts, passive adsorbers, and multi-zone catalysts.
- The apparent level of interest in HC-SCR continues to be low among OEMs, although there is more interest among the suppliers compared to the other groups.
- As expected, the highest priority in understanding 3-way catalyst kinetics and mechanisms was indicated by the gasoline group.
- Interest is widespread in system-level modeling that includes the engine and aftertreatment.
- Of all the groups, the heavy-duty diesel responders gave the highest priority to atomistic and micro-kinetics modeling.
- The highest priority for hybrid electric vehicle simulations was indicated by the supplier group.
- Interest in alternate fuels and their effects on emissions controls appear to be highest among the heavy-duty diesel OEMs and suppliers.

In light of the above, there are still important questions remaining about technology priorities which need to be further investigated. These include:

- Why did most industry responders assign low priorities for particulate oxidation kinetics, urea-SCR mechanisms and kinetics, and urea spray dynamics, when these processes are known to be highly important in low-temperature emissions controls?
- Why were there significant priority divergences between OEMs and suppliers in SCR and LNT catalyst mechanism modeling and also in system modeling of hybrid electric vehicles?
- Why did heavy-duty diesel OEMs indicate higher interest in atomistic and micro-kinetic modeling compared to the other groups?

Regarding CLEERS activities, the survey responses revealed that:

- The CLEERS public workshops and national lab coordination received the highest rankings across all the groups.
- Interest and participation in the monthly focus telecons are high, especially among the OEMs.
- The website has been moderately successful in serving the CLEERS community but there is room for improvement.
- CLEERS development of standardized catalyst characterization protocols was most highly ranked by gasoline OEMs but ranked relatively low by heavy-duty diesel OEMs.
- Access to unique national lab facilities was not highly ranked, but after the survey it was determined that many responders were confused by the language used in the questionnaire.
- Having CLEERS provide shared reference catalysts received a low ranking from all groups.

- Light-duty diesel OEMs and suppliers gave the highest support CLEERS to generate benchmark aftertreatment models and data that can be publicly shared. The lowest rankings for giving priority to this activity came from the heavy-duty diesel OEMs.

Remaining questions about CLEERS activities needing additional follow up include the following:

- Why are there significant differences in participation in the technical telecoms between the supplier and OEM groups?
- What specific improvements need to be made to the CLEERS website and shared databases to improve their value?
- How do national labs and universities respond to industry concerns about working with commercially relevant catalysts given the general lack of support for having CLEERS maintain shared commercial reference catalysts?

Acronyms

CLEERS Crosscut Lean Exhaust Emissions Simulation

CO Carbon monoxide

DOE Department of Energy

GDI Gasoline direct injection

HC Hydrocarbon

HDD Heavy-duty diesel

LDD Light-duty diesel

LNT Lean NO_x trap

NH₃ Ammonia

NO_x Nitrogen oxides

OEM Original equipment manufacturer

PM Particulate matter

SCR Selective catalytic reduction

Appendix A- 2013 CLEERS Questionnaire (Cover Letter)

Dear Colleague:

You are receiving this email because you have been identified as having a unique perspective on aftertreatment simulation and modeling. The CLEERS Planning Committee has been asked by the DOE Advanced Engine Crosscut Team to periodically survey the Crosscut Team members and their emission control equipment partners to ensure that CLEERS is doing everything we can to promote useful discussion and resolution of shared, pre-competitive aftertreatment technology issues. We would very much appreciate your filling out this form and returning it to Stuart Daw (dawcs@ornl.gov) at your earliest convenience. We have tried to design this form so that it should take no more than 10 minutes to complete. Our goal is to receive all the responses by Wednesday, May 1st. Your assistance in this process is greatly appreciated. Please feel free to contact me by email or phone (865-946-1341) if you have any questions or concerns. As in the past, all answers are kept in strictest confidence and are never associated with any specific individual or company.

Best Regards,

Stuart Daw for the CLEERS Planning Committee

Appendix A- 2013 CLEERS Survey Questionnaire (Instructions)

2013 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 your understanding of your organization’s specific needs/business interests. We recognize that not everyone may have the same perspective about some of the listed technologies or terminology. If you feel some of the listed questions are not clear or open to multiple interpretations, please feel free to provide additional explanations for your answer in the general comment section (see part 3 below).
- There are 3 separate parts in each questionnaire. In the first 2 parts, please indicate your level of interest in each option as “High (**H**), Medium (**M**), or Low (**L**)”. Be sure to check only one box (**H**, **M**, or **L**) for each option (unfortunately the form is not ‘smart’ enough to prevent multiple box checks for each option).
- Your responses regarding **Technology Priorities** (part 1) 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** (part 2) 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.
- The **Additional Comments** page (part 3) is provided for any additional comments or concerns you have beyond your High, Medium, and Low scores on the first 2 parts. As noted above, this is where you can comment on any of the previously listed ranking areas where you think additional explanations would be helpful or where you think important technology issues were missed.

Appendix A- 2013 CLEERS Survey Questionnaire (Page 1)

1. 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 -Characterization and modeling of filtration mechanisms
- H M L -Particulate/soot cake oxidation kinetics
- H M L -Particulate filter measurement, sensing, & diagnostics for OBD
- H M L -Multi-functional filters (including NOx and/or CO+HC controls)
- H M L -Discovery of new low-temperature regeneration strategies
- H M L -GDI particulate characterization (low & high temperature)
- H M L -Membrane layer filtration technology

NOx Emission Controls- NH₃ Selective Catalytic Reduction

- H M L -Urea SCR catalyst NOx reduction mechanisms & kinetics
- H M L -Urea SCR catalyst poisoning & aging mechanisms
- H M L -Urea injection dynamics & decomposition kinetics
- H M L -NH₃ storage, oxidation, & release on SCR catalysts
- H M L -Urea SCR catalyst measurement, sensing, & diagnostics for OBD
- H M L -Non-urea NH₃ sources
- H M L -Discovery of new low-temperature NH₃-SCR catalysts

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

- H M L -LNT catalyst NOx storage and reduction mechanisms & kinetics
- H M L -LNT catalyst poisoning & aging mechanisms
- H M L -LNT catalyst measurement, sensing, & diagnostics for OBD
- H M L -Discovery of lower PGM LNT formulations
- H M L -Discovery of new lower-temperature LNT catalysts

Other Emissions Control Categories

- H M L -Oxidation catalyst mechanisms & kinetics
- H M L -Discovery of new low-temperature oxidation catalysts
- H M L -Passive HC or NOx adsorbers and their kinetics
- H M L -HC SCR catalyst refinement or new materials discovery
- H M L -Three-way catalyst mechanisms & kinetics
- H M L -Multi-layer, multi-zone catalysts (e.g., LNT/SCR, TWC/SCR)
- H M L -Alternate fuel effects on emissions controls (e.g. biofuels, natural gas)

Multi-Scale Modeling and Simulation

- H M L -System level drive cycle simulation for transient emissions response
- H M L -Atomistic modeling to refine catalyst kinetic description
- H M L -Microkinetic catalyst modeling to understand rate limiting kinetics
- H M L -Shared lab & dyno models & data for relevant reference catalysts
- H M L -Vehicle simulations of advanced combustion + aftertreatment
- H M L -Vehicle simulations of hybrids + aftertreatment

Appendix A- 2013 CLEERS Survey Questionnaire (Page 2)

2. CLEERS Activities

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

- H M L -Public workshop on aftertreatment modeling and simulation.
- H M L -Monthly technical telecons.
- H M L -Website for announcements, data sharing, member interactions.
- H M L -Std. lab protocols for catalyst measurements.
- H M L -Coordination of national lab aftertreatment R&D.
- H M L -Access to unique experimental and/or computational DOE lab facilities.
- H M L -Shared commercially relevant referencecatalysts.
- H M L -Aftertreatment models & data from government sponsored projects.
- H M L -Public databases of lab & engine-out measured & simulated emissions.

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

Appendix A- 2013 CLEERS Survey Questionnaire (Page 3)

3. 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.

Appendix B- Summary Statistics for 2013 CLEERS Survey (All 24 responders)

1. Technology Priorities (Average score/Std. deviation)

Scores computed based on High=3, Medium=2, Low=1

Particulate Emissions Controls

Characterization and modeling of filtration mechanisms- **2.25/.794**

Particulate/soot cake oxidation kinetics- **1.96/.751**

Particulate filter measurement, sensing, & diagnostics for OBD- **2.67/.637**

Multi-functional filters (including NO_x and/or CO+HC controls)- **2.54/.588**

Discovery of new low-temperature regeneration strategies- **2.21/.779**

GDI particulate characterization (low & high temperature)- **2.25/.897**

Membrane layer filtration technology- **1.67/.761**

NO_x Emission Controls- NH₃ Selective Catalytic Reduction

Urea SCR catalyst NO_x reduction mechanisms & kinetics- **2.13/.797**

Urea SCR catalyst poisoning & aging mechanisms- **2.21/.721**

Urea injection dynamics & decomposition kinetics- **2.00/.834**

NH₃ storage, oxidation, & release on SCR catalysts- **2.50/.722**

Urea SCR catalyst measurement, sensing, & diagnostics for OBD- **2.46/.779**

Non-urea NH₃ sources- **1.88/.797**

Discovery of new low-temperature NH₃-SCR catalysts- **2.29/.859**

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

LNT catalyst NO_x storage and reduction mechanisms & kinetics- **1.83/.868**

LNT catalyst poisoning & aging mechanisms- **1.79/.833**

LNT catalyst measurement, sensing, & diagnostics for OBD- **1.83/.917**

Discovery of lower PGM LNT formulations- **2.00/.834**

Discovery of new lower-temperature LNT catalysts- **1.83/.868**

Other Emissions Control Categories

Oxidation catalyst mechanisms & kinetics- **1.96/.807**

Discovery of new low-temperature oxidation catalysts- **2.29/.751**

Passive HC or NO_x adsorbers and their kinetics- **2.21/.721**

HC SCR catalyst refinement or new materials discovery- **1.71/.807**

Three-way catalyst mechanisms & kinetics- **1.75/.847**

Multi-layer, multi-zone catalysts (e.g., LNT/SCR, TWC/SCR)- **2.17/.761**

Alternate fuel effects on emissions controls (e.g. biofuels, natural gas)- **2.04/.690**

Multi-Scale Modeling and Simulation

System level drive cycle simulation for transient emissions response- **2.21/.721**

Atomistic modeling to refine catalyst kinetic description- **1.75/.794**

Microkinetic catalyst modeling to understand rate limiting kinetics- **2.00/.780**

Shared lab & dyno models & data for relevant reference catalysts- **2.13/.797**

Vehicle simulations of advanced combustion + aftertreatment- **2.42/.776**

Vehicle simulations of hybrids + aftertreatment- **1.96/.624**

Appendix B- Summary Statistics for 2013 CLEERS Survey (All 24 responders)

2. CLEERS Activities (Avg. score/Std. deviation)

Scores computed based on High=3, Medium=2, Low=1

Public workshop on aftertreatment modeling and simulation- **2.63/.647**

Monthly technical telecons- **2.29/.807**

Website for announcements, data sharing, member interactions- **2.38/.576**

Std. lab protocols for catalyst measurements- **2.21/.658**

Coordination of national lab aftertreatment R&D- **2.54/.658**

Access to unique experimental and/or computational DOE lab facilities- **2.08/.830**

Shared commercially relevant reference catalysts- **1.92/.717**

Aftertreatment models & data from government sponsored projects- **2.46/.658**

Public databases of lab & engine-out measured & simulated emissions- **2.42/.717**