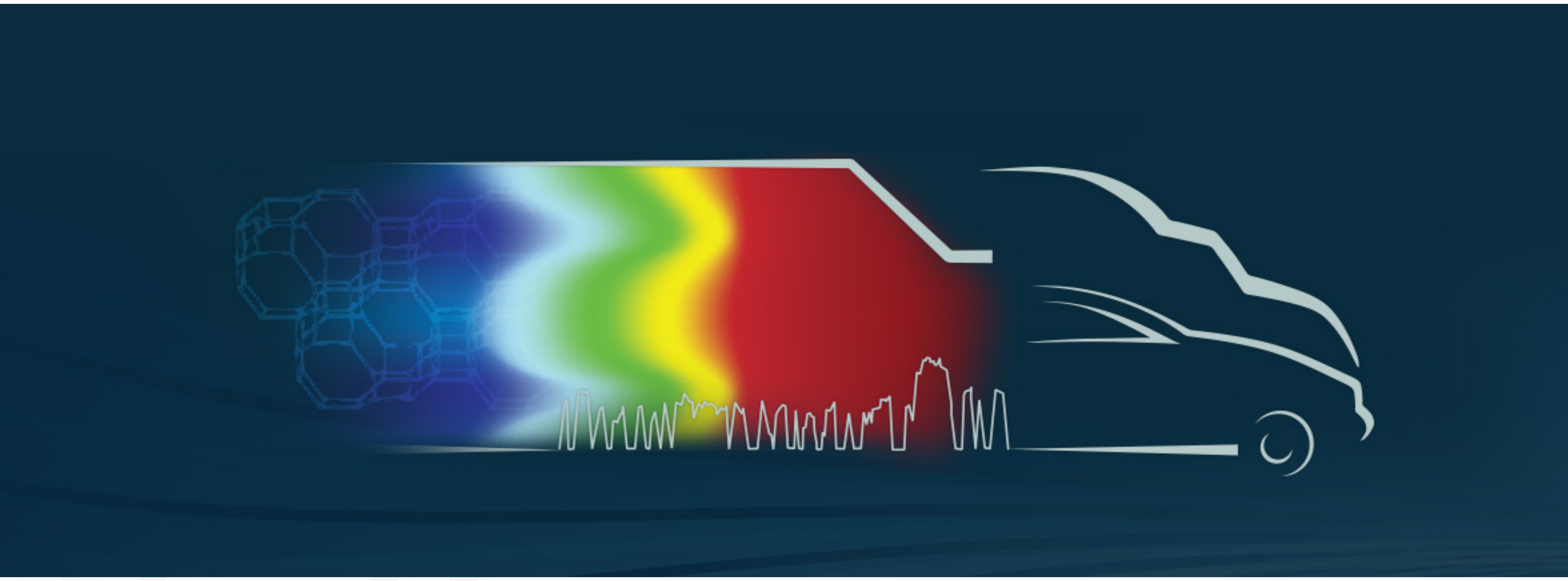
CLEERS
Cross Cut Lean
Exhaust Emissions
Reduction Simulations



2015 CLEERS Industry Priorities Survey Final Report

"A survey-based assessment of emission control research priorities based on input from 23 companies in the automotive and trucking industries"

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For the CLEERS Planning Committee
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CLEERS is an R&D focus project of the U.S. Department of Energy
Advanced Engine Cross-Cutting Technology Development Team

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Finally, we thank all of the CLEERS participants who responded to the survey questionnaire.

CONTENTS

ABBREVIATIONS

DOC	diesel oxidation catalyst
DOE	U.S. Department of Energy
DPF	diesel particulate filter
EPA	U.S. Environmental Protection Agency
GHG	greenhouse gas
GPF	gasoline particulate filter
HCT	hydrocarbon trap
HDD	heavy duty diesel
LDD	light duty diesel
LDG	light duty gasoline
LNT	lean NOx trap
MSD	multi-scale modeling, simulation, and data sets
NG	natural gas
NOx	oxides of nitrogen
PM	particulate matter
OBD	onboard diagnostics
OEC	other emissions control devices
PNA	passive NOx adsorber
SCR	selective catalytic reduction
TARDEC	U.S. Army Tank Automotive Research, Development, and Engineering Center
TWC	three-way catalyst

1. INTRODUCTION

1.1 CLEERS

CLEERS is an R&D focus project of the DOE Advanced Engine Cross-Cutting Technology Development Team (known as the Cross-Cut Team). The Cross-Cut Team is composed of representatives from heavy duty engine manufacturers, automotive companies, the U.S. Department of Energy (DOE), the U.S. Army Tank Automotive Research, Development and Engineering Center (TARDEC), and the U.S. Environmental Protection Agency (EPA). The primary function of the Crosscut Team is to coordinate development efforts for advanced, low-emission, high-efficiency combustion engines. This role includes identification and prioritization of specific R&D projects appropriate for government funding.

CLEERS was created in response to a key barrier to the commercialization of advanced high-efficiency engines identified by the Cross-Cut Team; specifically, the need for accurate simulation tools for use in designing, calibrating, and controlling the advanced aftertreatment systems needed to meet increasingly stringent U.S. emissions regulations in parallel with advancing fuel economy/greenhouse gas requirements. The mission of CLEERS is to accelerate the development of these simulation tools. It performs this mission through the pursuit of four key objectives: (1) supporting collaborations among industry, university and DOE National Laboratory partners; (2) developing and disseminating pre-competitive data, parameters, and models; (3) gathering feedback from industry on critical emissions control research needs; and (4) coordinating DOE National Laboratory research efforts.

1.2 SURVEY MOTIVATION

The CLEERS Industry Priority Survey was developed to support the third objective listed above: gathering feedback from industry on critical emissions control research needs. It was designed as a way to get a snapshot of the technology areas and development needs that are of highest importance to our industrial partners. The survey was initiated in 2007, and conducted in 2008, 2011, 2013. The survey has been modified with each iteration to best capture recent trends in directions in engine and aftertreatment development as identified by the CLEERS organizers. Reports from prior surveys are available through the CLEERS website. The results from the survey are used to guide the ongoing emissions control research programs at the DOE National Laboratories, and to inform DOE program managers and Cross-Cut Team members in planning new research activities.

2. SURVEY APPROACH

2.1 SURVEY STRUCTURE AND CONTENTS

The full survey text, including the cover letter and instructions for completing the survey, is included in Appendix A. As was done in previous surveys, the current survey questionnaire was separated into three sections: Technology Priorities, CLEERS Activities, and Additional Comments.

2.1.1 Technology Priorities

In the first section, respondents were asked to indicate the market perspective to which their responses applied. They were then asked to rate a series of technology priorities as High, Medium, or Low importance by selecting the appropriate check box next to each research priority listed. The 64 research priorities included in the survey were organized into 10 technology areas:

1. Particulate Emissions Controls: Diesel Particulate Filters (DPF)
2. Particulate Emissions Controls: Gasoline Particulate Filters (GPF)
3. NOx Emission Controls: NH_3 Selective Catalytic Reduction (SCR)
4. NOx Emission Controls: Lean NOx Trap (LNT) or NOx Storage/Reduction Catalysts
5. Oxidation Catalysts for Diesel (DOC) or Low Temperature Combustion Engines
6. Three-way Catalysts (TWC) for Stoichiometric Engine Exhaust
7. Low Temperature Adsorbers: Hydrocarbon Traps (HCT)
8. Low Temperature Adsorbers: Passive NOx adsorbers (PNA)
9. Other Emissions Control Devices and Issues (OEC)
10. Multi-Scale Modeling, Simulation, and Data Sets (MSD)

The specific research priorities listed were tailored to the individual technology areas under which they fell. However, where possible, the priorities were worded so as to reflect parallel research connections across multiple technology areas. For example, many of the technology areas included research topics that addressed formation of greenhouse gases, aging, poisoning, reaction kinetics, or discovery of novel low temperature formulations. The survey was structured in this manner in an effort to identify the emergence of consistent research themes across multiple technology areas.

2.1.2 CLEERS Activities

In the second section, respondents were asked to rate a list of CLEERS activities as High, Medium, or Low importance by selecting the appropriate check box next to each activity listed. There were a total of 11 CLEERS activities included in the survey, most of which are already conducted under CLEERS. However, two new activities were added to the list to gauge survey respondents' interest in their inclusion as part of the CLEERS organization's activities.

In addition to the priority ratings, this section of the survey included a text box in which respondents were given an opportunity to list up to three additional activities that they would want to see conducted by CLEERS.

2.1.3 Additional Comments

The third section of the survey included a text box in which respondents were asked to enter any additional comments or suggestions regarding the technology priorities or CLEERS activities. In addition, there was a question prompting respondents to share their perspectives on the "potential importance of emerging technologies that could directly or indirectly impact vehicle emissions controls, including:

Light-duty electric hybridization; Heavy-duty electric hybridization; Natural gas fueling; Gasoline vs. diesel heavy duty vehicles."

2.2 DISTRIBUTION

The survey was sent as an email attachment to a total of 23 organizations, which included manufacturers of light duty and heavy duty vehicles, engine manufacturers, emissions control suppliers, energy companies, and government agencies. In most instances, the survey was sent to three individuals at each organization. Typically these individuals had either replied to prior CLEERS Industry Priority Surveys, and/or were active in recent CLEERS-organized activities. Respondents were asked to indicate one of three market segments to which their responses applied: heavy duty diesel (HDD), light duty diesel (LDD), and gasoline (LDG). It should be noted that the survey did not differentiate between stoichiometric and lean-burn gasoline engines, so responses from the LDG market segment would include both of these technologies. The instructions for the survey requested that each organization submit a single response for each market segment, for a total of up to three questionnaire responses from each organization.

2.3 SUMMARY OF RESPONSES

A total of 29 survey responses were received from 16 organizations, which equates to at least one response from 70% of the organizations that were surveyed. Some of the survey responses indicated that they applied to more than one market segment; in these instances, the response was duplicated and counted as a separate response for each market segment. Some of the organizations submitted more than response for a single market segment; in those instances, the scores (as described in the analysis methodology section below) from that organization and market segment were averaged to create a single composite response from that organization for that market segment. After these separations and combinations were completed, a total of 34 independent survey responses remained. The distribution of responses across market segments is summarized in Figure 1.

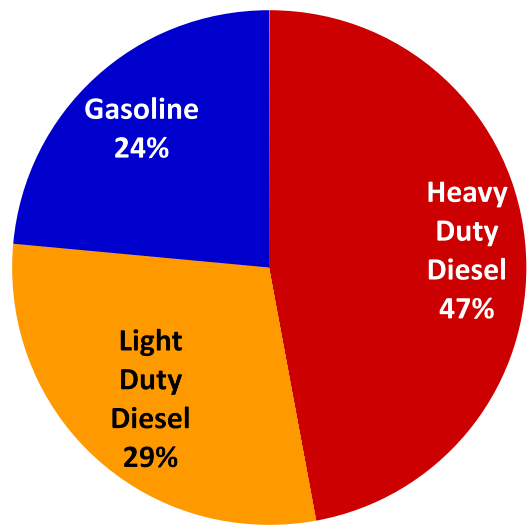

Figure 1. Distribution of survey responses by market perspective

2.4 ANALYSIS METHODOLOGY

As discussed in section 2.1, respondents were asked to rate research topics and CLEERS activities as High, Medium, or Low priority. To better summarize the survey responses and draw comparisons across technology areas and market perspectives, these ratings were assigned arbitrary individual scores of 10 for High, 5 for Medium, and 0 for Low. These scores were then averaged across various technology areas, market perspectives, and respondent classifications to identify overall trends in priorities. Based on the arbitrary scores, a topic which received a High priority rating from all respondents would receive an average score of 10, while a topic that was rated as Low priority by all respondents would have an average priority score of 0. Thus, higher average scores indicate a larger fraction of respondents rating a particular topic as high priority, and lower average scores signify a larger fraction of respondents rating the topic as low priority. For each average score, the fractions of High, Medium, and Low ratings underlying the score were also tracked to provide a measure of scatter (or disagreement) among the survey respondents.

The survey analysis methodology is illustrated in Figure 2, which demonstrates how a sample set of individual survey responses are converted into individual scores that are averaged to calculate an overall average priority score for a particular topic. The sample bar plot illustrates how the survey responses are graphically represented for most of the discussion that follows: the length of the bar is proportional to the average priority score, while the shaded areas are proportional to the fraction of respondents that rated the topic as Low (red), Medium (yellow), or High (green) importance. It should be noted that the survey distribution methodology and number of responses received do not represent a scientific sampling of the emissions control community. Furthermore, the number of responses received from each market perspective, and the limited response options in the survey, do not allow for an accurate assessment of whether or not the responses adhere to a normal (or other) distribution, preventing rigorous statistical analysis of the survey responses. However, the qualitative analysis outlined here still allows for extraction of useful insights on general trends in industrial emissions control research directions.

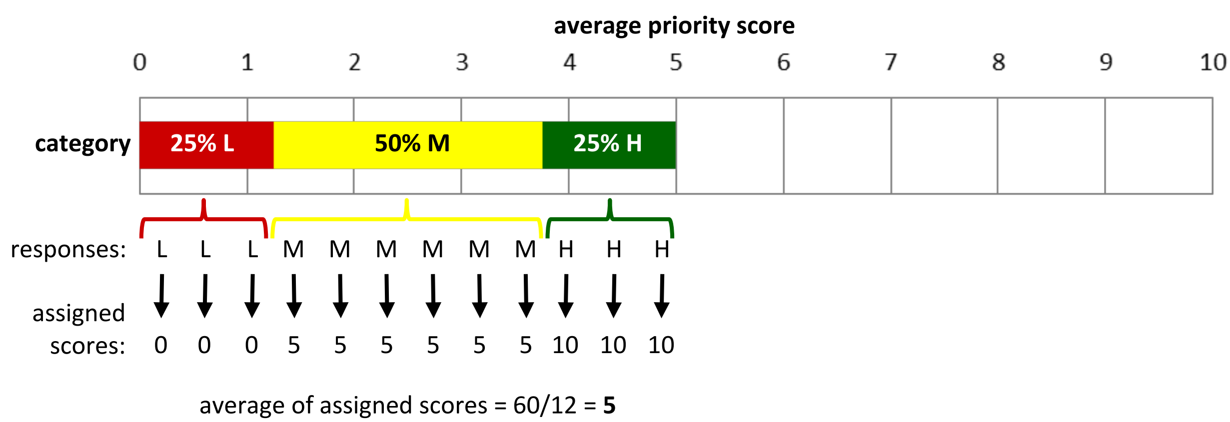

Figure 2. Illustration of survey analysis and plotting methodology showing how responses are assigned scores, scores are averaged to generate the average priority score for a given topic, and the distribution of responses is indicated with different fill colors on the bar chart.

3. SURVEY RESULTS

3.1 CLEERS ACTIVITIES

Figure 3 shows the priority scores for all of the CLEERS activities included in the survey averaged across all survey respondents. Three of the activities were ranked as a high priority by the vast majority of survey respondents, resulting in scores of greater than 8: the annual public CLEERS Workshop, monthly technical teleconferences, and coordination of national lab aftertreatment R&D. These three topics are the areas where the national labs focus most of the CLEERS coordination resources, and will remain as top priorities in the future.

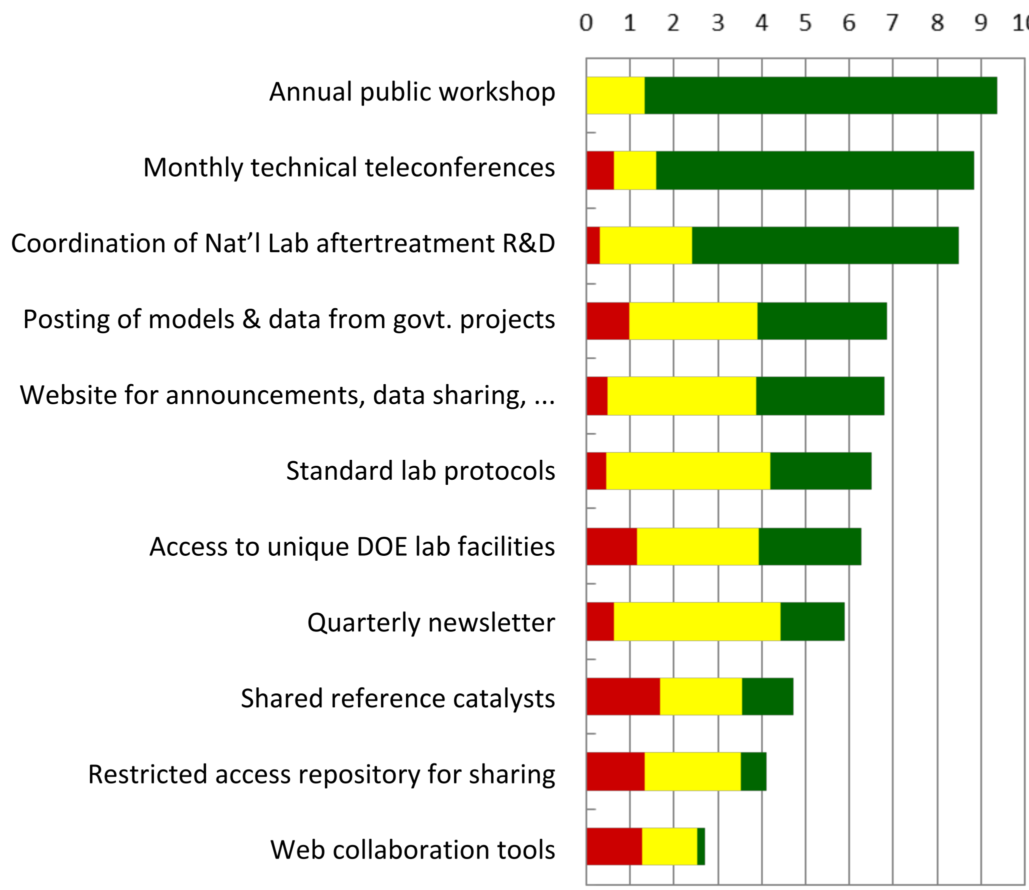

Figure 3. Average priority scores for CLEERS activities

A second group of activities was ranked as medium or high importance by most respondents, resulting in priority scores between 5 and 7: posting of models and data from government-funded projects, the CLEERS website, standard lab protocols for catalyst measurements, access to unique DOE lab facilities, and a quarterly CLEERS newsletter. Aside from the newsletter, these are ongoing activities, and will be continued in the future based on the moderate level of interest from respondents. The newsletter will be initiated in 2016.

The remaining CLEERS activities in the survey (shared commercially relevant reference catalysts, a restricted access repository for sharing of data and information, and web collaboration tools) were all ranked as medium or low importance by most respondents, resulting in priority scores below 5. Thus, these activities will not be a major emphasis of the CLEERS organization in the near future.

3.2 TECHNOLOGY PRIORITIES

3.2.1 Overall Trends

Figure 4 shows the priority scores for all 64 technical topics included in the survey averaged across all 34 independent survey responses. Please note that the technology priority topics are unlabeled, as Figure 4 is not intended to provide a ranking of specific topics. Instead, this plot highlights the diversity of opinions among the survey respondents, as well as the overall relative interest in all of the topics. Looking at each of the multicolor bars, every single topic was ranked high importance by at least one respondent and medium importance by multiple respondents, while all but one of the topics were ranked low importance by at least one respondent. Thus, for just about every topic surveyed, it is possible to find someone who considers it to be high importance, someone who considers it medium importance, and someone who considers it low importance.

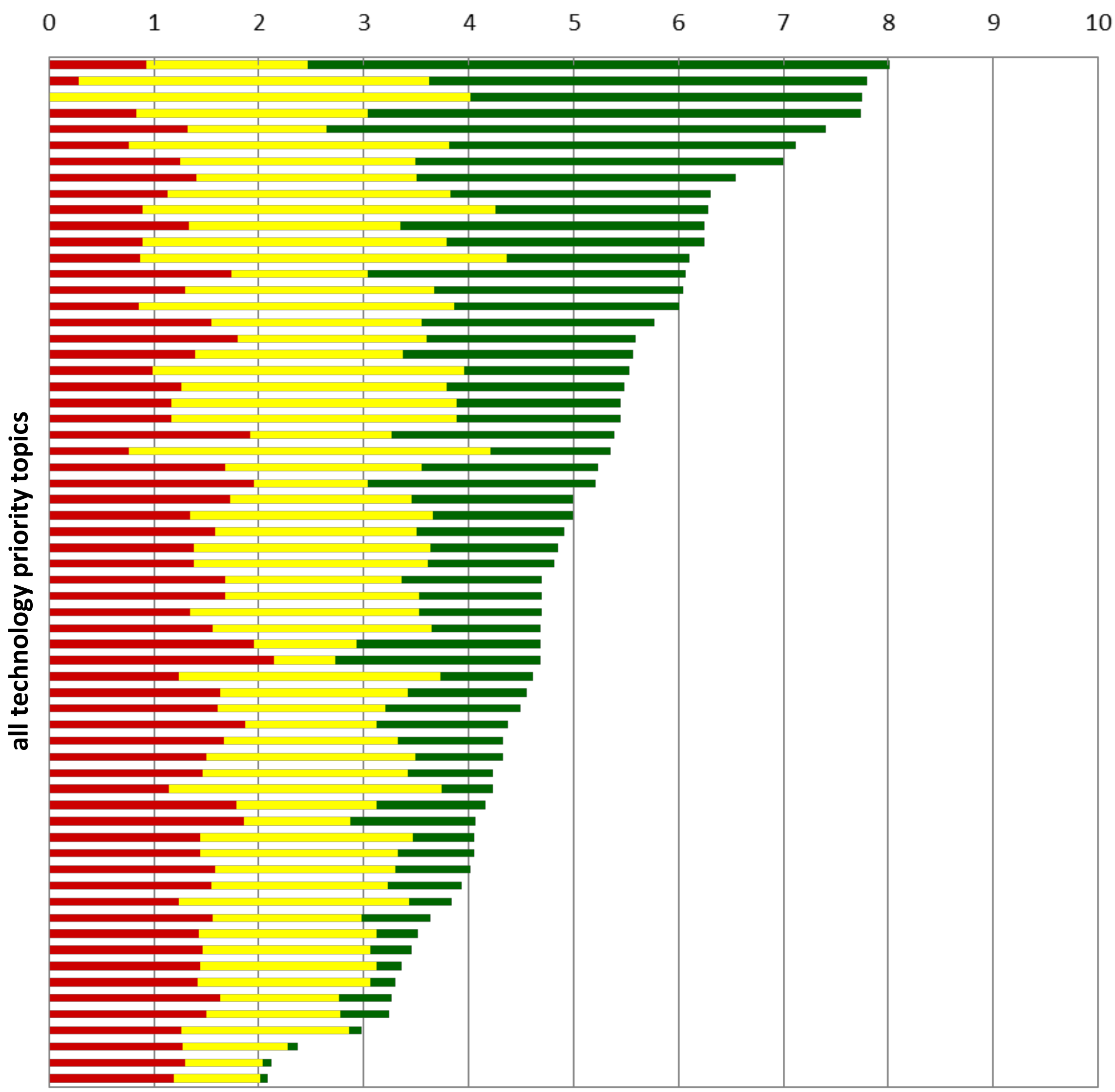

Figure 4. Priority scores for all 64 technical topics in the priority survey averaged across all survey respondents.

As discussed in Section 2.4, the survey sampling methodology and number of responses preclude rigorous statistical analysis of the results. However, a qualitative analysis of trends can still provide useful insights, particularly if the content and wording of the survey questions are chosen carefully. Figure 4 show that the technology priority scores, when averaged across all respondents, are spread across a wide range of potential scores. This spread increases further when the scores are grouped according to market segments, resulting in high scores greater than 9 and low scores below 1. Thus, from a composition sense, the survey topics spanned the interests of the respondents. As to whether or not the survey was sufficiently complete in capturing potential research topics, the responses to the open-ended questions at the end of the survey seemed to confirm that the survey was appropriately inclusive.

The diversity of opinions from survey respondents is also apparent when considering the survey results aggregated across technology areas. Figure 5 gives a graphical summary of the relative importance of the different technology areas across market perspectives. Each row shows the average score of all the topics surveyed for a particular technology area. For example, the top row indicates an average of all of the topics that fall under the Passive NOx Adsorber (PNA) technology area. The columns indicate the market perspective of the survey responses included in each average score: all responses, heavy duty diesel (HDD) responses, light duty diesel (LDD) responses, and gasoline (LDG) responses. The diameter of the circle is proportional to the average score for each technology area and market perspective: larger circles indicate a higher average priority score.

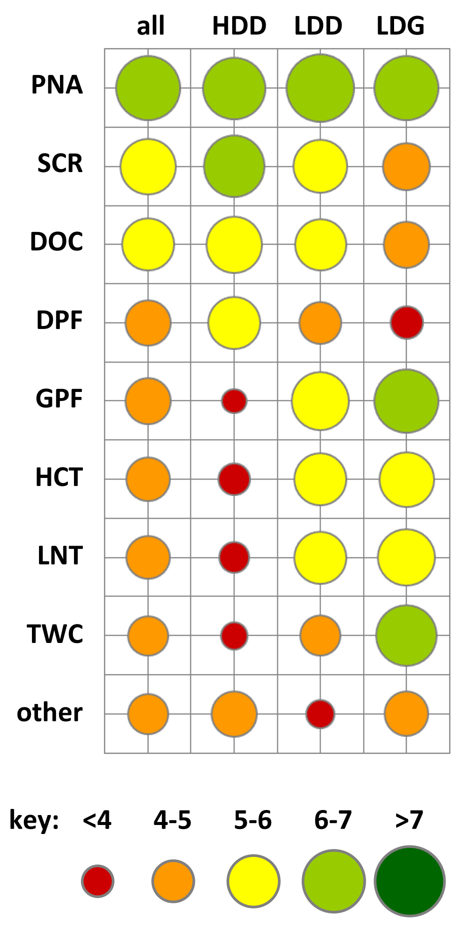

Figure 5. Average priority scores across technology areas and market perspectives. Note that circle diameter is proportional to priority score.

Looking across the rows in the chart gives an illustration of the breadth of interest from survey respondents: every technology area included in the survey was ranked at least medium importance (average priority score greater than 5) by respondents from at least one market perspective. Looking down the columns gives a snapshot of the relative importance of the various technology areas to each market perspective.

Responses from the HDD perspective ranked PNA, SCR, DOC, and DPF as the areas of highest importance. The importance of the latter three technologies is not surprising since most HDD aftertreatment systems include DOC, DPF, and SCR components. The HDD interest in PNA seems to indicate a new trend, and likely stems from the need for NOx conversion performance at temperatures lower than where SCR catalysts can operate.

As noted above, the gasoline market perspective encompassed both stoichiometric and lean-burn gasoline engines. Respondents from this market perspective prioritized GPF, PNA, TWC, HCT, and LNT as the most important technology areas. The high interest in TWCs is consistent with the majority of current gasoline-fueled engines running under stoichiometric air/fuel ratios, although these catalysts could also find use for lean-burn applications that require stoichiometric operation at high loads or that use a passive SCR strategy for NOx control. The interest in GPFs follows from the shift toward gasoline direct injection (GDI) engines for improving fuel efficiency. The high priorities for PNA and HCT likely stem from the need for better low temperature emissions control due to decreasing exhaust temperatures. Interest in LNT is consistent with a desire to run gasoline engines lean to improve efficiency. The LNT interest might also be due to some cross-over between LDD and LDG survey responses, as some survey respondents indicated more than one market perspective applied to their responses. This LDD/LDG cross-over is also likely the reason for GPF receiving a relatively high priority under responses from the LDD perspective.

The other technologies generating at least moderate interest from LDD respondents included PNA, SCR, DOC, HCT, and LNT. Unlike the HDD and LDG responses, the interests of LDD respondents appeared to be distributed across a larger number of technology areas, resulting in moderate priority scores across multiple technologies rather than higher priority scores concentrated on a few technologies. This could stem from less consistency in LDD emissions control system architectures due to differing corporate strategies and/or variations in emissions control regulations around the world.

Two key survey findings follow from the results shown in Figure 5. First, technologies that have been commercialized for a number of years are still considered important research topics by survey respondents. LDG respondents ranked TWCs as a relatively high priority technology area, while responses from the HDD market perspective included both DOC and SCR as areas of relatively high importance. Thus, even though TWC, DOC, and SCR devices have been on the road for years, survey respondents still see the need for further development in these areas. Second, PNA technology is considered high importance across all market perspectives. This is the only technology area that generated such broad interest.

As mentioned above, the technology priority topics in the questionnaire were intentionally selected to reveal parallel interest in research areas that span multiple technologies. For example, most technology areas included topics related to: discovery of novel low temperature formulations; formation of greenhouse gases; aging; poisoning; reaction mechanisms and kinetics; and measurement and sensing for onboard diagnostics (OBD). This survey structure made it possible to analyze the relative importance of these general research areas by averaging the priority scores for each research area across all of the technologies. The results of this analysis are included in Figure 6, which has the same format as Figure 5. The average priority scores for “Multi-scale modeling, simulation, and data sets,” which was included as an additional survey category separate from all of the technology areas, are also shown in Figure 6.

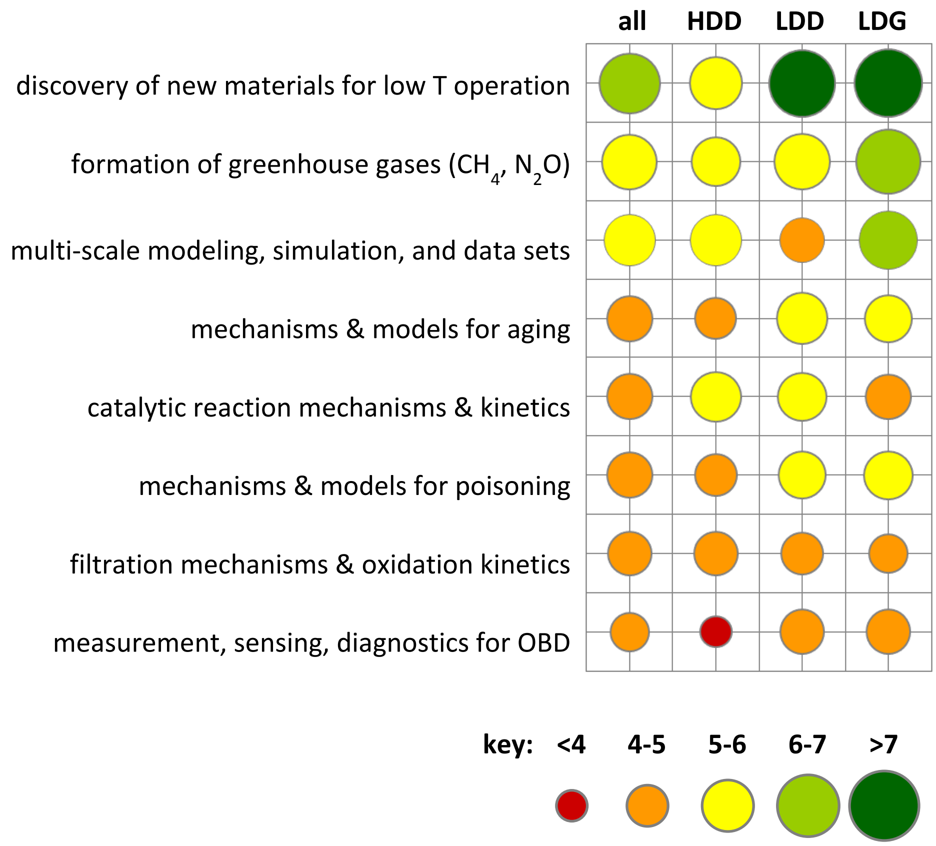

Figure 6. Average priority scores for general research areas across market perspectives

Two of the general research areas were given relatively high priority scores by respondents from multiple market perspectives: discovery of new catalysts that function at lower temperatures, and formation of greenhouse gas byproducts. The interest in low temperature catalysts is consistent with broader trends in emissions control development.[1] The relatively high importance placed on greenhouse gas production is likely related to the inclusion of greenhouse gases in emissions regulations. Under the U.S. EPA Greenhouse Gas Vehicle Standards, both CH_4 and N_2O are included in vehicle fuel economy calculations as CO_2 equivalent emissions if they exceed permitted levels (30 mg/mile for CH_4 and 10 mg/mile for N_2O).[2] The topics under the multi-scale modeling, simulation, and data sets also received relatively high priority scores, particularly from the LDG and HDD market perspectives.

The other general research areas all received average priority scores of around 5, meaning they were ranked as roughly medium importance. However, specific topics in these general research areas were ranked as high importance; these high priority topics will be highlighted below.

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[1] "Future Automotive Aftertreatment Solutions: The 150°C Challenge Workshop Report," ACEC Low Temperature Aftertreatment Group: Michael Zammit, Craig DiMaggio, Chang Kim, Christine Lambert, George Muntean, Chuck Peden, Jim Parks, Ken Howden, http://cleers.org/acec-lowt/includes/The_150C_Challenge_Workshop_Report.pdf

[2] Federal Register, "Environmental Protection Agency and Department of Transportation-National Highway Traffic Safety Administration 40 CFR Parts 85, 86, and 600; 49 CFR Parts 531, 533, 536, et al.", Vol. 75, No. 88, May 7, 2010 (pp. 25396, 25399).

3.2.2 Detailed Results by Technology Area

3.2.2.1 Diesel Particulate Filters (DPF)

The priority scores for all of the DPF-related survey technical topics are summarized in Figure 7 for the (a) HDD and (b) LDD market perspectives. Note that GPF was included as a separate topic, so the LDG perspective is covered under that technology. The most obvious trend apparent in Figure 7 is the high importance placed on SCR catalysts coated on DPFs in responses from both the heavy duty and light duty diesel market perspectives. Nearly all HDD respondents indicated that this topic was of high importance, as did a large majority of LDD respondents. The resulting high priority scores placed the SCR on DPF topic at or near the top of all technical priorities for both of the diesel market perspectives. The importance of this topic shows that packaging and cost remain challenges in aftertreatment system development, even for heavy duty applications. Beyond SCR on DPF, HDD respondents rated most of the remaining DPF topics (DOC on DPF, NOx oxidation kinetics, OBD, and filtration mechanisms) as, on average, medium priority. The last remaining topic, O_2 oxidation kinetics, was rated low importance by a majority of HDD respondents, which appears to be consistent with the currently predominant reliance on passive DPF regeneration by NOx in heavy duty applications. For the LDD perspective, OBD was the only other topic rated medium and high importance by most respondents; the other four DPF topics were rated low importance by a majority of respondents from the LDD market perspective.

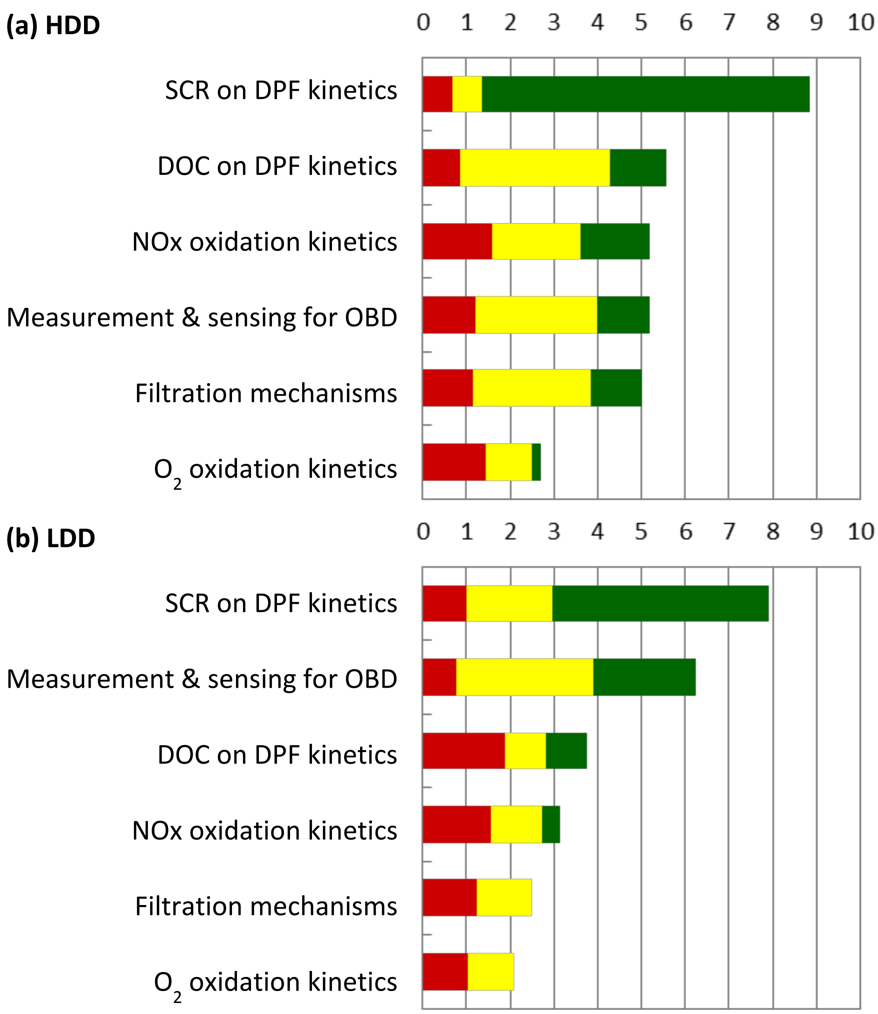

Figure 7. Priority Scores for DPF topics from (a) HDD and (b) LDD market perspectives

3.2.2.2 Gasoline Particulate Filters (GPF)

In contrast with the DPF responses, all four of the GPF-related topics were rated as high importance by a significant fraction of respondents from the LDG market perspective, consistent with GPFs being in an earlier stage of development and commercialization. There was particularly high interest in characterization and modeling of GPF filtration mechanisms, but the average priority scores for all four GPF topics fell in the moderate to high priority range.

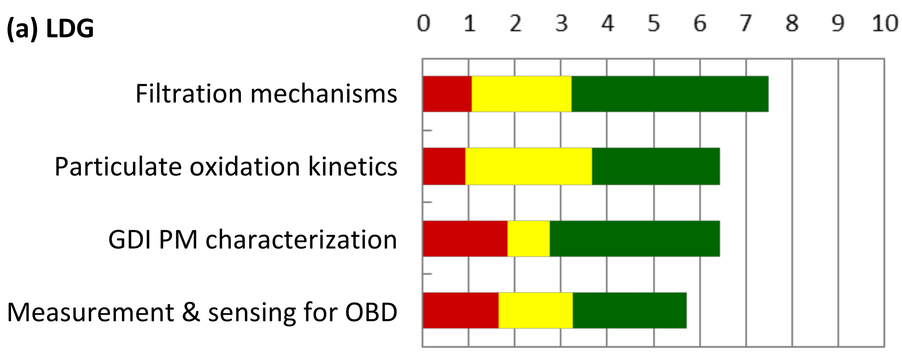

Figure 8. Priority scores for GPF topics from the LDG market perspective

3.2.2.3 NH_3 Selective Catalytic Reduction (SCR)

Figure 9 shows the priority scores from both heavy duty and light duty diesel market perspectives for the SCR topics included in the survey. The majority of respondents from the gasoline market perspective ranked most of the SCR topics as low or medium importance, resulting in lower priority scores than for the diesel market perspectives. The one topic ranked as a high priority by a majority of gasoline respondents was discovery of new lower temperature NH_3 SCR catalysts. This topic was also the highest priority SCR topic for both of the diesel market perspectives, and was one of the highest overall priorities of all the survey technical topics from both HDD and LDD market perspectives.

Beyond low temperature catalysts, a majority of HDD respondents rated four other SCR topics as high importance: aging mechanisms and models; poisoning mechanisms and models; formation of greenhouse gas byproducts; and NH_3 storage, release, and oxidation. The relatively high scores from the HDD market perspective for these topics placed them in the top ten highest priorities of all technical topics in the survey. Of the four remaining SCR topics, three still fell in the medium to high priority category: NOx reduction mechanisms and kinetics; measurement and sensing for OBD; and urea injection and decomposition. The only SCR topic rated as medium or low importance by all of the HDD respondents was non-urea NH_3 sources. This exception is somewhat interesting given the high level of importance placed on lower temperature NH_3 SCR formulations. Current urea dosing technology is typically limited at low temperatures by the potential for incomplete decomposition and deposit formation, so lower temperature SCR catalysts will likely require alternate methods for introducing NH_3 into the exhaust stream. However, such a method would not be needed unless new low temperature SCR formulations were developed, so perhaps the relatively low priority score stems from a desire among survey respondents to see the development of the catalysts first.

Aside from agreement on the high importance of new lower temperature SCR catalysts, the responses from the LDD market perspective were much more polarized than those from the HDD perspective. For many of the topic areas, there were roughly equal numbers of respondents giving ratings of low importance and high importance. The divergence of opinions from the LDD sector is consistent with the prior observation that LDD market participants are pursuing a wider range of strategies for meeting emissions regulations, perhaps due to differing corporate strategies or variations in global emissions regulations. This disagreement resulted in generally lower overall priority scores from the LDD market perspective compared to the HDD perspective, with the exception of non-urea NH_3 sources. Even so, most of the SCR topics were still rated medium to high priority overall by respondents from the LDD market perspective.

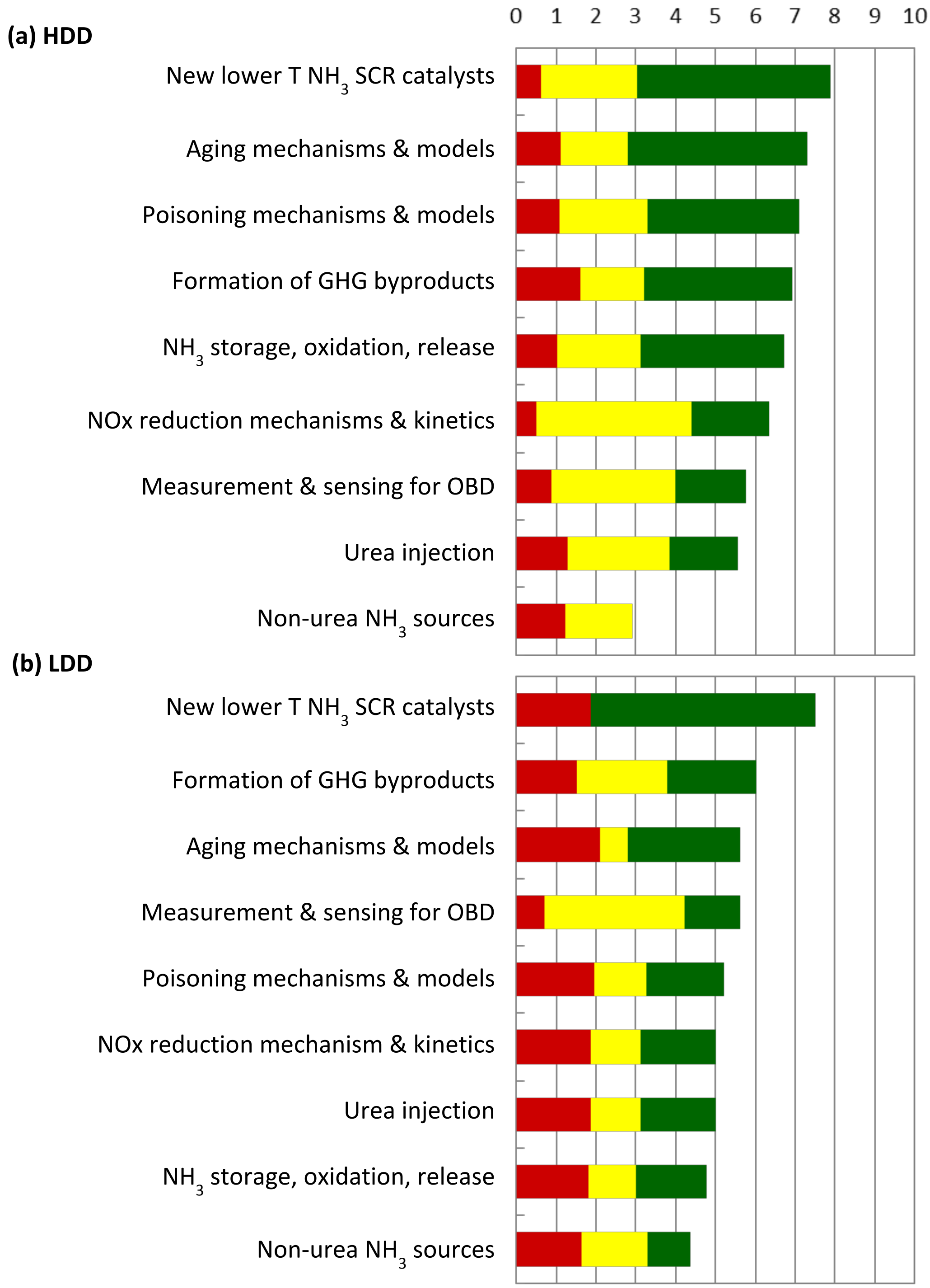

Figure 9. Priority Scores for SCR topics from (a) HDD and (b) LDD market perspectives

3.2.2.4 Lean NOx Traps (LNT)

Interest in LNTs has clearly dwindled in the heavy duty market, as shown in Figure 10(c). However, a number of respondents from light duty market perspectives, particularly the gasoline market segment, rated multiple LNT topics as medium or high importance. Interestingly, formation of greenhouse gas byproducts topped the list of LNT topics for all three market perspectives. LDG and LDD respondents also ranked aging mechanisms and models, poisoning mechanisms and models, and new lower temperature LNT formulations as, on average, medium to high importance. As with the SCR ratings, LDD responses were more polarized than for the other market perspectives, with a number of LNT topics showing roughly equal numbers of low importance and high importance ratings.

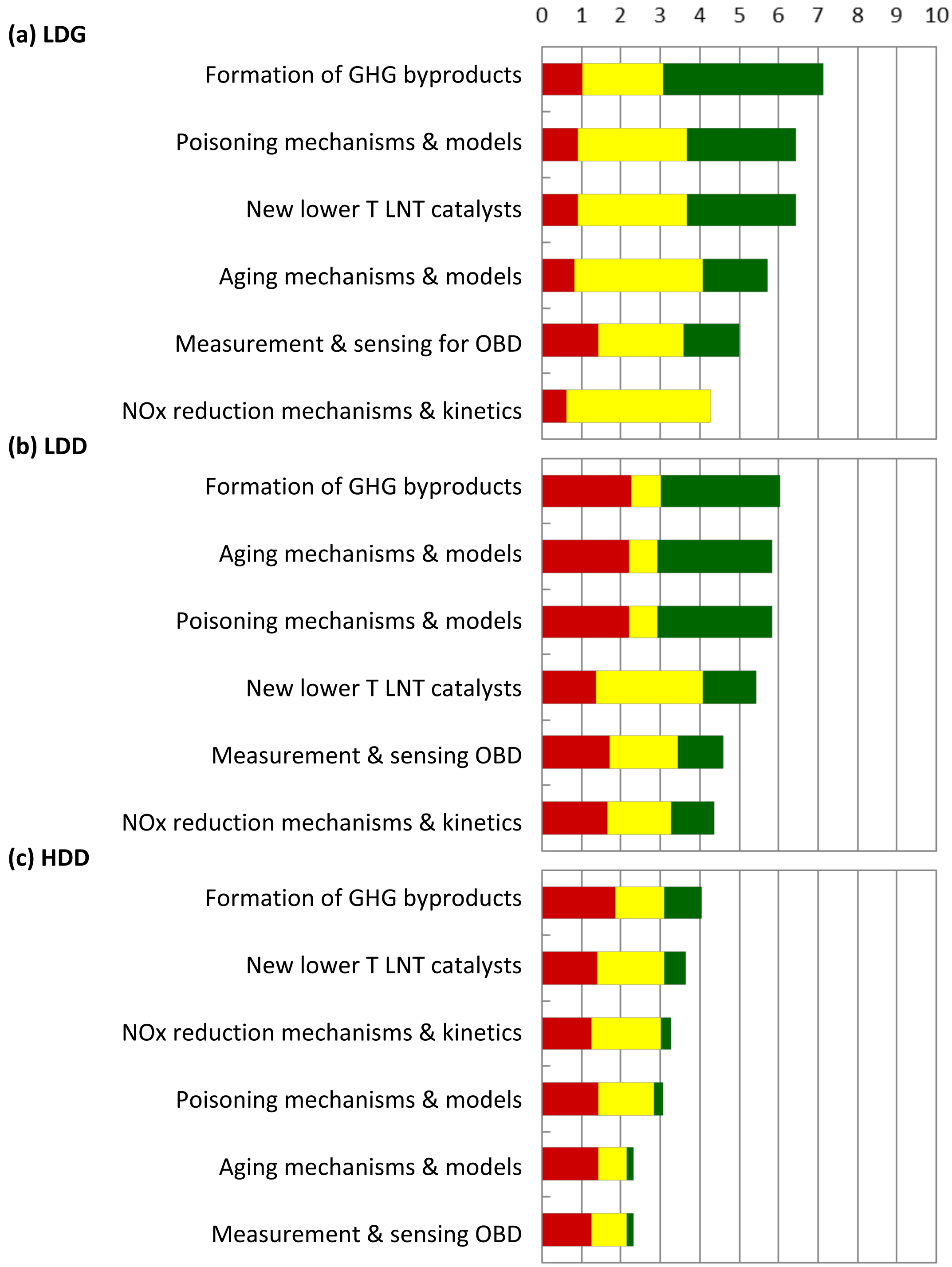

Figure 10. Priority Scores for LNT topics from (a) LDG, (b) LDD, and (c) HDD market perspectives

3.2.2.5 Oxidation Catalysts for Diesel (DOC) or Low Temperature Combustion Engines

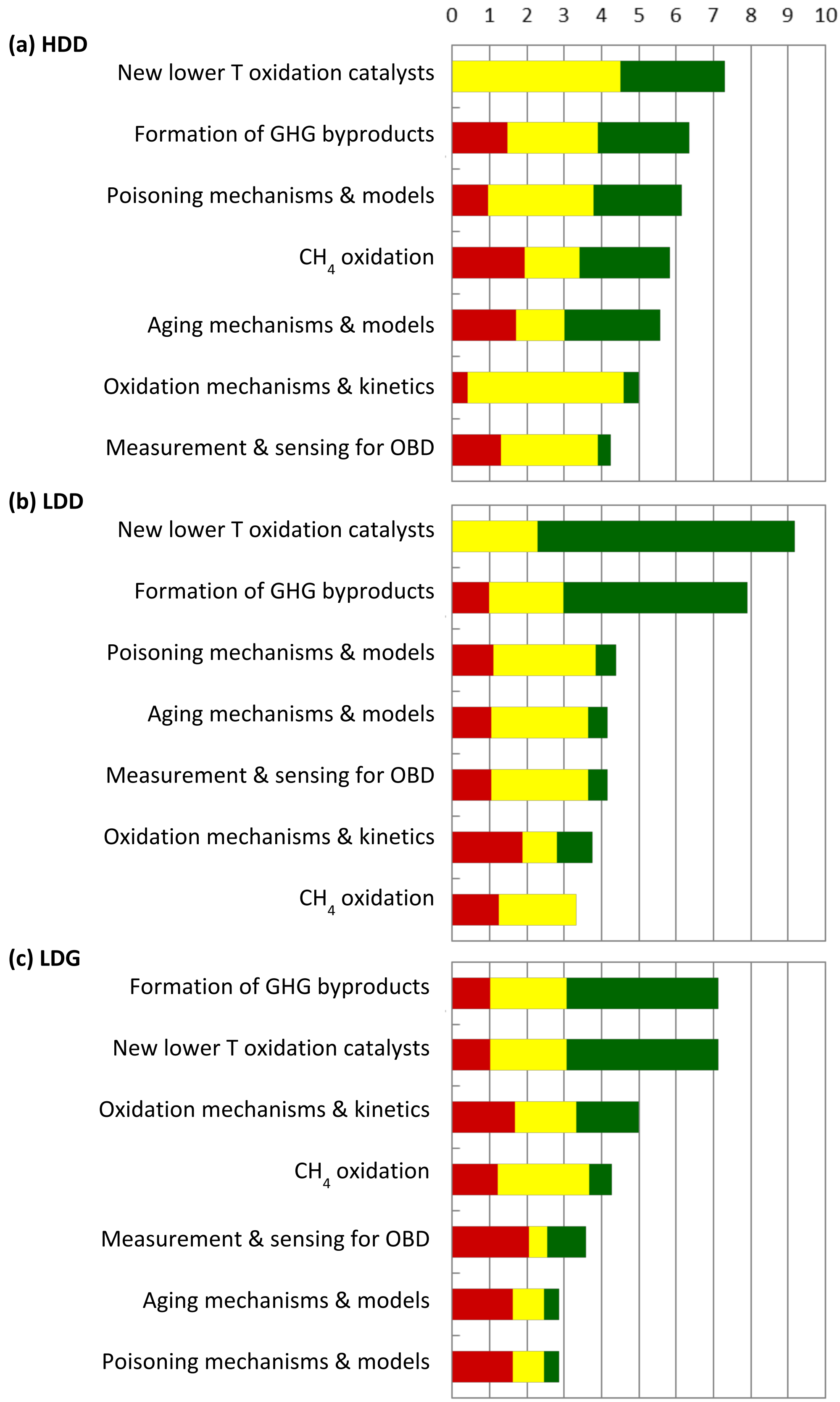

Figure 11. Priority Scores for DOC topics from (a) HDD, (b) LDD, and (c) LDG market perspectives

Much as for the SCR results, a significant fraction of HDD respondents rated many of the DOC topics as high or medium importance (Figure 11(c)), resulting in relatively high priority scores for most of the DOC-related items in the survey: new lower temperature oxidation catalysts; formation of greenhouse gas byproducts; poisoning mechanisms and models; CH_4 oxidation; and aging mechanisms and models. Respondents from the light duty market perspectives (Figure 11(a-b)) were much more focused on two topics consistent with the general research trends discussed in section 3.2.1: new lower temperature oxidation catalysts and formation of greenhouse gases.

3.2.2.6 Three-way Catalysts (TWC)

Since three-way catalysts are primarily designed to operate under stoichiometric conditions, only priority scores from the gasoline market perspective are included in Figure 12. However, it should be noted that TWCs may find application for lean gasoline and other advanced combustion engines to control emissions when the engine operates under stoichiometric conditions over portions of the operating map, or to perform other roles (such as NH_3 generation) in the aftertreatment system. All LDG respondents ranked four of the TWC topics as either high or medium priority: formation of greenhouse gas byproducts; new lower temperature TWC catalysts; CH_4 conversion; and measurement and modeling of TWC dynamics. The first two of these topics reflect the general research area trends discussed previously. The high importance of CH_4 conversion to respondents from the gasoline market perspective was an interesting result, and perhaps reflects growing interest in natural gas fueled vehicles. Beyond these top ranked items, three more topics received, on average, medium priority scores: aging mechanisms and models, poisoning mechanisms and models, and TWC reaction mechanisms and kinetics. Only measurement and sensing for OBD received a relatively low average priority score, likely due to the commercial maturity of oxygen sensor technology.

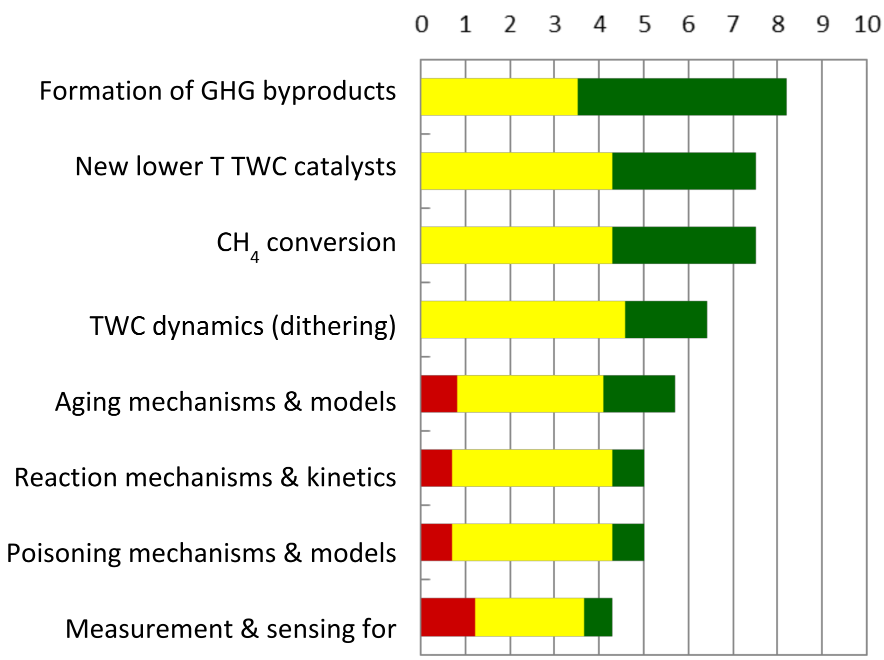

Figure 12. Priority scores for TWC topics from the LDG market perspective

3.2.2.7 Hydrocarbon Traps (HCT)

Heavy duty diesel respondents showed relatively low interest in hydrocarbon traps, as illustrated in Figure 13. However, the majority of light duty respondents (both LDG and LDD) ranked new hydrocarbon trap materials as high importance, consistent with the general trend emphasizing new low temperature formulations. The majority of LDD respondents also ranked mechanisms for hydrocarbon storage, release, and conversion as a topic of medium or high importance, while LDG respondents ranked mechanisms, aging, and poisoning all as medium priority on average. While the priority scores for HCT were not quite as high as for some of the other technology areas, they still reflect at least moderate interest in this technology from light duty market perspectives.

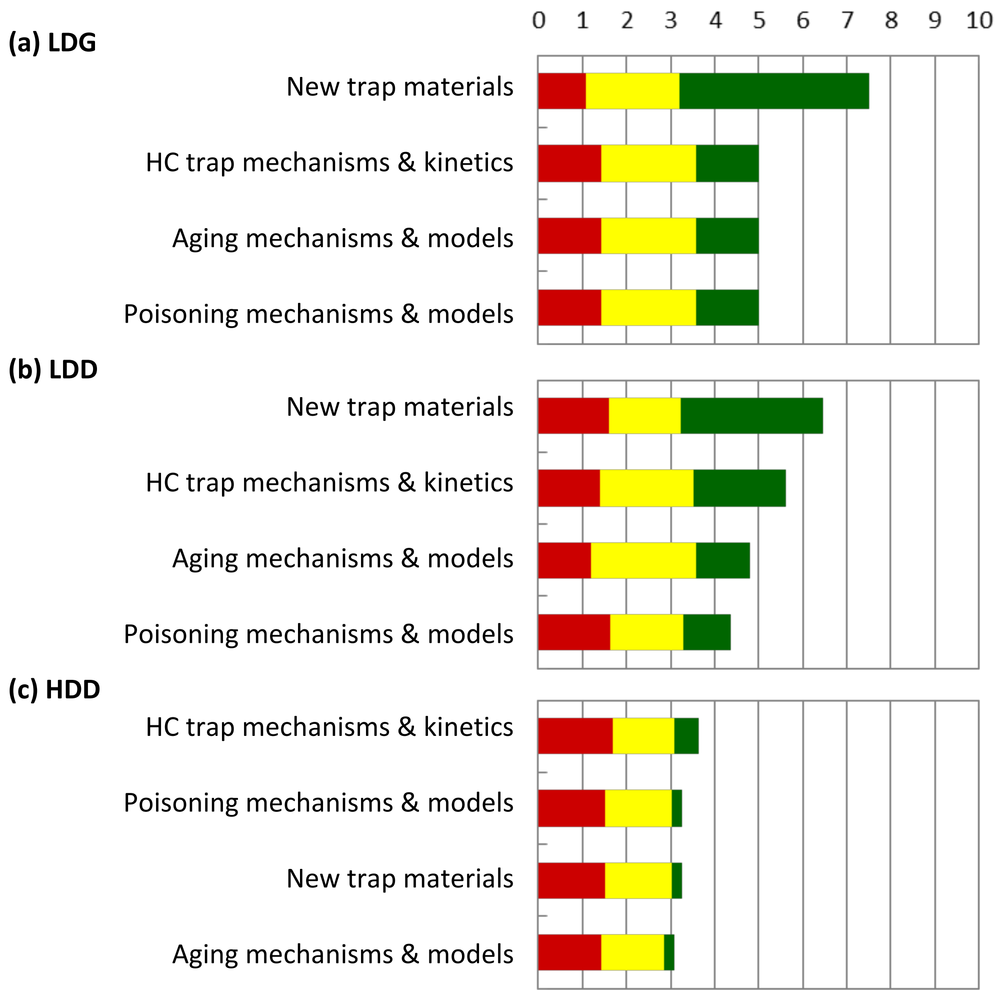

Figure 13. Priority Scores for HCT topics from (a) LDG, (b) LDD, and (c) HDD market perspectives

3.2.2.8 Passive NOx Adsorbers (PNA)

A majority of survey respondents from all three market perspectives rated all of the PNA-related topics as high to medium importance (Figure 14). This breadth of interest across both market perspectives and research areas was not observed for any other technology included in the survey. Survey respondents showed particular interest in discovery of new PNA materials and PNA mechanisms and kinetics, but the other three topics (poisoning mechanisms and models; aging mechanisms and models; and formation of greenhouse gas byproducts) all received average priority scores greater than five, with some variations in relative importance across market perspectives.

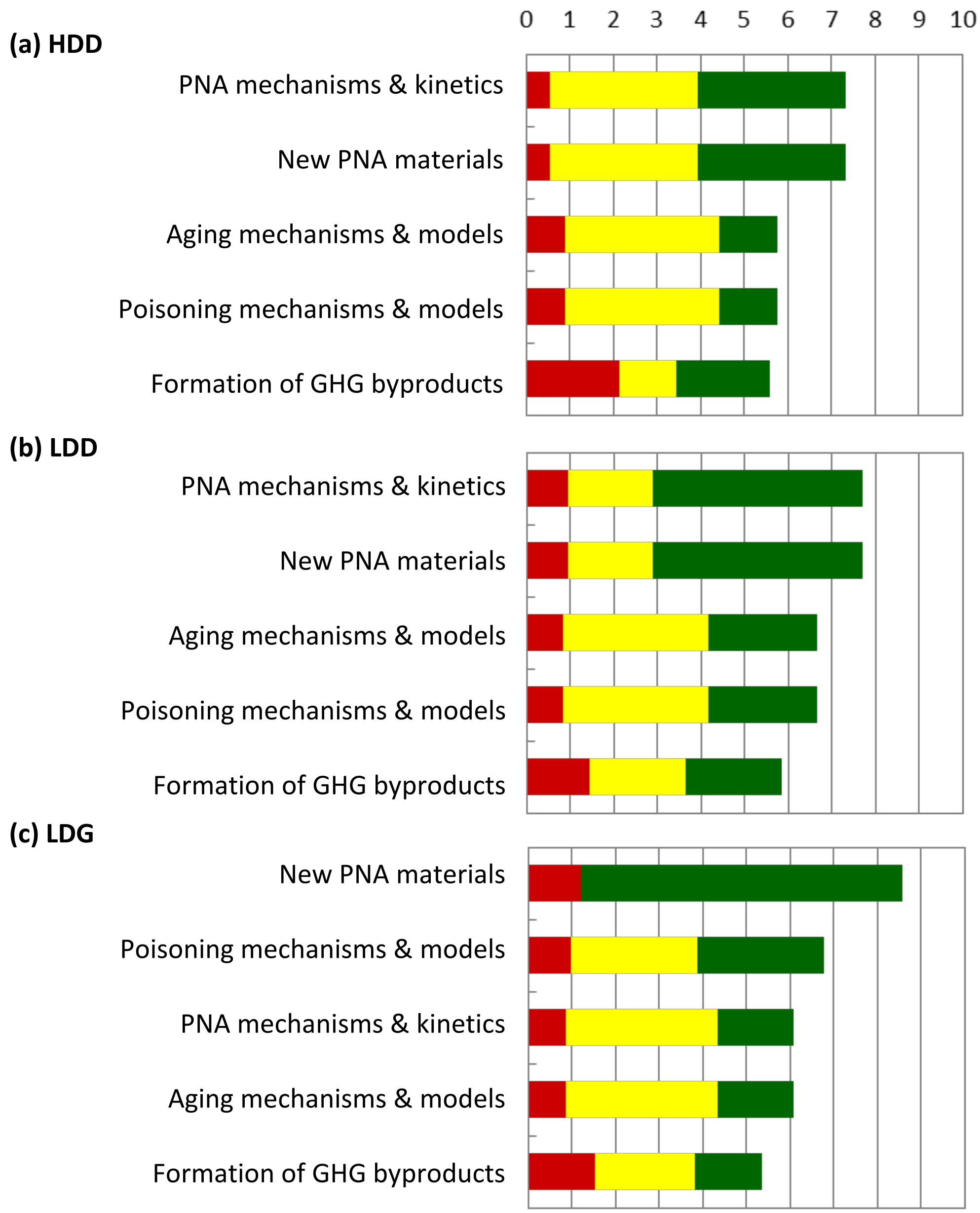

Figure 14. Priority Scores for PNA topics from (a) HDD, (b) LDD, and (c) LDG market perspectives

3.2.2.9 Other Emissions Control Devices and Issues (OEC)

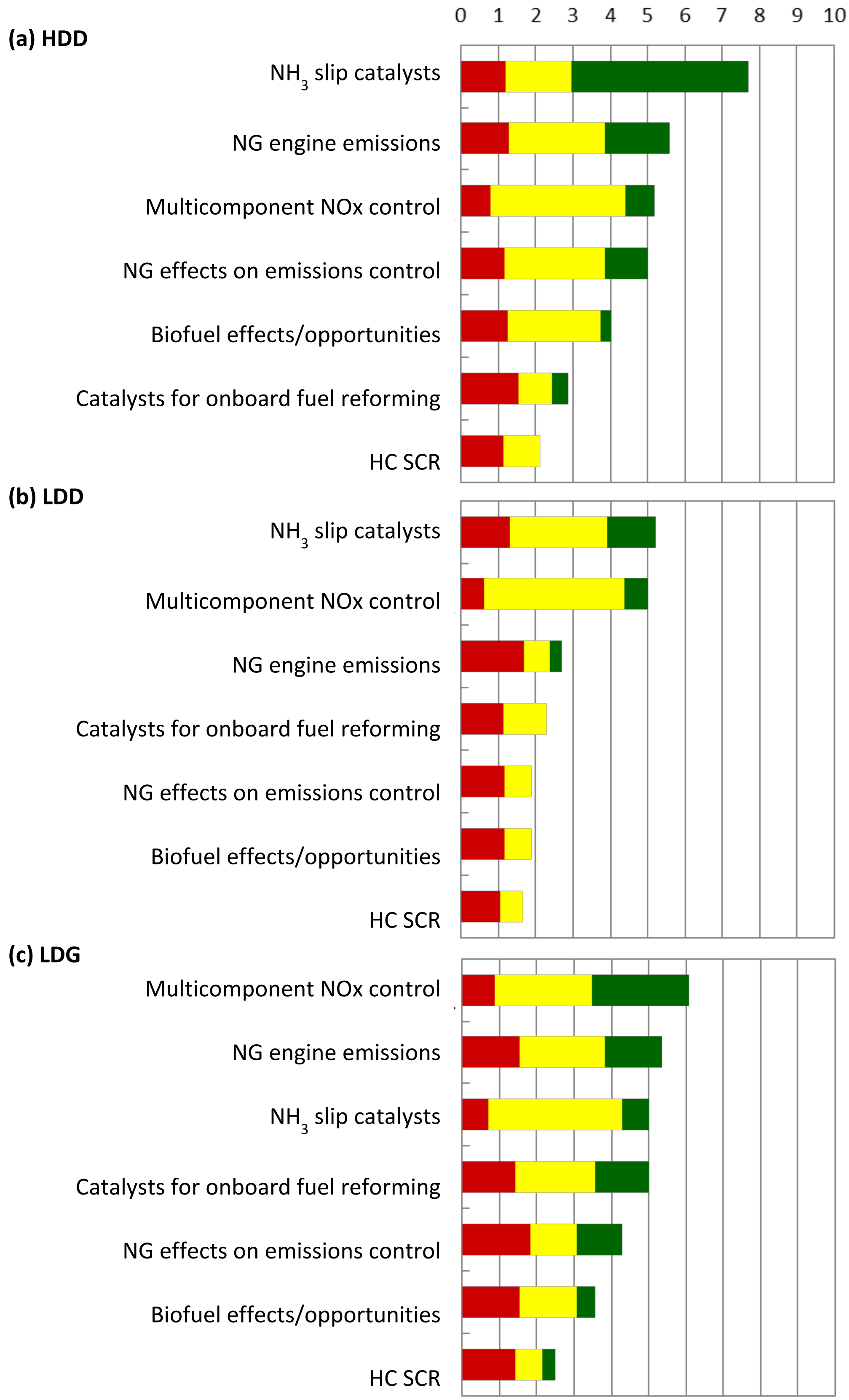

Figure 15. Priority Scores for other emission control topics from (a) HDD, (b) LDD, and (c) LDG market perspectives

The section on “Other emissions control devices and issues” was included in the survey in an attempt to capture interest in any technologies outside the eight technology areas covered in detail in the survey, so it is a fairly broad and unrelated list. Of the other topics listed, NH_3 slip catalysts stood out as it received a rating of high importance from a majority of HDD respondents, and moderate interest levels from both of the light duty market perspectives. “Multilayer, multizone, or multicomponent NOx control strategies (LNT/NH_3 SCR, TWC/NH_3 SCR, HC SCR/NH_3 SCR)” received ratings of medium to high importance from a majority of respondents from all three market perspectives, with higher interest from the LDG perspective. “Natural gas engine emissions” received, on average, medium importance ratings from both the HDD and LDG market perspectives. This result seems to indicate at least moderate interest in emissions control for natural-gas-fueled vehicles, particularly when combined with the priority scores for CH_4 conversion under the DOC and TWC sections of the survey. “Catalysts for onboard fuel reforming” generated moderate interest from LDG respondents, but minimal support from the two diesel market perspectives. Biofuel effects/opportunities received relatively low priority scores. HC SCR was rated low importance from a majority of survey respondents across all three market perspectives, giving it the lowest average priority score of all of the technical topics surveyed.

3.2.2.10 Multi-scale Modeling, Simulation, Data Sets (MSD)

Unlike the technical topics covered so far, the Multi-scale Modeling, Simulation, and Data Sets category is not specific to a particular emissions control technology. Instead, it was included to capture potential interest in models and experimental data focused on larger (vehicle) or smaller (atomistic or microkinetic) scales than the device-specific topics already listed.

Figure 16 shows the average priority scores for all of the MSD topics surveyed for the LDG and LDD market perspectives, and Figure 17 shows the scores for the same topics from the HDD perspective. The top scoring MSD topic for all three market perspectives was “Steady state & transient emissions data for advanced combustion engines and hybrid powertrains.” The average priority scores for this topic were high enough to make it the highest LDG priority of all the topics surveyed, and placed it in the top quarter of all surveyed topics for the LDD and HDD market perspectives. Clearly, survey respondents see a critical need for this type of data. There was also fairly broad interest in drive cycle simulations of transient emissions response, as a significant fraction of respondents from all three market perspectives rated this topic as high importance. Light duty respondents, and in particular LDG respondents, also gave fairly high ratings to vehicle simulations of hybrids + aftertreatment and advanced combustion + aftertreatment. The high ratings for system level data sets and simulations may reflect the importance of control system calibration for meeting emissions regulations, and the calibration challenges created by advanced powertrain technologies. A majority of HDD and LDG respondents rated microkinetic models as medium to high importance, though this topic did not receive as much interest from the LDD market perspective. Reference catalyst data, models, and parameters received somewhat mixed ratings, while atomistic modeling received some of the lowest priority scores for technical topics in the survey.

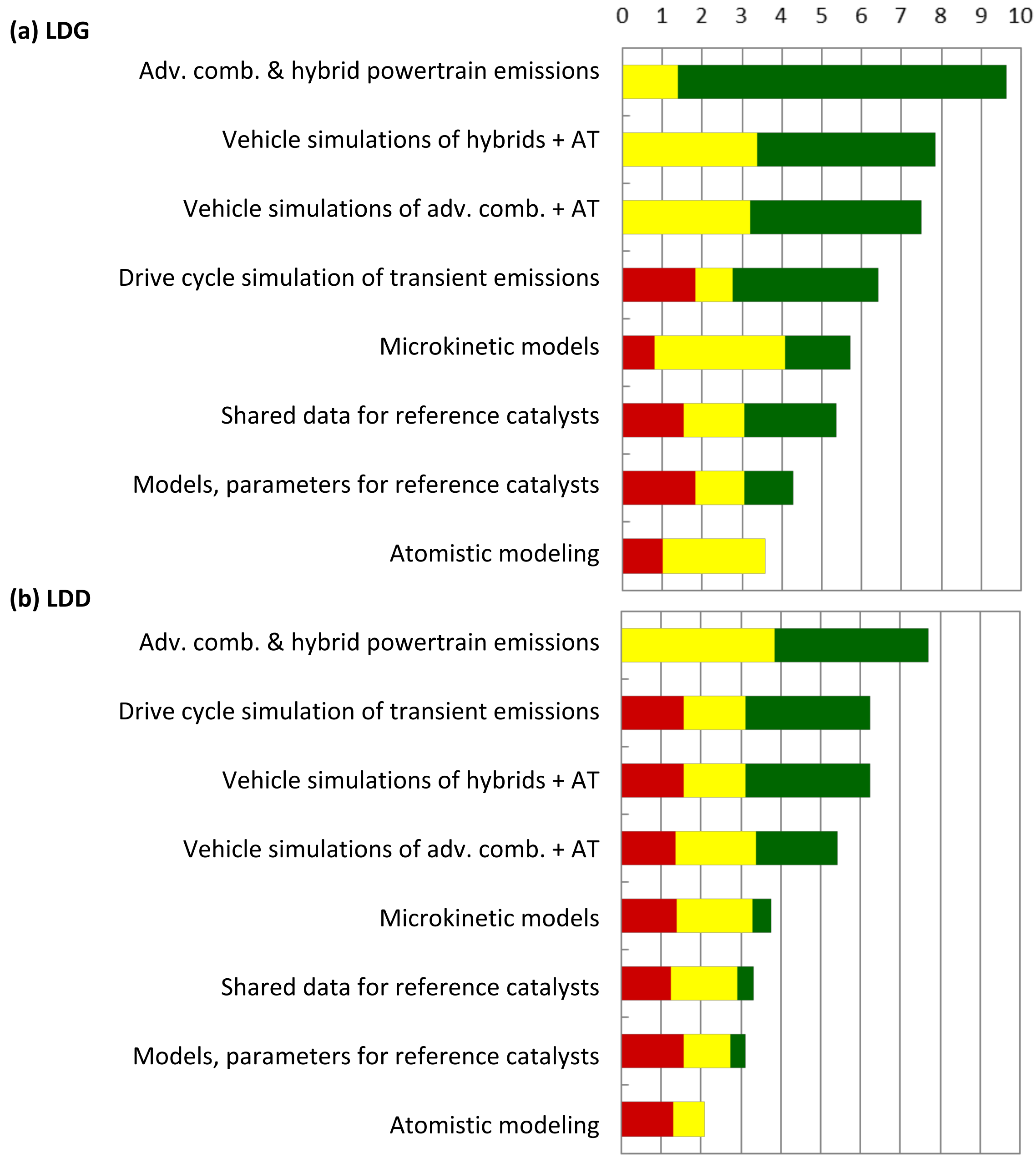

Figure 16. Priority Scores for multiscale modeling, simulation, and data set topics from (a) LDG and (b) LDD market perspectives

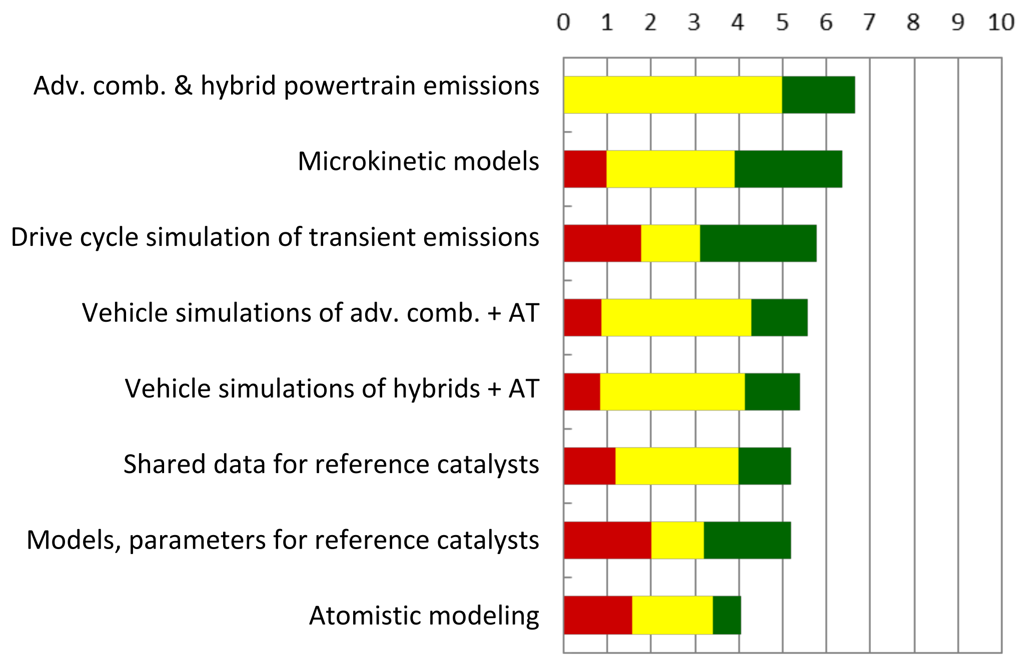

Figure 17. Priority Scores for multiscale modeling, simulation, and data set topics from HDD market perspective

3.2.3 Top Priorities by Market Perspective

In addition to consideration of the priority scores by technology area, the survey results were processed to determine the top technical priorities across all technologies for each of the three market perspectives. The 16 topics with the highest average priority scores (representing the top 25% of the 64 topics surveyed) are shown for each of the market perspectives below. While the trends in the top 16 lists were consistent with the overall themes discussed in section 3.2.1, and the individual scores were embedded in the technology area results discussed in section 3.2.2, it is still instructive to consider how the individual priorities ranked relative to each other.

3.2.3.1 HDD

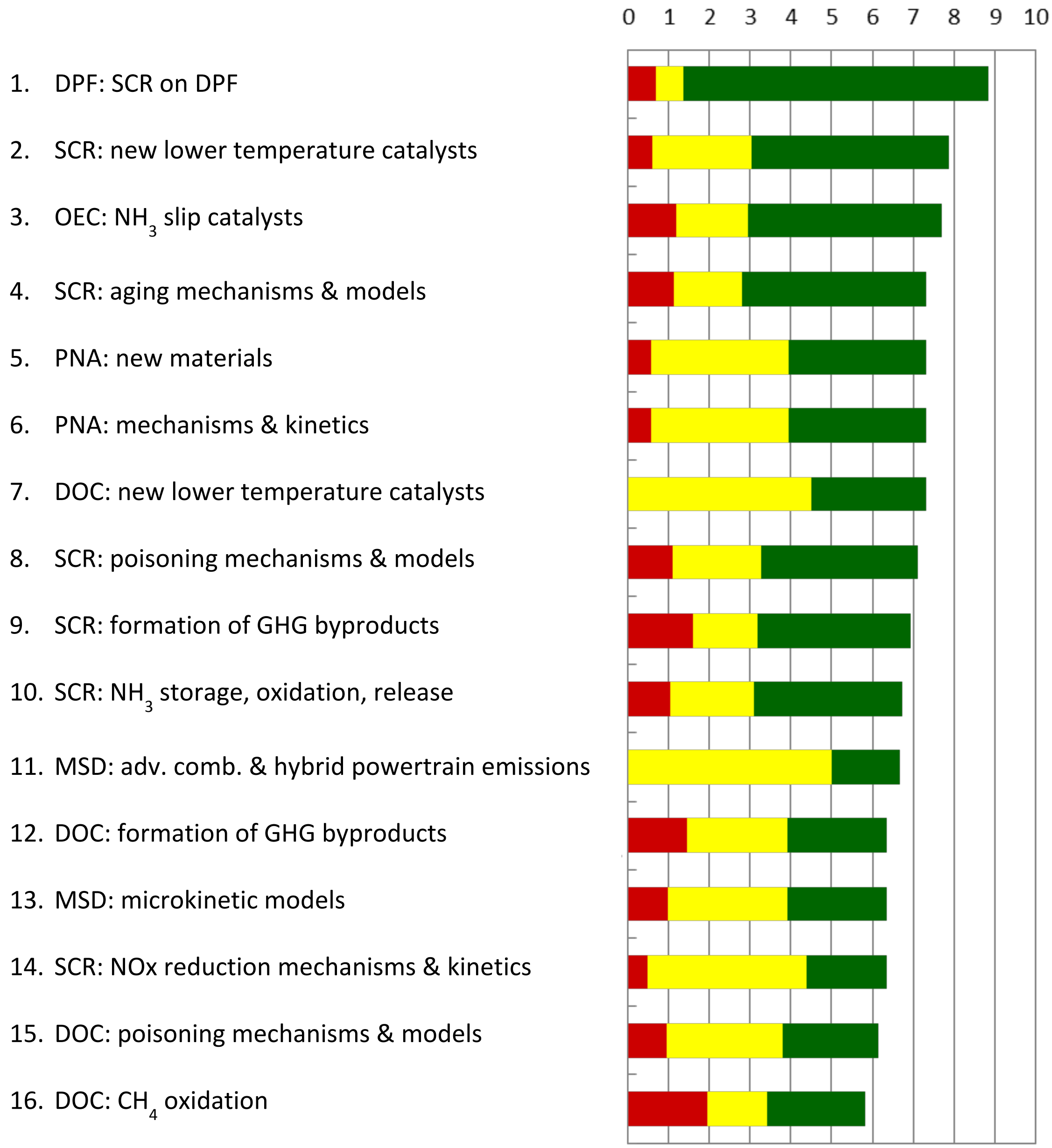

Figure 18. Top 16 technical topics ranked by average priority score for the HDD market perspective

Figure 18 shows the top 16 technical priorities from the heavy duty diesel perspective. SCR-related topics dominated the list, accounting for fully half of the top 16. Another quarter of the list related to DOCs, and PNAs were prominent near the top of the list. Interestingly, SCR on DPF was the only DPF topic that appeared in the top 16. Overall, the top priorities demonstrated a consensus among HDD respondents that SCR, DOC, and PNA will be the key technologies requiring additional development to meet future emissions regulations with high efficiency diesel engines. Two MSD topics also made it into the top 16 priorities: emissions measurements from advanced combustion engines and hybrid powertrains, and microkinetic models for generalized prediction of catalyst performance. Among other key survey trends, new low temperature formulations (SCR, PNA, DOC) and formation of greenhouse gas byproducts (SCR, DOC) both appeared in the top HDD priorities.

3.2.3.2 LDD

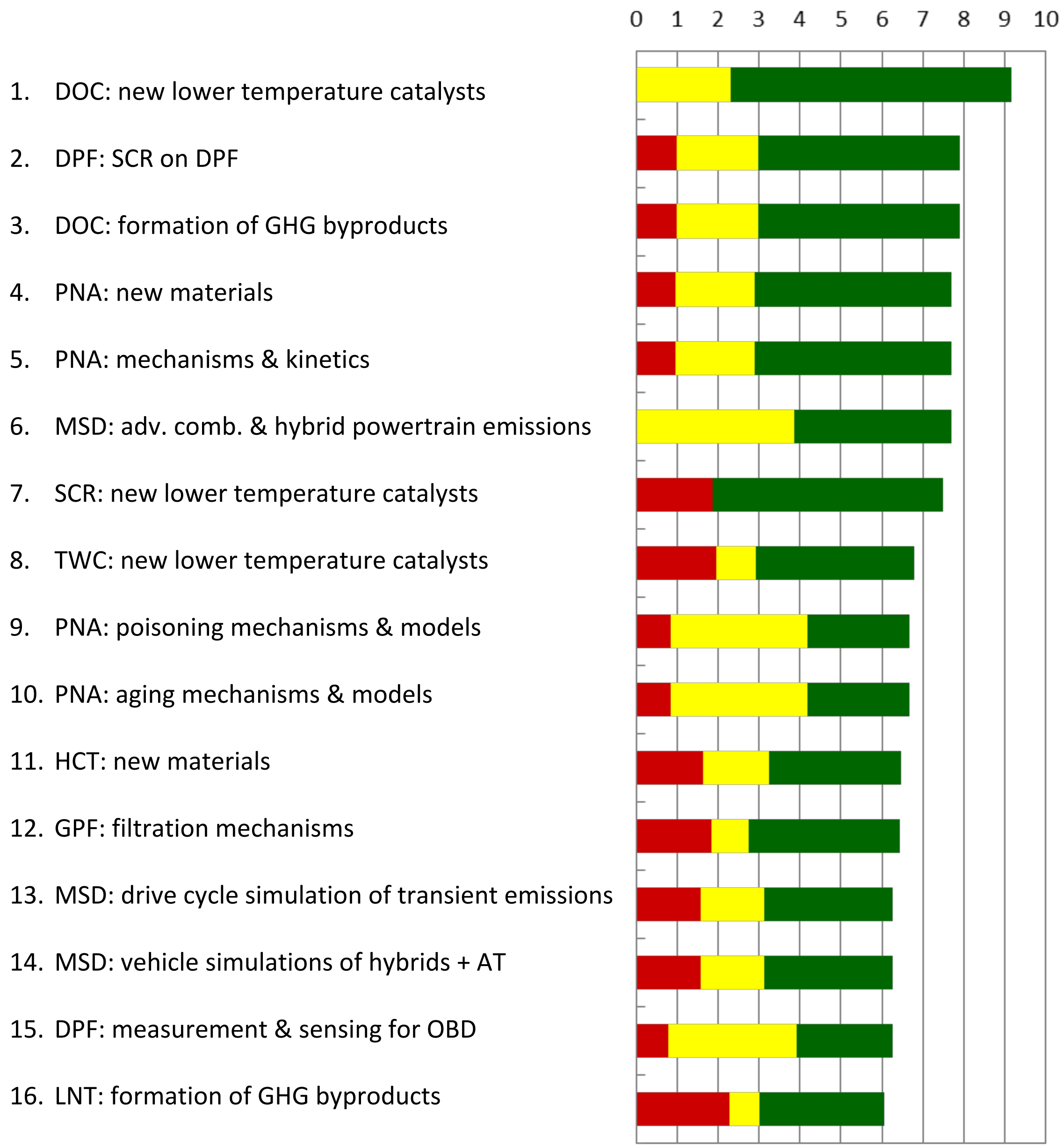

Figure 19. Top 16 technical topics ranked by average priority score for the LDD market perspective

Unlike the HDD market perspective, there seems to be less consensus regarding the key emissions control technologies among LDD respondents. The top 16 priorities from the LDD perspective (Figure 19) included topics related to seven different technologies (DOC, DPF, PNA, SCR, TWC, HCT, and LNT) along with multiscale measurements and simulations of emissions. New materials for low temperature emissions control (DOC, PNA, SCR, TWC, HCT) appeared prominently among the top LDD priorities. PNA-related topics represented the largest fraction of top LDD priorities, with four separate topics appearing in the top 16.

3.2.3.3 LDG

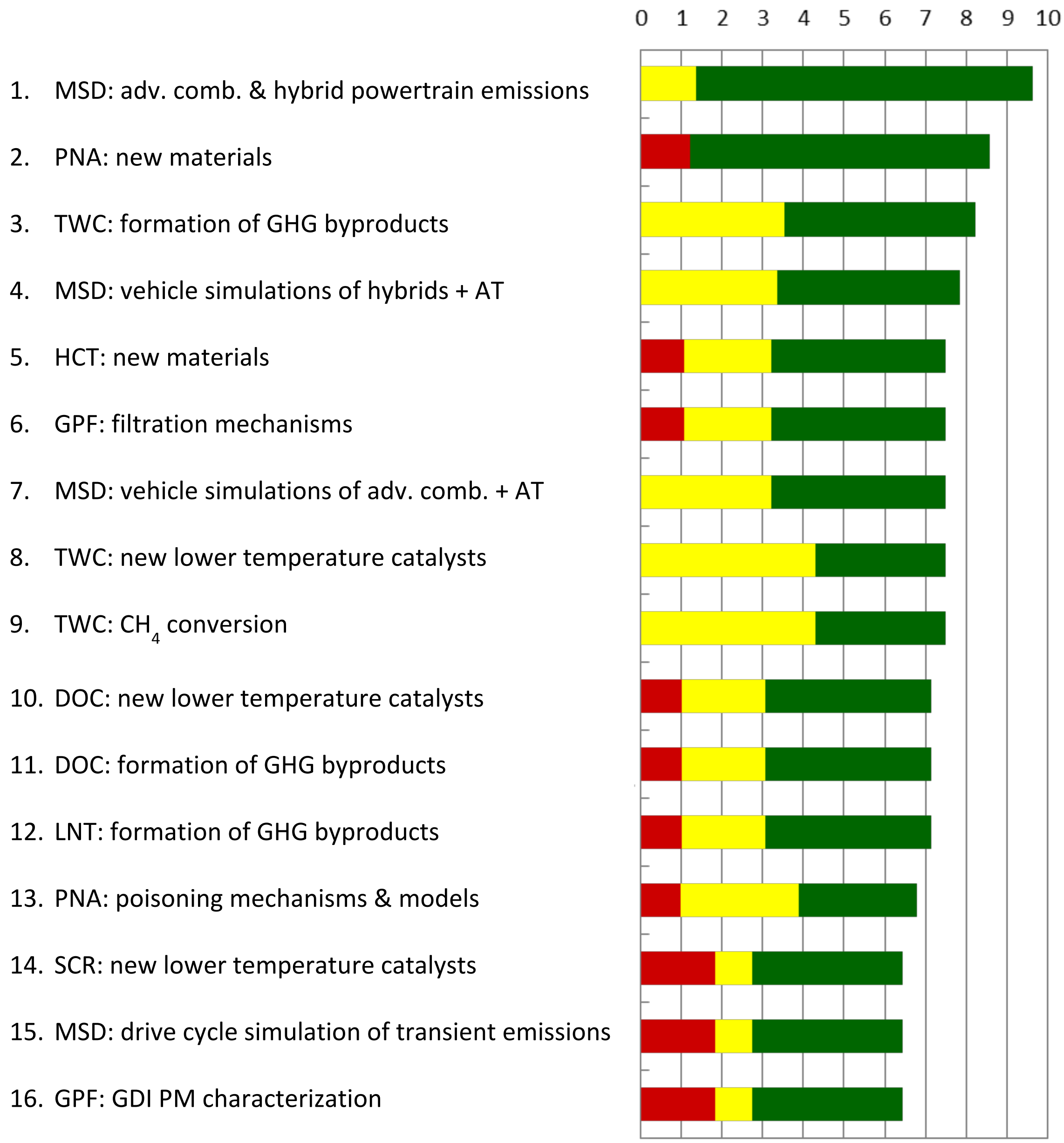

Figure 20. Top 16 technical topics ranked by average priority score for the LDG market perspective

The top ranked topics from the LDG market perspective showed some parallels with the LDD perspective: a wide array of technologies (PNA, TWC, HCT, GPF, DOC, LNT, SCR) appeared in the top 16 list, and many of the topics related to new low temperature formulations (PNA, HCT, TWC, DOC, SCR). Multiscale modeling, simulation, and data generation topics were a particularly high priority for LDG respondents: one fourth of the top 16 LDG topics came from this area (more than for any technology), including the overall top LDG priority. Formation of greenhouse gas byproducts (TWC, DOC, LNT) also appeared prominently in the top LDG priorities.

3.3 WRITE-IN COMMENTS

All of the comments entered by respondents into the survey text boxes, along with the market perspectives from which they were written, are included in a table in APPENDIX B: Full Write-in Comments. This section summarizes a few of the themes from those comments.

Overall, many of the comments echoed the general trends from the rest of the priority survey.

- Three different respondents mentioned the importance of greenhouse gas regulations, and one of those highlighted N_2O as a particular challenge.
- Several commenters discussed how improving fuel economy will require increased hybridization and/or low temperature combustion engines, which will create emissions control challenges. New catalyst formulations that are active at lower temperatures will be required. Also, simulation tools have a role to play in the design of new formulations and in predicting exhaust properties and catalyst performance for use in designing emissions control architectures for next generation vehicles.
- Two respondents highlighted the need for more focus on emissions control for natural gas vehicles, particularly discovery of new lower temperature catalysts (both oxidation and three-way) for converting CH.

In addition to these comments that were more or less in line with the general trends observed elsewhere in the survey, there were a few commenters who listed specific issues that were not heavily covered elsewhere in the survey.

- Two commenters from the HDD market perspective highlighted urea deposits as a critical issue, with one emphasizing the need to understand the thermodynamic driving force behind the formation of solid deposits rather than the desired products of urea decomposition and NOx reduction.
- One of the commenters addressed the need to understand aging mechanisms for the sensors used in feedback control (such as NOx sensors), with a particular emphasis on models that could capture those aging processes.
- Commenters from the light duty market perspectives listed TWC with NOx storage, HC speciation for gasoline-based low temperature combustion modes, and multi-functional GPF devices as areas of interest.

Finally, one commenter discussed the timing of the CLEERS Workshop relative to SAE World Congress, and inquired about changing the workshop dates or adding a teleconferencing option.

4. COMPARISON WITH PRIOR SURVEY RESULTS

The structure and content of the CLEERS Industry Priority Survey has evolved considerably over the years since it was first conducted in 2007. Changes were made to better reflect current aftertreatment development needs; to account for lessons learned from previous surveys in making sure that wording of the questions is clear; to make it easier for respondents to complete the survey; and to better support planning decisions at the DOE National Laboratories. As a result, the list of technical topics and even the ranking methodology changed significantly between the 2007 and 2015 versions of the survey. However, it is still possible to compile a list of the top-ranked priorities from each of the surveys to look for general trends regarding how the relative importance of various technologies and research areas has evolved over the years.

Table 1 summarizes the top ranked technical topics from each market perspective for all the surveys conducted since 2007. In general, the top three topics were selected from each market perspective for each year. Note that there were only two market perspectives included in the 2007 and 2008 surveys; the heavy duty and light duty distinctions for the diesel market segment were not added until 2011. Also, in instances where multiple topics received the same priority score resulting in a tie within the top 3 topics, all of those topics were included in Table 1. This was particularly common in the earlier years of the survey under the gasoline market perspective, when a limited number of survey responses resulted in a large number of topics receiving the same average priority score.

Looking first at the general mix of technologies that appeared in the top priorities over the years, the diesel market perspectives showed a consistent focus on urea SCR and DPF, with a few DOC topics. The high priority topics for the gasoline market perspective, on the other hand, have changed completely in the past eight years. The initial mix of technologies receiving high priority scores included LNT, HC SCR, and urea SCR. In more recent years, those technology areas have been completely displaced by particulate filters, low temperature adsorbers, TWCs, and vehicle simulations and emissions data generation.

Considering the broader research areas appearing in the top ranked topics, there was a strong emphasis on OBD-related topics for all of the prior surveys up until the most recent installment, which had zero OBD topics ranked in the top technical topics. In fact, only a single OBD-related topic made it into the top 25% of technical topics for any of the market perspectives (see Figure 19). This seemingly abrupt shift away from OBD topics was somewhat remarkable, and it will be interesting to see if it continues going forward. The increased emphasis on new low temperature catalyst formulations in the results from the last two surveys is consistent with ongoing trends in engine and aftertreatment development toward lower exhaust temperatures. There was also a new emphasis on vehicle simulations and data generation in the recent surveys, particularly from light duty market perspectives, but the source for this trend is not clear. Finally, the top priorities from the most recent survey included two topics related to formation of greenhouse gas byproducts. These topics were only included in the most recent survey, so it is not clear if their high ranking reflects a new focus on greenhouse gases due to changing emissions regulations, or if the interest in those areas was already there and just not captured in prior surveys. Multifunctional filters fall into a similar category: they appear in the top priorities for the 2013 and 2015 surveys, but they were not included in the prior survey topics.

Table 1. Top technical priorities by market perspective for all of the CLEERS Industry Priority Surveys conducted since 2007

Year	HDD	LDD	Gasoline
2007	• Urea SCR poisoning • DPF OBD • Urea SCR aging	(not separated from HDD)	• LNT aging • LNT chemistry, kinetics
2008	• Urea SCR OBD • DPF OBD • DPF soot oxidation kinetics	(not separated from HDD)	• HC-SCR activity • HC-SCR durability & poisoning • LNT activity • LNT poisoning • Urea SCR activity • Urea SCR durability • Urea SCR OBD
2011	• Urea SCR catalyst properties, poisoning, aging • Filter measurement, sensing, diagnostics • Urea SCR kinetics • Oxidation catalyst properties	• Urea SCR catalyst properties, poisoning, aging • Urea SCR kinetics • Filter measurement, sensing, diagnostics	• NH_3 oxidation & storage • particulate properties • particulate filter coating • LNT measurement, sensing, diagnostics • HC traps • LNT-SCR • LNT-TWC
2013	• NH_3 storage, oxidation • New low T NH_3 SCR catalysts • Measurement & sensing for urea SCR OBD	• NH_3 storage, oxidation • Measurement & sensing for particulate OBD • Vehicle simulations of adv. comb. + aftertreatment	• Nano-PM characterization • Vehicle simulations of adv. comb. + aftertreatment • Filtration mechanisms • Measurement & sensing for filter OBD • Multifunction filters
2015	• SCR on DPF • New low T NH_3 SCR catalysts • NH_3 slip catalysts	• New low T oxidation catalysts • SCR on DPF • Formation of GHG byproducts from DOC	• Data for adv. comb. and hybrid powertrain emissions • New PNA materials • Formation of GHG byproducts from TWC

5. SUMMARY OF FINDINGS

This section contains a brief summary of the key findings from the 2015 CLEERS Industry Priority Survey.

Regarding CLEERS activities:

- The core activities of the CLEERS organization (annual public workshop, regular technical teleconferences, national laboratory research coordination) are all still very important to survey respondents, and should remain the primary focus of the CLEERS coordinators.
- The information and resources sharing capabilities provided by CLEERS (the CLEERS website, posting of data sets and models, standard laboratory protocols for catalyst measurements, access to unique DOE lab facilities) were ranked medium to high importance and should continue to be supported.

Regarding technical priorities:

- The survey responses reflect a diversity of opinions in the CLEERS community:
    - Nearly every technical topic was ranked low priority by at least one respondent, medium priority by multiple respondents, and high priority by at least one respondent.
    - Every technology included in the survey was ranked (on average) medium priority or higher for at least one market segment.
- Technology priorities vary significantly among different market segments, and responders from each market segment identified multiple high priority technology areas:
    - HDD: SCR, PNA, DOC, DPF
    - LDD: PNA, SCR, LNT, DOC, HCT
    - LDG: GPF, PNA, TWC, LNT, HCT
- Technologies that have been on the road for some time still generated high priority ratings in specific market segments:
    - TWC topics were ranked high priority by gasoline respondents.
    - SCR and DOC topics were ranked high priority by diesel respondents.
- Passive NOx adsorbers were the only technology ranked as a high priority by all three market segments.
- Two cross-cutting high priority themes emerged repeatedly in the questionnaire responses and write-in comments and concerns:
    - New low temperature catalysts
    - Formation of greenhouse gas byproducts
- Systems level experimental data and drive-cycle simulations generated significant interest, particularly from the light duty responders.
- Of the "other" topics included in the survey, two generated significant interest:
    - NH_3 slip catalysts were ranked a high priority by HDD respondents.
    - Multilayer, multizone, or multicomponent NOx control strategies (LNT/NH_3 SCR, TWC/NH_3 SCR, HC SCR/NH_3 SCR) received medium to high ratings, with more interest from the LDG perspective.
- Multifunctional filters (particularly SCR on DPF) remain a high priority topic.
- Natural gas engine emissions appear to be a growing issue based on ratings for topics related to CH_4 conversion by both DOCs and TWCs, as well as write-in comments from two separate respondents.
- The relative importance of OBD-related topics decreased significantly compared to prior surveys, although one respondent submitted a comment specifically addressing aging of onboard sensors.

APPENDIX A: Full Survey Text

Dear Colleague:

You are receiving this email because you have been identified as having a unique perspective on aftertreatment development, application and simulation. 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. This survey is used to prioritize emissions control technology development needs and occasionally identifies new opportunities for technology development. The results of this survey could impact both ongoing DOE-funded work as well as future DOE funding opportunities.

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 to minimize the amount of time required to complete it. Since the invitation list for this questionnaire is relatively small, your response is especially important in order to get reasonable statistics for the conclusions abstracted from this survey. Additionally, while absolute rankings across the technology areas are of primary importance, please try to provide as much differentiation as possible within the subtopics so that we may focus our resources in areas that are of highest importance. Our goal is to receive all the responses by Friday, 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

2015 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 3 separate parts in each questionnaire. On the first 2 parts, please indicate your level of interest in each option as "High (**H**), Medium (**M**), or Low (**L**)". On the 3rd part, 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** (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. Please try to answer the questions with a single application area in mind so that we may clearly differentiate the priorities by application. As mentioned above, each company can submit a separate response for each application area.
- 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 input and comments you might have beyond that covered in the previous pages.

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: Diesel Particulate Filters (DPF)

H☐ **M**☐ **L**☐ -Characterization and modeling of DPF filtration mechanisms
H☐ **M**☐ **L**☐ -Diesel particulate O_2 oxidation kinetics
H☐ **M**☐ **L**☐ -Diesel particulate NOx oxidation kinetics
H☐ **M**☐ **L**☐ -DPF measurement, sensing & diagnostics for OBD
H☐ **M**☐ **L**☐ -DOC coated on DPF: HC, CO, and NO oxidation kinetics
H☐ **M**☐ **L**☐ -SCR coated on DPF: effects of multiple functions on reaction kinetics

Particulate Emissions Controls: Gasoline Particulate Filters (GPF)

H☐ **M**☐ **L**☐ -Characterization and modeling of GPF filtration mechanisms
H☐ **M**☐ **L**☐ -Gasoline particulate oxidation kinetics
H☐ **M**☐ **L**☐ -GPF measurement, sensing & diagnostics for OBD
H☐ **M**☐ **L**☐ -Characterization of gasoline direct injection engine particulate matter

NOx Emission Controls: NH_3 Selective Catalytic Reduction

H☐ **M**☐ **L**☐ -NH_3 SCR catalyst NOx reduction reaction mechanisms & kinetics
H☐ **M**☐ **L**☐ -NH_3 storage, oxidation, & release on NH_3 SCR catalysts
H☐ **M**☐ **L**☐ -Formation of greenhouse gas byproducts (N_2O) on SCR catalysts
H☐ **M**☐ **L**☐ -Mechanisms & models for NH_3 SCR catalyst aging
H☐ **M**☐ **L**☐ -Mechanisms & models for NH_3 SCR catalyst poisoning
H☐ **M**☐ **L**☐ -Discovery of new lower temperature NH_3 SCR catalysts
H☐ **M**☐ **L**☐ -NH_3 SCR catalyst measurement, sensing & diagnostics for OBD
H☐ **M**☐ **L**☐ -Urea injection dynamics & decomposition kinetics
H☐ **M**☐ **L**☐ -Non-urea NH_3 sources

NOx Emission Controls: Lean NOx Trap (LNT) or NOx Storage/Reduction Catalysts

H☐ **M**☐ **L**☐ -NOx storage, release, and reduction mechanisms & kinetics
H☐ **M**☐ **L**☐ -Formation of greenhouse gas byproducts (N_2O, CH_4) on LNT catalysts
H☐ **M**☐ **L**☐ -Mechanisms & models for LNT catalyst aging
H☐ **M**☐ **L**☐ -Mechanisms & models for LNT catalyst poisoning
H☐ **M**☐ **L**☐ -Discovery of new lower temperature LNT catalysts
H☐ **M**☐ **L**☐ -LNT catalyst measurement, sensing & diagnostics for OBD

Oxidation Catalysts for Diesel (DOC) or Low Temperature Combustion Engines

H☐ **M**☐ **L**☐ -Oxidation catalyst reaction mechanisms & kinetics
H☐ **M**☐ **L**☐ -Formation of greenhouse gas byproducts (N_2O, CH_4) on oxidation cats
H☐ **M**☐ **L**☐ -Mechanisms & models for oxidation catalyst aging
H☐ **M**☐ **L**☐ -Mechanisms & models for oxidation catalyst poisoning
H☐ **M**☐ **L**☐ -Discovery of new lower temperature oxidation catalysts
H☐ **M**☐ **L**☐ -Oxidation catalyst measurement, sensing & diagnostics for OBD
H☐ **M**☐ **L**☐ -CH_4 oxidation

Three-way Catalysts (TWC) for Stoichiometric Engine Exhaust

H ☐ **M** ☐ **L** ☐ -TWC catalyst reaction mechanisms & kinetics
H ☐ **M** ☐ **L** ☐ -Formation of greenhouse gas byproducts (N_2O, CH_4) on TWCs
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for TWC catalyst aging
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for TWC catalyst poisoning
H ☐ **M** ☐ **L** ☐ -Discovery of new lower temperature TWC catalysts
H ☐ **M** ☐ **L** ☐ -TWC catalyst measurement, sensing & diagnostics for OBD
H ☐ **M** ☐ **L** ☐ -Measurement and modeling of TWC dynamics (dithering)
H ☐ **M** ☐ **L** ☐ -CH_4 conversion

Low Temperature Adsorbers: Hydrocarbon Traps

H ☐ **M** ☐ **L** ☐ -Mechanisms & kinetics for HC storage, release, and conversion
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for HC trap aging
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for HC trap poisoning
H ☐ **M** ☐ **L** ☐ -Discovery of new HC traps

Low Temperature Adsorbers: Passive NOx adsorbers (PNA)

H ☐ **M** ☐ **L** ☐ -Mechanisms & kinetics for NOx storage, release, and conversion
H ☐ **M** ☐ **L** ☐ -Formation of greenhouse gas byproducts (N_2O) on PNAs
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for PNA aging
H ☐ **M** ☐ **L** ☐ -Mechanisms & models for PNA poisoning
H ☐ **M** ☐ **L** ☐ -Discovery of new PNAs

Other Emissions Control Devices and Issues

H ☐ **M** ☐ **L** ☐ -NH_3 slip catalysts
H ☐ **M** ☐ **L** ☐ -HC SCR
H ☐ **M** ☐ **L** ☐ -Catalysts for onboard fuel reforming
H ☐ **M** ☐ **L** ☐ -Multilayer, multizone, or multicomponent NOx control strategies (LNT/NH_3 SCR, TWC/NH_3 SCR, HC SCR/NH_3 SCR)
H ☐ **M** ☐ **L** ☐ -Natural gas engine emissions
H ☐ **M** ☐ **L** ☐ -Natural gas effects on emissions control devices and strategies
H ☐ **M** ☐ **L** ☐ -Biofuel effects on/opportunities in emissions control devices

Multi-Scale Modeling, Simulation, and Data Sets

H ☐ **M** ☐ **L** ☐ -Drive cycle simulation for transient emissions response
H ☐ **M** ☐ **L** ☐ -Atomistic modeling (e.g., DFT) to refine catalyst kinetic descriptions
H ☐ **M** ☐ **L** ☐ -Microkinetic models for generalized prediction of catalyst performance
H ☐ **M** ☐ **L** ☐ -Shared reactor & dynamometer data for relevant reference catalysts
H ☐ **M** ☐ **L** ☐ -Component models & associated parameters for reference catalysts
H ☐ **M** ☐ **L** ☐ -Vehicle simulations of advanced combustion + aftertreatment
H ☐ **M** ☐ **L** ☐ -Vehicle simulations of hybrids + aftertreatment
H ☐ **M** ☐ **L** ☐ -Steady state & transient emissions data for advanced combustion engines and hybrid powertrains

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

H☐ **M**☐ **L**☐ -Annual public workshop on aftertreatment modeling and simulation.
H☐ **M**☐ **L**☐ -Monthly technical teleconferences.
H☐ **M**☐ **L**☐ -Website for announcements, data sharing, member interactions.
H☐ **M**☐ **L**☐ -Quarterly CLEERS newsletter covering recent activities, upcoming events, database postings, funding opportunities, job postings, etc.
H☐ **M**☐ **L**☐ -Web collaboration tools (such as Zotero sharing functions).
H☐ **M**☐ **L**☐ -Standard 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 reference catalysts.
H☐ **M**☐ **L**☐ -Posting of aftertreatment models & data from govt. sponsored projects.
H☐ **M**☐ **L**☐ -Restricted access repository for sharing of data and information with selected membership groups.

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

3. Additional Comments

Please use the space below to add any additional comments or suggestions you might have regarding any of the technology priorities covered in the previous pages or other specific feedback you might have regarding how CLEERS might become more directly useful to you. We would also be interested in hearing your perspectives on the potential importance of emerging technologies that could directly or indirectly impact vehicle emissions controls, including:

- Light-duty electric hybridization;
- Heavy-duty electric hybridization;
- Natural gas fueling;
- Gasoline vs. diesel heavy duty vehicles.

You may also contact Stuart Daw directly at dawcs@ornl.gov , 865-946-1341 if you have questions.

Add comments here:

APPENDIX B: Full Write-in Comments

Appendix B. Full Write-in Comments

HDD	LDD	LDG	Comments
○			• Understanding aging mechanisms for sensors which are used for feedback control (e.g. NOx sensor for HD diesel). • Associated mathematical models for said aging mechanisms would be very useful for controls development to meet end-of-life requirements.
○			• New SCR catalyst formulations using fundamental reaction kinetics as the basis for design. Periodic table cation zeolites. Can't we do better than Cu? • California low-NOx rule is changing everything. We're looking at PNA's, SCR+F, better slip catalysts, all in the context of durability. Models should direct us on integrating components. • N_2O is emerging as a key issue. It is being capped and there seems to be a CO_2 - N_2O trade-off for SCR systems.
○			• Medium - TWC reaction mechanisms and kinetics for natural gas fueled engines • High - Discovery of new lower temperature TWC catalysts for natural gas fueled engines • High - Discovery of new lower temperature oxidation catalysts for natural gas fueled engines
○			• Urea deposit formation and removal
○			• For the next 10 years heavy duty diesel will focus primarily on improved fuel economy and reduced greenhouse gas (GHG) emissions. There is a fundamental conflict in achieving these goals while simultaneously meeting the current 0.2 g/hp.hr NOx target (even more so if this limit is lowered). Better understanding of the thermodynamic limits of the various competing reactions (NOx reduction versus nitrate formation; urea conversion into ammonia versus deposit formation) is as important as understanding the kinetics of the aftertreatment reactions.
○			• With CLEERS being right after SAE World Congress, it is often challenging to attend both from a financial perspective for companies outside of the Detroit area. On hindsight this may foster attendance by people who continue to stay in the area after SAE. In any case are there proposals to change the dates for CLEERS or include a Webex type connection where people can dial-in and actively participate in the conference? Thank you!
○		○	• Important to give priority to creating lower temperature fast light-off catalysts recognizing increasing reg. emphasis on cold start emissions • We would like to see high priority given to the aftertreatment issues associated with all types of Natural Gas fueled vehicles; especially cold start CH_4 emissions

HDD	LDD	LDG	Comments
	○		• LD is headed into very low CO_2 in the 2025 timeframe yet the industry is very conservative. It will want to keep the ICE. We will see increasing LTC and HEV with all the synergies and emissions issues.
	○		• Increased hybridization is adding complexity to vehicles and the design of emissions control systems. Systems modeling of different types of hybridization would give guidance to the emissions community on the impact on the catalyst requirements. Will hybridization change the temperatures and space velocities seen by the catalyst? Are there unique operation modes that are beneficial or harmful for emissions?
	○	○	• TWC + NOx Storage Catalyst Drive cycle analysis would be higher if it fell more in line with production intent not just this is possible • Light duty GHG standards are of importance with all new powertrain options
		○	• HC speciation for gasoline-based low-temperature combustion modes • GPF based multi-functional devices • TWC with high temperature NOx storage functionality