CLEERS Research Prioritization

Analysis of Focus Areas from CLEERS Members

May 2007

Introduction

The Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) activities began in 2001, with the intention to enhance collaboration among OEMs, emission control suppliers, national laboratories, and universities for emission control research. CLEERS provides a framework for sharing non-proprietary data and simulations and also provides a mechanism for industry feedback to the Department of Energy. The activities are overseen by a CLEERS Planning Committee that implements rules and procedures, updates reports and recommendations to the Crosscut Team, and coordinates CLEERS Focus Groups.

In late 2006, the Department of Energy requested that CLEERS collect information from its partners on recommended research and development priorities for emission controls. The CLEERS Planning Committee undertook the design of the survey questions, the complete list of R&D priorities, and the list of partners to be surveyed (including Crosscut Team members and emission control suppliers), with a view toward understanding the most important focus areas for which the CLEERS group should apply future resources. The CLEERS Planning Committee engaged the services of an independent third party, New West Technologies LLC, to conduct the survey in January 2007, analyze the results, and report the results back to the CLEERS group.

In this work, the CLEERS partners were asked to review and prioritize a list of possible future activities and to highlight their three choices for the top priority items. Respondents were also asked to provide suggestions on the recommended balance of funding across several general areas of research. Results were collected separately for diesel and lean gasoline applications (although the lean gasoline work is outside the Crosscut scope). New West developed the electronic survey tools with the assistance of the CLEERS Planning Committee, distributed the tools to the respondents, collected and analyzed responses, and presented the results anonymously to the Committee to protect the identities of the responding companies. This report outlines the procedures and results of the study in more detail.

Summary of Findings

Gasoline Priorities

The top priorities for CLEERS focus areas for gasoline are:

- **Commercial Relevance:** (tie) ISS-1e: Integrated Systems Simulation (ISS)/oxidation catalysts/multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit AND LNT-2b: Lean NOx Traps (LNT)/Determination and characterization of limiting chemical or physical mechanisms for precious metal aging
- **Importance to National Energy Strategy:** (tie) ISS-1e: Integrated Systems Simulation (ISS)/oxidation catalysts/multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit AND LNT-1a: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for NO, NO_2, and O_2 storage and release
- **Scientific Importance/Challenge:** LNT-1d: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates
- **Utilization of Special National Lab Capabilities:** LNT-1d: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates.

Diesel Priorities

The top priorities for CLEERS focus areas for diesel are:

- **Commercial Relevance:** DPF-5a: Diesel Particulate Filters (DPF)/Improved sensor concepts and sensor utilization/Accurate estimation of soot loading and prediction of regeneration exotherm.
- **Importance to National Energy Strategy:** ISS-1e: Integrated Systems Simulation (ISS)/Oxidation catalysts/Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit

- **Scientific Importance/Challenge:** DPF-2b: Diesel Particulate Filters (DPF)/Kinetics - oxidation mechanisms, detailed kinetics, global rates/Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)
- **Utilization of Special National Lab Capabilities:** ISS-3a: Integrated Systems Simulation (ISS)/Device-device interactions (both dynamic and steady-state)/DPF & SCR

Resource Allocation

Respondents recommended that resources for gasoline applications be chiefly focused on lean NOx traps, and recommended that resources for diesel applications be focused about equally on integrated systems simulations, selective catalytic reduction, and diesel particulate filters, with a minor investment in lean NOx traps.

Respondents

Prioritization requests were sent electronically via e-mail in Excel format to 22 government and industrial partners. A total of 14 partners provided responses. The overall response rate from the partners was thus 64 percent.

Responses received were from light-duty and heavy-duty vehicle OEMs, Tier 1 suppliers, heavy-duty engine OEMs, and energy companies. Respondents were asked to provide separate responses for emission control prioritization for gasoline applications and for diesel applications. A total of six (6) gasoline and twelve (12) diesel prioritization responses were received (several partners provided both, while some provided only gasoline or only diesel responses).

Prioritization Questions and Procedures

Questions

Respondents were sent an Excel spreadsheet including a sheet of instructions on completing the prioritization and three sheets of response areas. First, respondents were asked to prioritize the complete list of CLEERS focus targets into high priority, medium priority, and low priority items. Second, they were asked to provide their top three choices for CLEERS activities in four categories: commercial relevance; importance to national energy strategy; scientific importance/challenge; and utilization of special national laboratory capabilities. Third, respondents were asked to identify their recommended resource allocation percentages (totaling to 100 percent) across the four major CLEERS activity categories: integrated systems simulation (ISS); diesel particulate filters (DPF); selective catalytic reduction (SCR); and lean-NOx traps (LNT). Screen shots of the individual pages of the form appear at the end of this document.

For convenience, each CLEERS focus target in the list was provided with a unique identifier indicating the overall category, the subcategory, and the activity. Respondents then used these unique identifiers to assign their top priorities without retyping the entire category/subcategory/activity text.

Analysis

Analysis of the responses was conducted using Excel as the main tool, and proceeded in the following manner with gasoline applications and for diesel applications reviewed separately but using the same procedures. For the complete prioritization of CLEERS focus targets, each response was placed into a single spreadsheet and the low, medium, and high priorities were assigned numeric values of 1 (low), 2 (medium), or 3 (high). The overall prioritization of the focus targets was then determined simply by totaling the numeric values from all responses across each focus target, and then sorting the list from highest to lowest based on the total numeric score.

For the top three choices for CLEERS activities, respondents were asked to provide their first, second, and third choices from the complete list of targets in the categories of commercial relevance; importance to national energy strategy; scientific importance/challenge; and utilization of special national laboratory capabilities. The choices from each respondent were placed into a single spreadsheet and each choice was assigned a numeric weight of 3 (top choice), 2 (middle choice), or 1 (bottom choice). These weighted choices were then arranged by the focus area and the weighted scores were totaled. For example, if focus area A was noted as a top choice by one respondent and a middle choice for a second, then the total score for focus area A would be 3 (top) plus 2 (middle), or 5 total. This was repeated for each category, and the choice list was sorted by weighted score.

For the recommended allocation percentages, the numeric percentage allocations for each respondent were arrayed in a matrix for both gasoline and diesel applications. The numeric percentages for each of the four categories (ISS, DPF, SCR, and LNT) were then averaged to provide the summary of responses.

In this report analysis, the individual respondents will be anonymous, and no company name will be attached to any of the responses provided.

Prioritization Results

Prioritization of Technical Focus Targets

As noted above, respondents were asked to review the list of technical focus targets and prioritize them with high, medium, or low importance. The overall procedure described above was used to produce the prioritizations in Tables 1 and 2 below.

Gasoline

For gasoline applications, respondents placed the technical focus targets in the priority list shown below in Table 1.

Table 1. Gasoline Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
LNT-2b	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Precious metal aging	17
LNT-3d	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Consumption of H_2, CO, and HC during rich conditions and lean-rich transients	17
LNT-1a	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO, NO_2,and O_2 storage and release	16
LNT-1b	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO, NO_2 and O transport between PGM adsorption and storage sites	16
LNT-3b	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Release of stored NO, NO_2, and O_2 during rich conditions	16
LNT-3c	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Reduction of NO and NO_2 by CO, H_2, and HC during rich conditions	16
LNT-1d	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	Formation of NH_3, N_2O, HCN, and isocyanates	15
LNT-3e	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Production of NH_3 and N_2O during rich conditions and lean-rich transitions	15
LNT-1c	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO and NO_2 reduction by CO, H_2, and HC (separately)	14
LNT-1e	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	Formation and decomposition of sulfates	14
LNT-2a	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	H_2O and CO_2 inhibition	14
LNT-2c	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Formation of non-regenerable sulfur	14
LNT-2e	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Degree of contacting between precious metals and NOx storage sites	14
LNT-3a	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NO, NO_2, and O_2 storage during lean conditions	13
LNT-3h	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Capture of SO_2 and SO_3 during lean conditions	13

Table 1. Gasoline Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
LNT-3i	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Release of SO_2, SO_3, and H_2S during desulfation	13
SCR-4a	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Thermal degradation due to cycling	13
LNT-2d	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Microstructural changes in the support materials with aging	12
LNT-3f	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NOx storage by ceria	12
LNT-3g	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NOx/CO_2 diffusion in/out of sorbent as a function of sorbent state/composition	12
ISS-1e	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	11
ISS-2a	Integrated Systems Simulation (ISS)	2.Reformer catalysts	Modeling for applications to LNT	11
SCR-1b	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	NH_3 surface adsorption/desorption	11
SCR-1c	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	NH_3 reaction with NO, NO_2	11
SCR-4b	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Poisoning by S, P, HC's	11
ISS-4b	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	LNT regeneration and desulfation maps for reference engines	10
SCR-1a	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	Urea thermolysis (gas and surface)	10
SCR-1d	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	Role of different HC components (e.g., alkanes, alkenes, aromatics)	10
SCR-3a	Selective Catalytic Reduction (SCR)	3.Transport effects	Pore/washcoat diffusion	10
ISS-3f	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)	9
SCR-1g	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HNCO formation/decomposition	9
SCR-1h	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	N_2O formation/reduction	9
SCR-2a	Selective Catalytic Reduction (SCR)	2.Dosing system	Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet	9
DPF-1a	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Variation with time, engine design, operating conditions and fuel formulation.	8
DPF-1d	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Capture, generation, and release of nano-particles.	8
DPF-2a	Diesel Particulate Filters (DPF)	2.Kinetics - oxidation mechanisms, detailed kinetics, global rates.	Reaction rates for passive and active regeneration of the soot.	8
DPF-2b	Diesel Particulate Filters (DPF)	2.Kinetics - oxidation mechanisms, detailed kinetics, global rates.	Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)	8
DPF-3a	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for soot regeneration control studies.	8
DPF-3b	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for component interaction studies.	8
DPF-4b	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Practical simulations capturing structural and flow effects.	8
DPF-4c	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Evolution of temperature distributions and gradients combined with filter stability/survivability	8
DPF-5a	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	Accurate estimation of soot loading and prediction of regeneration exotherm.	8
DPF-5b	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.	8

Table 1. Gasoline Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
DPF-5c	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	More reliable, less operation-specific DPF state assessment.	8
ISS-1b	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Hydrocarbon storage effects	8
ISS-2b	Integrated Systems Simulation (ISS)	2.Reformer catalysts	Modeling for applications to SCR	8
ISS-3b	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/LNT	8
ISS-3c	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	LNT/SCR	8
ISS-3d	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/Oxycat	8
ISS-3e	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	LNT/Oxycat	8
ISS-4c	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	Standard methods for triggering regenerations during simulations	8
SCR-1f	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HC reaction with NO, NO_2	8
SCR-2b	Selective Catalytic Reduction (SCR)	2.Dosing system	Effect of mixers	8
SCR-2c	Selective Catalytic Reduction (SCR)	2.Dosing system	Aerosol quality	8
SCR-2d	Selective Catalytic Reduction (SCR)	2.Dosing system	Atomizer placement	8
SCR-2e	Selective Catalytic Reduction (SCR)	2.Dosing system	Exhaust gas temperature effects	8
SCR-3b	Selective Catalytic Reduction (SCR)	3.Transport effects	Droplet vaporization	8
SCR-4c	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Effects of soot, ash, coking	8
DPF-1c	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Longer term effects of ash accumulation on DPF durability.	7
DPF-3c	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for trade-off assessments between higher precious metal loading vs. engine torque/speed modifications.	7
DPF-4a	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Higher order models for design and optimization of DPF substrates and systems.	7
ISS-1c	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	NO to NO_2 inter-conversion	7
ISS-4a	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	DPF regeneration maps for reference engines (e.g., 1.9L GM engine)	7
SCR-1e	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HC reaction with O_2	7
DPF-1b	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Local effects of ash loading on filter cake.	6
DPF-4d	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Micro-mechanical models to predict strength degradation and part failure due to thermal cycling	6
ISS-1a	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Shifts in hydrocarbon species distribution with oxycat transit	6
ISS-1d	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Shifts in particulate characteristics with oxycat transit	6
ISS-3a	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/SCR	6

Diesel

For diesel applications, respondents placed the technical focus targets in the priority list shown below in Table 1.

Table 2. Diesel Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
SCR-4b	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Poisoning by S, P, HC's	37
SCR-4c	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Effects of soot, ash, coking	36
DPF-5a	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	Accurate estimation of soot loading and prediction of regeneration exotherm.	35
DPF-5b	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.	34
SCR-4a	Selective Catalytic Reduction (SCR)	4.Deactivation mechanisms	Thermal degradation due to cycling	34
DPF-2a	Diesel Particulate Filters (DPF)	2.Kinetics - oxidation mechanisms, detailed kinetics, global rates.	Reaction rates for passive and active regeneration of the soot.	32
DPF-5c	Diesel Particulate Filters (DPF)	5.Improved sensor concepts and sensor utilization	More reliable, less operation-specific DPF state assessment.	32
SCR-1c	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	NH_3 reaction with NO, NO_2	32
DPF-3a	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for soot regeneration control studies.	31
ISS-1c	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	NO to NO_2 inter-conversion	31
ISS-3a	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/SCR	31
DPF-1a	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Variation with time, engine design, operating conditions and fuel formulation.	30
ISS-1e	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	30
SCR-2e	Selective Catalytic Reduction (SCR)	2.Dosing system	Exhaust gas temperature effects	30
DPF-2b	Diesel Particulate Filters (DPF)	2.Kinetics - oxidation mechanisms, detailed kinetics, global rates.	Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)	29
DPF-4c	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Evolution of temperature distributions and gradients combined with filter stability/survivability	29
SCR-2a	Selective Catalytic Reduction (SCR)	2.Dosing system	Spatial and temporal distribution of urea/NH3 or HCs at monolith inlet	29
LNT-2b	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Precious metal aging	28
SCR-1a	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	Urea thermolysis (gas and surface)	28
DPF-1c	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Longer term effects of ash accumulation on DPF durability.	27
ISS-3d	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/Oxycat	27
LNT-2c	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Formation of non-regenerable sulfur	27
LNT-3b	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Release of stored NO, NO_2, and O_2 during rich conditions	27
LNT-3i	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Release of SO_2, SO_3, and H_2S during desulfation	27
SCR-1b	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	NH_3 surface adsorption/desorption	27
SCR-2b	Selective Catalytic Reduction (SCR)	2.Dosing system	Effect of mixers	27
SCR-3b	Selective Catalytic Reduction (SCR)	3.Transport effects	Droplet vaporization	27

Table 2. Diesel Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
DPF-3b	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for component interaction studies.	26
LNT-3c	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Reduction of NO and NO_2 by CO, H_2, and HC during rich conditions	26
LNT-3d	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Consumption of H_2, CO, and HC during rich conditions and lean-rich transients	26
LNT-3e	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Production of NH_3 and N_2O during rich conditions and lean-rich transitions	26
SCR-1g	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HNCO formation/decomposition	26
SCR-2c	Selective Catalytic Reduction (SCR)	2.Dosing system	Aerosol quality	26
DPF-4a	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Higher order models for design and optimization of DPF substrates and systems.	25
ISS-3f	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)	25
ISS-4c	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	Standard methods for triggering regenerations during simulations	25
LNT-1e	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	Formation and decomposition of sulfates	25
SCR-1h	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	N_2O formation/reduction	25
DPF-4d	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Micro-mechanical models to predict strength degradation and part failure due to thermal cycling	24
LNT-1c	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO and NO_2 reduction by CO, H_2, and HC (separately)	24
SCR-2d	Selective Catalytic Reduction (SCR)	2.Dosing system	Atomizer placement	24
SCR-3a	Selective Catalytic Reduction (SCR)	3.Transport effects	Pore/washcoat diffusion	24
DPF-3c	Diesel Particulate Filters (DPF)	3.1-D device models (using local properties and kinetics sub-models) for systems simulation.	Models for trade-off assessments between higher precious metal loading vs. engine torque/speed modifications.	23
ISS-2a	Integrated Systems Simulation (ISS)	2.Reformer catalysts	Modeling for applications to LNT	23
ISS-2b	Integrated Systems Simulation (ISS)	2.Reformer catalysts	Modeling for applications to SCR	23
ISS-4a	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	DPF regeneration maps for reference engines (e.g., 1.9L GM engine)	23
LNT-1a	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO, NO_2,and O_2 storage and release	23
LNT-2e	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Degree of contacting between precious metals and NOx storage sites	23
LNT-3f	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NOx storage by ceria	23
SCR-1d	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	Role of different HC components (e.g., alkanes, alkenes, aromatics)	23
DPF-1b	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Local effects of ash loading on filter cake.	22
DPF-1d	Diesel Particulate Filters (DPF)	1.Models for local properties of the filter cake (e.g., permeability, density, morphology).	Capture, generation, and release of nano-particles.	22
DPF-4b	Diesel Particulate Filters (DPF)	4.Detailed 3-D device models for understanding capture and oxidation phenomenon.	Practical simulations capturing structural and flow effects.	22
ISS-3b	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	DPF/LNT	22
ISS-3e	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	LNT/Oxycat	22

Table 2. Diesel Prioritization of Technical Focus Targets

ID Number	Major Category	Subcategory	Activity	Total Score
LNT-1b	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	NO, NO_2 and O transport between PGM adsorption and storage sites	22
LNT-1d	Lean NOx Traps (LNT)	1.Determination of the elementary reaction steps for:	Formation of NH_3, N_2O, HCN, and isocyanates	22
LNT-3h	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	Capture of SO_2 and SO_3 during lean conditions	22
ISS-1b	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Hydrocarbon storage effects	21
ISS-3c	Integrated Systems Simulation (ISS)	3.Device-device interactions (both dynamic and steady-state)	LNT/SCR	21
LNT-3a	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NO, NO_2, and O_2 storage during lean conditions	21
SCR-1f	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HC reaction with NO, NO_2	21
ISS-4b	Integrated Systems Simulation (ISS)	4.Reference regeneration strategies for drive cycle simulations	LNT regeneration and desulfation maps for reference engines	20
ISS-1a	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Shifts in hydrocarbon species distribution with oxycat transit	19
LNT-2d	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	Microstructural changes in the support materials with aging	19
LNT-3g	Lean NOx Traps (LNT)	3.Chemistry and kinetics common to LNT's and 3-way catalysts	NOx/CO_2 diffusion in/out of sorbent as a function of sorbent state/composition	19
ISS-1d	Integrated Systems Simulation (ISS)	1.Oxidation catalysts	Shifts in particulate characteristics with oxycat transit	18
SCR-1e	Selective Catalytic Reduction (SCR)	1.Global reaction rate equations, including hybrid mechanisms	HC reaction with O_2	18
LNT-2a	Lean NOx Traps (LNT)	2.Determination/characterization of limiting chemical or physical mechanisms for:	H_2O and CO_2 inhibition	17

Top Priority Project Recommendations

Once the respondents had developed their full prioritization of all the CLEERS focus areas, they were asked to provide the top three choices relative to four major categories: commercial relevance; importance to national energy strategy; scientific importance/challenge; and utilization of special national laboratory capabilities. The procedure described above was used to produce the weighted scores and top priorities listed in Tables 3 and 4 below.

Gasoline

The complete results of the top priority choices from the respondents providing information for gasoline applications are listed in Table 3 for the four categories listed above.

Table 3. Top Priority Choices for Gasoline Applications

Category	Weighted Score
COMMERCIAL RELEVANCE	
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts, Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	6
LNT-2b: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	6
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Thermal degradation due to cycling	4
LNT-1a: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2,and O_2 storage and release	3
LNT-1c: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO and NO_2 reduction by CO, H_2, and HC (separately)	3
ISS-2a: Integrated Systems Simulation (ISS), Reformer catalysts , Modeling for applications to LNT	2
LNT-1b: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2 and O transport between PGM adsorption and storage sites	2

Table 3. Top Priority Choices for Gasoline Applications

Category	Weighted Score
LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates	2
LNT-2c: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for formation of non-regenerable sulfur	2
LNT-3a: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts , NO, NO_2, and O_2 storage during lean conditions	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	2
LNT-3h: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts , Capture of SO_2 and SO_3 during lean conditions	1
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	1
IMPORTANCE TO NATIONAL ENERGY STRATEGY	
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts, Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	6
LNT-1a: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2,and O_2 storage and release	6
LNT-2b: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	4
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Thermal degradation due to cycling	4
LNT-3c: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Reduction of NO and NO_2 by CO, H_2, and HC during rich conditions	3
DPF-1d: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles.	2
LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates	2
LNT-3a: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts , NO, NO_2, and O_2 storage during lean conditions	2
LNT-3d: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Consumption of H_2, CO, and HC during rich conditions and lean-rich transients	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms , Poisoning by S, P, HC's	2
ISS-2a: Integrated Systems Simulation (ISS), Reformer catalysts , Modeling for applications to LNT	1
LNT-3h: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts , Capture of SO_2 and SO_3 during lean conditions	1
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	1
SCIENTIFIC IMPORTANCE/CHALLENGE	
LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates	5
LNT-2b: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	4
ISS-3f: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state) , Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)	3
LNT-1b: Lean NOx Traps (LNT), Determination of the elementary reaction steps for, NO, NO_2 and O transport between PGM adsorption and storage sites	3
LNT-1c: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO and NO_2 reduction by CO, H_2, and HC (separately)	3
LNT-3d: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Consumption of H_2, CO, and HC during rich conditions and lean-rich transients	3
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms , Thermal degradation due to cycling	3
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts , Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	2
ISS-4c: Integrated Systems Simulation (ISS), Reference regeneration strategies for drive cycle simulations, Standard methods for triggering regenerations during simulations	2
LNT-3g: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, NOx/CO_2 diffusion in/out of sorbent as a function of sorbent state/composition	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	2
ISS-2a: Integrated Systems Simulation (ISS), Reformer catalysts , Modeling for applications to LNT	1
LNT-1a: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2,and O_2 storage and release	1
LNT-2a: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for H_2O and CO_2 inhibition	1
LNT-3i: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Release of SO_2, SO_3, and H_2S during desulfation	1
UTILIZATION OF SPECIAL NATIONAL LAB CAPABILITIES	
LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates	4
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts , Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	3

Table 3. Top Priority Choices for Gasoline Applications

Category	Weighted Score
LNT-1a: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2,and O_2 storage and release	3
LNT-1c: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO and NO_2 reduction by CO, H_2, and HC (separately)	3
LNT-2b: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	3
LNT-3e: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Production of NH_3 and N_2O during rich conditions and lean-rich transitions	3
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Thermal degradation due to cycling	3
ISS-4b: Integrated Systems Simulation (ISS), Reference regeneration strategies for drive cycle simulations LNT regeneration and desulfation maps for reference engines	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	2
ISS-2a: Integrated Systems Simulation (ISS), Reformer catalysts , Modeling for applications to LNT	1
LNT-3i: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Release of SO_2, SO_3, and H_2S during desulfation	1
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	1
SCR-1d: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Role of different HC components (e.g., alkanes, alkenes, aromatics)	1

As Table 3 illustrates, the top priorities for CLEERS topics for gasoline applications are:

- **Commercial Relevance:** (tie) ISS-1e: Integrated Systems Simulation (ISS)/oxidation catalysts/multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit AND LNT-2b: Lean NOx Traps (LNT)/Determination and characterization of limiting chemical or physical mechanisms for precious metal aging
- **Importance to National Energy Strategy:** (tie) ISS-1e: Integrated Systems Simulation (ISS)/oxidation catalysts/multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit AND LNT-1a: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for NO, NO_2, and O_2 storage and release
- **Scientific Importance/Challenge:** LNT-1d: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates
- **Utilization of Special National Lab Capabilities:** LNT-1d: Lean NOx Traps (LNT)/Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates

Diesel

The complete results of the top priority choices from the respondents providing information for diesel applications are listed in Table 4 for the four categories listed above.

Table 4. Top Priority Choices for Diesel Applications

Category	Weighted Score
COMMERCIAL RELEVANCE	
DPF-5a: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Accurate estimation of soot loading and prediction of regeneration exotherm.	9
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts, Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	8
DPF-5b: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.	7
ISS-3a: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state), DPF/SCR	6
SCR-2a: Selective Catalytic Reduction (SCR), Dosing system, Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet	6
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	5
LNT-1e: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation and decomposition of sulfates	4
DPF-1a: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Variation with time, engine design, operating conditions and fuel formulation.	3

Table 4. Top Priority Choices for Diesel Applications

Category	Weighted Score
DPF-2a: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Reaction rates for passive and active regeneration of the soot.	3
DPF-4a: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Higher order models for design and optimization of DPF substrates and systems.	3
LNT-2e: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for degree of contacting between precious metals and NOx storage sites	3
SCR-1b: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 surface adsorption/desorption	3
SCR-1c: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 reaction with NO, NO_2	3
SCR-3b: Selective Catalytic Reduction (SCR), Transport effects, Droplet vaporization	3
DPF-1d: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles.	2
DPF-3b: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for component interaction studies.	2
ISS-3c: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state), LNT/SCR	2
LNT-2c: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for formation of non-regenerable sulfur	2
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Thermal degradation due to cycling	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	2
DPF-3c: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for trade-off assessments between higher precious metal loading vs. engine torque/speed modifications.	1
ISS-4c: Integrated Systems Simulation (ISS), Reference regeneration strategies for drive cycle simulations, Standard methods for triggering regenerations during simulations	1
SCR-1g: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, HNCO formation/decomposition	1
IMPORTANCE TO NATIONAL ENERGY STRATEGY	
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts, Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	15
SCR-1c: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 reaction with NO, NO_2	6
DPF-1d: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles.	4
DPF-5a: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Accurate estimation of soot loading and prediction of regeneration exotherm.	4
DPF-5b: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.	4
SCR-1b: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 surface adsorption/desorption	4
DPF-1a: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Variation with time, engine design, operating conditions and fuel formulation.	3
DPF-2a: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Reaction rates for passive and active regeneration of the soot.	3
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	3
DPF-3a: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for soot regeneration control studies.	2
DPF-4a: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Higher order models for design and optimization of DPF substrates and systems.	2
ISS-4a: Integrated Systems Simulation (ISS), Reference regeneration strategies for drive cycle simulations, DPF regeneration maps for reference engines (e.g., 1.9L GM engine)	2
SCR-2a: Selective Catalytic Reduction (SCR), Dosing system, Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet	2
SCR-2e: Selective Catalytic Reduction (SCR), Dosing system, Exhaust gas temperature effects	2
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms Thermal degradation due to cycling	2
SCR-4c: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Effects of soot, ash, coking	2
DPF-3b: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for component interaction studies.	1
DPF-4d: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Micro-mechanical models to predict strength degradation and part failure due to thermal cycling	1
LNT-1e: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation and decomposition of sulfates	1

Table 4. Top Priority Choices for Diesel Applications

Category	Weighted Score
LNT-2b: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	1
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	1
SCIENTIFIC IMPORTANCE/CHALLENGE	
DPF-2b: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)	10
DPF-2a: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Reaction rates for passive and active regeneration of the soot.	9
LNT-3i: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Release of SO_2, SO_3, and H_2S during desulfation	5
LNT-2e: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for degree of contacting between precious metals and NOx storage sites	4
SCR-1b: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 surface adsorption/desorption	4
DPF-4a: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Higher order models for design and optimization of DPF substrates and systems.	3
DPF-5a: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Accurate estimation of soot loading and prediction of regeneration exotherm.	3
DPF-5b (1) DPF-5b: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.	3
ISS-2a: Integrated Systems Simulation (ISS), Reformer catalysts, Modeling for applications to LNT	3
ISS-3a: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state), DPF/SCR	3
LNT-1c: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO and NO_2 reduction by CO, H_2, and HC (separately)	3
LNT-3c: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Reduction of NO and NO_2 by CO, H_2, and HC during rich conditions	3
LNT-3h: Lean NOx Traps (LNT), Chemistry and kinetics common to LNT's and 3-way catalysts, Capture of SO_2 and SO_3 during lean conditions	3
SCR-3b: Selective Catalytic Reduction (SCR), Transport effects, Droplet vaporization	3
DPF-1d: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles.	2
DPF-3b: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for component interaction studies.	2
DPF-5c: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, More reliable, less operation-specific DPF state assessment.	2
ISS-1e: Integrated Systems Simulation (ISS), Oxidation catalysts, Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	2
ISS-2b: Integrated Systems Simulation (ISS), Reformer catalysts, Modeling for applications to SCR	2
LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH_3, N_2O, HCN, and isocyanates	2
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	2
DPF-3c: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for trade-off assessments between higher precious metal loading vs. engine torque/speed modifications.	1
DPF-4c: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Evolution of temperature distributions and gradients combined with filter stability/survivability	1
DPF-4d: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Micro-mechanical models to predict strength degradation and part failure due to thermal cycling	1
LNT-1e: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation and decomposition of sulfates	1
UTILIZATION OF SPECIAL NATIONAL LAB CAPABILITIES	
ISS-3a: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state) , DPF/SCR	6
SCR-4b: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Poisoning by S, P, HC's	6
DPF-1d: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles.	5
DPF-4a: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Higher order models for design and optimization of DPF substrates and systems.	5
DPF-1a: Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Variation with time, engine design, operating conditions and fuel formulation.	3
DPF-2a: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Reaction rates for passive and active regeneration of the soot.	3
LNT-2e: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for degree of contacting between precious metals and NOx storage sites	3

Table 4. Top Priority Choices for Diesel Applications

Category	Weighted Score
SCR-1a: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Urea thermolysis (gas and surface)	3
SCR-1d: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, Role of different HC components (e.g., alkanes, alkenes, aromatics)	3
SCR-3a: Selective Catalytic Reduction (SCR), Transport effects, Pore/washcoat diffusion	3
DPF-2b: Diesel Particulate Filters (DPF), Kinetics - oxidation mechanisms, detailed kinetics, global rates, Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)	2
DPF-3a: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for soot regeneration control studies.	2
DPF-3b: Diesel Particulate Filters (DPF), 1-D device models (using local properties and kinetics sub-models) for systems simulation, Models for component interaction studies.	2
DPF-5a: Diesel Particulate Filters (DPF), Improved sensor concepts and sensor utilization, Accurate estimation of soot loading and prediction of regeneration exotherm.	2
ISS-3f: Integrated Systems Simulation (ISS), Device-device interactions (both dynamic and steady-state), Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)	2
SCR-2a: Selective Catalytic Reduction (SCR), Dosing system, Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet	2
SCR-4c: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Effects of soot, ash, coking	2
DPF-4b: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Practical simulations capturing structural and flow effects.	1
DPF-4d: Diesel Particulate Filters (DPF), Detailed 3-D device models for understanding capture and oxidation phenomenon, Micro-mechanical models to predict strength degradation and part failure due to thermal cycling	1
ISS-1d: Integrated Systems Simulation (ISS), Oxidation catalysts , Shifts in particulate characteristics with oxycat transit	1
LNT-1e: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation and decomposition of sulfates	1
LNT-2c: Lean NOx Traps (LNT), Determination/characterization of limiting chemical or physical mechanisms for formation of non-regenerable sulfur	1
SCR-1b: Selective Catalytic Reduction (SCR), Global reaction rate equations, including hybrid mechanisms, NH_3 surface adsorption/desorption	1

As Table 4 illustrates, the top priorities for CLEERS topics for diesel applications are:

- **Commercial Relevance:** DPF-5a: Diesel Particulate Filters (DPF)/Improved sensor concepts and sensor utilization/Accurate estimation of soot loading and prediction of regeneration exotherm.
- **Importance to National Energy Strategy:** ISS-1e: Integrated Systems Simulation (ISS)/Oxidation catalysts/Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit
- **Scientific Importance/Challenge:** DPF-2b: Diesel Particulate Filters (DPF)/Kinetics - oxidation mechanisms, detailed kinetics, global rates/Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)
- **Utilization of Special National Lab Capabilities:** ISS-3a: Integrated Systems Simulation (ISS)/Device-device interactions (both dynamic and steady-state)/DPF & SCR

Additional Suggested Priorities: Gasoline

Respondents were given the opportunity to suggest additional focus areas that were not included in the existing list. The additional suggested priorities for gasoline applications are listed below.

- LNT—R&D on high-temperature NOx storage catalysts (non-alkali metal)
- LNT or SCR—Particulate emissions from stratified gasoline direct injection engines
- LNT—Platinum group metal utilization/minimization
- LNT—Direct reduction of stored nitrate versus decomposition followed by NOx reduction over platinum group metals
- LNT—Platinum group metal and NOx storage site temperature measurements
- LNT—Incorporation of oxygen storage capacity chemical and thermal effects into LNT models
- LNT—Optimization of oxygen storage capacity between three-way catalyst and LNT
- LNT—Platinum group metal and NOx storage site temperature measurements

- LNT—Analysis of radial and axial aging effects (inhomogeneity as measured by Spaci-MS)
- SCR—Catalysts that work well for gasoline applications
- SCR—Alternatives to urea for NH_3 generation/ supply
- SCR—Impact of high-temperature rich aging conditions on zeolite-SCR durability
- SCR—Catalyst deactivation under gasoline operating conditions (stoichiometric or rich, high temperature of 700°C)
- SCR—Induction period required when NH_3 injection initialized
- SCR—Redox aging mechanisms for SCR catalysts

Additional Suggested Priorities: Diesel

The additional suggested priorities for diesel applications are listed below.

- Non platinum group metals, non NH_3-based NOx reduction systems
- DPF regeneration maps for reference engines (e.g., 1.9L GM engine)
- LNT regeneration and desulfation maps for reference engines
- Lowering the temperature window of LNT and SCR performance without increasing fuel consumption
- Deterioration of passive soot regeneration rates due to DPF aging (thermal and chemical)
- DPF soot cake formation and structure—impact on oxidation and exhaust gas flow

Resource Allocations

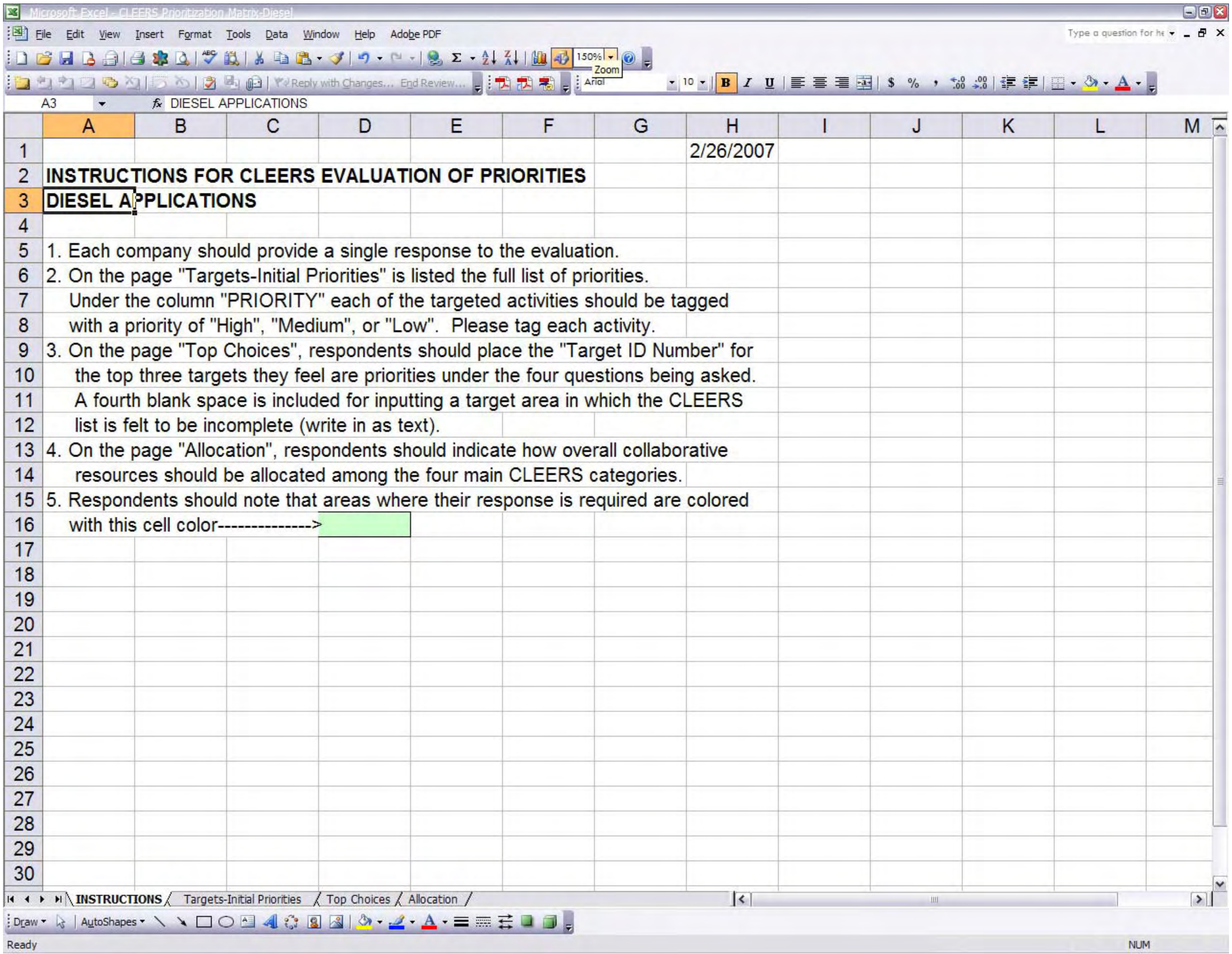
Table 5 illustrates the results of the analysis of the allocation responses for both gasoline and diesel. Note that gasoline respondents recommended that the majority of funds be allocated to lean NOx traps, with some funding for ISS and DPFs but very little for SCR. Diesel respondents felt that roughly equal resources should be allocated to ISS, SCR, and DPFs, with a slight advantage to SCR: fewer resources should be allocated to lean NOx traps.

Table 5. Resource Allocations (Percent of Total Resources)

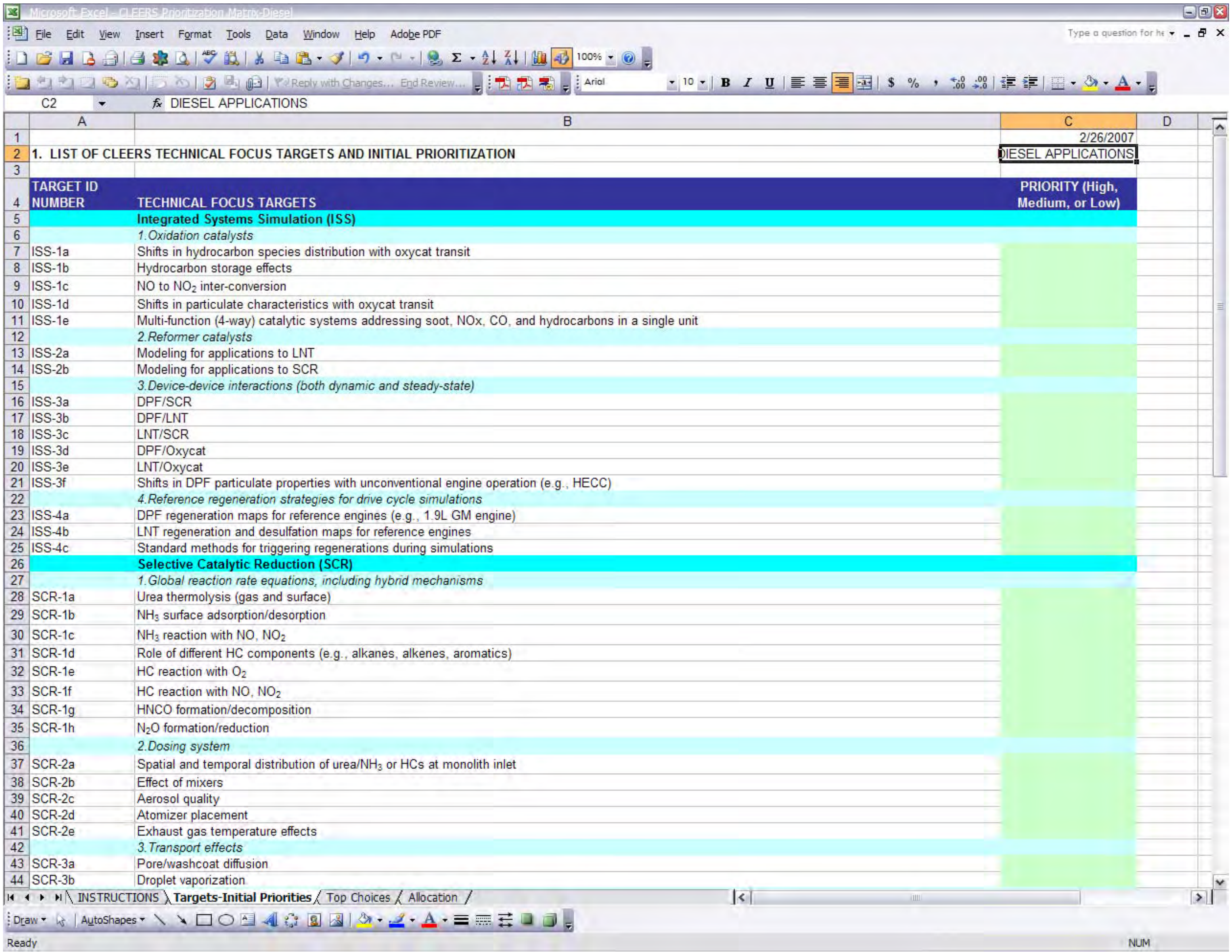
	Integrated Systems Simulation (ISS)	Selective Catalytic Reduction (SCR)	Diesel Particulate Filters (DPF)	Lean NOx Traps (LNT)
Gasoline	15.8	3.8	19.6	60.8
Diesel	25.4	30.0	29.2	15.4

Screen Shots of Prioritization Forms

Instructions

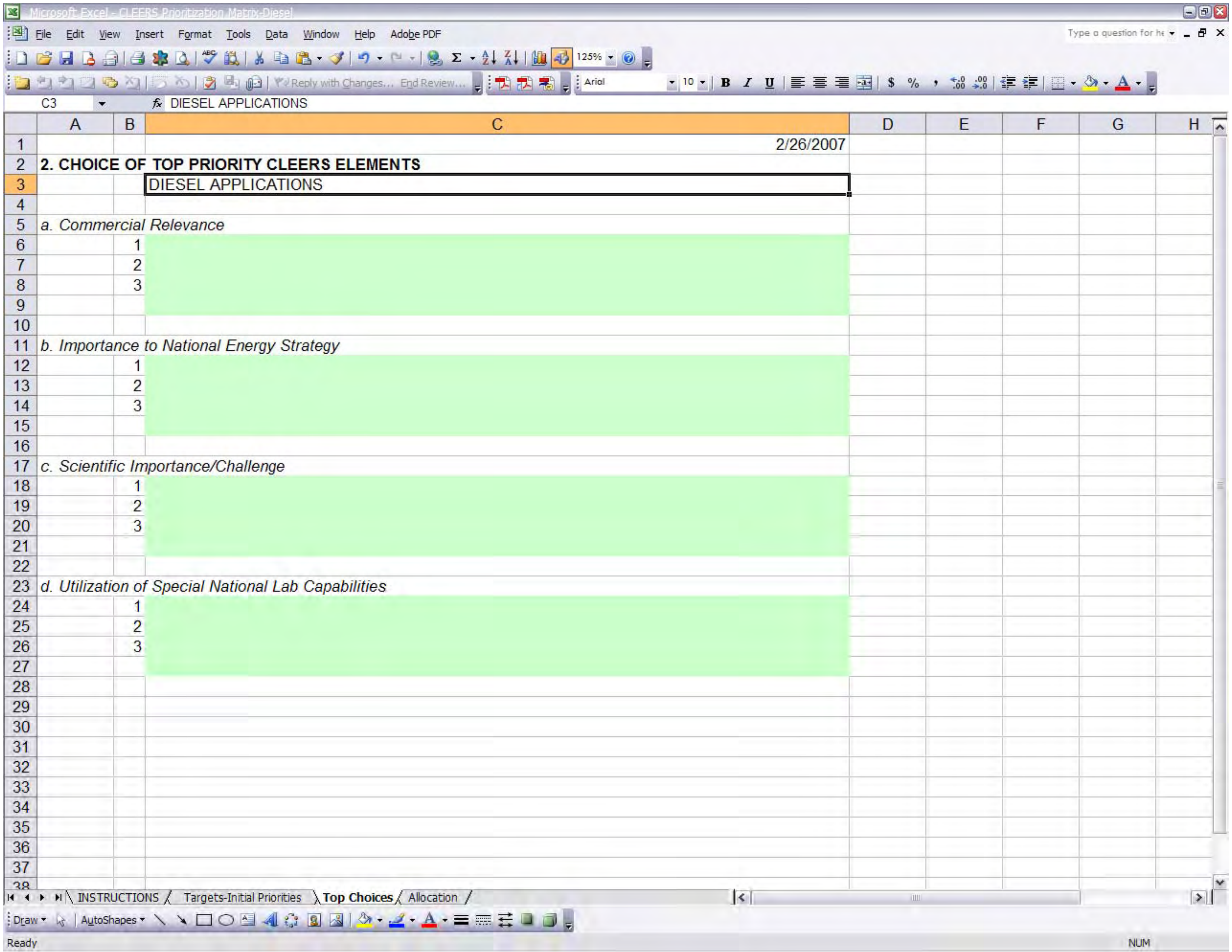


Overall Prioritization of CLEERS Focus Elements



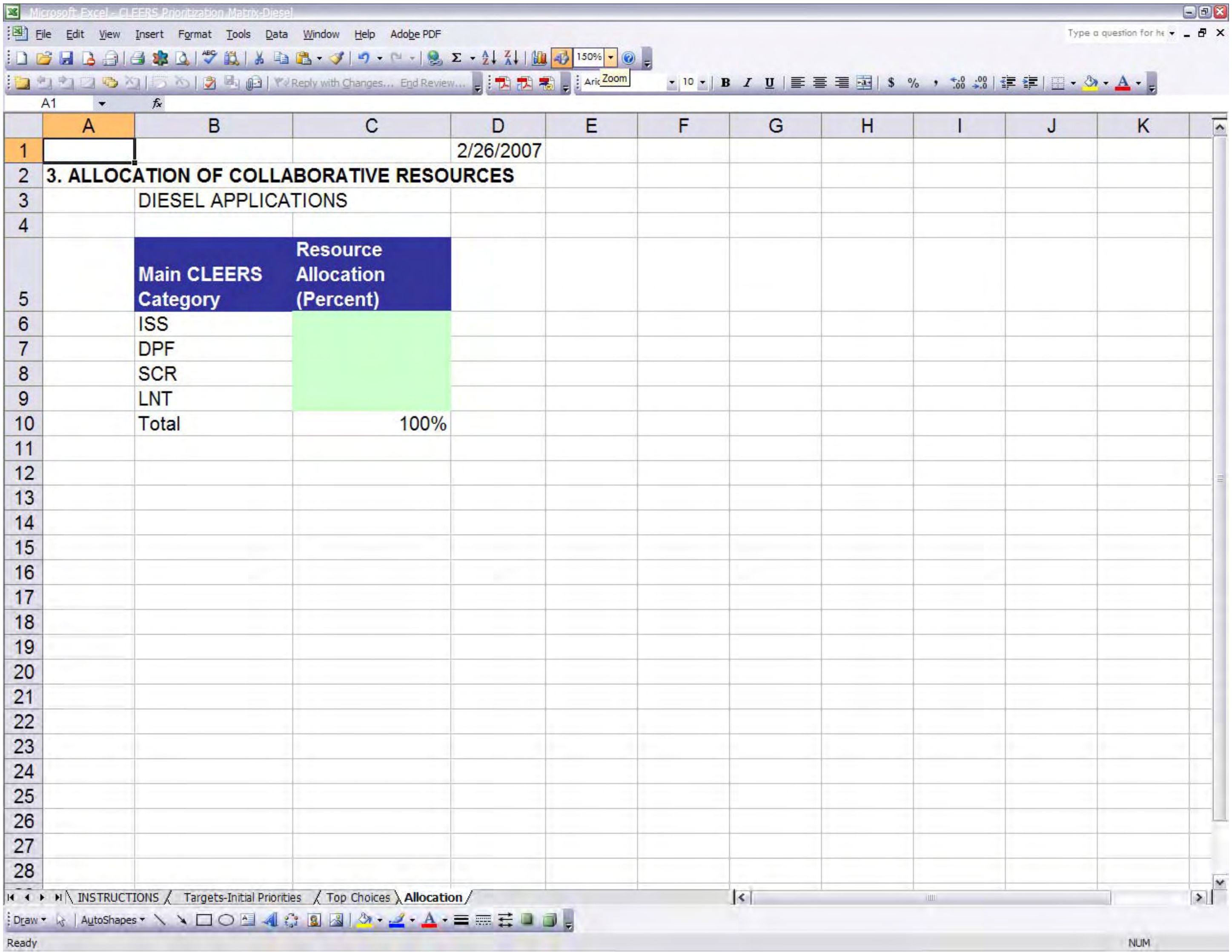
	A	B	C
1			2/26/2007
2	1. LIST OF CLEERS TECHNICAL FOCUS TARGETS AND INITIAL PRIORITIZATION		DIESEL APPLICATIONS
3			
4	**TARGET ID NUMBER**	**TECHNICAL FOCUS TARGETS**	**PRIORITY (High, Medium, or Low)**
5		**Integrated Systems Simulation (ISS)**	
6		*1.Oxidation catalysts*	
7	ISS-1a	Shifts in hydrocarbon species distribution with oxycat transit	
8	ISS-1b	Hydrocarbon storage effects	
9	ISS-1c	NO to NO_2 inter-conversion	
10	ISS-1d	Shifts in particulate characteristics with oxycat transit	
11	ISS-1e	Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit	
12		*2.Reformer catalysts*	
13	ISS-2a	Modeling for applications to LNT	
14	ISS-2b	Modeling for applications to SCR	
15		*3.Device-device interactions (both dynamic and steady-state)*	
16	ISS-3a	DPF/SCR	
17	ISS-3b	DPF/LNT	
18	ISS-3c	LNT/SCR	
19	ISS-3d	DPF/Oxycat	
20	ISS-3e	LNT/Oxycat	
21	ISS-3f	Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)	
22		*4.Reference regeneration strategies for drive cycle simulations*	
23	ISS-4a	DPF regeneration maps for reference engines (e.g., 1.9L GM engine)	
24	ISS-4b	LNT regeneration and desulfation maps for reference engines	
25	ISS-4c	Standard methods for triggering regenerations during simulations	
26		**Selective Catalytic Reduction (SCR)**	
27		*1.Global reaction rate equations, including hybrid mechanisms*	
28	SCR-1a	Urea thermolysis (gas and surface)	
29	SCR-1b	NH_3 surface adsorption/desorption	
30	SCR-1c	NH_3 reaction with NO, NO_2	
31	SCR-1d	Role of different HC components (e.g., alkanes, alkenes, aromatics)	
32	SCR-1e	HC reaction with O_2	
33	SCR-1f	HC reaction with NO, NO_2	
34	SCR-1g	HNCO formation/decomposition	
35	SCR-1h	N_2O formation/reduction	
36		*2.Dosing system*	
37	SCR-2a	Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet	
38	SCR-2b	Effect of mixers	
39	SCR-2c	Aerosol quality	
40	SCR-2d	Atomizer placement	
41	SCR-2e	Exhaust gas temperature effects	
42		*3.Transport effects*	
43	SCR-3a	Pore/washcoat diffusion	
44	SCR-3b	Droplet vaporization	

Choice of Top Priority CLEERS Elements



	A	B	C
1			2/26/2007
2	**2. CHOICE OF TOP PRIORITY CLEERS ELEMENTS**		
3			DIESEL APPLICATIONS
4			
5	*a. Commercial Relevance*		
6		1	
7		2	
8		3	
9			
10			
11	*b. Importance to National Energy Strategy*		
12		1	
13		2	
14		3	
15			
16			
17	*c. Scientific Importance/Challenge*		
18		1	
19		2	
20		3	
21			
22			
23	*d. Utilization of Special National Lab Capabilities*		
24		1	
25		2	
26		3	
27			

Allocation of Collaborative Resources



			2/26/2007
3. ALLOCATION OF COLLABORATIVE RESOURCES			
	DIESEL APPLICATIONS		
	Main CLEERS Category	Resource Allocation (Percent)	
	ISS		
	DPF		
	SCR		
	LNT		
	Total	100%	