Aftertreatment Research Prioritization: A CLEERS Industrial Survey

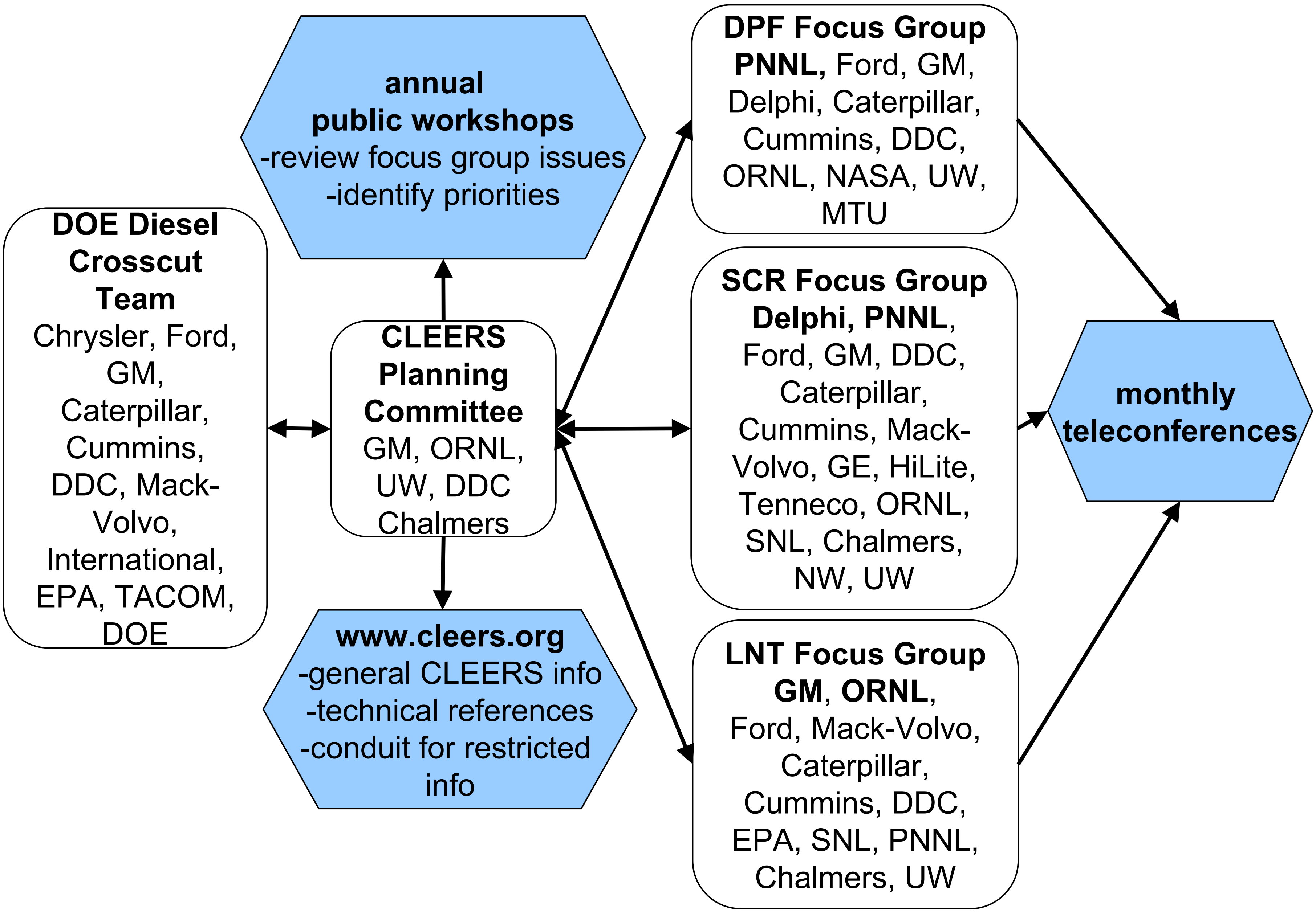
Stuart Daw, Michael Laughlin
and Richard Blint

CLEERS: Crosscut Lean Exhaust Emissions Reduction Simulation

- **Initial activities began mid-FY 2001**
- **Main benefit of CLEERS is to enhance emissions controls (EC) collaboration**
  - **Network among OEM's, EC suppliers, national labs, and universities (focus groups and workshops)**
  - **Collective forums for identifying critical technology bottlenecks and sharing with DOE and industry (i.e.; Cross Cut Team)**
  - **Mechanism for sharing non-proprietary data/understanding and simulations**
  - **Mechanism for industry feedback to DOE**
- **CLEERS not intended to fund software development**

- **Technical Challenges & Barriers from FCVT MYPP:**
  - ***3.3.1.8.C. Emission control. Meeting EPA requirements for oxides of nitrogen and particulate matter emissions standards with little or no fuel economy penalty will be a key factor for market entry of advanced combustion engines. NOx adsorbers appear to be the most viable NOx reduction devices for light-duty vehicles, but they are very sulfur-sensitive, resulting in an increasingly greater energy penalty over time to compensate for loss of activity.***
  - ***3.3.1.8.E. Durability. The emission control system has to perform effectively for 120,000 miles ....***

- **FreedomCAR ACEC Tech Team 2006 Roadmap:**
  - ***Development and optimization of catalyst-based aftertreatment systems are inhibited by the lack of understanding of catalyst fundamentals (e.g., surface chemistry, deactivation mechanisms...) and catalysts modeling capabilities.***


annual public workshops
-review focus group issues
-identify priorities
DOE Diesel Crosscut Team
Chrysler, Ford, GM, Caterpillar, Cummins, DDC, Mack-Volvo, International, EPA, TACOM, DOE
CLEERS Planning Committee
GM, ORNL, UW, DDC Chalmers
www.cleers.org
-general CLEERS info
-technical references
-conduit for restricted info
DPF Focus Group
PNNL, Ford, GM, Delphi, Caterpillar, Cummins, DDC, ORNL, NASA, UW, MTU
SCR Focus Group
Delphi, PNNL, Ford, GM, DDC, Caterpillar, Cummins, Mack-Volvo, GE, HiLite, Tenneco, ORNL, SNL, Chalmers, NW, UW
LNT Focus Group
GM, ORNL, Ford, Mack-Volvo, Caterpillar, Cummins, DDC, EPA, SNL, PNNL, Chalmers, UW
monthly teleconferences

Focus Groups

- Monthly telecoms/webcasts on key technical topics
  - participation is limited because sensitive material maybe included
- Input and reviews for proposed standard testing and measurement protocols used by industry, national labs
  - LNT sorbent/catalyst characterization protocol
  - SCR catalyst characterization protocol
  - Standardized reference materials
- Reviews of ongoing work at national labs
  - Rapid feedback to labs on data, model usefulness
  - Rapid data/results transfer from labs to industry
  - Recommendations from industry for redirecting DOE effort
    - Informal
    - Formal polling
- Workshop organization
  - Each session organized by specific Focus Group
  - Groups define invited speakers, major topics

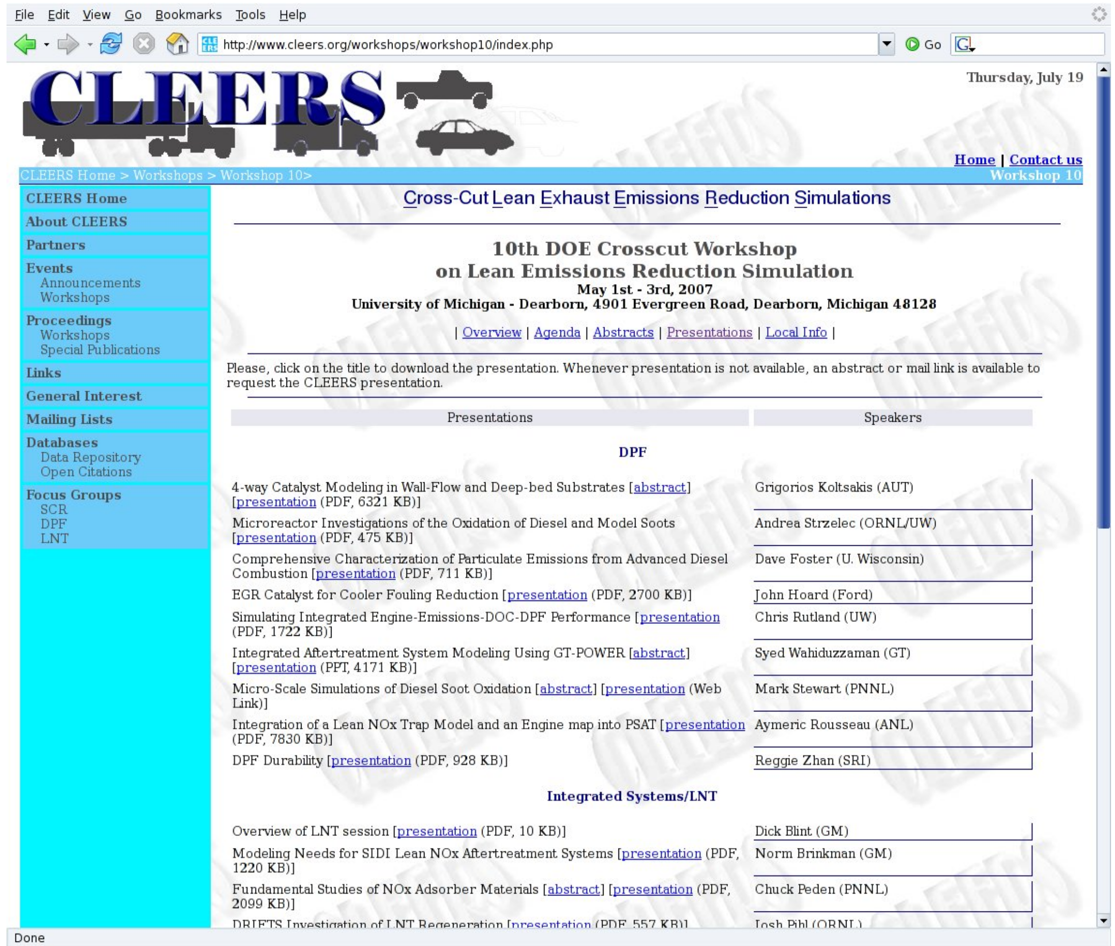
Workshops are forum for discussing common emissions control simulation issues

- Mechanism for CLEERS to interface with wider community
  - Two-way feedback on terminology, bottlenecks, priorities
- Max 120 participants (promotes informal discussions)
  - 85% U.S./15% International
- Single session each day
  - Emphasis on NOx and PM control, system integration
  - Typically 6 invited speakers (2-3 international)
  - 28-30 contributed technical talks
- Open to anyone interested; participants typically include:
  - OEMs (30%)
  - Emissions controls suppliers (20%)
  - Emission controls R&D companies/consultants (10%)
  - Software suppliers (6%)
  - Universities (17%)
  - Government agencies (4%)
  - National labs (13%)

CLEERS Website (http://www.cleers.org:)

- Basic information (organization, workshop agendas, downloads etc.)
  - ~10,000 visits per month
- Experimental database
  - 9 data categories
  - 9 technology areas
  - ~5000 downloads
  - Links to other relevant data (e.g., data from non-CLEERS DOE activities)
- Articles database (with search capability)
  - Over 600 citations
- Focus Group area
- Event calendar
- Mailing lists

Site Visits



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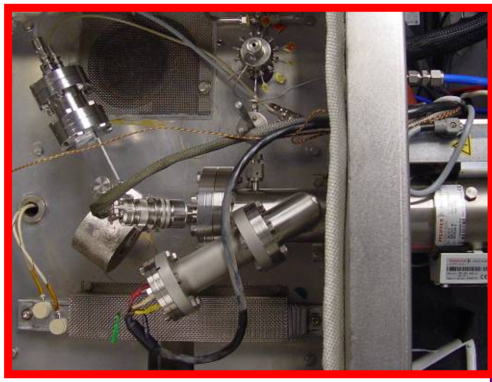
Emissions Control R&D Priorities survey

- **Recommended in November 2006 by Cross Cut Team (Diesel emphasis) and DOE (Gurpreet Singh and Ken Howden)**
- **Designed by CLEERS planning committee (<u>including a high fidelity topic list</u>), conducted January 2007 by independent third party (Mike Laughlin, New West Technologies)**
- **Limited to only Crosscut members and emissions controls suppliers with complete anonymity & single response from each company**
- **Lean gasoline (outside the CrossCut scope) was also polled**
- **Polled:**
  - **Technical priorities**
  - **Four perspective areas:**
    - **Commercial relevance;**
    - **Importance to national energy strategy;**
    - **Scientific importance/challenge;**
    - **Utilization of special national lab capabilities.**
  - **Allocation of resources**

ORNL utilizes diverse capabilities and collaborations with other DOE labs for fundamental understanding of aftertreatment devices

Collaborations with national labs:

- SNL: mechanism development, modeling
- PNNL: unique experimental capabilities, complementary catalysis expertise



SpaciMS

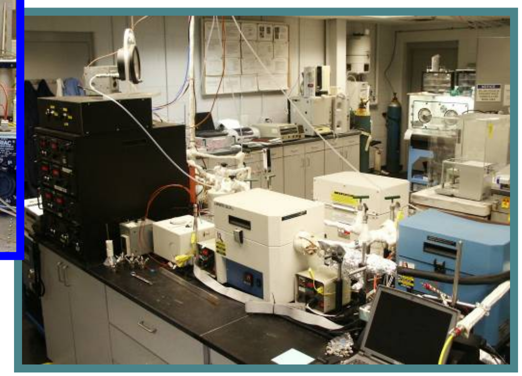
- capillary inlet mass spec.
- concentration profiles inside monoliths
- magnetic sector detector: H_2

Microreactor

- powders
- surface areas
- TPR/TPO
- performance eval.

DRIFTS reactor

- powders, washcoated wafers
- quantify adsorbates
- identify intermed.



Bench reactor

- monolith cores
- performance eval.
- SpaciMS

Other capabilities

- microscopy, XRD
- engine dynamometers

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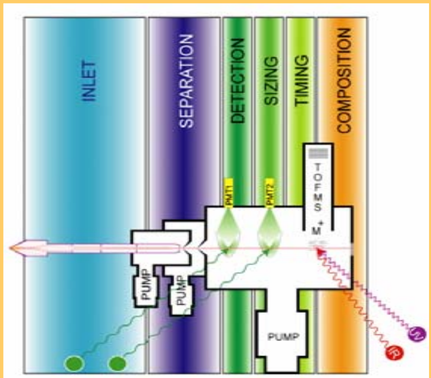
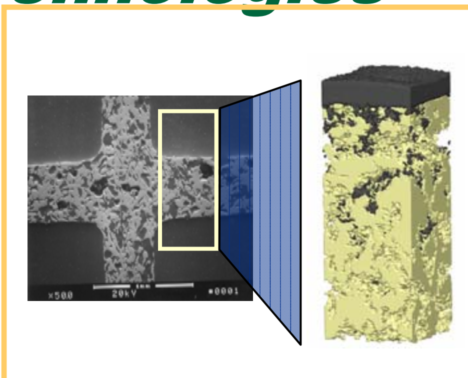
PNNL Utilizes Science of Particles and Catalyst Material Surfaces at All Scales to enable Emission Technologies



- **Single Particle Laser Ablation Time-of-flight MS (SPLAT)**
- **Size, density and molecular composition of particles**
- **Proton Transfer Reaction MS - gaseous HC's**

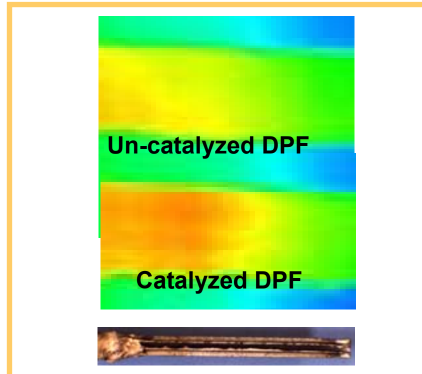


- **Micro-scale filtration and regeneration models**
- **Digital mapping of microstructure**
- **Models include species transport, soot oxidation and kinetics**

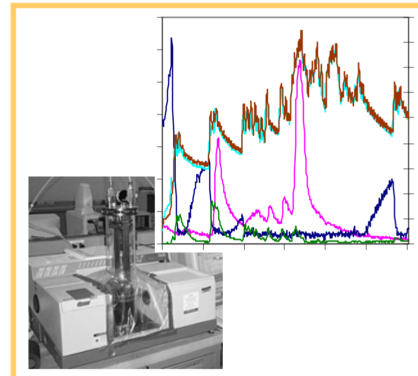
Collaborations

SNL: SCR after-treatment

ORNL: engine dynamometer testing, catalyst aging protocols



- **Dual single channel DPF and SCR experiments**
- **Infrared thermography**



- **Transient thermal reactor – gaseous transients**
- **Multiple *in-situ* FTIR reactors – catalyst surface transients**

Other Capabilities for Catalysis R&D

Synchrotron XANES, EXAFS (collaboration with BNL)

Catalytic Reactors: laboratory, pilot, engine test benches

Catalyst Characterization: XPS, TPR, XRD, TEM, Raman

Example choices for Selective Catalytic Reduction (SCR)

1. Global reaction rate equations, including hybrid mechanisms (a-h); e.g.,
   a. Urea thermolysis (gas and surface)
2. Dosing system (a-e); e.g.,
   a. Spatial and temporal distribution of urea/NH_3 or HCs at monolith inlet
3. Transport effects (a-b); e.g.,
   a. Pore/washcoat diffusion
4. Deactivation mechanisms (a-c); e.g.,
   a. Thermal degradation due to cycling

Example choices for Diesel Particulate Filters (DPF)

1. Models for local properties of the filter cake (e.g., permeability, density, morphology) (a-d); e.g.,
   a. Variation with time, engine design, operating conditions and fuel formulation.
2. Kinetics - oxidation mechanisms, detailed kinetics, global rates (a-b); e.g.,
   a. Reaction rates for passive and active regeneration of the soot.
3. 1-D device models (using local properties and kinetics sub-models) for systems simulation (a-c); e.g.,
   a. Models for soot regeneration control studies.
4. Detailed 3-D device models for understanding capture and oxidation phenomenon. (a-d); e.g.,
   a. Higher order models for design and optimization of DPF substrates and systems.
5. Improved sensor concepts and sensor utilization (a-c); e.g.,
   a. Accurate estimation of soot loading and prediction of regeneration exotherm.

Example choices for Lean NOx Traps (LNT)

1. **Determination of the elementary reaction steps (a-e); e.g.,**
   a. **NO, NO_2,and O_2 storage and release**
2. **Determination/characterization of limiting chemical or physical mechanisms (a-e); e.g.,**
   a. **H_2O and CO_2 inhibition**
3. **Chemistry and kinetics common to LNT's and 3-way catalysts (a-i); e.g.,**
   a. **NO, NO_2, and O_2 storage during lean conditions**

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Example choices for Integrated Systems Simulation (ISS)

1. Oxidation catalysts (a-e); e.g.,
   a. Shifts in hydrocarbon species distribution with oxycat transit
2. Reformer catalysts (a-b); e.g.,
   a. Modeling for applications to LNT
3. Device-device interactions (both dynamic and steady-state) (a-f); e.g.,
   a. DPF/SCR
4. Reference regeneration strategies for drive cycle simulations (a-c); e.g.,
   a. DPF regeneration maps for reference engines

Prioritization Responses

- Requests sent to 22 organizations
- Total of fourteen (14) organizations responded (64% response rate
- Total of eighteen (18) individual responses
  - Twelve responses for diesel
  - Six responses for gasoline
- Responses received from
  - LD Vehicle OEMs
  - HD Vehicle OEMs
  - HD Engine OEMs
  - Tier 1 Suppliers
  - Energy Companies

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Prioritization Methodology

- Resource Allocation
  - Respondents provide allocations by work area
  - Responses averaged to provide overall conclusion
- Overall Prioritization
  - Responses given as low, medium, high priority for each focus area
  - Numeric scores assigned to low (1), medium (2), high (3) and totaled for each focus area
  - Focus areas sorted by total numeric score
- Top Priority
  - Responses given as list of top three choices of focus area for four categories
  - Responses weighted by whether the choice was top, middle, or bottom
  - Weighted total for each chosen focus area developed, list sorted by weighted total

Diesel Topic Prioritization

Score	Id Code	Comment
37, 36, 34	SCR-4b, SCR-4c, SCR-4a	Deactivation mechanisms
35, 34, 32	DPF-5a, DPF-5b, DPF-5c	Soot loading (estimating and sensor)
32, 31	DPF-2a, DPF-3a	Reaction rates for passive and active regeneration of the soot.
32	SCR-1c	NH_3 reaction with NO, NO_2
31	ISS-1c, ISS-3a	Oxidation catalysts & DPF/SCR

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Diesel Topic Prioritization Comments

- **DPF**
  - **Oxidation characteristics of soot cakes ranked high also DPF-1a and DPF-2b (30, 29)**
- **SCR**
  - **Dosing system effects had priority numbers of 30, 29, 27 and lower**
- **LNTs**
  - **First occurrence of an LNT priority (28), LNT-2b (Precious metal aging)**
  - **Aging and NOx regeneration kinetics were the most highly rated categories**
- **ISS**
  - **Ranked 31 and below**
  - **DOC components pushed up the ranking**
  - **First device interactions occurred at 27**

Gasoline Topic Prioritization

Score	Id Code	Comment
17-14	LNT-3d, 1a, 1b, 3b, 3c, 1d, 3e, 1c, 2a, 2e, 3a,	Kinetic issues
17, 14-12	LNT-2b, 1e, 2c, 3h, 3i, 2d	Precious metal aging and sulfur poisoning
13	SCR-4a	Thermal degradation through cycling
12	ISS-1e	4-way catalytic systems

Gasoline Topic Prioritization Comments

- DPF
  - Came in low at 8
  - Mostly questions about morphology of gasoline particles
- SCR
  - Almost all came in below the LNT issues
- LNT
  - Kinetics...kinetics....kinetics
- ISS
  - Typically low

Commercial Relevance-Diesel

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

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Importance to National Energy Strategy-Diesel

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, DPF-5a DPF-5b : Diesel Particulate Filters (DPF), Models for local properties of the filter cake (e.g., permeability, density, morphology), Capture, generation, and release of nano-particles. Improved sensor concepts and sensor utilization,	4
SCR-1b: Selective Catalytic Reduction (SCR), Global reaction rate equations, including mechanisms, NH3 surface adsorption/desorption	4

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Scientific Importance/Challenge-Diesel

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

Utilization of National Lab Capabilities-Diesel

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

Commercial Relevance-Gasoline

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, NO2,and O2 storage and release	3
LNT-1c: Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO and NO2 reduction by CO, H2, and HC (separately)	3

Importance to National Energy Strategy-Gasoline

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, NO2,and O2 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 NO2 by CO, H2, and HC during rich conditions	3

Scientific Importance/Challenge-Gasoline

LNT-1d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for formation of NH3, N2O, 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, LNT-1c, LNT-3d: Lean NOx Traps (LNT), Determination of the elementary reaction steps for, NO, NO2 and O transport between PGM adsorption and storage sites; reaction steps for NO and NO2 reduction by CO, H2, and HC; Consumption of H2, 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

Utilization of National Lab Capabilities-Gasoline

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
LNT-1a, LNT-1c, LNT-2b : Lean NOx Traps (LNT), Determination of the elementary reaction steps for NO, NO_2,and O_2 storage and release; for NO and NO_2 reduction by CO, H_2, and H; Determination/characterization of limiting chemical or physical mechanisms for precious metal aging	3
SCR-4a: Selective Catalytic Reduction (SCR), Deactivation mechanisms, Thermal degradation due to cycling	3

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Summary & Future

- Question: Allocate resources across four areas of work
  - For diesel, recommend small LNT activity (15% of resources) with remainder about equally distributed among ISS, SCR, and DPF (slightly more to SCR)
  - For gasoline, majority (about 60%) of resources should be on LNT, very limited SCR, balance about equally divided between ISS and DPF
- Commercial relevance & National Energy Strategy: DPF & SCR for diesels and LNT & 4-way for lean gasoline
- Scientific Importance/Challenge: Kinetics for both diesel and gasoline
- Utilization of National Labs: Kinetics & materials analysis
- Consider the possibility of an annual survey

Acknowledgments

- PNNL team (Darrell Herling, George Muntean, Mark Stewart, Jonathan Male)
- ORNL team (Ron Graves)
- Crosscut team
- DOE (Gurpreet Singh, Ken Howden)

Backup Slides

CLEERS Planning Committee

- Oversees detailed CLEERS operation
  - Implementation of rules, procedures
  - Update reports, recommendations to Crosscut Team
  - Coordination of Focus Groups
- Current members:
  - Dick Blint (GM)
  - Stuart Daw (ORNL)
  - Houshun Zhang (DDC)
  - Chris Rutland (UW)
  - Louise Olsson (Chalmers)

CLEERS Focus Groups are organized into three main categories

- Diesel Particulate Filters (DPF)
  - Leaders: Mark Stewart, George Muntean (PNNL)
  - PM characterization, oxidation kinetics
  - Filter media and cake modeling
  - Integral reaction and heat transfer
- Lean NOx Traps (LNT)
  - Leaders: Dick Blint (GM), Stuart Daw (ORNL)
  - NOx capture, release, reduction kinetics
  - S poisoning and desulfation
  - Integral reaction and heat transfer
- Selective Catalytic NOx Reduction (SCR)
  - Leaders: Jonathon Male (PNNL), Joe Bonadies (Delphi)
  - Zeolite catalyst characterization
  - NH3 and HC species storage, NOx reduction
  - Urea thermolysis, spray modeling
- Issues related to oxidation catalysts, systems integration, standardized testing shared by all three groups

10 CLEERS public workshops held to date

- **#1- May 7-8, 2001, National Transportation Research Center, Knoxville**
- **#2,3- October 16-18, 2001, Ford Scientific Research Lab, Dearborn**
- **#4,5- April 30-May 2, 2002, University of Michigan, Ann Arbor**
- **#6- September 23-24, 2003, General Motors R&D Center, Warren**
- **#7- June 16-17, 2004, Detroit Diesel R&D Center, Detroit**
- **#8- May 17-19, 2005, University of Michigan, Dearborn**
- **#9- May 2-4, 2006, University of Michigan, Dearborn**
- **#10- May 1-3, 2007, University of Michigan, Dearborn**

➢ **3 day meetings now held annually in Detroit area**

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General Comments

- Overall agreement from the participants that the limited size of the workshop is a plus
- Oversea attendees came from
  - Sweden
  - Canada (BC, Ontario)
  - India
  - Greece
  - Korea
  - Italy
  - Austria
- 75 industrial, 18 academic, 17 National Laboratory & ? EPA

Selective Catalytic Reduction (SCR)

1. Global reaction rate equations, including hybrid mechanisms
    a. Urea thermolysis (gas and surface)
    b. NH3 surface adsorption/desorption
    c. NH3 reaction with NO, NO_2
    d. Role of different HC components (e.g., alkanes, alkenes, aromatics)
    e. HC reaction with O_2
    f. HC reaction with NO, NO2
    g. HNCO formation/decomposition
    h. N_2O formation/reduction
2. Dosing system
    a. Spatial and temporal distribution of urea/NH3 or HCs at monolith inlet
    b. Effect of mixers
    c. Aerosol quality
    d. Atomizer placement
    e. Exhaust gas temperature effects
3. Transport effects
    a. Pore/washcoat diffusion
    b. Droplet vaporization
4. Deactivation mechanisms
    a. Thermal degradation due to cycling
    b. Poisoning by S, P, HC's
    c. Effects of soot, ash, coking

Diesel Particulate Filters (DPF)

1. Models for local properties of the filter cake (e.g., permeability, density, morphology).
   a. Variation with time, engine design, operating conditions and fuel formulation.
   b. Local effects of ash loading on filter cake.
   c. Longer term effects of ash accumulation on DPF durability.
   d. Capture, generation, and release of nano-particles.
2. Kinetics - oxidation mechanisms, detailed kinetics, global rates.
   a. Reaction rates for passive and active regeneration of the soot.
   b. Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion)
3. 1-D device models (using local properties and kinetics sub-models) for systems simulation.
   a. Models for soot regeneration control studies.
   b. Models for component interaction studies.
   c. Models for trade-off assessments between higher precious metal loading vs. engine torque/speed modifications.
4. Detailed 3-D device models for understanding capture and oxidation phenomenon.
   a. Higher order models for design and optimization of DPF substrates and systems.
   b. Practical simulations capturing structural and flow effects.
   c. Evolution of temperature distributions and gradients combined with filter stability/survivability
   d. Micro-mechanical models to predict strength degradation and part failure due to thermal cycling
5. Improved sensor concepts and sensor utilization
   a. Accurate estimation of soot loading and prediction of regeneration exotherm.
   b. Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure.
   c. More reliable, less operation-specific DPF state assessment.

Lean NOx Traps (LNT)

1. Determination of the elementary reaction steps for:
   a. NO, NO_2,and O_2 storage and release
   b. NO, NO_2 and O transport between PGM adsorption and storage sites
   c. NO and NO_2 reduction by CO, H_2, and HC (separately)
   d. formation of NH_3, N_2O, HCN, and isocyanates
   e. formation and decomposition of sulfates
2. Determination/characterization of limiting chemical or physical mechanisms for:
   a. H_2O and CO_2 inhibition
   b. precious metal aging
   c. formation of non-regenerable sulfur
   d. microstructural changes in the support materials with aging
   e. degree of contacting between precious metals and NOx storage sites
3. Chemistry and kinetics common to LNT's and 3-way catalysts
   a. NO, NO_2, and O_2 storage during lean conditions
   b. Release of stored NO, NO_2, and O_2 during rich conditions
   c. Reduction of NO and NO_2 by CO, H_2, and HC during rich conditions
   d. Consumption of H_2, CO, and HC during rich conditions and lean-rich transients
   e. Production of NH_3 and N_2O during rich conditions and lean-rich transitions
   f. NOx storage by ceria
   g. NOx/CO_2 diffusion in/out of sorbent as a function of sorbent state/composition
   h. Capture of SO_2 and SO_3 during lean conditions
   i. Release of SO_2, SO_3, and H_2S during desulfation

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Integrated Systems Simulation (ISS)

1. Oxidation catalysts
   a. Shifts in hydrocarbon species distribution with oxycat transit
   b. Hydrocarbon storage effects
   c. NO to NO2 inter-conversion
   d. Shifts in particulate characteristics with oxycat transit
   e. Multi-function (4-way) catalytic systems addressing soot, NOx, CO, and hydrocarbons in a single unit
2. Reformer catalysts
   a. Modeling for applications to LNT
   b. Modeling for applications to SCR
3. Device-device interactions (both dynamic and steady-state)
   a. DPF/SCR
   b. DPF/LNT
   c. LNT/SCR
   d. DPF/Oxycat
   e. LNT/Oxycat
   f. Shifts in DPF particulate properties with unconventional engine operation (e.g., HECC)
4. Reference regeneration strategies for drive cycle simulations
   a. DPF regeneration maps for reference engines (e.g., 1.9L GM engine)
   b. LNT regeneration and desulfation maps for reference engines
   c. Standard methods for triggering regenerations during simulations