

Opening Remarks: CLEERS Workshop on LNT and DPF Technology

**General Motors Technical Center
Warren, Michigan
September 23 and 24, 2003**

**Dick Blint (GM)
Stuart Daw (ORNL)**

CLEERS

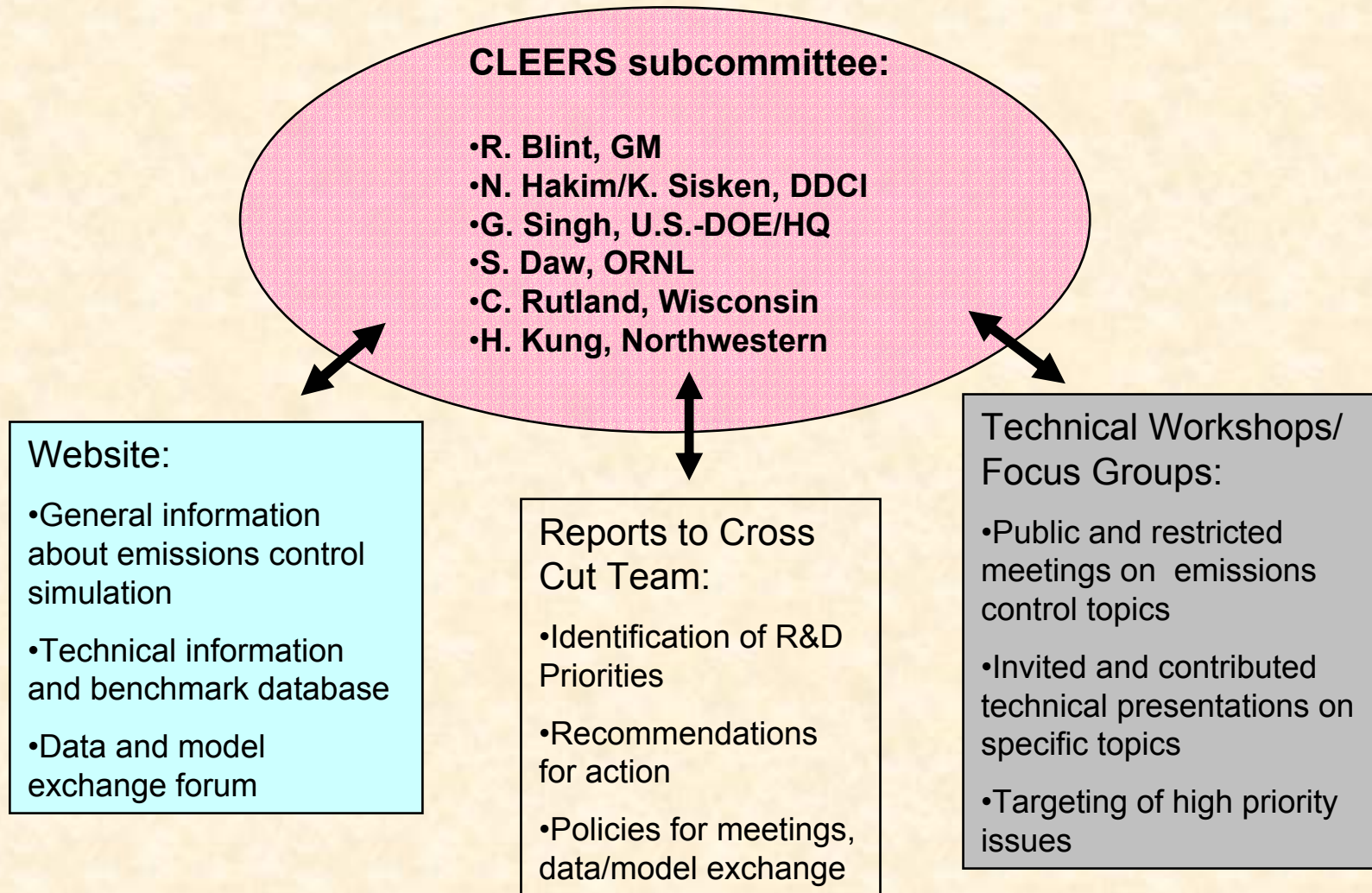
- **Crosscut Lean Exhaust Emissions Reduction Simulation**
- **Overall objective to promote development of improved simulation capabilities for control of lean-burn emissions**
- **Relevance:**
 - **Lean-burn engines are key technology for achieving major near term increases in transportation energy efficiency**
 - **Utilization of lean-burn engines requires new NOx and particulate emissions control technologies**
 - **Existing capabilities for optimizing these control technologies largely empirical, costly in \$ and time**
 - **Strong interest among OEM community in leveraging simulation capabilities to supplement device testing**

Expected CLEERS Benefits

- Framework for collaboration among OEM's, emission controls suppliers, national labs, and universities
- Collective forum for identifying critical technology bottlenecks and demonstrating simulation value
- Mechanism for sharing non-proprietary basic data/understanding among the community
- Mechanism for direct industry feedback to DOE R&D
- Definition of common technical terminology/standards to facilitate communication (e.g., between researchers, between OEM's and suppliers)
- **CLEERS not intended to fund software development**

CLEERS Approach

Directed by Diesel Crosscut Team (Daimler Chrysler, Ford, GM, Caterpillar, Cummins, DDC, Mack/Volvo, DOE, International, EPA, TACOM)



CLEERS Public Workshops (FY 01,02)

Topics were:

- 1) Full system modeling, NTRC, May 7-8, 2001**
- 2) Lean NOx Traps (LNTs), Ford SRL, October 16-17, 2001**
- 3) Diesel Particulate Filters (DPFs), Ford SRL, October 17-18, 2001**
- 4) Urea/Ammonia Selective Catalytic Reduction (SCR), UM, April 30-May 1, 2002**
- 5) Non-Urea SCR, UM, May 1-2, 2002**

Each workshop had 70-80 attendees, OEM's, component/software suppliers, labs, academia

- Invited and contributed presentations**
- Review panel discussions**
- Wrap-up/conclusion discussions**
- Reports to Crosscut Team**

Full System Workshop (FY 01)

Major conclusions were:

- Highest priority should be predictive simulation tools for post-engine NOx/PM conversion efficiency, catalyst aging
- Two major simulation types needed:
 - 0-D and 1-D component device models
 - Mechanistic models to study reaction pathways, rate limiting steps
- Emissions control technology priorities:
 - Lean NOx traps
 - Diesel particulate filters
 - Urea/ammonia SCR
 - Sulfur traps
 - Engine exhaust heaters/conditioners
 - Fuel reformers

} most important

LNT/DPF/SCR Workshops (FY 02)

Critical priorities for each technology area:

- **LNT**

- Aging/S poisoning
- NOx reduction/adsorption kinetics
- Desulfation chemistry (including the heat and mass transfer effects)

- **DPF**

- Particle morphology, oxidation characteristics
- PM spatial distribution and impact on maximum temperature
- Ash creation, composition, and transport vs. operation
- Gas emissions during regeneration

- **SCR**

- Non-Urea

- Non-Pt catalyst additives
- Non-standard HC reductants
- NOx and reductant storage
- Engine-out speciation
- Fuel reformer kinetics

- Urea/ammonia

- Ammonia storage
- Urea decomposition
- Catalyst degradation
- Effects of NO/NO2 split
- NOx reaction pathways, rate

Overall Workshop Summary (FY 02)

Cross-cutting issues:

- **Kinetics, kinetics, kinetics!!!**
 - Heterogeneous catalytic reactions including NO_x reduction, poisoning, degradation, and regeneration rates
 - Global reactions based on lumped chemistry
 - Single-step (elementary) reactions
 - Physio-chemical solid phase processes contributing to storage
 - Gas-phase reactions, including pre-cat reductant, NO_x reactions
- **Controlled lab data to support above**
- **Accurate transient engine-out data with ≤ 1 s resolution**
- **Adaptive computation of multi-step kinetic rates**
- **Standard software/data interfacing**

The Next Step (FY 03)

Formation of CLEERS Focus Groups:

- **Recommended by subcommittee**
 - Address identified public workshop priorities
 - Promote direct collaboration, leveraging among Cross Cut team
 - Continue public workshops at reduced frequency (e.g., 1/yr)
- **Approach**
 - Three initial groups targeting LNT's, DPF's, SCR
 - Consist of Crosscut members and sponsored participants
 - Two co-leaders (industry, national lab) do coordination, reporting
 - Monthly net meetings
 - Discussion of benchmark data, simulation results
 - Details on protected website, summary reports to Cross Cut team
 - Open results shared via joint publications/public disclosure via website

CLEERS Focus Group Status

Each technology area proceeding in parallel:

- **LNT**

- Group formed, co-leaders Dick Blint (GM)/Stuart Daw (ORNL)
- 6 Crosscut companies, 2 national labs, 1 sponsored university
- Web meetings held monthly since March

- **DPF**

- Group formed, co-leaders Cornelius Opris (Cat)/George Muntean (PNNL)
- 5 Crosscut companies, 2 national labs, 1 university
- Web meetings held monthly since June

- **SCR**

- Group still in formation, co-leaders Darrell Herling (PNNL)/Joe Bonadies (Delphi)
- 4 companies, 1 university expected to participate

This Workshop (#6)

- **Organized by CLEERS Planning Committee, LNT and DPF Focus Groups**
- **Theme is LNT and DPF modeling/simulation**
 - **Status of kinetics**
 - **Key experimental needs**
 - **Aging**
 - **Systems issues**
 - **Common LNT/DPF issues**
- **Contributed and invited talks**
- **Emphasis on technical results, details**

Workshop #6 Objectives

- **Highlight what tools/data are currently available for LNT and DPF modeling and simulation**
- **Highlight current research efforts**
 - **Experimental**
 - **Analytical**
- **Consider current research priorities and discuss if they need updating**
- **Review/feedback to ongoing discussion about developing standardized kinetic maps**
 - **Benchscale characterizations**
 - **Engine-dyno measurements**
 - **Rapid aging protocol**
- **Really dig into technical details and get our hands dirty!**

Goals and Objectives for the 6th CLEERS workshop

- **Update on the state of technology for modeling LNTs and DPFs.**
- **An opportunity for the focus group members to meet face to face**
- **A forum for non-Cross cut team members to participate in device simulation discussions**
- **An forum to provide additional input to the DOE on priorities for device simulations**

Focus Groups

- **Focus groups are active for LNT's, DPF's and SCR modeling activities.**
- **These are industry groups with restricted membership that:**
 - **Are working groups that share sensitive information**
 - **Develop modeling/validation priorities and distribute them to the industry and the DOE**
 - **Organize and promote research and development for the devices on which they are developing simulations**
 - **Report to the Diesel Cross Cut Team**

Focus Group Membership

- **Focus groups are industry groups working on aftertreatment modeling. Participation is determined by the Diesel Cross Cut team. Participation is:**
 - **Automatic for diesel cross team members who chose to participate**
 - **National laboratory participation is defined as one of the co-leaders of each group. The national laboratory co-leader has funding to provide administrative support for the focus group.**
 - **Non-cross cut membership is allowed with the sponsorship of a cross cut member. Sponsorship implies that the non-cross cut member will adhere to the proper confidentiality practices and will provide appropriate work to the focus group.**

LNT Focus Group

- **Net meetings held monthly**
- **Present membership 11 participants**
- **Major emphasis: Kinetic maps**

LNT Focus Participation

- **Ed Jobson** Mack/Volvo
- **Josh Driscoll** Cat
- **Dick Blint (co-leader), Yongsheng He** GM
- **John Hoard** Ford ;
- **Houshun Zhang, Kevin Sisken** Detroit Diesel
- **Neal Currier** Cummins
- **Stuart Daw (co-leader)** ORNL
- **Tony McDaniel** Sandia

DPF Focus Group

- **Monthly phone meetings held**
- **Present membership 9**
- **Major emphasis: Kinetic maps**

DPF Focus Participation

- **Aleksey Yezerets** Cummins
- **Bruce Bunting, Kalyana Chakravarthy** ORNL
- **Charles Salter** Mack
- **Chris Rutland** University of Wisconsin (CLEERS subcommittee member)
- **Cornelius Opris (co-leader)** Cat
- **Yongsheng He, Dick Blint** GM
- **George Muntean** PNNL
- **Kevin Sicken** Detroit Diesel

SCR Focus Group

- **Co-leaders are Darrel Hebbeling (PNNL) and Joe Bonadies* (Delphi)**
- **No meetings held so far**
- **Scope includes all reductants**

Objectives for CLEERS

- **Since CLEERS has no research funding, just organizational funding, CLEERS promotes development of lean aftertreatment devices by:**
 - **Gathering the interested parties via workshops and focus groups**
 - **Encourages the funding of supporting projects via appropriate agencies, primarily the Department of Energy**
 - **Is considering the development of industry standard for the sharing of device activity data; specifically the definition of kinetic maps**

Objectives of Standardized Testing

- **Develop data for model development**
 - Decouple functional steps
 - Cover a broad range of conditions
 - High quality data
 - **NO, NO₂, ...**
 - **High fidelity time series data**
- **Catalyst Mapping/Characterization**
 - Cover the important variable
 - Characterize performance
 - Minimal standard data set

Communication

- **Focus group communication comes through the net meetings and a secure website**
- **General communication comes through the website and workshops**

Closure

- **Feedback on the directions and effectiveness of CLEERS approach are solicited**
 - **One on one comments**
 - **E-mail to members of the CLEERS subcommittee**
 - **Input on specific approaches (e.g.; LNT kinetic maps) should be directed to the co-leaders of the focus groups**