Wrap-Up Discussion : CLEERS Workshop on LNT and DPF Technology

General Motors Technical Center
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Background

The following slides are from the wrap-up discussion for the workshop. They are provided here both as a summary of the discussion and also to invite further comment from the CLEERS community. It was agreed in the wrap up that further opportunities for feedback to the CLEERS planning committee and Focus Groups would be made available.

Please feel free to send your comments to:
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or to the comments area for the 6th CLEERS workshop at http://lists.cleers.org/wws/arc/work6-disc

E mail comments to Stuart Daw or Dick Blint will be kept confidential if requested, but comments submitted to the CLEERS website will be publicly available.

Wrap Up Outline

- **Review of previous LNT/DPF priorities**
- **Plans for development of ‘kinetic maps or templates’**
- **Plans for future workshops**
- **General comments/feedback**

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**

  } most important

  - **Sulfur traps**
  - **Engine exhaust heaters/conditioners**
  - **Fuel reformers**

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 NOx 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, NOx 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**

Updated Priorities (this workshop)

New priorities indicated in red

- **LNT**
  - **Aging/S poisoning (#1)**
  - **NOx reduction/adsorption kinetics (#3)**
  - **Desulfation chemistry (including heat and mass transfer effects) (#2)**
- **DPF**
  - **Maximum temperature during uncontrolled regeneration (#1) NEW!**
  - **Particle morphology, oxidation characteristics (#3)**
  - **PM spatial distribution and impact on maximum temperature (#2)**
  - **Ash creation, composition, and transport vs. operation**
  - **Gas emissions during regeneration**
- **SCR**
  - **Non-Urea (#2)**
  - **Urea/Ammonia (#1)**
- **DPNR (4-way) NEW!**
- **System Integration NEW!**

Development of Kinetic 'Maps/Templates'

- **Objective is to provide OEM's with information needed to simulate performance of candidate LNT/DPF/SCR materials**
- **Requires collaboration among OEM's, suppliers**
- **CLEERS Focus Groups provide mechanism for development**
- **Examples of similar previous standards available (applied with appropriate caution):**
  - **Turbocharger maps**
  - **Stationary power SCR catalyst specifications**

Kinetic 'Maps' for LNT's

Example proposed definition: A set of standard characterization data for washcoated monolith materials that can be used to estimate NOx storage and reduction rates for devices incorporating this material. The included characteristics are direct or indirect measures of intrinsic chemical and physical properties (including geometry) that account for the material response to variations in inlet gas flow, inlet gas composition, inlet gas temperature, and previous operating history. No direct information about washcoat formulation or manufacture is included.

Kinetic ‘Maps’ for DPF’s

Example proposed definition: A set of standard characterization data for catalyzed and uncatalyzed filter materials that can be used to estimate PM storage and oxidation rates for devices incorporating this material. The included characteristics are direct or indirect measures of intrinsic chemical and physical properties (including geometry) that account for the material response to variations in inlet gas flow, inlet gas composition, inlet gas temperature, inlet PM loading and previous operating history. No direct information about filter medium formulation or manufacture is included.

Proposed Map/Template Features

- **Based on realistic range of conditions (exhaust, operation)**
- **Consistent with global physics, chemistry**
- **Model independent**
- **Can be implemented near term (relevant to production)**
- **Flexible (can be improved)**
- **Minimal set (reasonable to generate in cost, time)**
- **Utilized existing data as much as possible**
- **Well-defined, reproducible**
- **Entries include error estimates**
- **Intrinsic to material, not system or configuration dependent**

Example Specific Applications for 'Maps/Templates'

- **LNT**
  - **Predict local rates of NOx/SOx adsorption, release, reduction in monolith with time**
  - **Predict local surface temperatures during NOx/SOx regeneration**
  - **Determine impact of previous operating history on above**
- **DPF**
  - **Predict local rates of soot deposition, oxidation in filter with time**
  - **Predict local surface temperatures during PM regeneration**
  - **Determine impact of previous operating history on above**
- **LNT/DPF**
  - **Predict NOx/SOx/PM interactions in separate devices and combined DPNR**
  - **Couple devices to full system (including engine, post-engine injection, oxidation catalysts, O2 and NOx sensors, etc.)**

Future CLEERS Workshops

- **SCR Workshop planned for sometime in next 6 months**
- **Feedback on workshop and Focus Group structure**
  - **Are they still useful?**
  - **Is current timing ok?**
  - **Do we need a significantly different format?**
  - **Are there ways to improve the interface with the Focus Groups for non-Crosscut members?**