2008 DOE OVT Merit Review

Diesel Soot Filter Characterization and Modeling for Advanced Substrates
(CRADA with DOW Automotive)

February 2008

Presenter Darrell Herling

Tom Gallant, Program Manager
Pacific Northwest National Laboratory

"**This presentation does not contain any proprietary or confidential information**"

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Overall Objective:

Adapt the micro-modeling capabilities _developed by the CLEERS Program_ to investigate substrate characteristics and spatial location of catalyzed washcoat on back pressure and soot regeneration

'08 Objective:
Validate the regeneration micro-model and optimize washcoat deposition by:

• Determine kinetics of catalyzed washcoat from reactor experiments,

• Incorporate kinetics into a micro-model to predict regeneration, and

• Validation reactor experiments.

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy

Acknowledgements

Technical Team

PNNL

Mark Stewart, Gary Maupin, Heather Dillon and Do Heui Kim

### Dow Automotive

Frank Mao, Alek Pyzik, Steven Martin and Rob Ziebarth

Support

DOE Office of Vehicle Technology
Ken Howden

Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the
U.S. Department of Energy

- Comment …. the research team needs to address the higher-level system and catalyst effects and compare to other technologies.
  - The micro-model will address catalyst effects, however, micro-modeling techniques are best for understanding the fundamentals which make the higher level models more robust..

- Comment….. still no plan to put this technology in context against other technologies…
  - The focus of the CRADA is to explore the performance of complex ACM structures to DPF performance. However, pressure drop comparisons have been presented in DOW sponsored society papers, e. g., American Ceramic Society, *'Porous Acicular Mullite for Diesel Particulate Filter Application'*, January, 2007, and micro modeling comparisons at CLEERS workshops.
  - Regeneration experiments will be conducted on other commercial substrates.
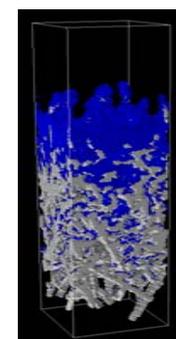
Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Approach

- ## Substrate reconstruction
  - Develop sectioning techniques and digitize acicular ceramic structure.
  - Characterize different acicular ceramic monoliths.

- ## Micro-modeling
  - Develop pressure versus loading curves and identify key substrate characteristics for reduced backpressure.
  - Predict soot structure and spatial location

- ## Experimental Validation
  - Backpressure versus loading curves.
  - Document spatial location of soot with SEM and other advance surface analysis techniques.

20kV   X100 100μm   05s971a
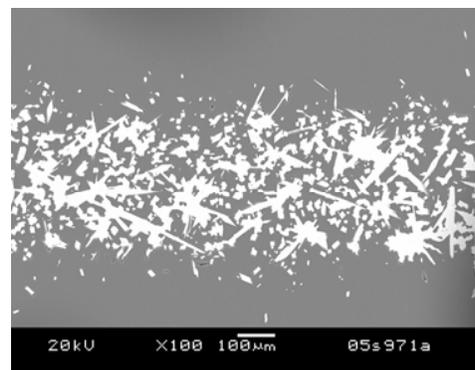
Micrographs
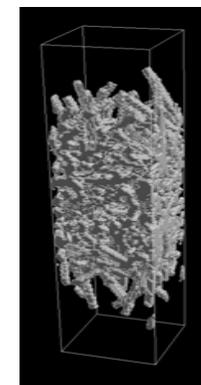
Digitized
3D reconstruction

Soot loaded substrate and pressure drop model

800 cc/min 2400 RPM 20 ft-lbs
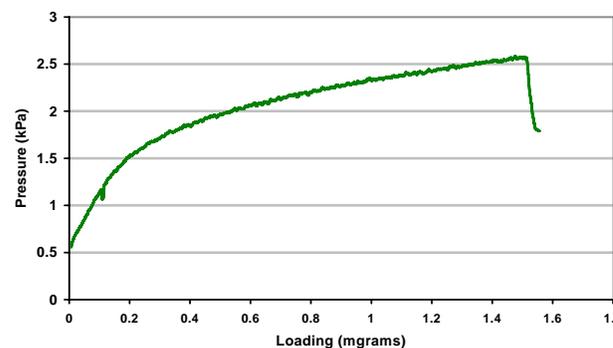
Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Performance Measures

2006

✓ ΔP characterization of clean filter substrate

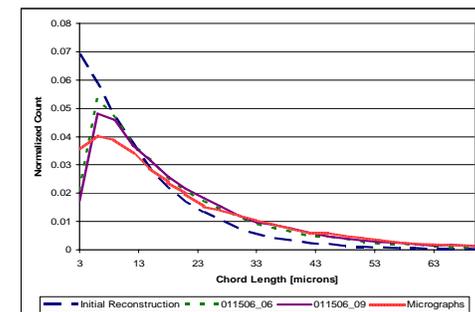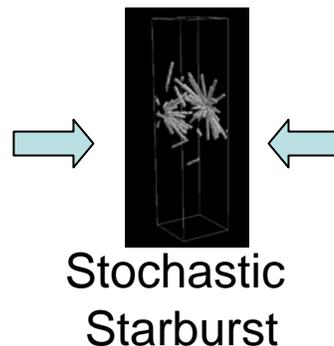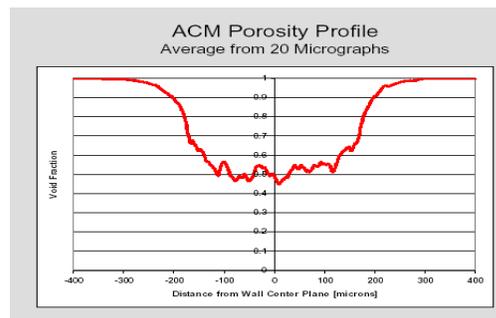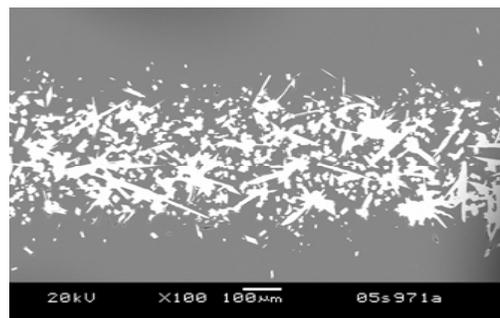✓ ΔP characterization of soot loaded filter.

2007

✓ ΔP characterization of a washcoated single channel filter (SCF).
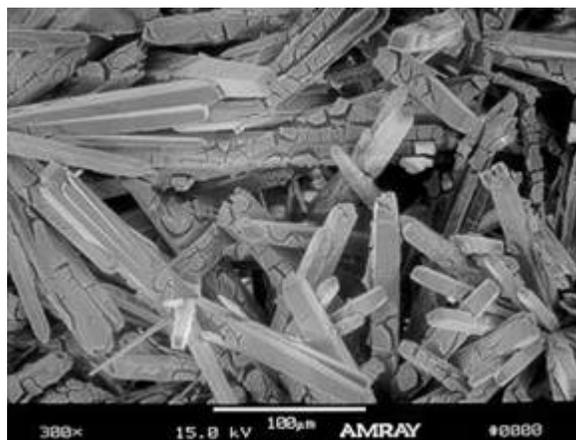
✓ ΔP characterization of a washcoated SCF loaded with soot

2008

• Reactor regeneration of soot loaded catalyzed SCF

• Micro-model of soot oxidation versus spatial catalyst loading.

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Barriers

✓ Accurate representation of the substrate

Stochastic
Starburst

➢ Accurate representation of a catalyzed washcoat ?

Uniform catalyst coating and evenly dispersed throughout the substrate.
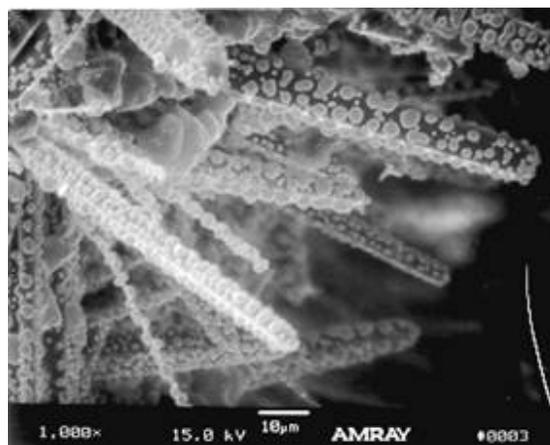
Adhesion of catalyst coating has been characterized.

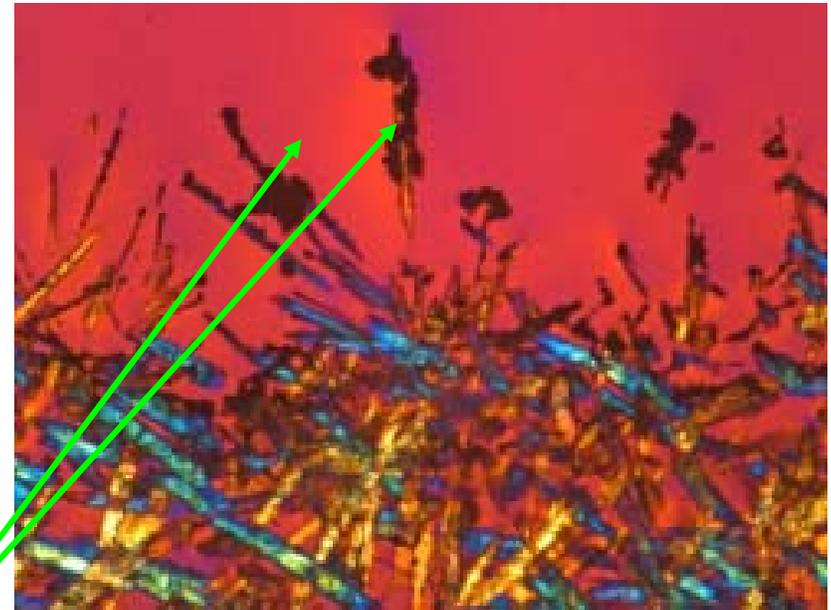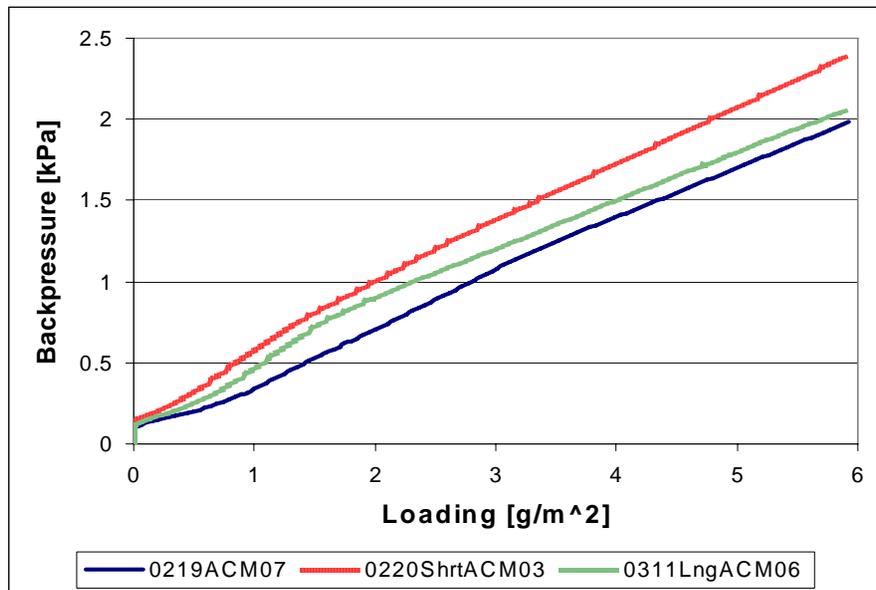**What metrics need to be developed to accurately describe the catalyzed washcoat?**

Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Previous '06 Accomplishments
Needle Geometry and Soot Deposition

The pressure drop for the long needle case increases at a slower rate than the other cases for loading greater than about 1.5 g/m^2, suggesting that longer needles might be better at higher loading..

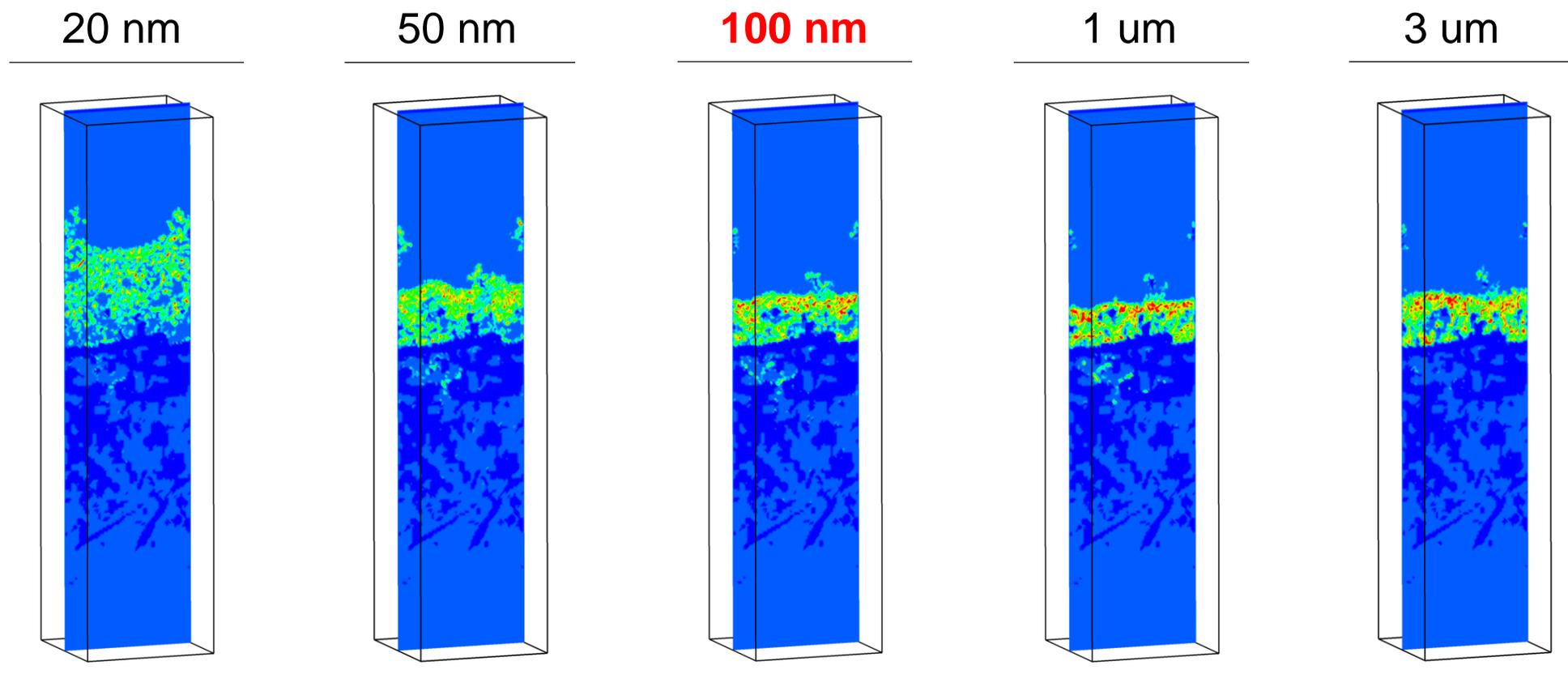Thin-section micrograph of soot loaded substrate

However, micro-modeling was not accurately capturing the soot collection on the needles using 100nm aerodynamic diameter.

Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Previous '07 Accomplishments
Simulations with Aerodynamic Diameters

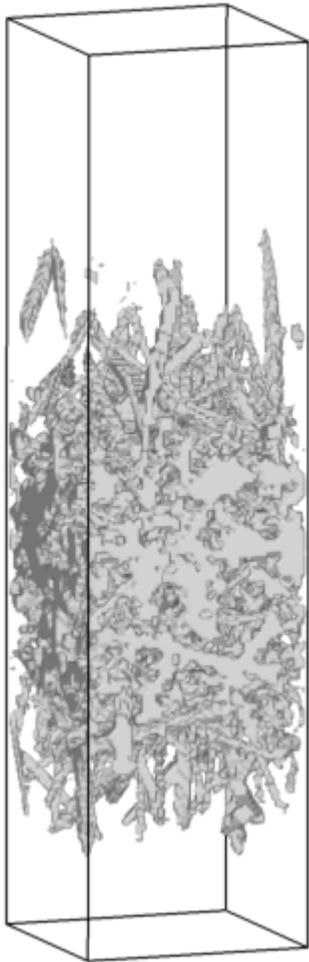| 20 nm	50 nm	**100 nm**	1 um	3 um

Smaller aerodynamic soot particles more accurately describe the soot captured by the needles as indicated by the thin section micrograph

Diesel Soot Filter Characterization and Modeling for Advanced Substrates
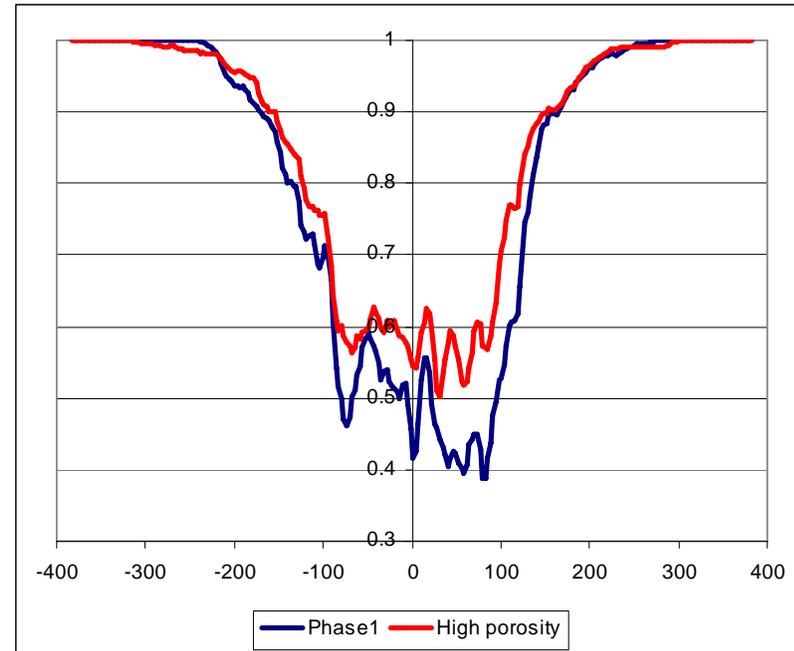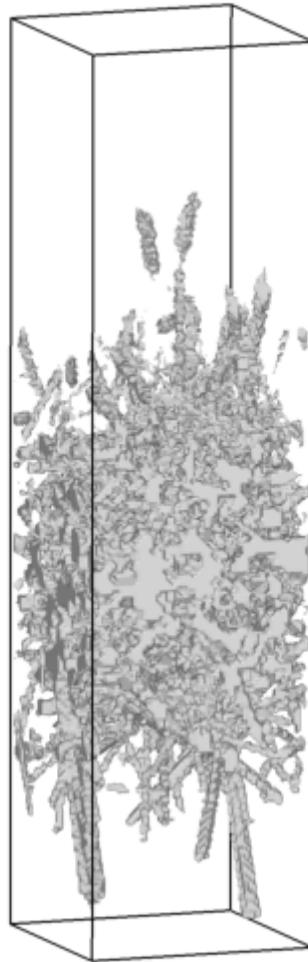
Battelle

Pacific Northwest National Laboratory
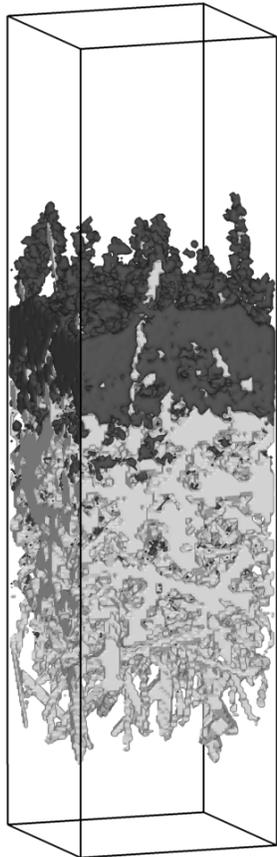Operated by Battelle for the U.S. Department of Energy

Phase1   High porosity

- Reconstruction similar to phase 1 with 20% less solid material

- Closer to 60% porosity at wall center as opposed to 50% for phase 1

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Simulation Results

Phase1   High porosity

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Soot Cake Surface Area
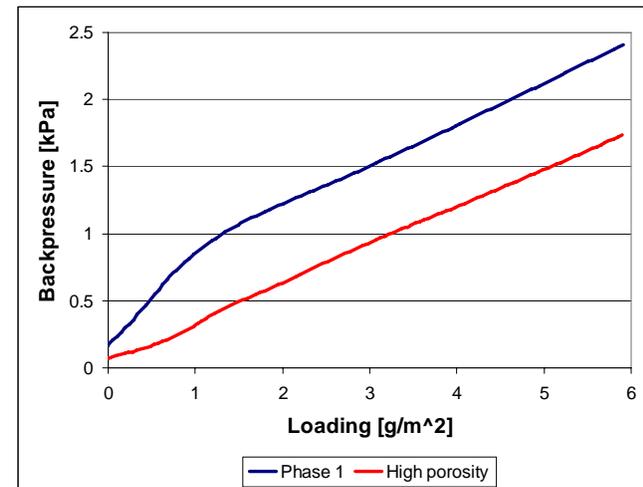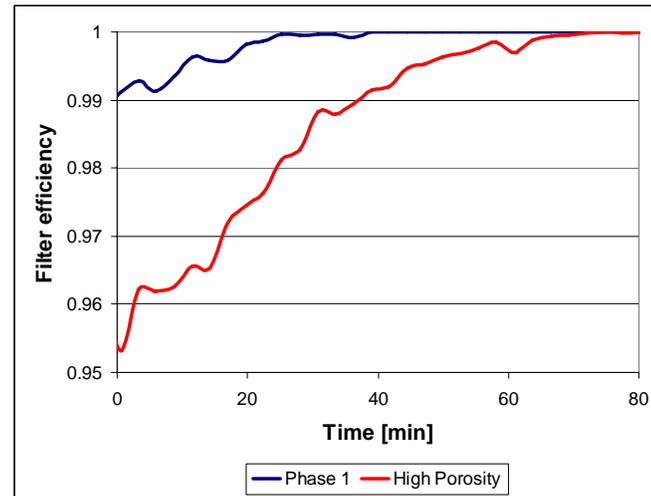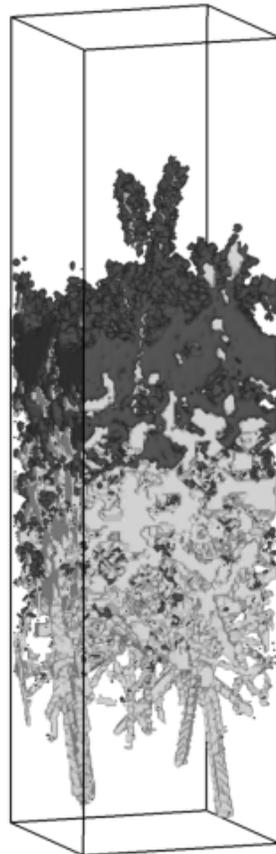
Model Predictions
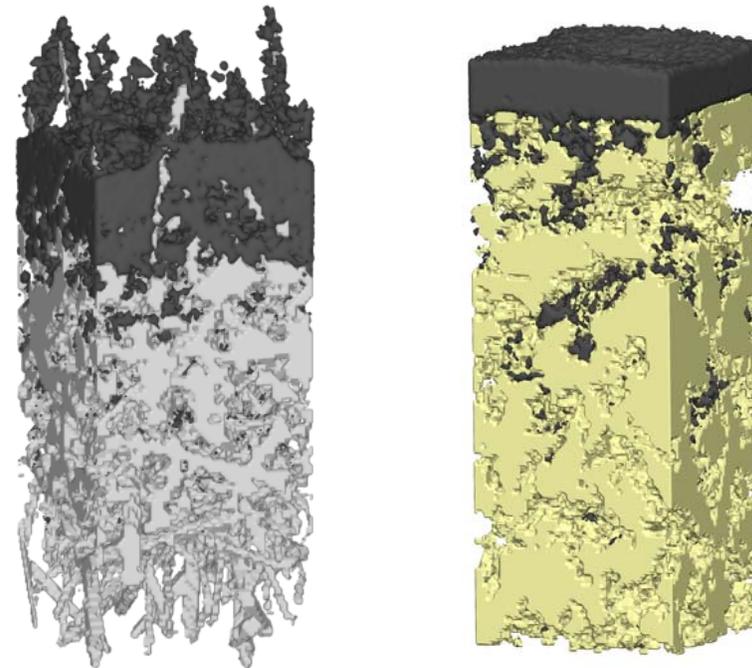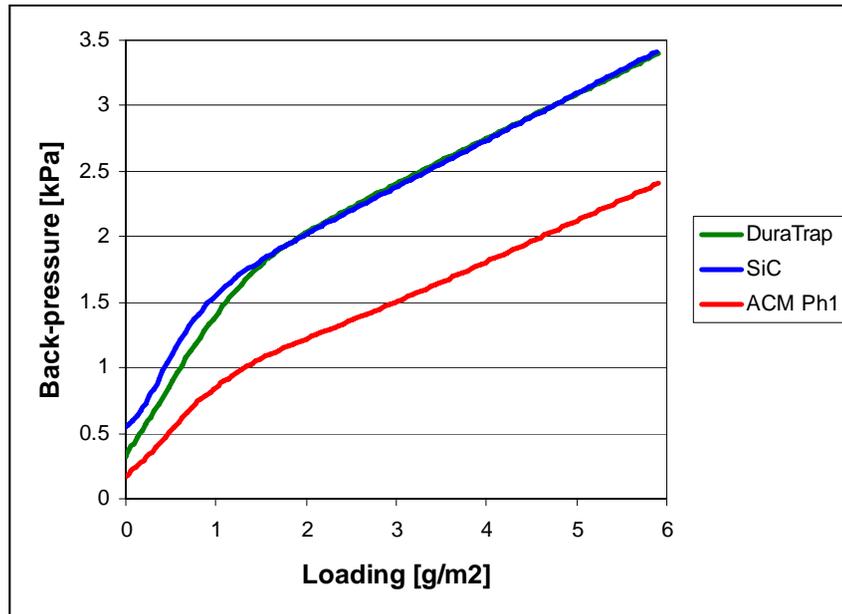
▶ Backpressure decreases somewhat more slowly for ACM than for SiC or Cordierite

▶ Clearly soot is spread over larger surface in ACM

▶ Can we draw a direct connection?

Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

- Catalyst is considered to be a perfectly even and infinitesimally thin layer

- Kinetics for alumina-supported Pt used initially – model will later be tuned using kinetic data from Dow's catalyst

- These simulations correspond to a set done last year for cordierite

- Four simulations:

  1. No catalyst
  2. Catalyst distributed over entire filter wall
  3. Catalyst distributed over top quarter of wall
  4. Catalyst distributed over top eighth of wall

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Regeneration Conditions for Simulation
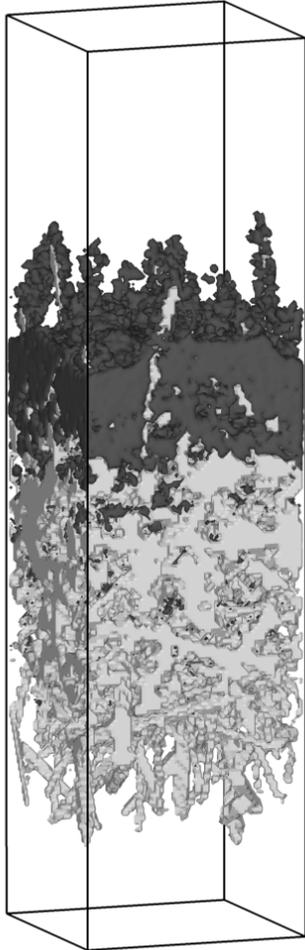
- Loaded to about 5.9 g soot /m^2 (5.3 g/L)
- Regeneration subsequent to loading
- 350°C
- 550 ppm NO
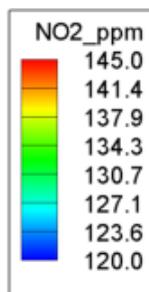- 150 ppm NO_2
- 10% O2
- Platinum loading: 120 g Pt/ft3

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Effect of Catalyst Distribution on NO$_2$ Concentration
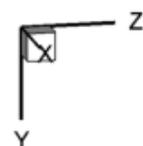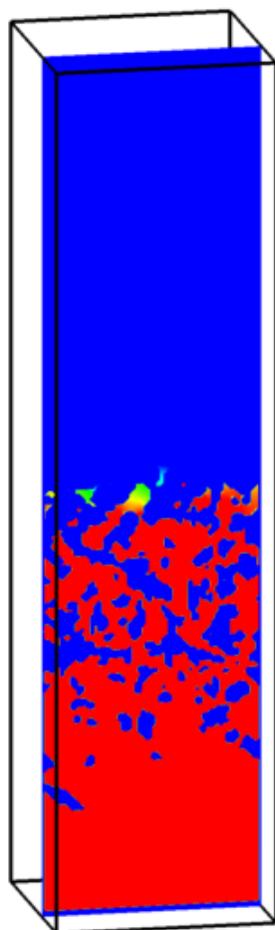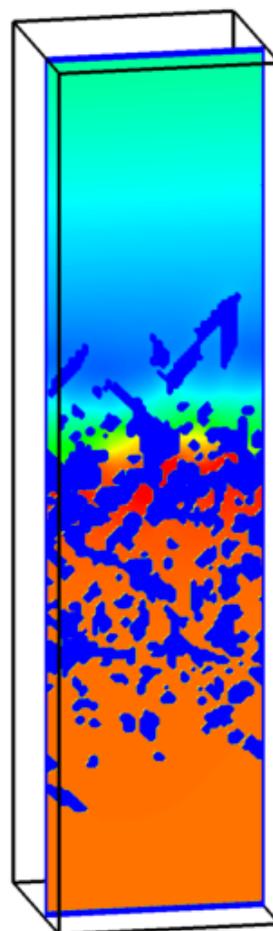
Entire Wall · Top Quarter · Top Eighth
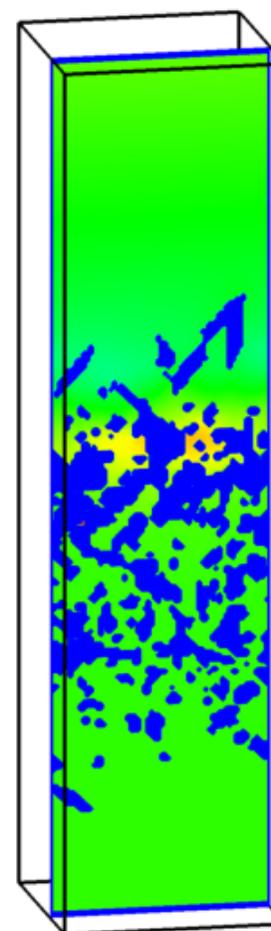
NO2_ppm
145.0
141.4
137.9
134.3
130.7
127.1
123.6
120.0

Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Battelle

Pacific Northwest National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Technology Transfer

- CLEERS Workshop

- Society papers and presentations

- Dow Automotive has contacted both light and heavy duty OEMs.

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Publications/Patents

- DEER 06, Stabilization of Soot in the Single Channel
- SAE 2007-01-1126, Visualization Techniques for Single Channel DPF Systems
- SAE 2007-01-1124, Optimizing the Advanced Ceramic Material for Diesel Particulate Filter Applications
- Microscopy and Microanalysis 2007 Conference Poster, *'Advanced Metallographic Techniques applied to Diesel Particulate Filters'*, 1St prize award.
- Microscopy Today, Advanced Metallographic Techniques applied to Diesel Particulate Filters
- American Ceramic Society, **Porous Acicular Mullite for Diesel Particulate Filter Application, January, 2007**

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Plans for Next Fiscal Year

- This is the final year of the CRADA.

- With OEM support, it is recommended that the ACM structure be optimized for a 4 way catalyst system (high washcoat loading) and spatial catalyst deposition using the micro model.

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy

Summary

- Micro-Modeling can identify the critical characteristics of a DPF substrate as it relates to back pressure.

- The high surface area provided by the needles, in conjunction with the high porosity, minimizes the exhaust backpressure.

- Micro modeling is tuned and validated by unique single channel experiments.

- Micro modeling techniques can be applied to various substrates which can be characterizes by digitized micrographs or stochastic models.

- Extend CRADA to optimize structure to maximum washcoat loading for a 4 way system.

Battelle

Pacific Northwest
National Laboratory
Operated by Battelle for the
U.S. Department of Energy