

2008 DOE OVT Merit Review

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

February 2007

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

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.

Technical Team

PNNL

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

Dow Automotive

Frank Mao, Alek Pyzik,
Steven Martin and Rob
Ziebarth

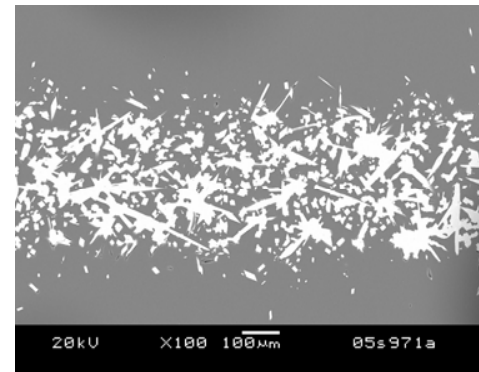
Support

DOE Office of Vehicle Technology

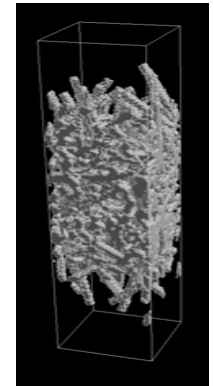
Ken Howden

- **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.

- 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.

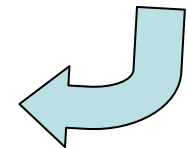
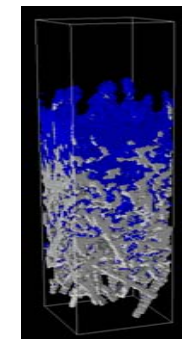


Micrographs

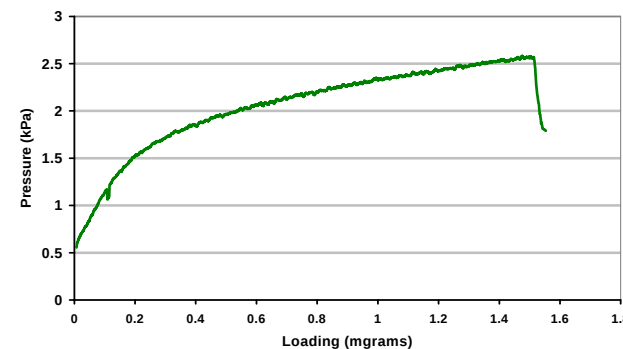


Digitized
3D reconstruction

Soot loaded
substrate and
pressure drop
model



800 cc/min 2400 RPM 20 ft-lbs



Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

2006

- ✓ ΔP characterization of clean filter substrate
- ✓ ΔP characterization of soot loaded filter.

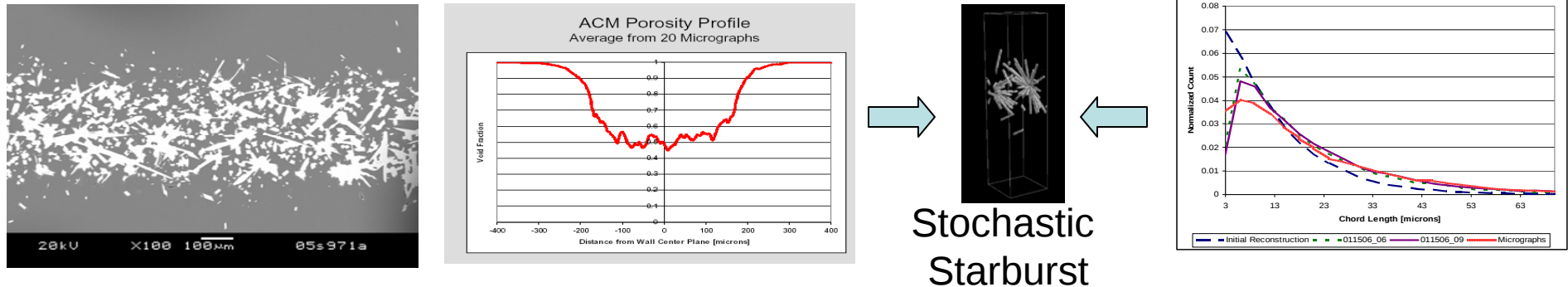
2007

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

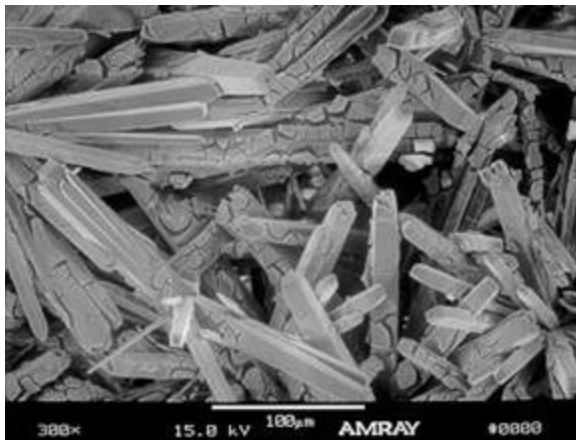
2008

- Reactor regeneration of soot loaded catalyzed SCF
- Micro-model of soot oxidation versus spatial catalyst loading.

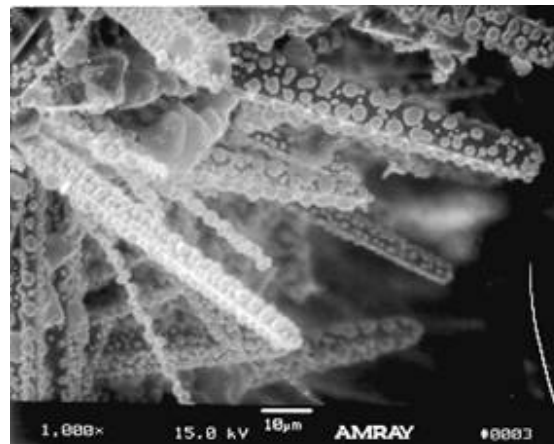
✓ Accurate representation of the substrate



➤ 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?

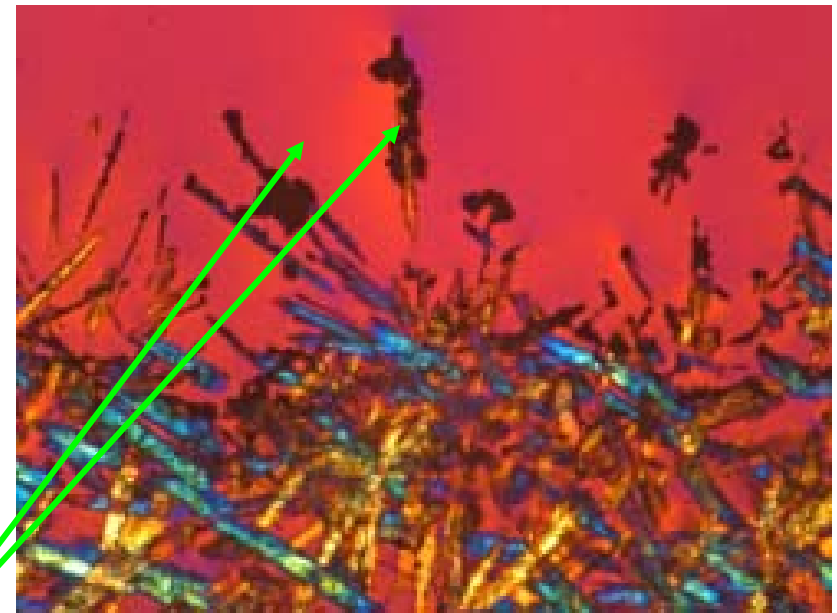
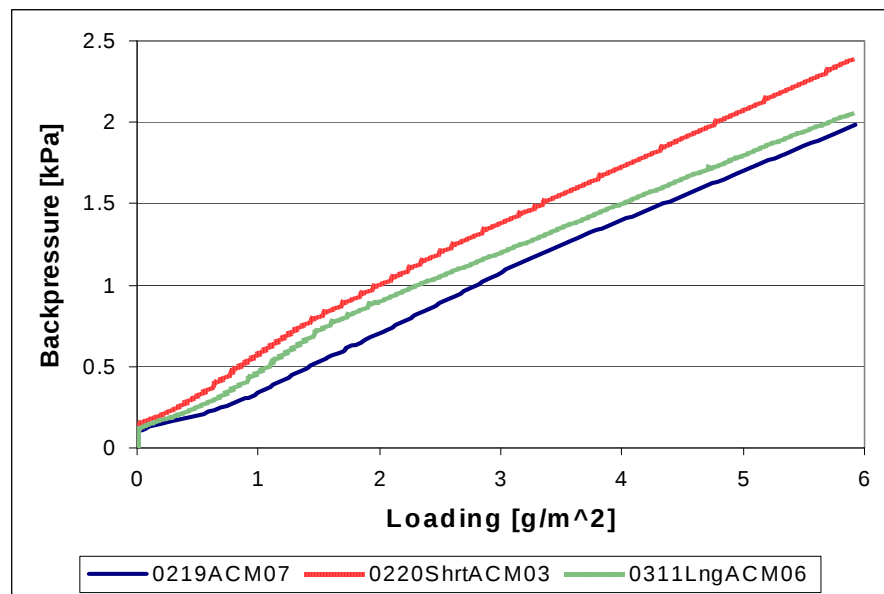
Diesel Soot Filter Characterization and Modeling for Advanced Substrates

Previous '06 Accomplishments

Needle Geometry and Soot Deposition

2008 DOE OVT
Merit Review

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

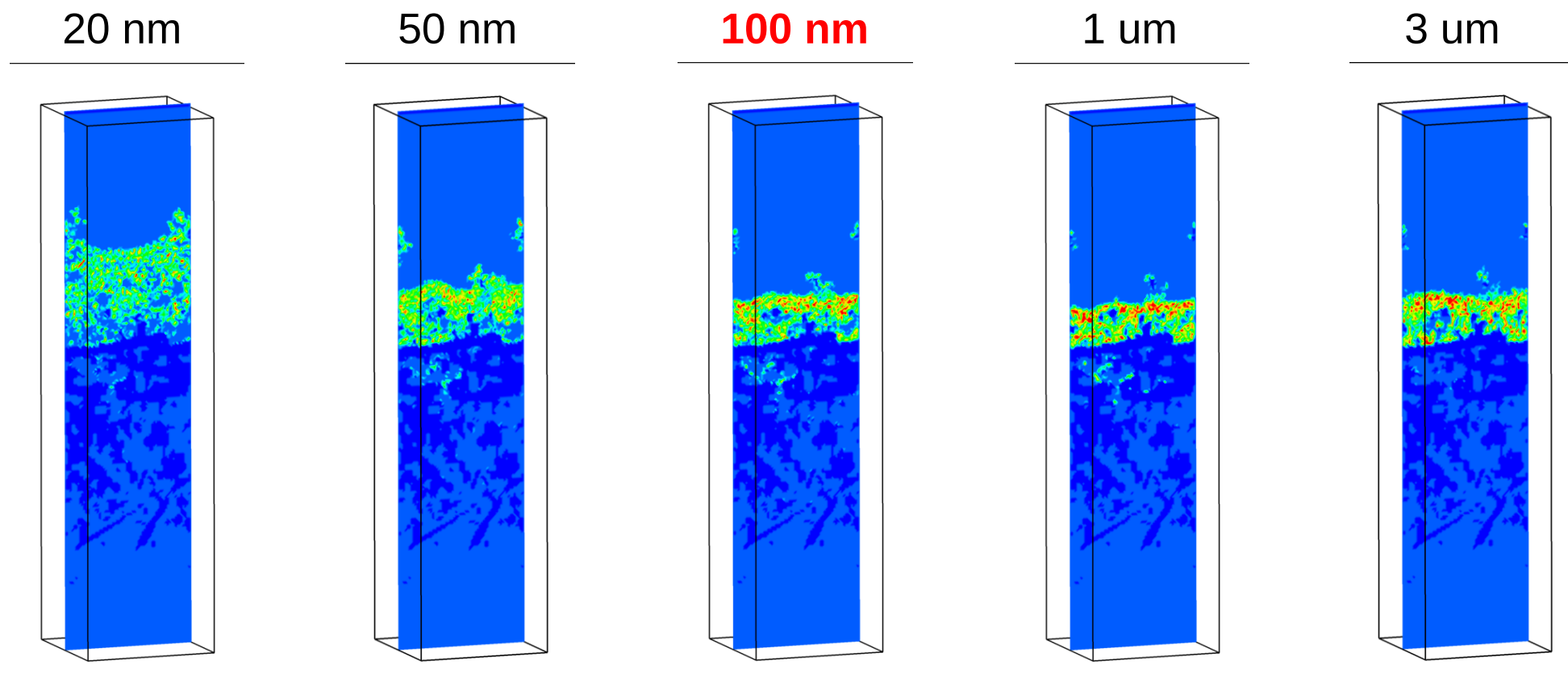
However, micro-modeling was not accurately capturing the soot collection on the needles using 100nm aerodynamic diameter.

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

Previous '07 Accomplishments

Simulations with Aerodynamic Diameters

2008 DOE OVT
Merit Review



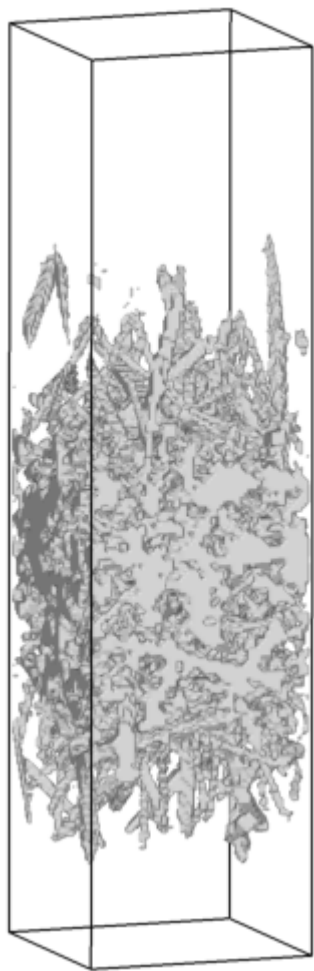
Smaller aerodynamic soot particles more accurately describe the soot captured by the needles as indicated by the thin section micrograph

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

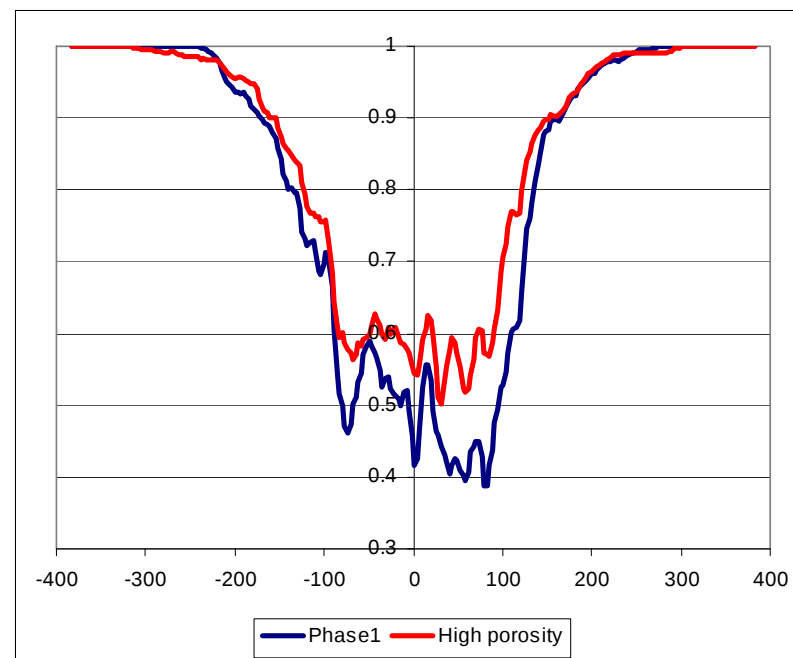
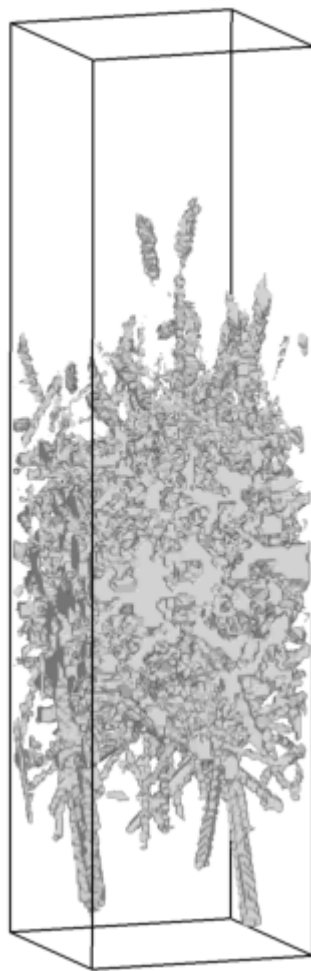
Hypothetical High Porosity ACM

2008 DOE OVT
Merit Review

Phase1



High porosity



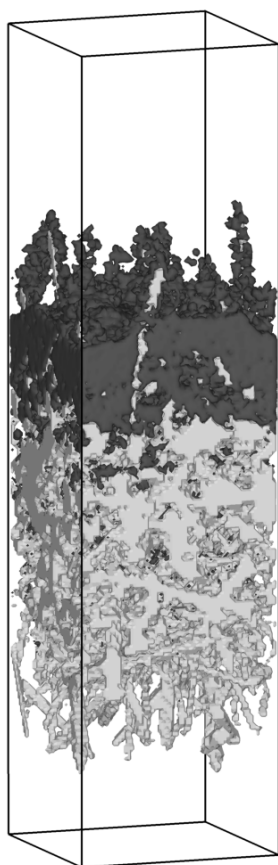
- Reconstruction similar to phase 1 with 20% less solid material
- Closer to 60% porosity at wall center as opposed to 50% for phase 1

Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

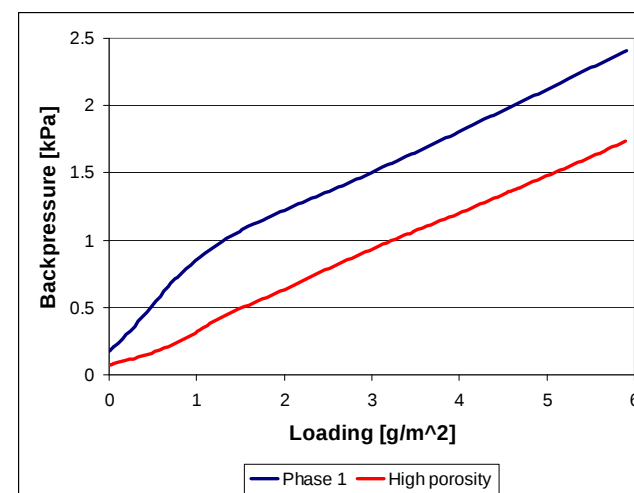
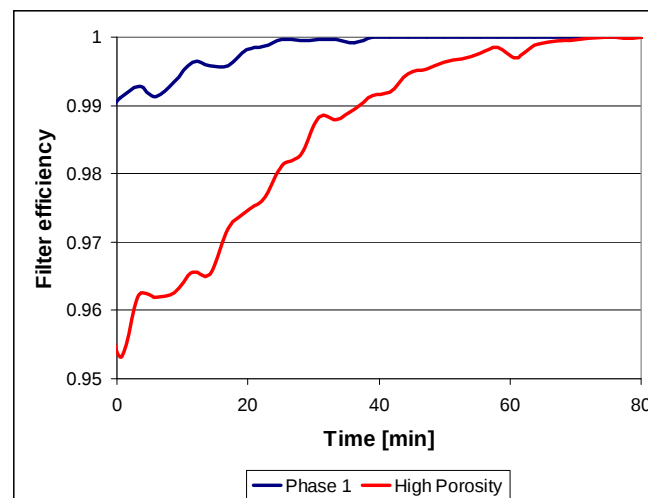
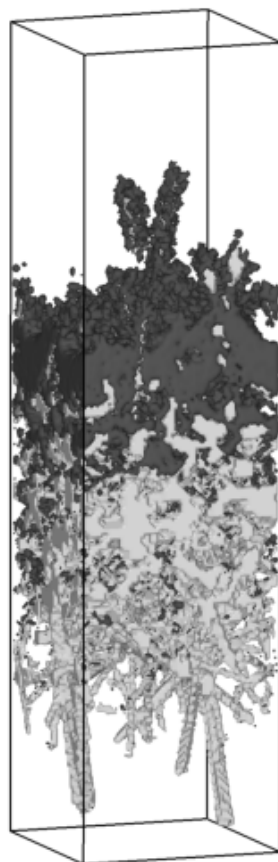
Simulation Results

2008 DOE OVT
Merit Review

Phase1

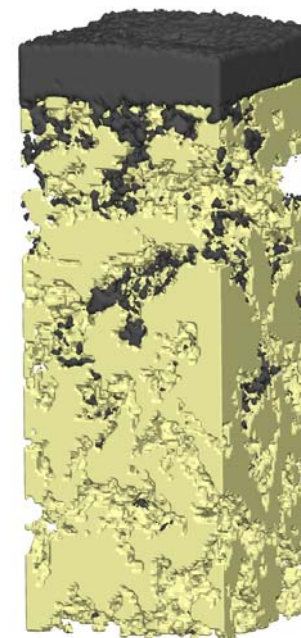
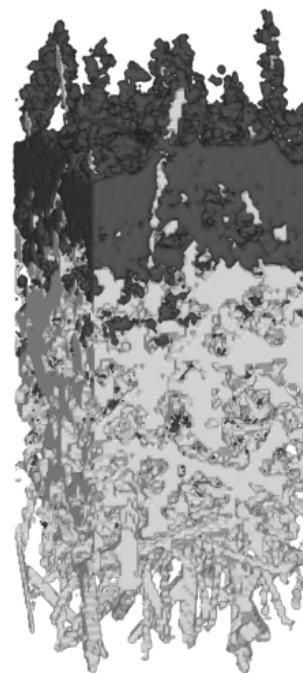
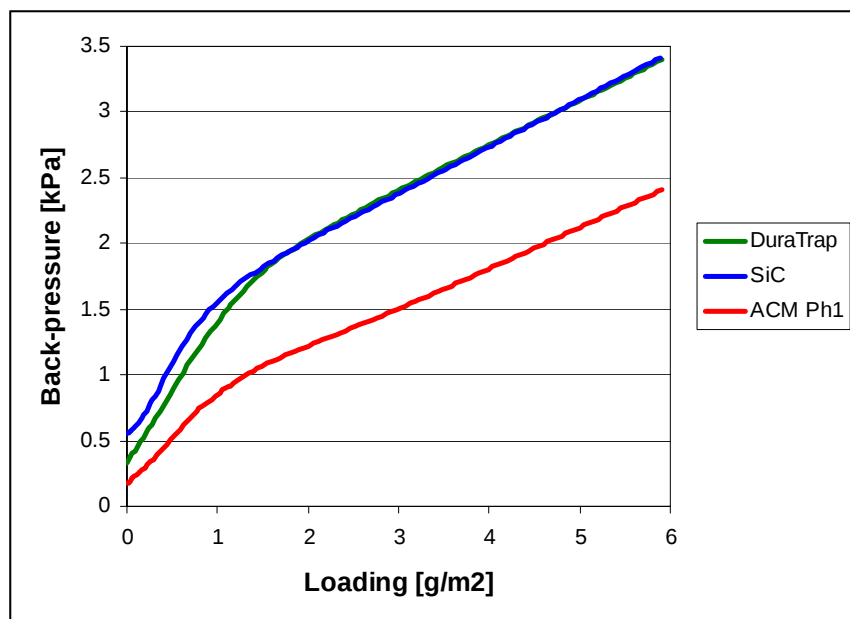


High porosity



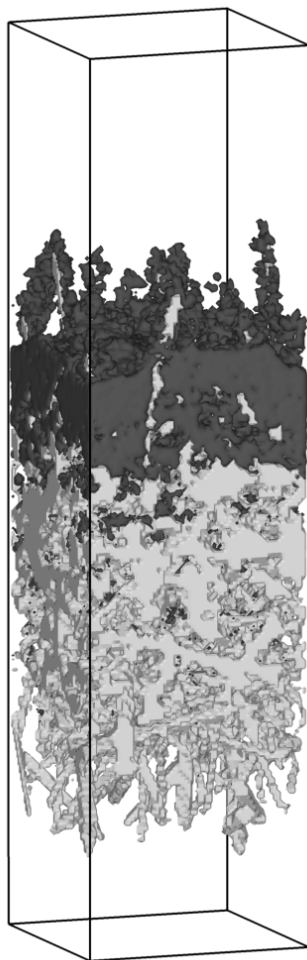
Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

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?

- 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

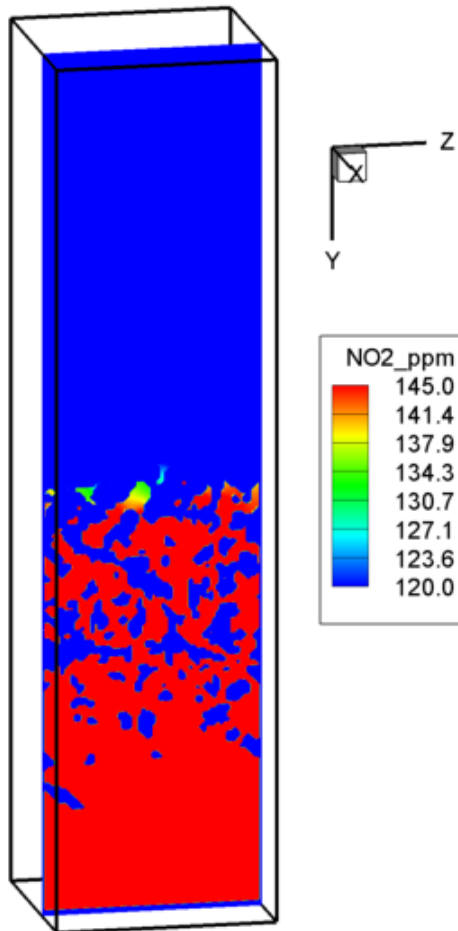


- Loaded to about 5.9 g soot /m² (5.3 g/L)
- Regeneration subsequent to loading
- 350°C
- 550 ppm NO
- 150 ppm NO₂
- 10% O₂
- Platinum loading: 120 g Pt/ft³

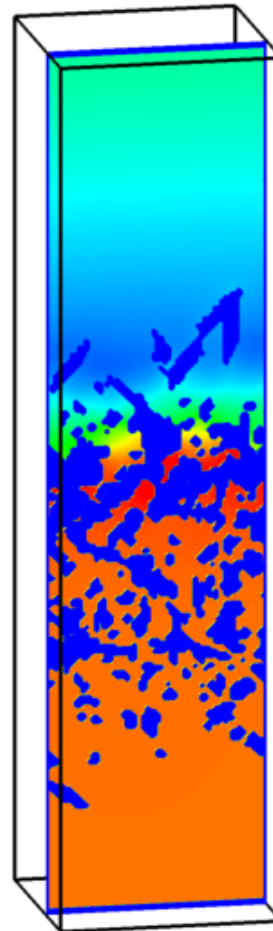
Effect of Catalyst Distribution on NO₂ Concentration

2008 DOE OVT
Merit Review

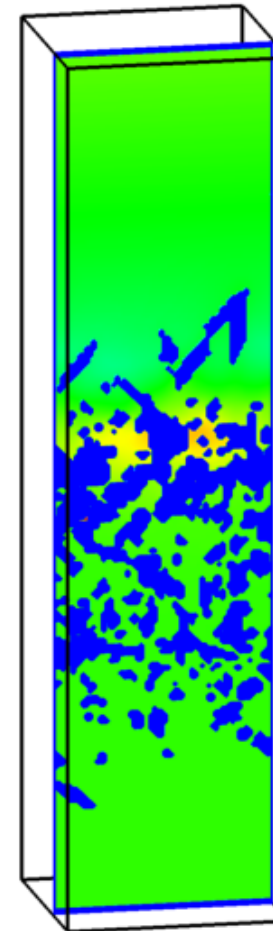
Entire Wall



Top Quarter



Top Eighth



Diesel Soot Filter Characterization and Modeling for
Advanced Substrates

- CLEERS Workshop
- Society papers and presentations
- Dow Automotive has contacted both light and heavy duty OEMs.

- **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**

- 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.

- 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.