Advanced Engine/Aftertreatment System R&D

CRADA with Navistar, Inc.

Josh Pihl (PI), Todd Toops

Oak Ridge National Laboratory

Vadim Strots, Ed Derybowski

Navistar, Inc.

DOE sponsors:

Ken Howden, Gurpreet Singh

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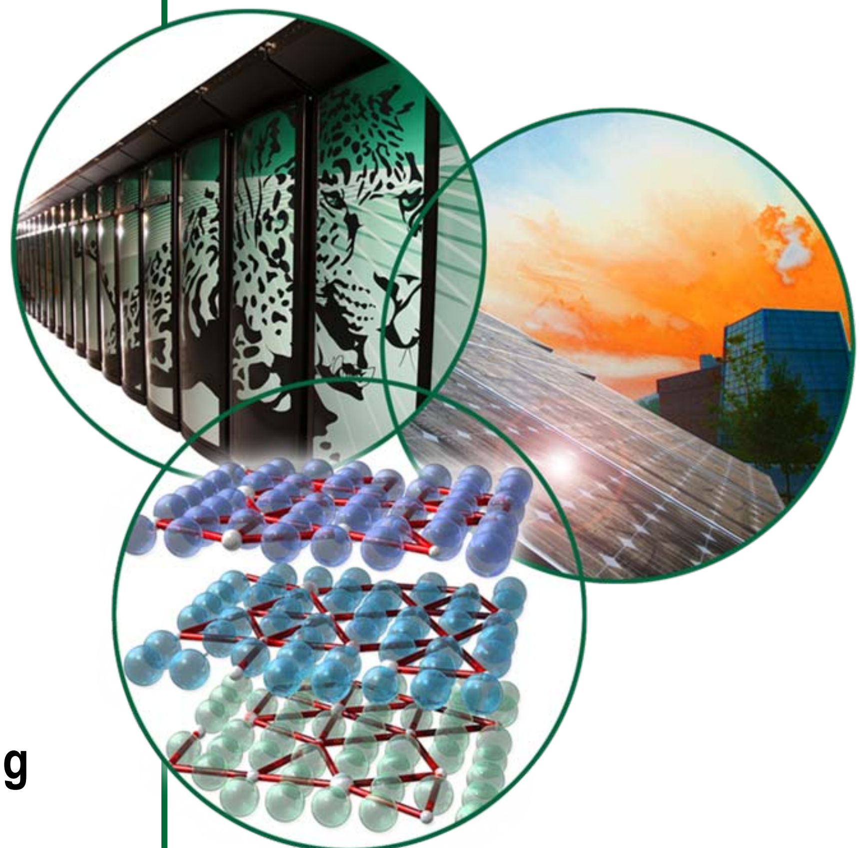

Project ID: ACE034

U.S. DEPARTMENT OF ENERGY

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Overview

Timeline

- Start: March 2001
- End: ongoing…
  - working toward CRADA renewal by end of 2011

Barriers

- Emission control. *"Meeting EPA requirements for oxides of nitrogen and particulate matter emissions standards with little or no fuel economy penalty…" (ACE MYPP 3.3.1.8.C)*
- Durability. *"The emission control system has to perform effectively for 120,000 miles…" (ACE MYPP 3.3.1.8.E)*

Budget

- Funding received FY09: $125k
- Funding expected FY10: $125k

Partners

- Navistar, Inc. (CRADA partner)
  - Exova (engine tests)
  - Michigan Tech (modeling)
- Collaborators:
  - CLEERS participants

Relevance: Objectives

- Overall Goal: Develop engine/aftertreatment system configurations and control strategies that meet stringent EPA emissions standards while improving overall vehicle efficiency
- Overall Objectives:
  - Enhance understanding of aftertreatment device operating principles to enable development of fuel-optimal control strategies
  - Measure reaction kinetics and operating parameters of aftertreatment devices required for accurate simulation tools and control strategy development
  - Characterize response of sensors for OBD and control applications
- Objectives for FY10:
  - Measure reaction kinetics required for accurate simulation of DPF regeneration
  - Evaluate impact of non-traditional or non-optimal operating regimes on DPF fuel penalty and durability
    - high soot loading
    - high hydrocarbon content
    - partial regenerations
    - alternative means to achieve regeneration temperatures

Approach: Milestones

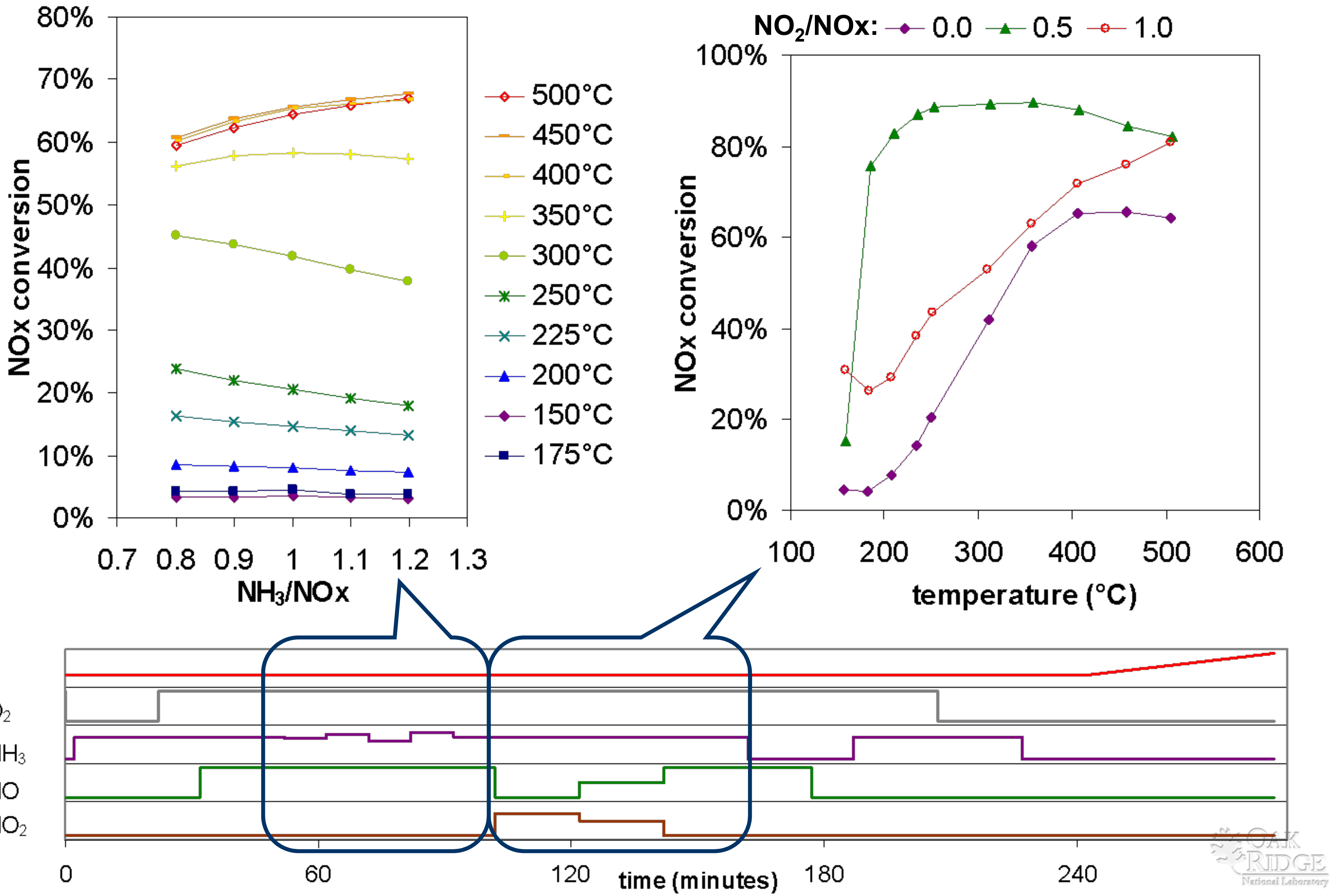
- FY09: Evaluate NH_3 storage and reactivity on fresh and aged fully-formulated urea SCR catalysts (completed)

- FY10: Evaluate soot oxidation kinetics with miniature DPFs that have been loaded under a range of high-efficiency combustion regimes on Navistar production-intent engines (on track for completion by September 30, 2010)

Approach: Project plans

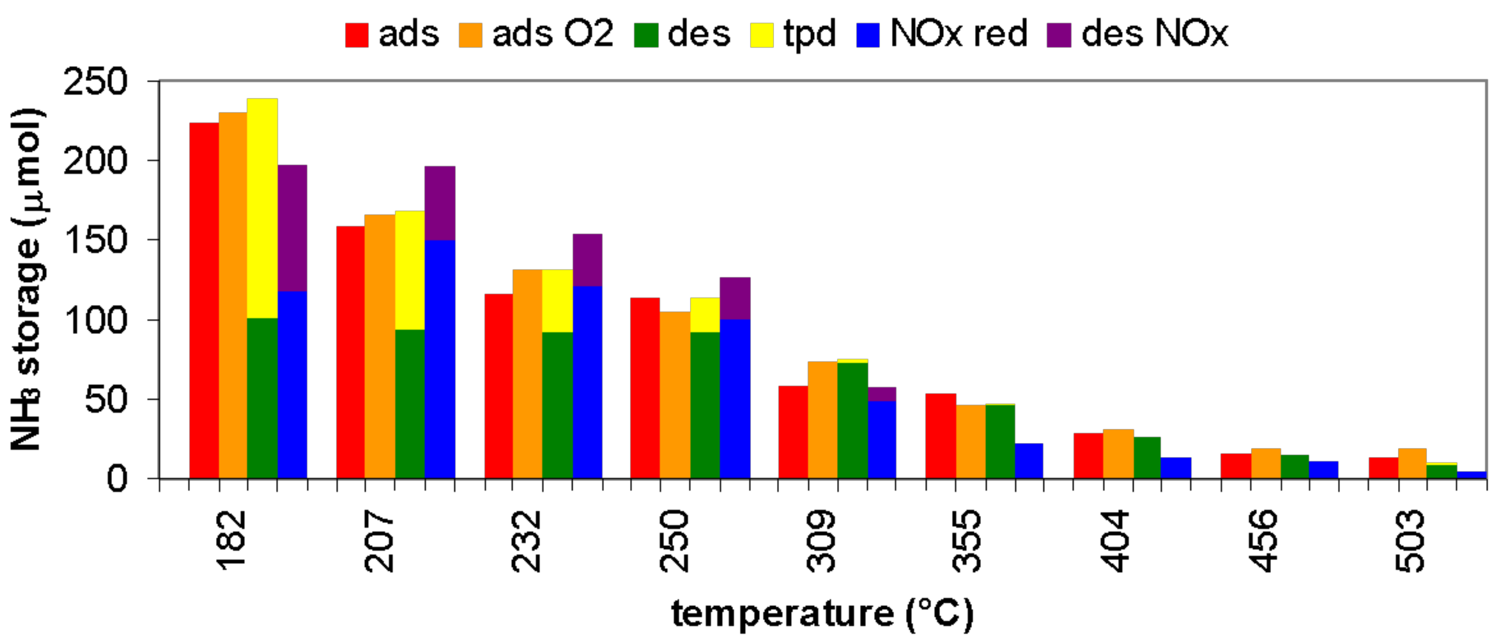
1. Navistar obtains mini-DPFs from suppliers
2. Navistar/Exova load filters with soot in engine exhaust
3. ORNL measures global reaction rates in flow reactor
   - temperature programmed oxidations:
     - O_2, NOx, NOx + O_2, O_2 + HC
   - steady state measurements of HC and NO oxidation over regenerated samples
4. Navistar identifies most promising formulation(s)
5. ORNL conducts isothermal pulsed oxidation experiments
   - measure kinetics as a function of T, gas composition, and soot burnout under differential conditions
   - evaluate correlations between soot structure, composition, and surface area and their effect on oxidation kinetics
6. MTU utilizes data for DPF model development & calibration
7. Team evaluates fuel optimal regeneration strategies through combination of experiments and simulation

Accomplishments (FY09): Developed & utilized a transient protocol for measurement of SCR kinetics



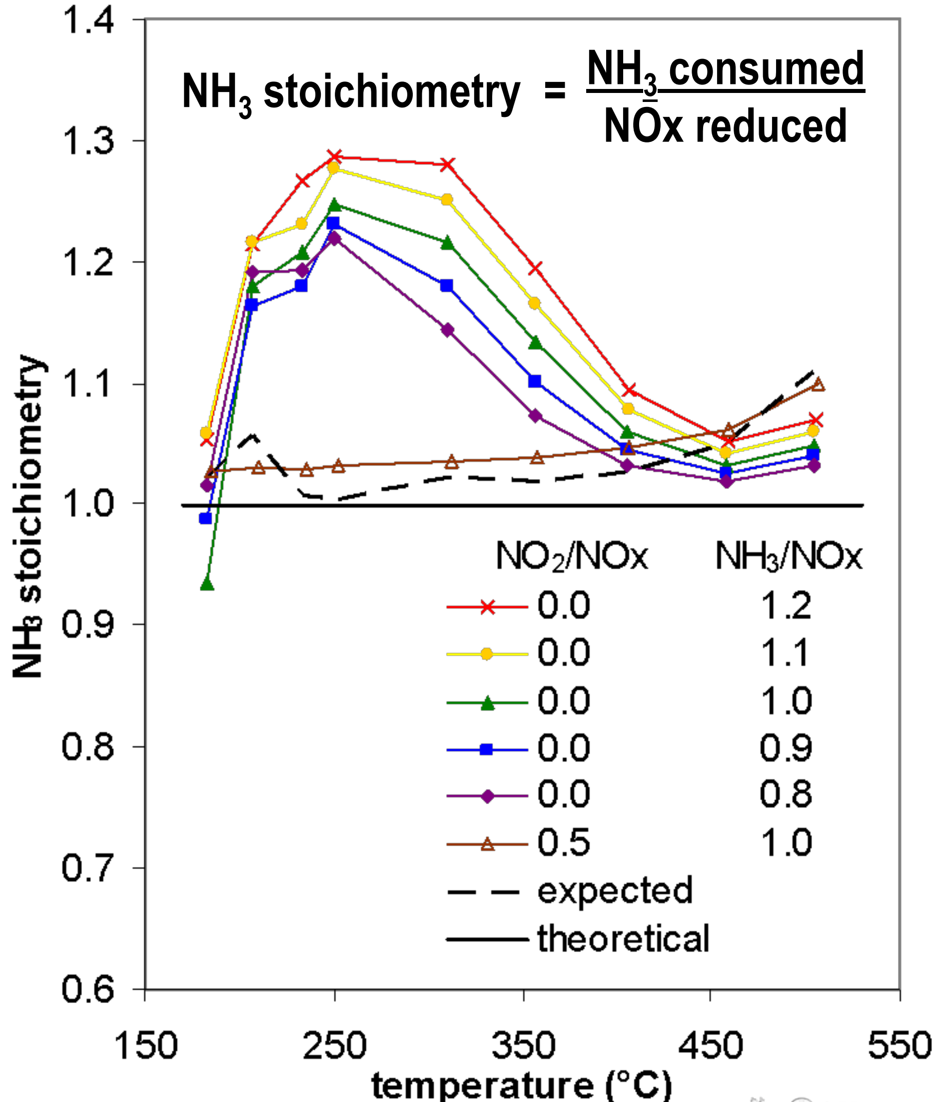
Accomplishments: Calculated consistent NH_3 storage capacities from several protocol segments

- Four segments allow measurement of NH_3 storage:
  1. NH_3 adsorption under inert conditions
  2. NH_3 adsorption in presence of O_2
  3. isothermal and subsequent temperature programmed desorption
  4. NOx reduced and NH_3 released after removal of NH_3 from feed gas
- All four steps yield relatively consistent values => measuring one probably sufficient
- Not all NH_3 on surface useful for subsequent NOx reduction
  - disparity depends on imbalances between rates of NH_3 release and SCR reaction



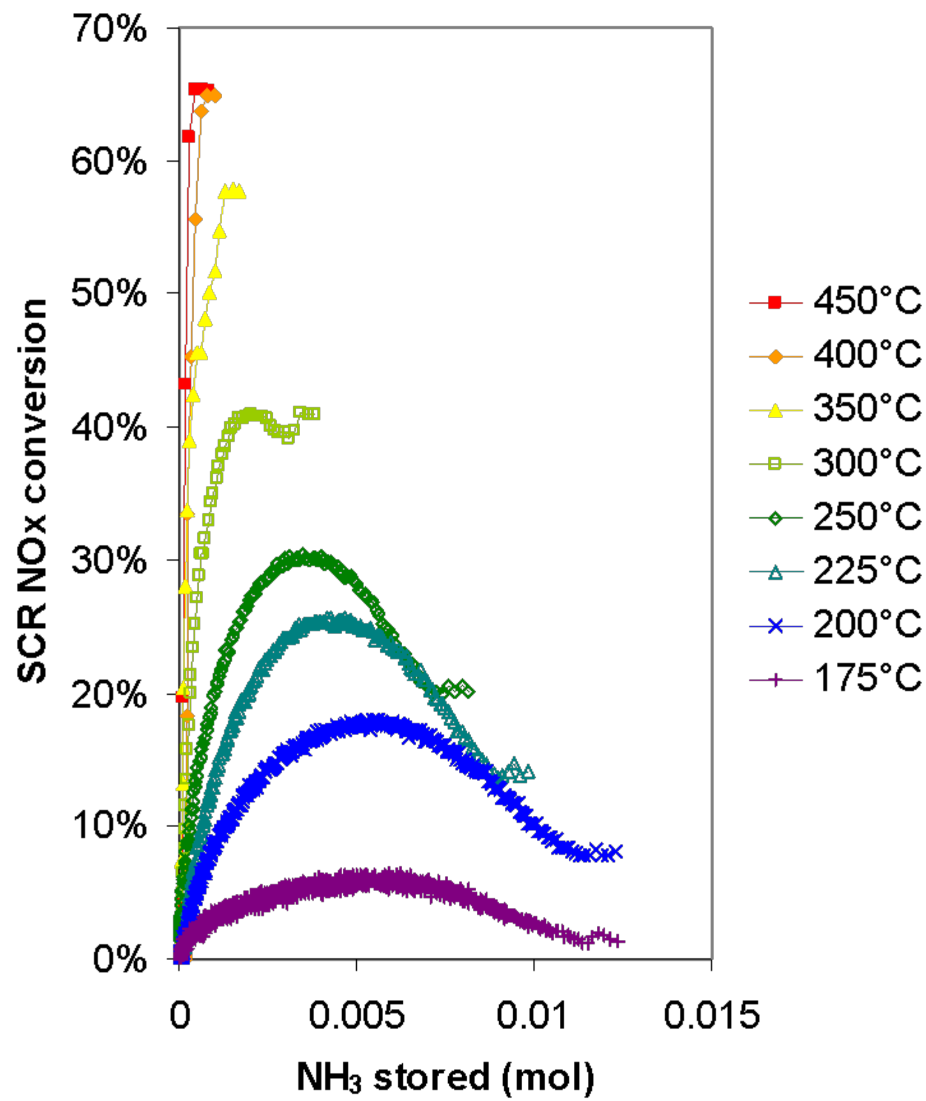
Accomplishments: Observed substantial parasitic NH_3 losses under NO SCR conditions

- NH_3 stoichiometry:
  - theoretically 1 for NO_2/NOx <= 0.5
  - expected to be slightly > 1 due to NH_3 oxidation
- "Fast" (NO_2/NOx = 0.5) SCR stoichiometry close to prediction
- NO SCR NH_3 stoichiometry much higher than expected at moderate Ts (200-350C)
  - increases with increasing NH_3 dose
- Possible causes:
  - coverage/spatial dependence of NH_3 oxidation kinetics
  - alternate surface redox cycle
- Problematic for model development, parameter estimation, and controls
- Additional characterization of parasitic NH_3 losses will be conducted under MTU aftertreatment project (ACE028)



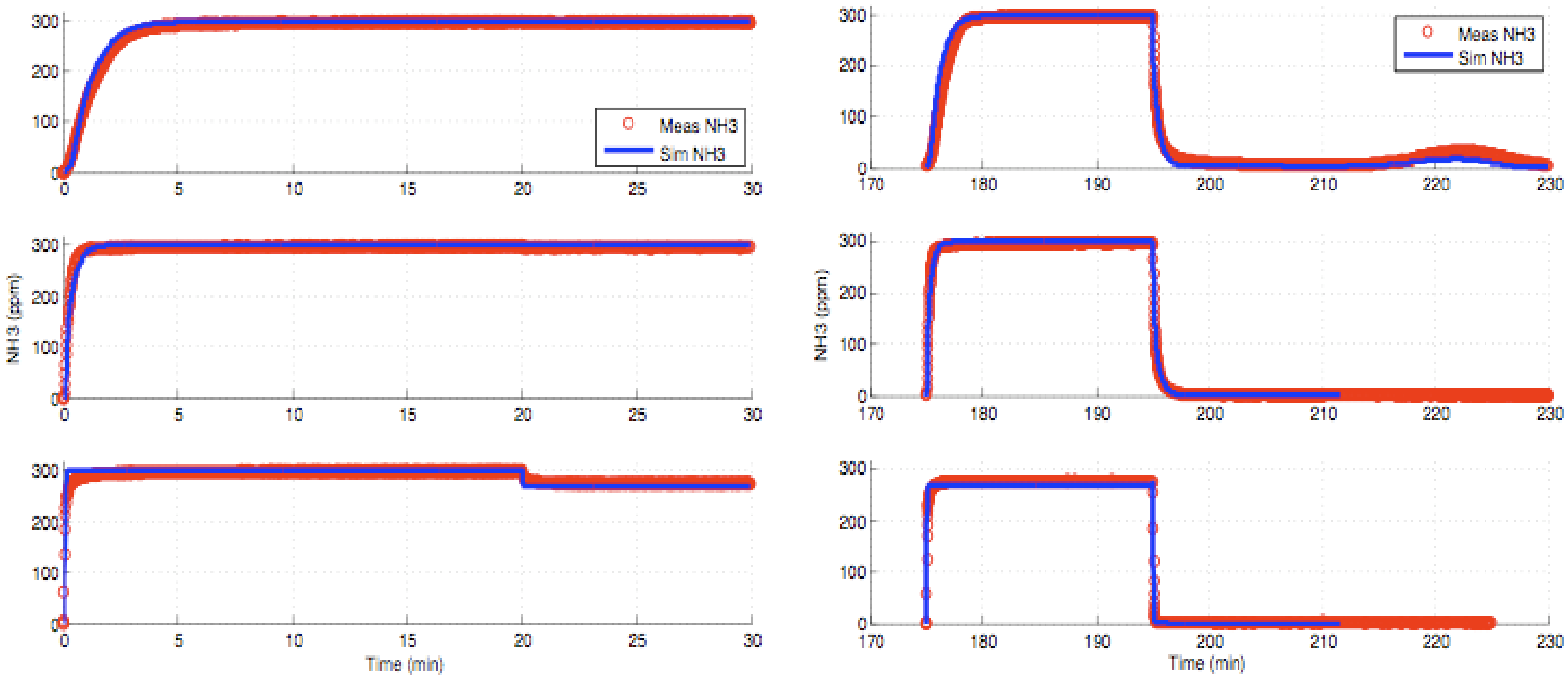
Accomplishments: Measured coverage-dependent SCR reaction kinetics

- NO conversion as a function of surface NH_3
  - NO SCR to steady state, shut off NH_3
  - incoming NO reacts with stored NH_3
- Low T (<300C) conversion profiles reflect NH_3 inhibition of NO SCR:
  - low coverage: insufficient surface NH_3 limits rate
  - high coverage: NH_3 blocks SCR active sites
- Achieving optimum NH_3 coverage would improve NOx conversion of Fe zeolite catalysts
  - difficult to achieve due to changes in optimal coverage and reaction rates with temperature
  - requires state-based control algorithms that track NH_3 storage

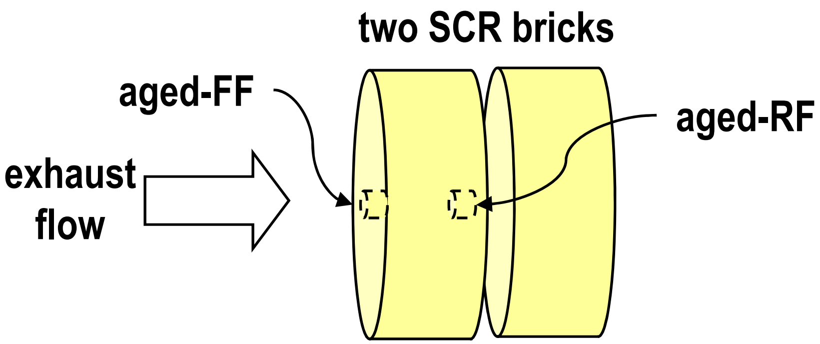


Accomplishments: SCR model development and parameter estimation proceeding at MTU

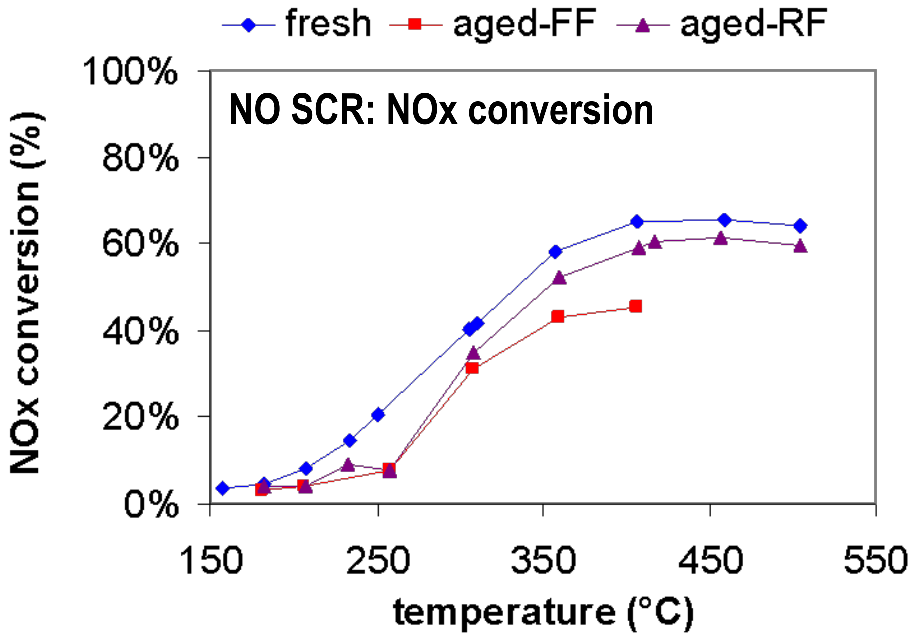
- **Modeling objective: create a predictive model with sufficient accuracy and computational efficiency to be used in model-based urea control system design**
- **Selected segments of protocol used to fit NH_3 storage and oxidation parameters**
- **Simulations fit calibration experiments well**

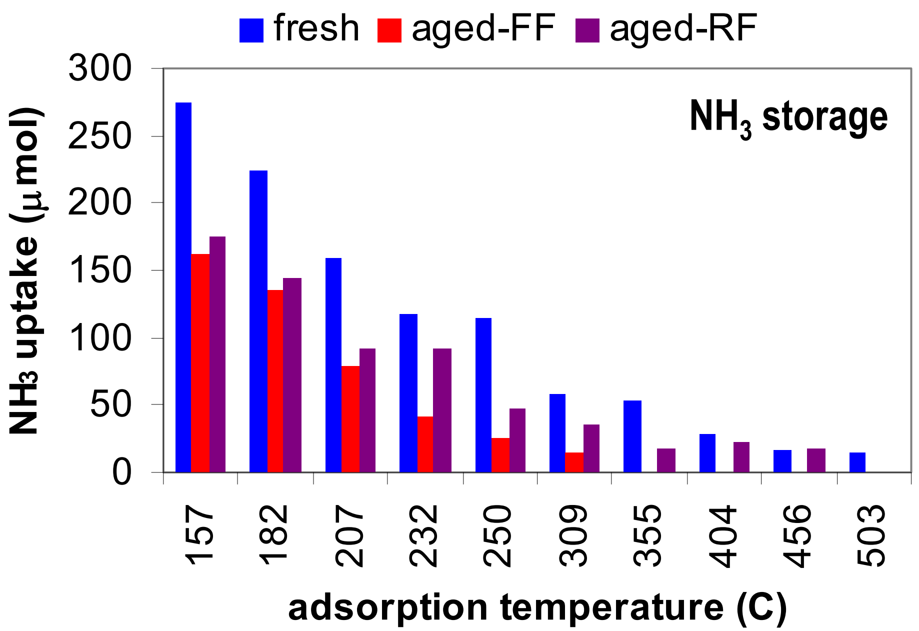


Accomplishments: Used SCR protocol to quantify impacts of engine aging

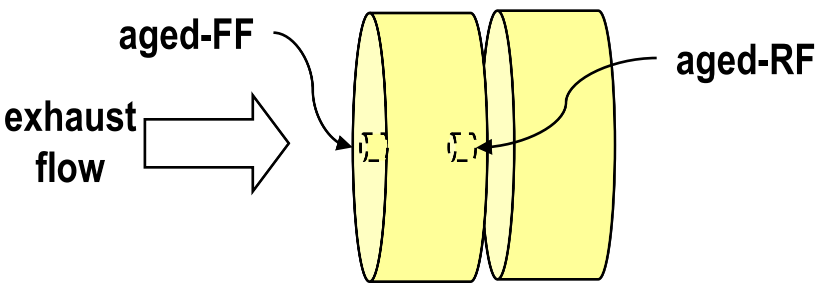


- Cut 25 mm OD x 25 mm L core samples from engine-aged Fe zeolite SCR bricks
- Evaluated performance with SCR protocol
- Aging decreased NOx reduction performance over entire T range
  – aged-FF much worse at high T
- Aged samples lost NH_3 storage capacity (by any measure) at all Ts
  – storage losses worse in aged-FF
  – due to higher T at front face of brick?





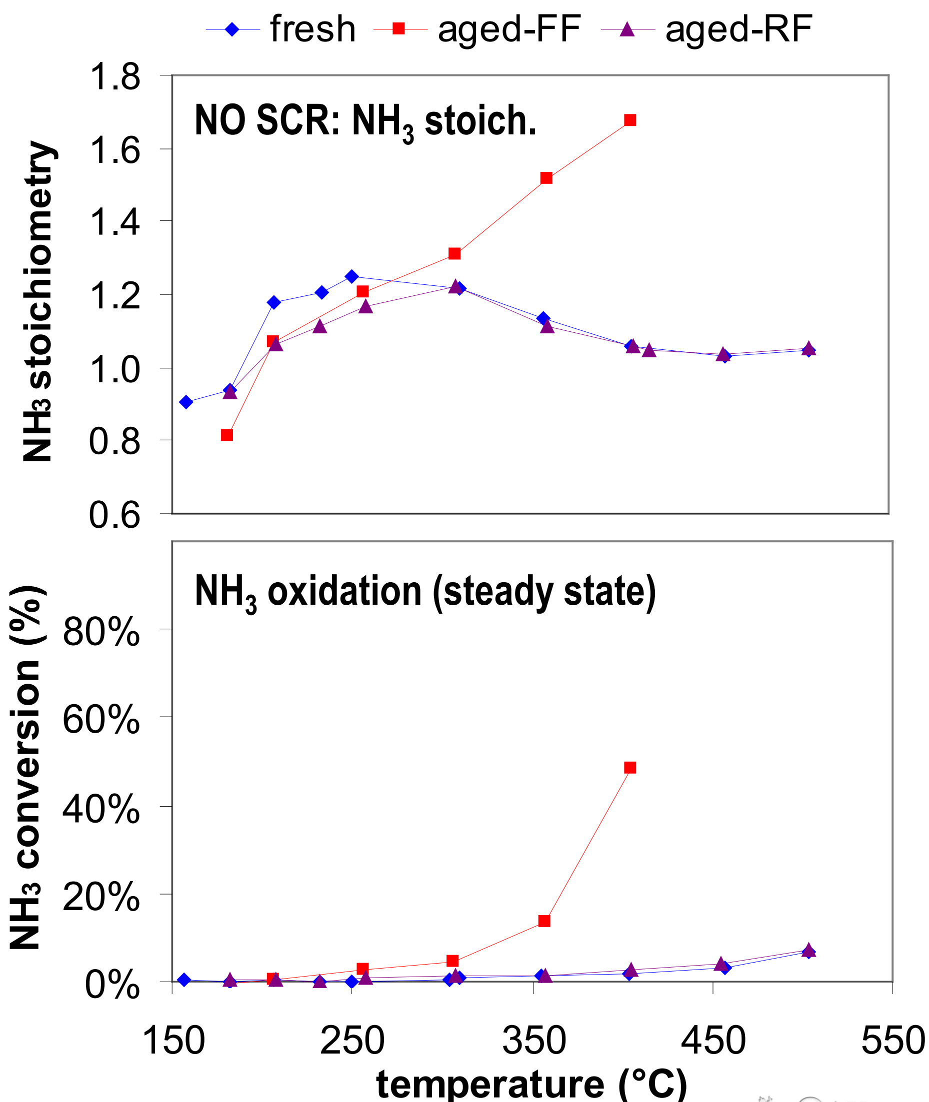
Accomplishments: SCR protocol experiments reveal two distinct degradation mechanisms



Aging mechanisms:

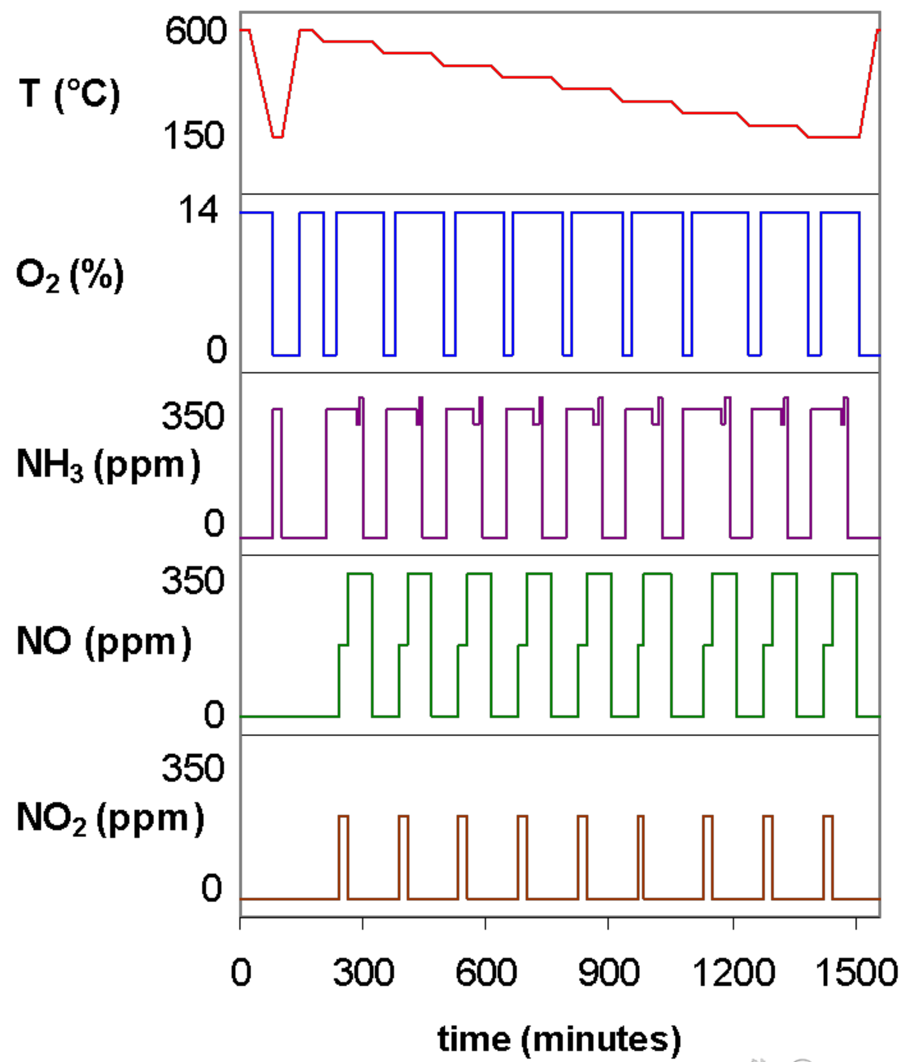
1. Loss of surface area and/or Brønsted acid sites after aging as evidenced by:
   - loss of NH_3 storage
   - drop in NOx performance
   - no change in NO oxid. (Fe unchanged)
2. Trace Pt deposition from upstream DOC onto face of SCR brick (sample aged-FF) during engine operation as evidenced by:
   - increase in NO SCR NH_3 stoichiometry
   - increase in NH_3 oxidation at high T

- MTU model calibration with aged sample data should yield additional insights.



Accomplishments: CRADA SCR protocol used as basis for new CLEERS transient SCR protocol

- Selected most useful steps from CRADA SCR protocol; eliminated redundancies where possible
- New protocol provides critical information needed for constructing accurate SCR device models at minimum time and expense
- Specifically reveals:
  - NH_3 storage and release
  - NH_3 and NO oxidation
  - NO SCR kinetics (and NH_3/NO impact)
  - NO + NO_2 SCR kinetics
- Presented at the CLEERS Workshop and in the CLEERS Focus Groups
- Undergoing experimental validation and utilization for systems simulations



Accomplishments: mini DPFs loaded in engine exhaust at Exova and shipped to ORNL

- 25 mm OD x 75 L mm mini-filters
- First batch included a total of 30 samples:
  - 6 formulations
    - 3 different substrate materials
    - with and without washcoat
  - 5 samples of each formulation with 3 soot loadings
    - 1 x 3 g/L, 1 x 5 g/L, 3 x 7g/L
  - shipped on dry ice and stored in a freezer at ORNL
- Engine operating conditions:
  - speed 1950 rpm
  - load: 350lb/ft
  - EGR: to achieve AVL smoke number of 2.7

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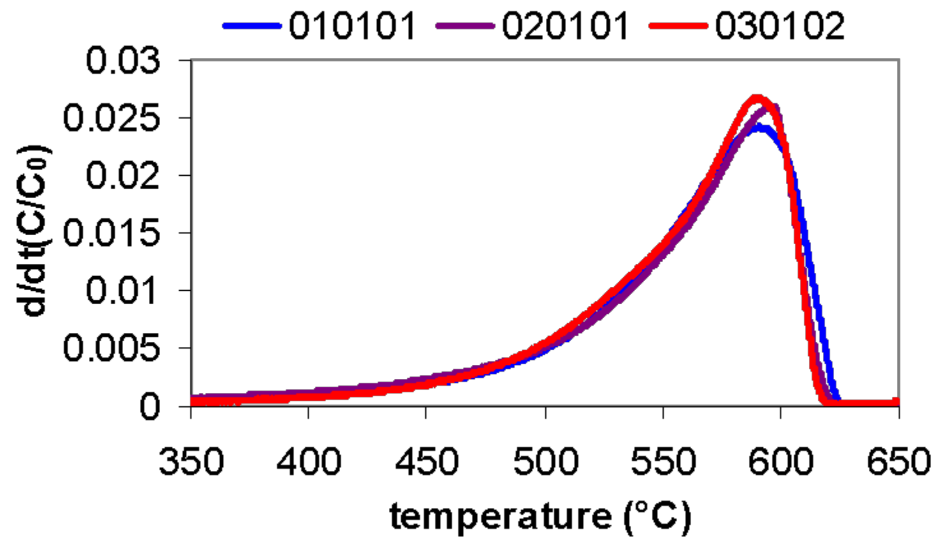
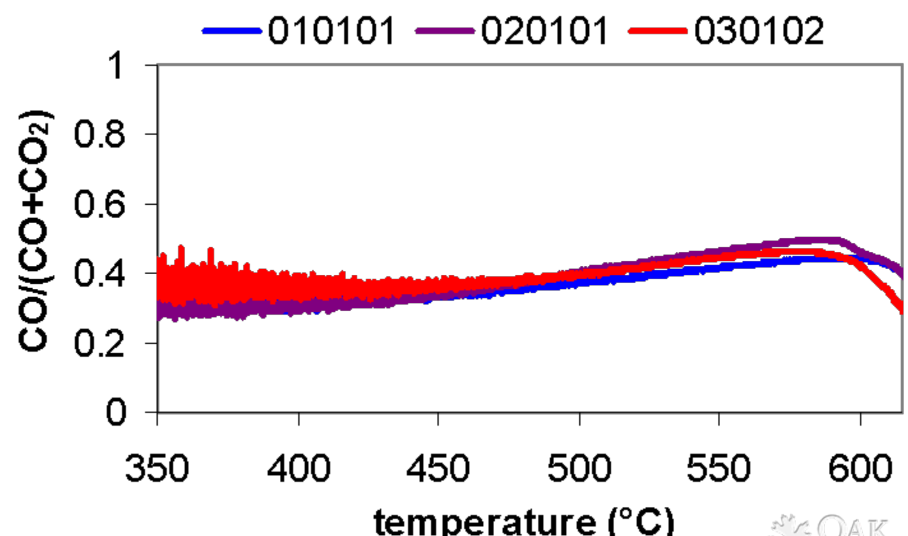
Accomplishments: Initial O_2 TPOs show minimal impact of substrate material on regeneration

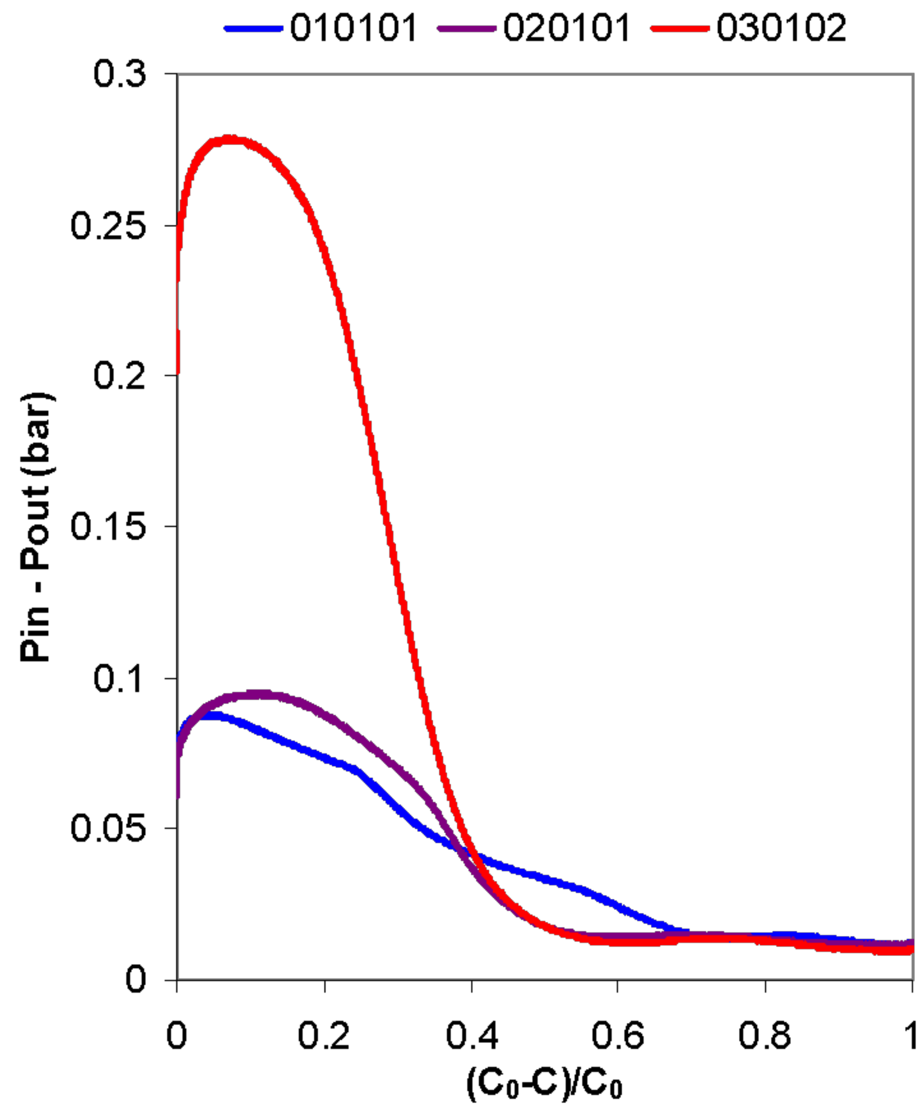
- three different substrate materials
- 7g/L soot loaded in engine exhaust
- Flow reactor TPO:
  - SV: 40,000 hr^{-1}
  - T ramp: 200-650°C @ 2°C/min
  - 10%O_2, 5%H_2O
- Carbon oxidation rate normalized to initial soot mass
- Burnout profiles and CO/CO_2 ratios nearly identical for all three samples





Accomplishments: Substrate materials impact backpressure evolution during DPF regeneration

- Substrate composition & structure impact:
  - initial backpressure of loaded filter
  - backpressure evolution during burnout
- Substrate 1: different backpressure profile
  - starts to decrease at <10% burnout
  - rate of decrease more gradual
- Substrates 2 and 3 reach nearly "clean" backpressure at ~50% burnout
  - potential for partial regen strategy?
- Next step: correlate backpressure changes with soot location/distribution
  - destructive evaluation after partial burnout?



Collaborations

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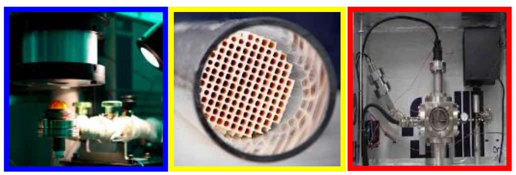
- develop experimental protocols
- perform detailed device characterization
- analyze and interpret results



CRADA

NAVISTAR

- identify relevant system configurations & components
- guide modeling & experiments
- obtain device samples (fresh & aged)

Exova

- load mini-DPFs on Navistar engine

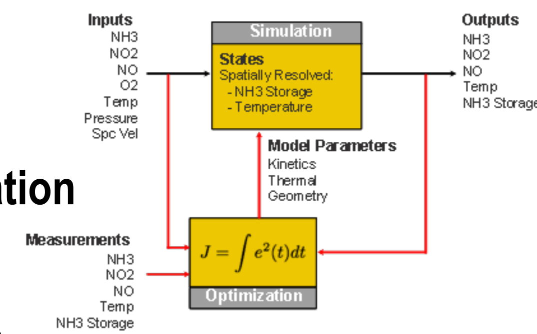
Device Suppliers

- fabricate samples

CLEERS

MichiganTech

- develop model code
- perform parameter estimation
- validate model
- identify experiment needs



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Proposed Future Work

- Publish investigation of aging impact on SCR catalyst characteristics and model parameters
- Complete TPOs on soot-loaded mini-DPFs
- Measure steady state HC and NO oxidation kinetics over regenerated washcoated mini-DPFs
- Conduct isothermal pulsed oxidation experiments on selected DPF formulations loaded with soot in engine exhaust
- Transfer data to Navistar and MTU for model calibration and validation
- Investigate alternate approaches to DPF regeneration to reduce fuel penalty

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Summary

Relevance

- Objective: Enhance understanding of aftertreatment device operating principles to enable development of fuel optimal control strategies

Approach

- Load mini-DPFs in engine exhaust, regenerate in an automated flow reactor to measure reaction kinetics, transfer data to MTU for model calibration and validation
- Evaluate impacts of high soot loads, large volatile fractions, and alternate regeneration strategies on soot oxidation kinetics

Accomplishments

- Identified parasitic NH_3 losses as key issue for future study
- Observed two distinct aging mechanisms on engine-aged SCR samples
- Provided starting point for new CLEERS transient SCR protocol
- Loaded mini-DPFs with engine soot and began TPOs; quantified DPF substrate impact on backpressure evolution during regeneration

Collaborations

- Partners: Navistar, Michigan Technological University, Exova
- Informal collaborations: CLEERS participants

Proposed Future Work

- Complete TPOs on soot-loaded mini-DPFs and begin isothermal pulsed oxidations