Combination & Integration of DPF-SCR Aftertreatment

PNNL:
Ken Rappe, Mark Stewart, Gary Maupin

PACCAR:
Rich Bergstrand (PTC), Mansour Masoudi (PTC),
Wim Evers (DAF), Bram Hakstege (DAF)

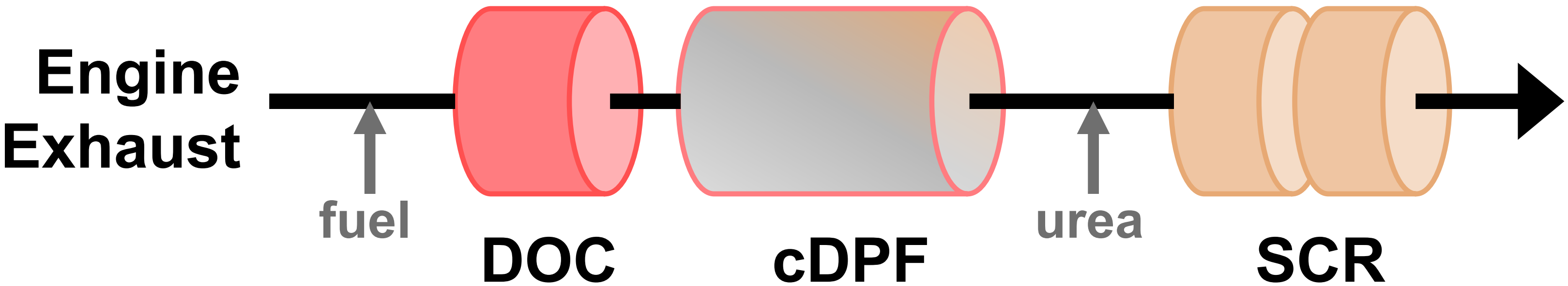
BASF:
Patrick Burk

DEER 2012

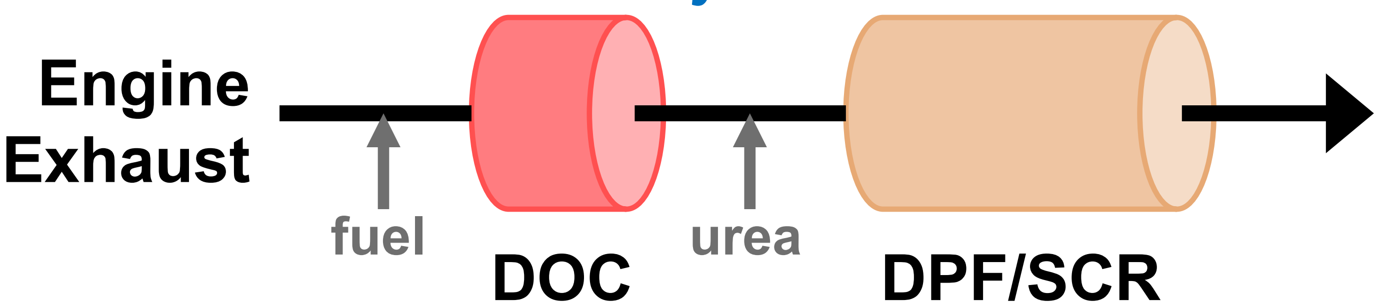
Pacific Northwest
NATIONAL LABORATORY

Integrating DPF & SCR functionalities for reducing cost and volume of engine after-treatment

Typical HDD EPA 2010 Layout



Possible Future HDD Layout



SCR – DPF INTEGRATION

OBJECTIVE: Fundamentally understand the integration of SCR & DPF technologies for HDD to provide a pathway to the next generation of emissions control systems

- CRADA with PACCAR, working closely with DAF Trucks

- *Highly* evolving field of work (mostly LDD, some HDD); this effort focused on:
  1. Optimizing SCR catalyst wash coat
  2. Facilitating passive soot oxidation
- BASF (HD Systems Development)
  - Providing SCR catalyst (Cu/Z) expertise
  - Washcoating, manufacturability
- Corning
  - Developmental UHP cordierite

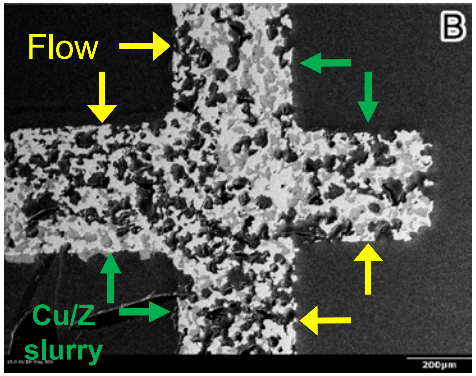
SCR – DPF INTEGRATION

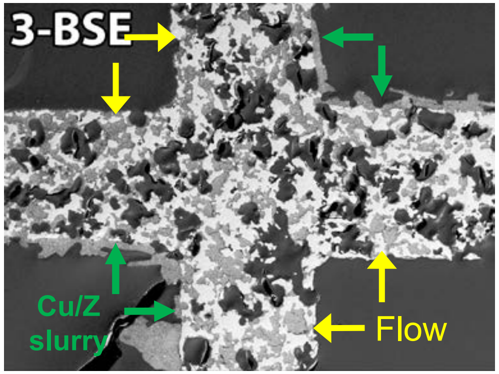
OBJECTIVE: Fundamentally understand the integration of SCR & DPF technologies for HDD to provide a pathway to the next generation of emissions control systems

- CRADA with PACCAR, working closely with DAF Trucks

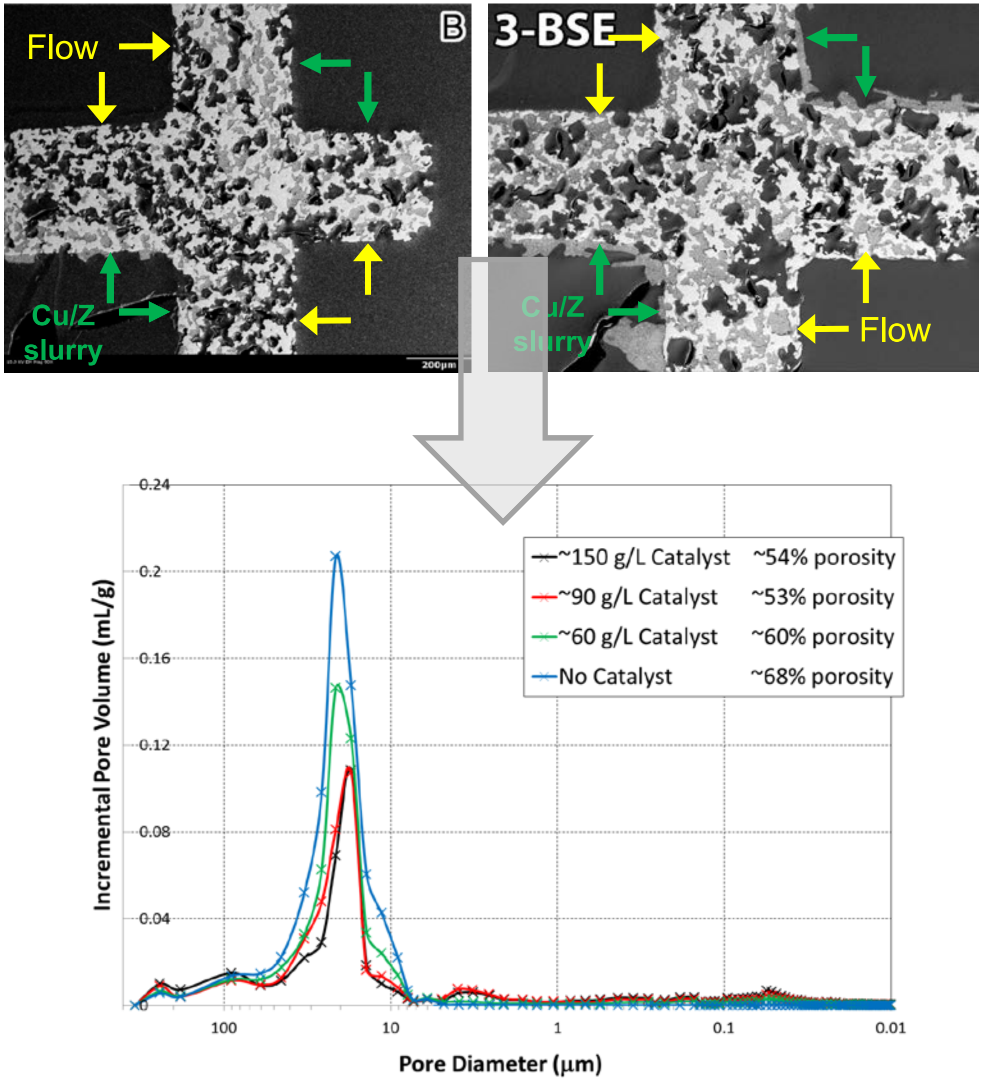
- *Highly* evolving field of work (mostly LDD, some HDD); this effort focused on:
  1. Optimizing SCR catalyst wash coat
  2. Facilitating passive soot oxidation
- BASF (HD Systems Development)
  - Providing SCR catalyst (Cu/Z) expertise
  - Washcoating, manufacturability
- Corning
  - Developmental UHP cordierite

OPTIMIZING SCRF WASHCOAT

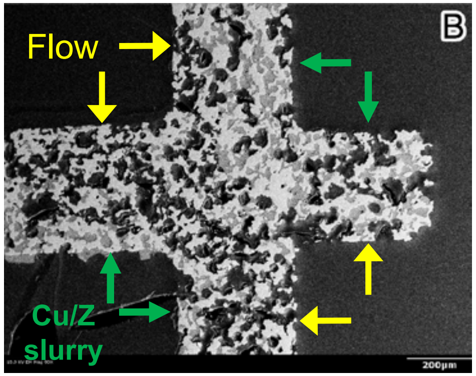


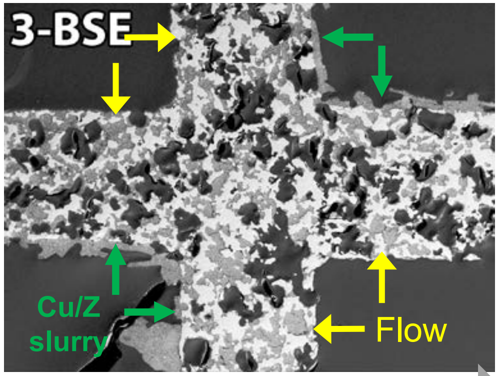


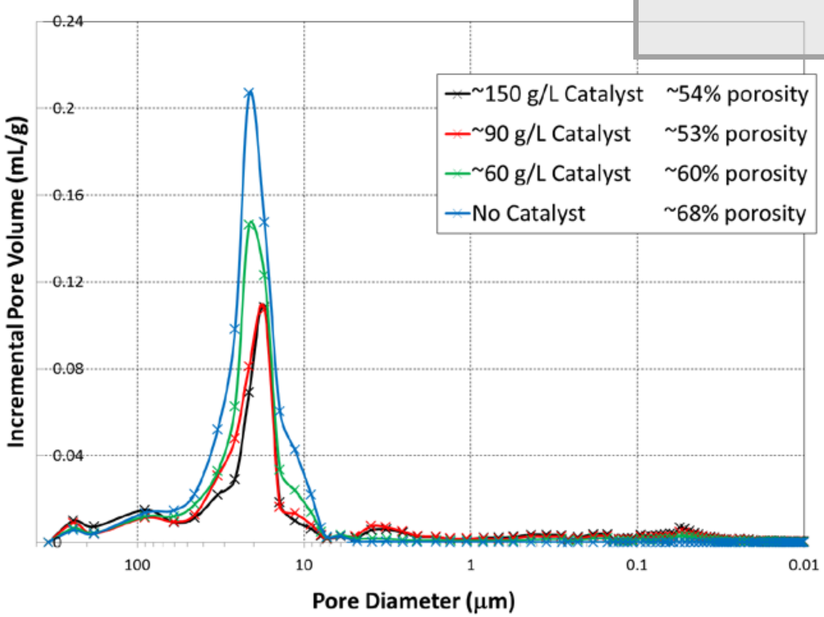
OPTIMIZING SCRF WASHCOAT

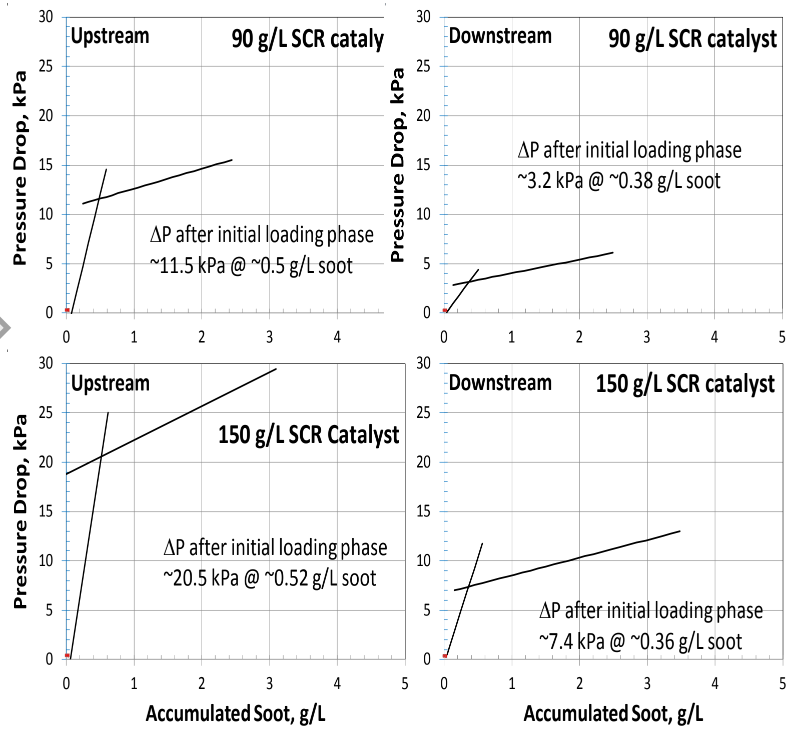


OPTIMIZING SCRF WASHCOAT









Pacific Northwest
NATIONAL LABORATORY

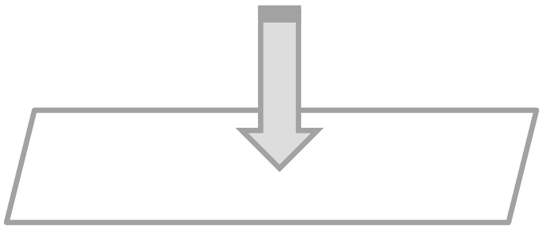
REACTION STUDIES

- Reaction competition
  - Passive soot oxidation vs. Selective catalytic reduction (SCR)
- Passive soot oxidation – NO_2 driven
  - The presence of SCR reaction(s) in a wall-flow filter ***WILL*** have a detrimental effect on passive soot oxidation
  - SCRF integration will NOT have oxidation component on filter, thus no NO_2 'recycle' component present
  - Reaction competition: passive soot oxidation vs. SCR
- GOAL: maximize the passive soot oxidation feasibility of an SCRF
  - Minimize adverse effect of SCR on passive soot oxidation process
  - No additional downstream SCR
    - cannot sacrifice acceptable de-NO_x performance

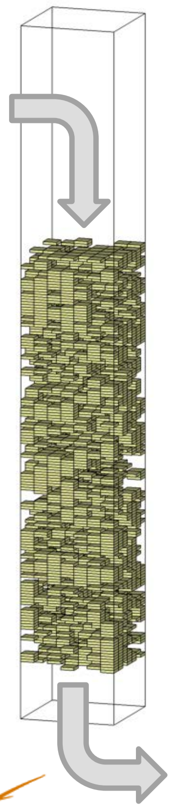
▶ MODELING WALL-SCALE SCRF

MODELING WALL-SCALE SCRF

- Single flat wall; exhaust flow in the normal direction
- Channel scale transport effects, axial variations are ignored
- Simplified SCR reaction network developed at PNNL
- Simplified porous media with similar porosity and tortuosity of the SCRF used in experiments
- 90 g/L of catalyst distributed evenly throughout the porous wall + 60 g/L placed on down-stream wall surface
- Lattice-Boltzmann model used to solve gas flow field
- Soot oxidation kinetic model by Messerer et al, 2006
- Soot present as cake layer on top of wall; assumed 50% oxidized soot
- *Conclusions dependent upon validity of assumptions and kinetics used*



exhaust flow



Standard Conditions

4 g/L soot
150 g/L catalyst
500 ppm NO_X
35,000 GHSV
ANR = 1

MODELING WALL-SCALE SCRF

- Simplified SCR kinetics model

  Developed under CLEERS in cooperation with ORNL using bench-scale experiments with a current commercial cu-CHA catalyst

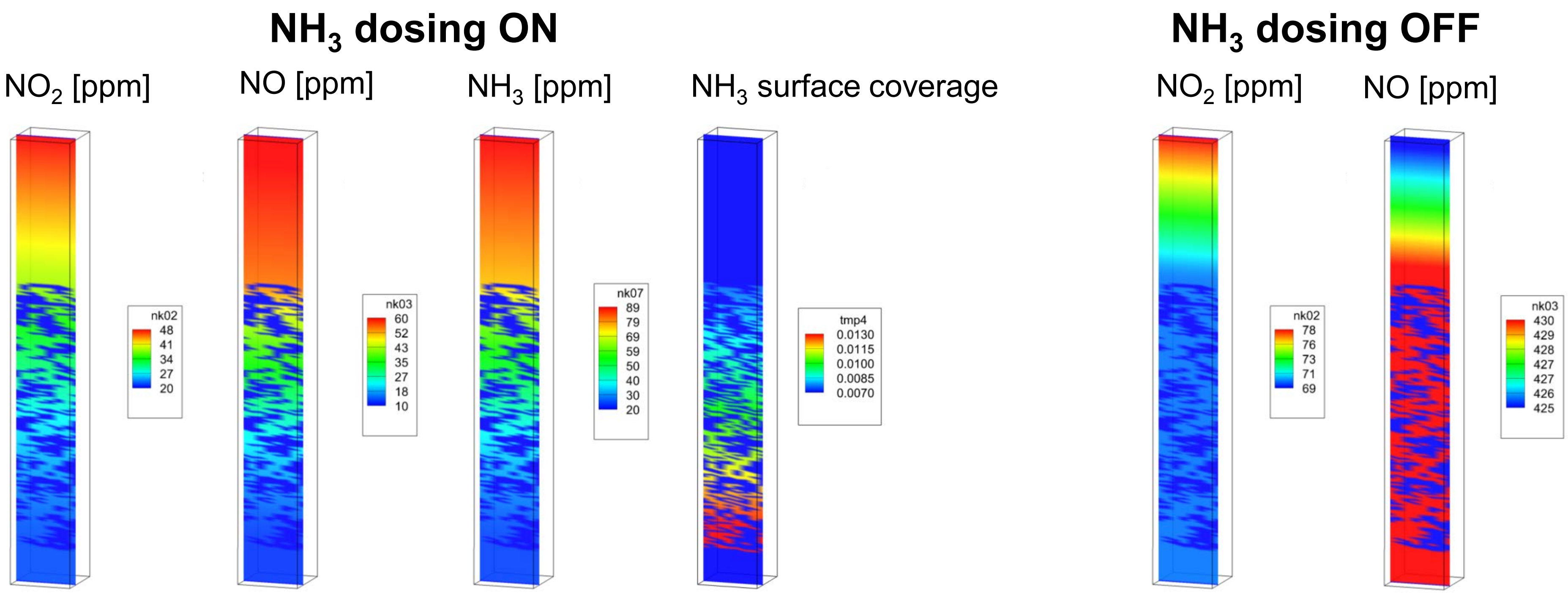
  - **NH_3 oxidation** $2NH_3 + 3/2O_2 \rightarrow N_2 + 3H_2O$
  - **Standard SCR** $4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$
  - **Fast SCR** $4NH_3 + 2NO + 2NO_2 \rightarrow 4N_2 + 6H_2O$

- Parametric matrix
  - 250°C, 300°C, 350°C, 400°C, 450°C
  - NO_2/NO_x = 0.33, 0.50, 0.67; NH_3/NO_x = 1.0, 0.85
  - DPF versus SCRF

- Diffusivity adjusted for temperature (Massman, 1998)

MODELING WALL-SCALE SCRF

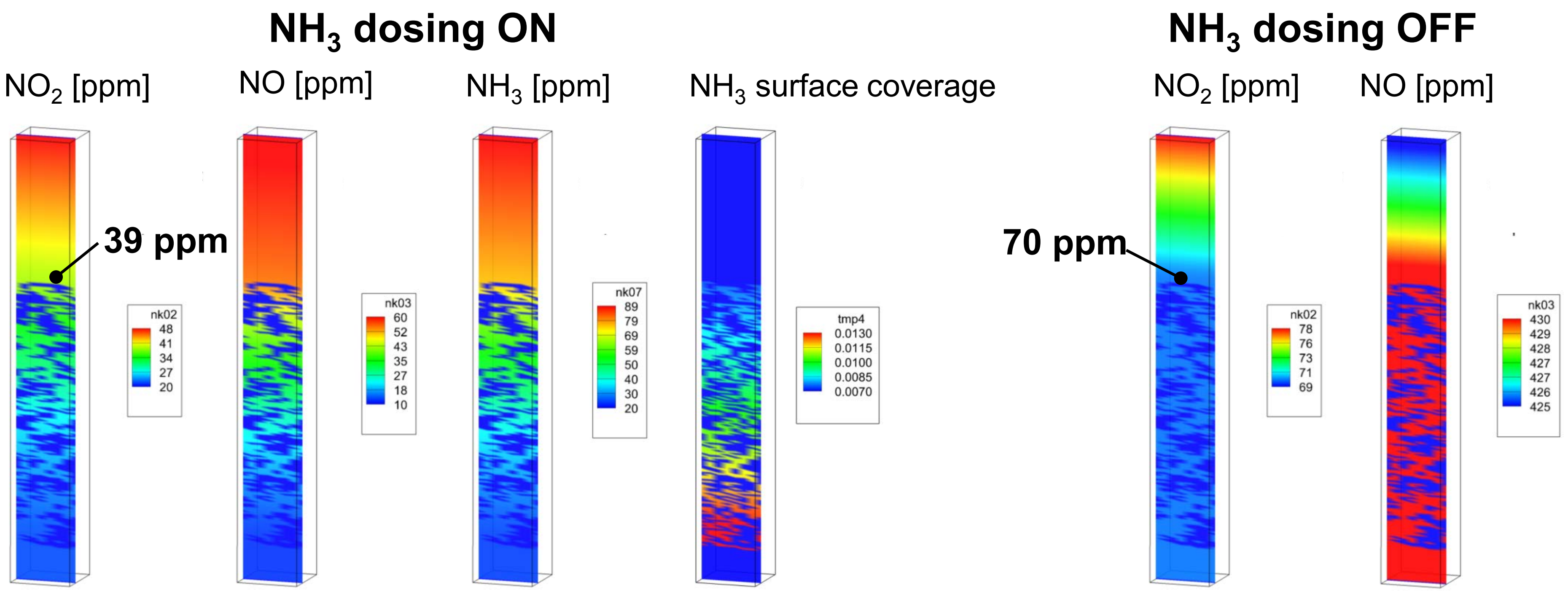
- Example species fields – 350°C



- In all SCRF cases: SCR catalyst creates gradients in active species concentrations and NH_3 surface coverage across the wall thickness

MODELING WALL-SCALE SCRF

- Example species fields – 350°C

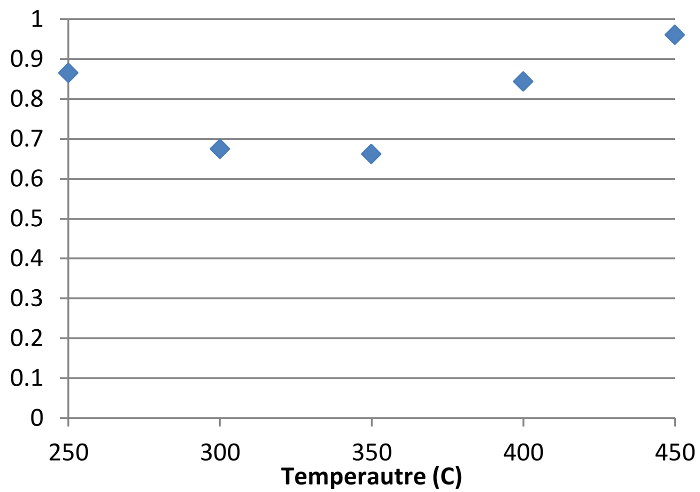


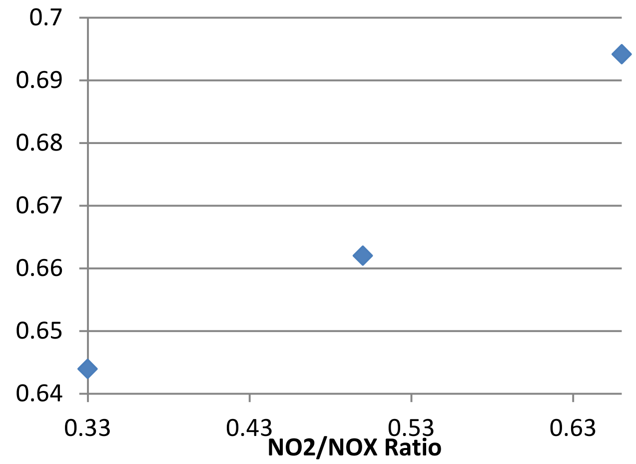
- Gradients in active species concentrations facilitate diffusion effects that are significant and effect concentrations upstream
- Of particular interest: NO_2

MODELING WALL-SCALE SCRF

- Passive soot oxidation (ANR = 1)

Ratio of soot oxidation rates [w/NH_3 dosing / w/o NH_3 dosing]





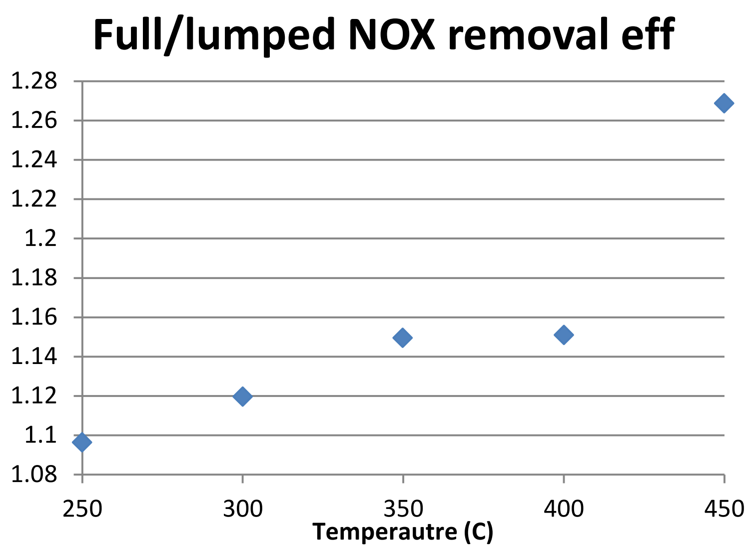
- Impact of SCR on soot oxidation is temperature dependent
  - SCR reactions decrease oxidation rate by about 35% at intermediate temperatures, but only 4% at higher temperatures
- Increased NO_2 fraction decreases inhibiting effect of SCR

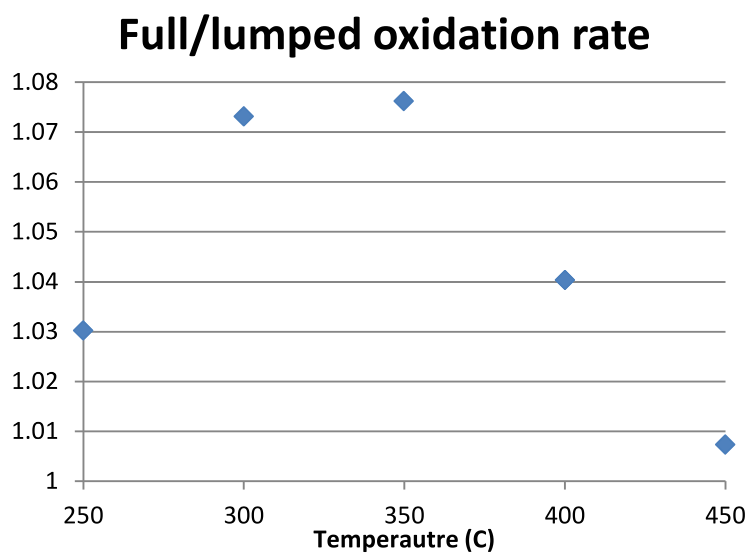
MODELING WALL-SCALE SCRF

- Full simulation (as described in initial model description)
  - Simplified porous media with similar porosity and tortuosity of the SCRF used in experiments
  - 90 g/L of catalyst distributed evenly throughout the porous wall + 60 g/L placed on down-stream wall surface
  - Soot present as cake layer on inlet channel surface of porous media
- Lumped simulation
  - Soot & SCR catalyst co-located
  - No porous media
  - Provides initial guesses for SS concentrations and NH_3 coverage
- Comparison provides a means of evaluating effect of spatial separation within wall-flow filter
  - Soot oxidation and SCR reaction components the same
  - Bulk-flow (i.e. convective) component the same
  - Allows evaluation of effect of concentration gradient(s) and resulting conductive transport (i.e. diffusive) effects

MODELING WALL-SCALE SCRF

- Spatial separation within wall-flow filter



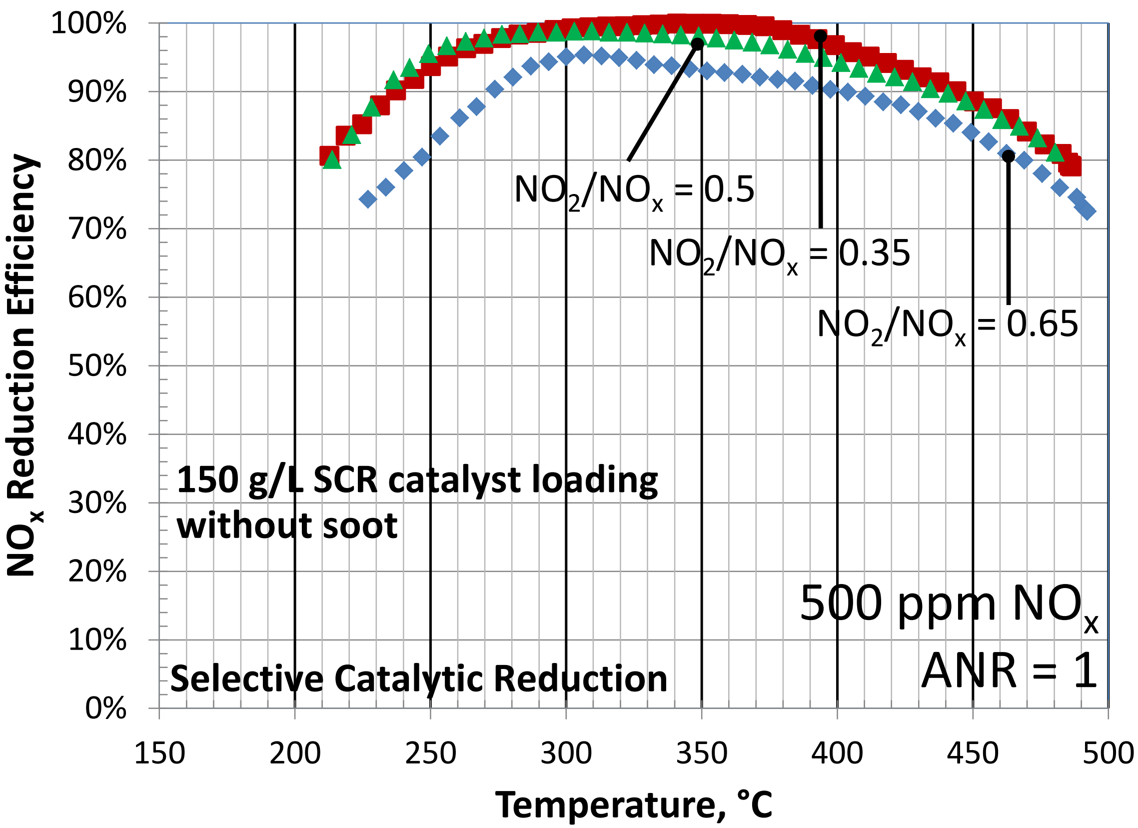


- Spacial separation (of SCR from soot) results in a small benefit for soot oxidation and NRE
  - Benefit for soot oxidation smaller
- Effect is small: kinetics of competing reactions and resulting conductive transport effects dominant for all cases

- **BENCH-SCALE REACTION STUDIES**

NO_X REDUCTION EFFICIENCY

- Effect of NO_2 fraction on NRE



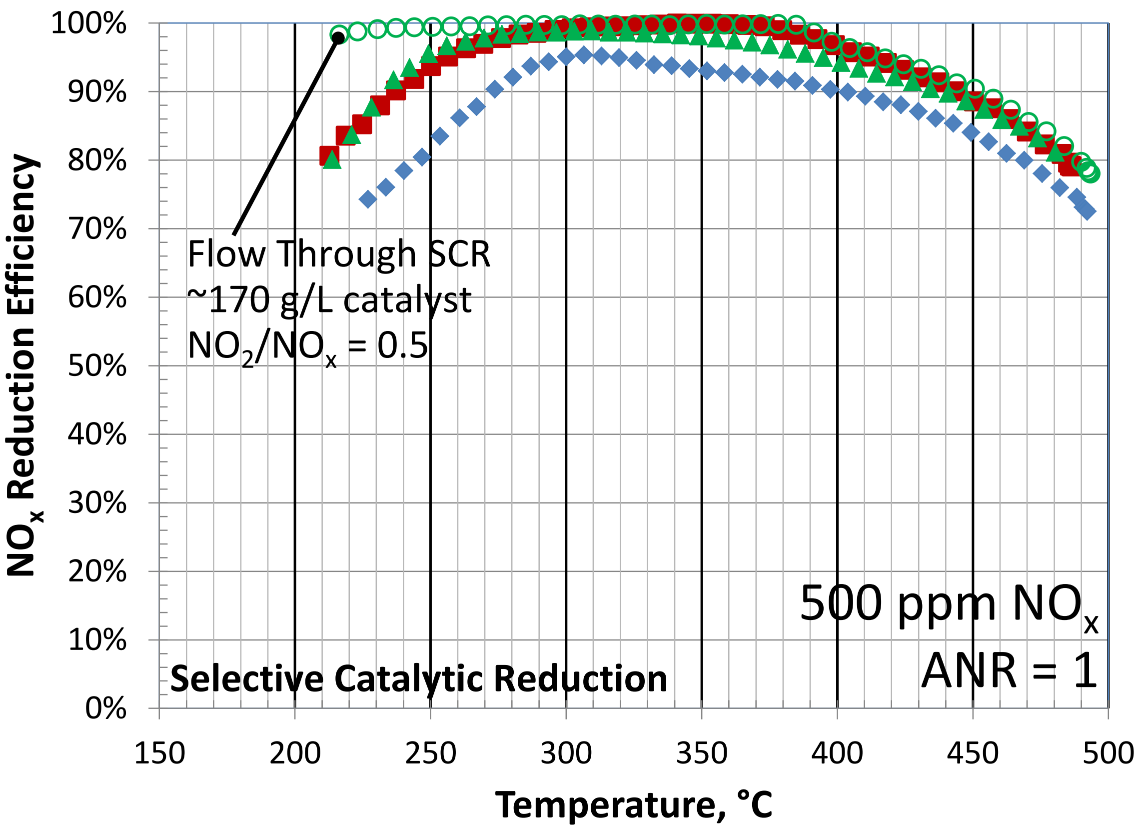
SCR performance:

Minimally affected at NO_2 /NO_x < 0.5

Detrimental effect at NO_2 /NO_x > 0.5

NO_x REDUCTION EFFICIENCY

- Effect of NO_2 fraction on NRE

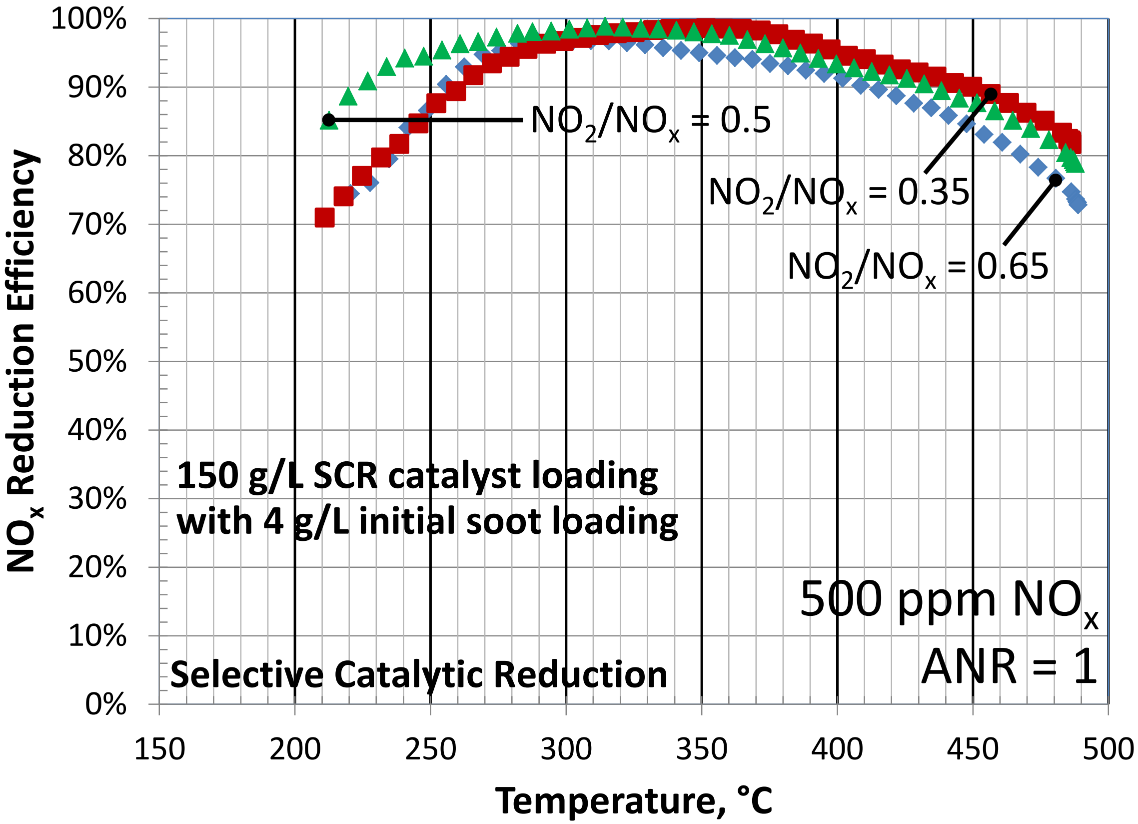


Detrimental effect of wall flow versus flow through

Especially at temp < ~275°C

NO_X REDUCTION EFFICIENCY

- Effect of NO_2 fraction on NRE



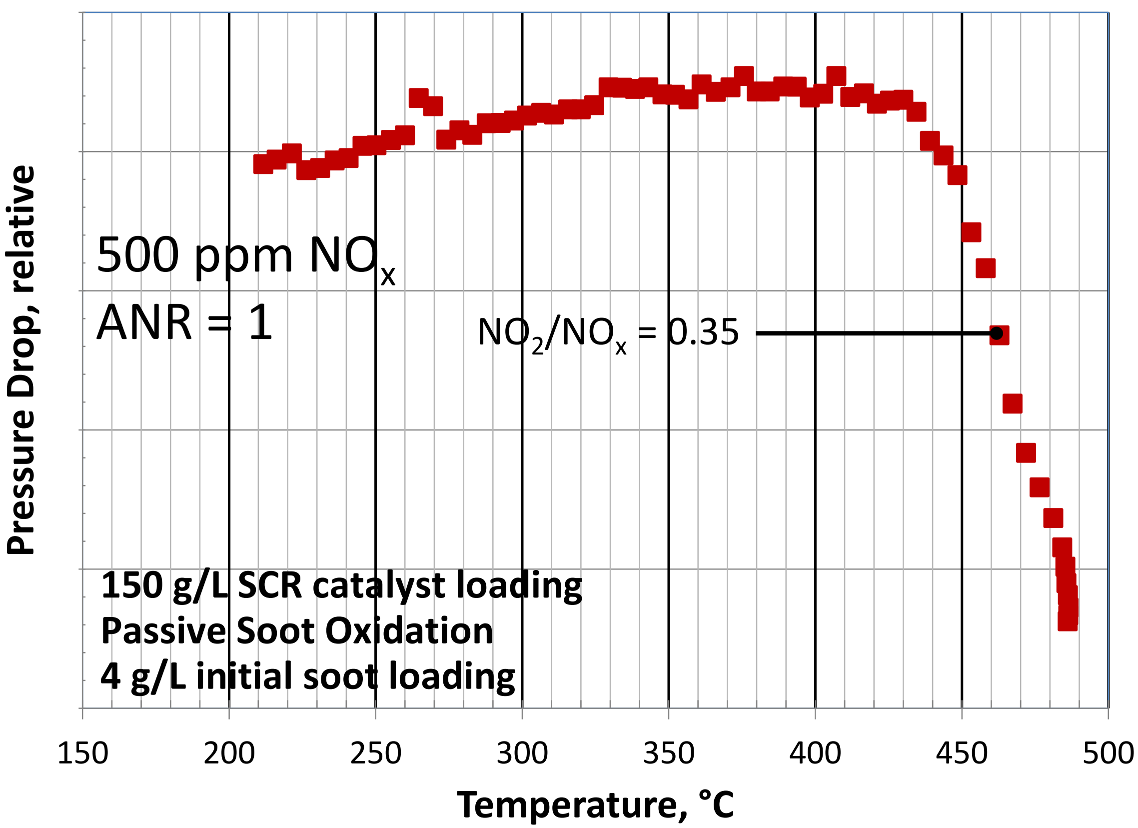
SCR performance not significantly affected by soot

NO_2 /NO_x > 0.5 improved

Contribution of passive soot oxidation

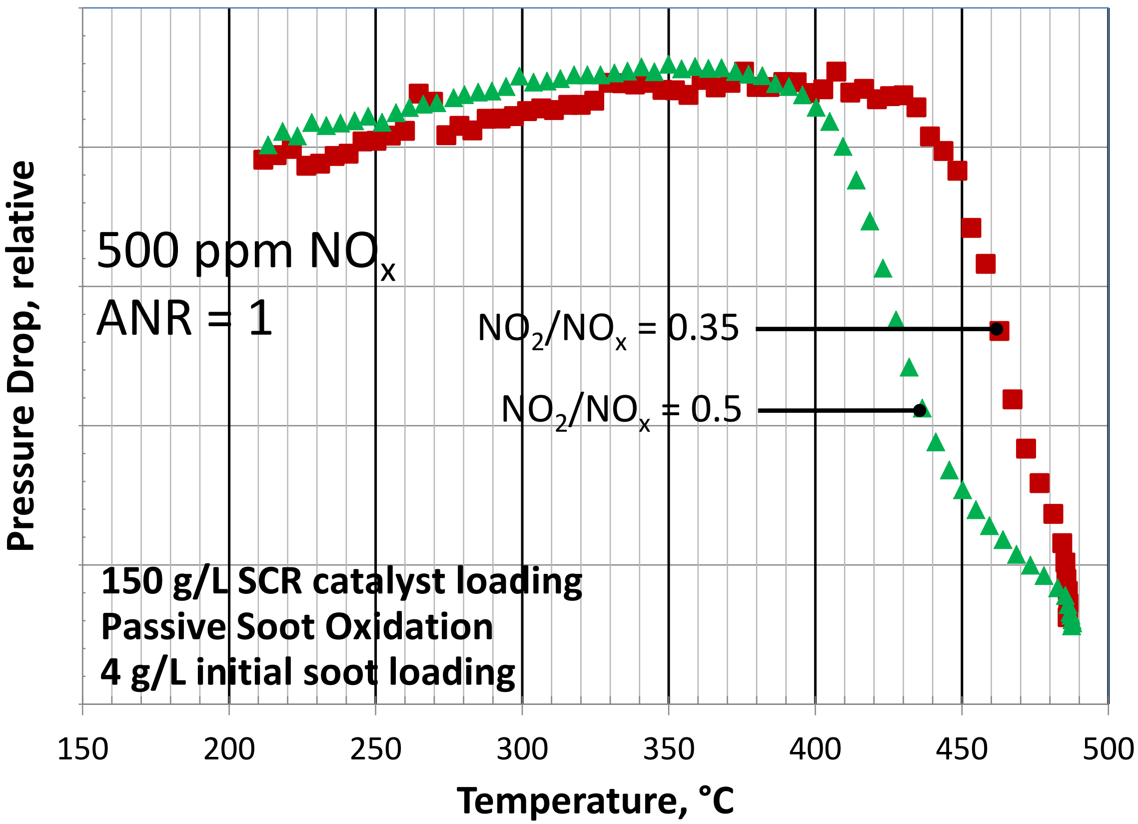
PASSIVE SOOT OXIDATION

- Effect of NO_2 fraction on soot oxidation rate



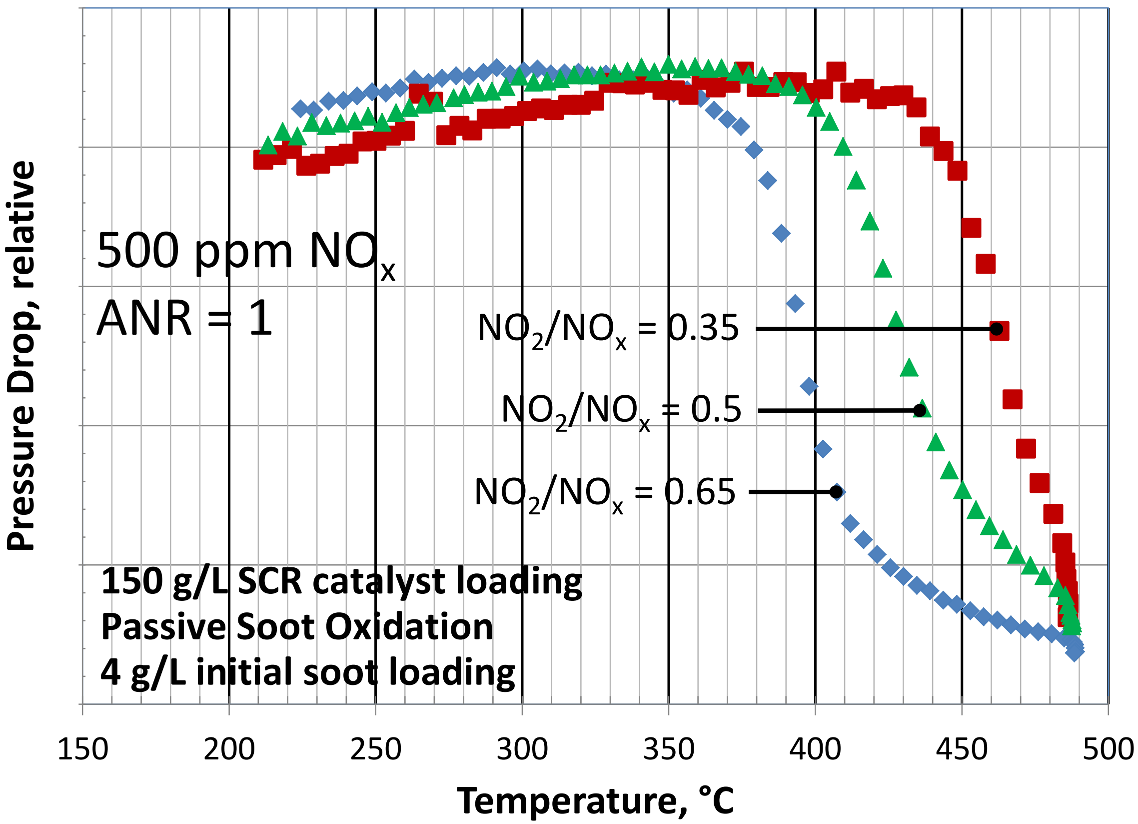
PASSIVE SOOT OXIDATION

- Effect of NO_2 fraction on soot oxidation rate



PASSIVE SOOT OXIDATION

- Constant NO_x: effect of NO_2 fraction on soot oxidation rate

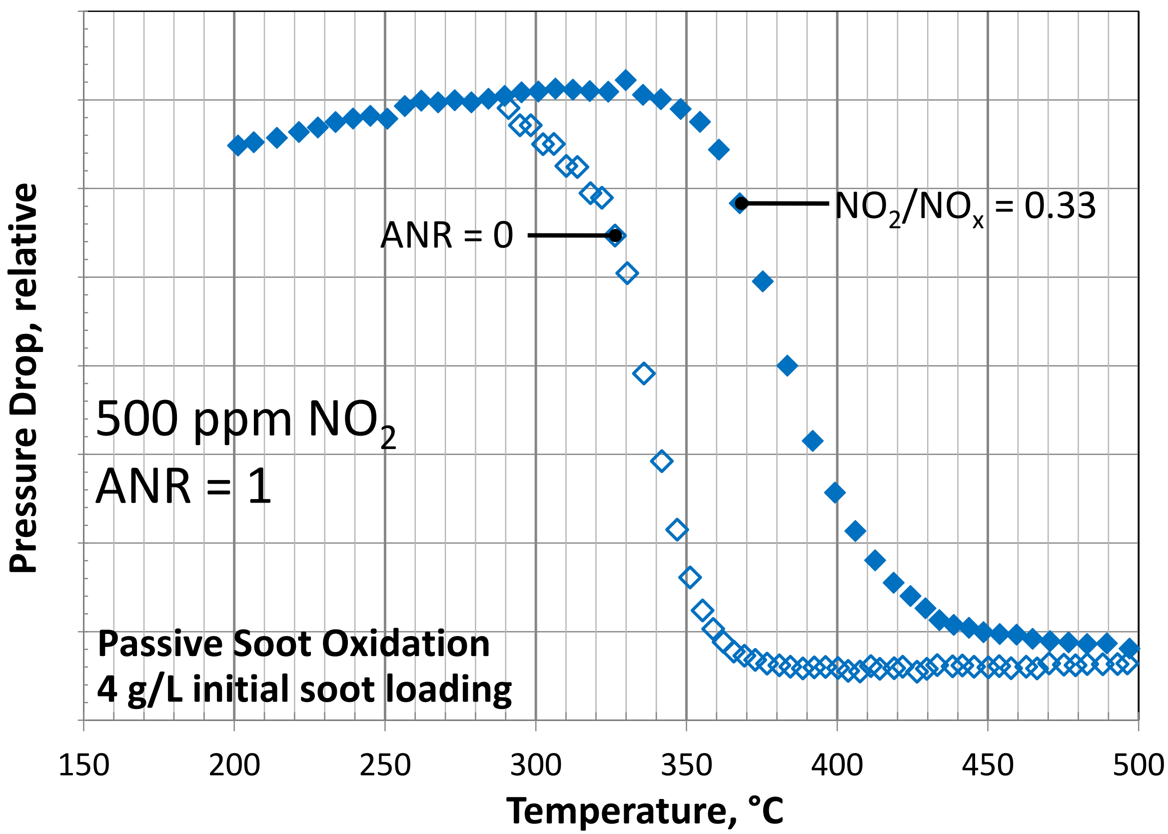


Increased NO_2 facilitates increased soot oxidation

Combined effect of more NO_2 and increased NO_2 fraction

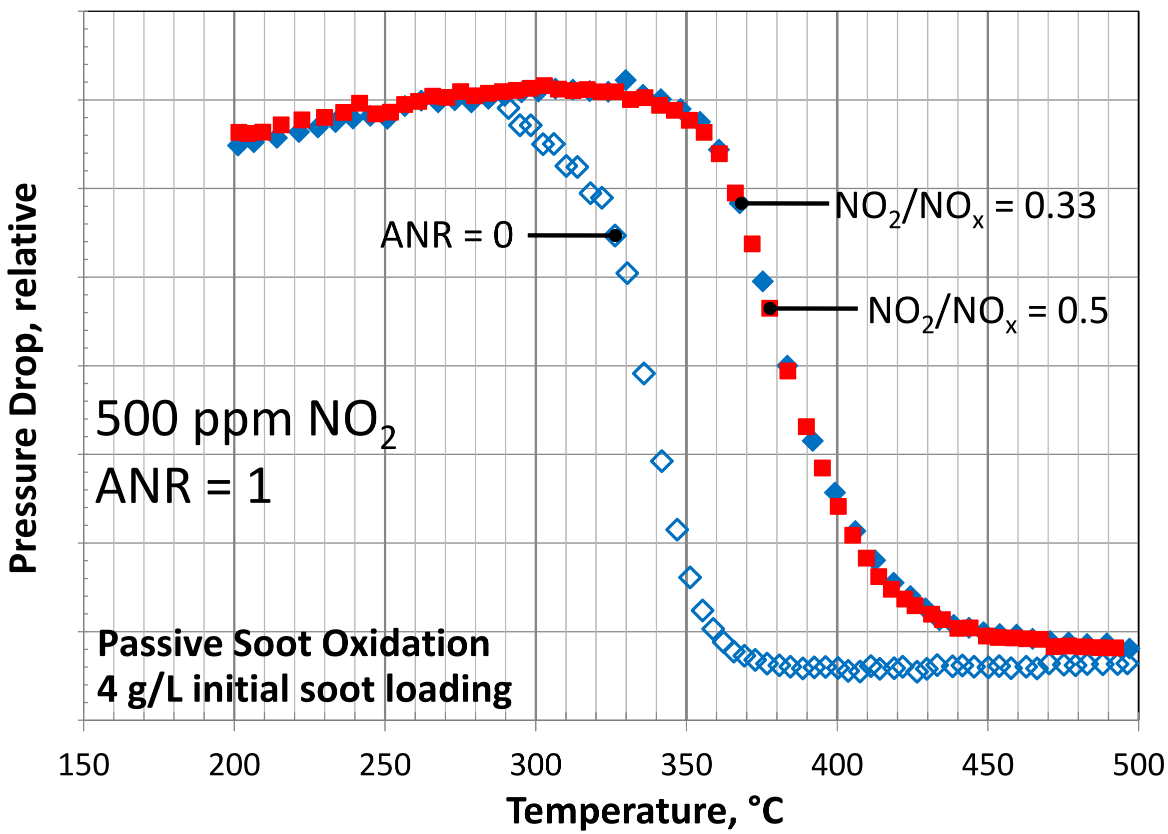
PASSIVE SOOT OXIDATION

- Separating NO_2 fraction



PASSIVE SOOT OXIDATION

- Separating NO_2 fraction
  - NO_2 constant, varying total NO_x



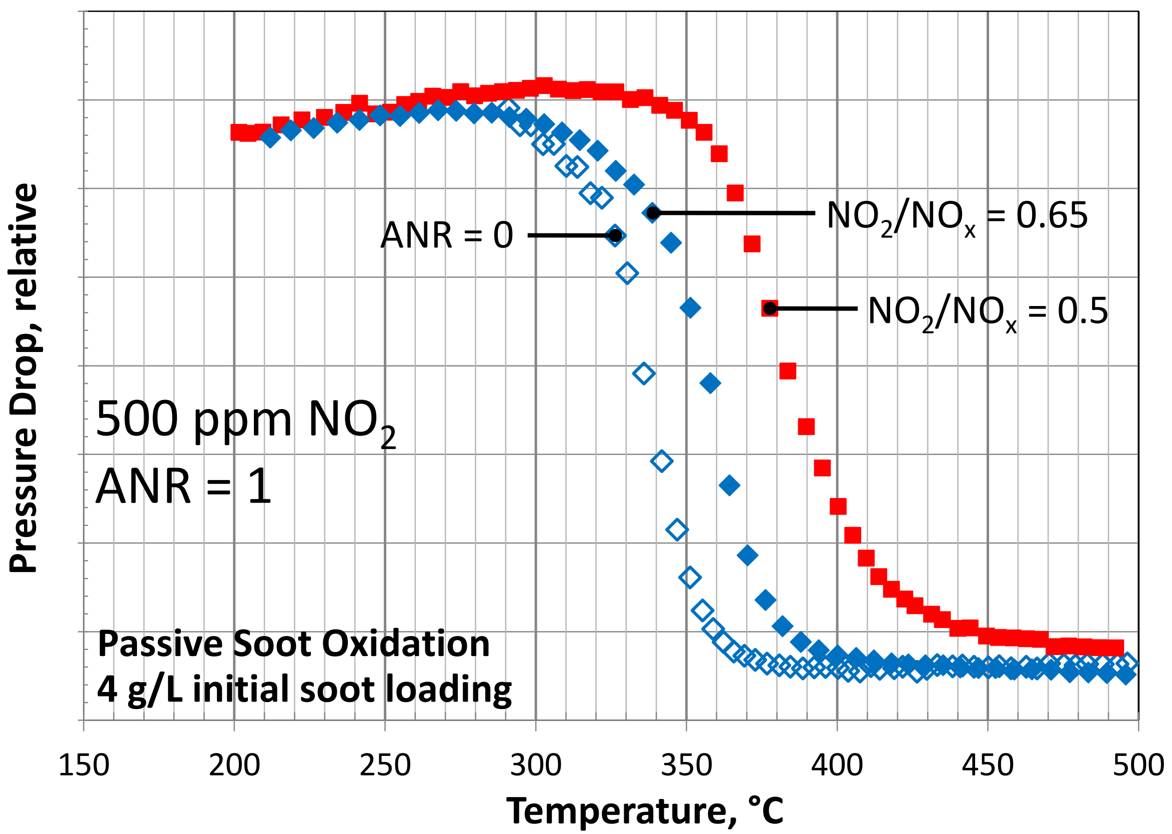
NO_2/NO_x 0.33 → 0.5

No improvement in passive oxidation

Pacific Northwest NATIONAL LABORATORY

PASSIVE SOOT OXIDATION

- Separating NO_2 fraction
  - NO_2 constant, varying total NO_x

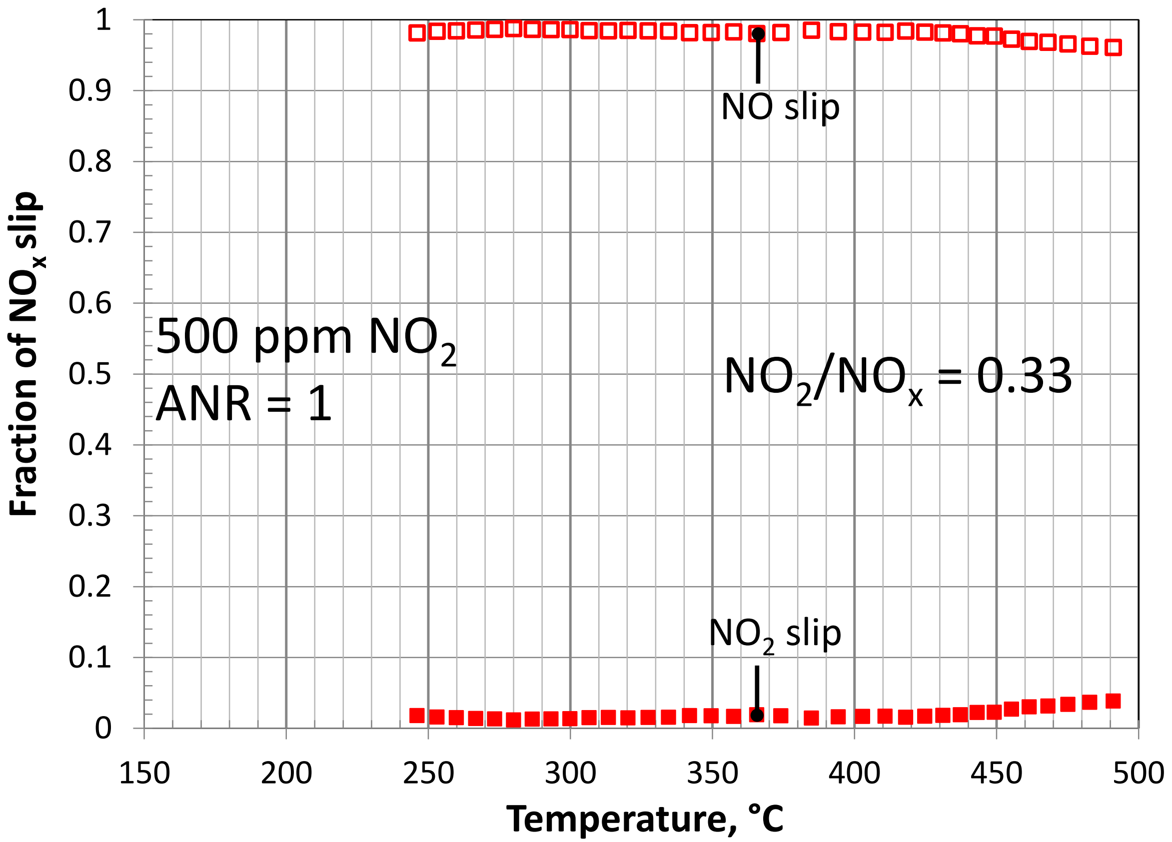


Fast SCR dominating

KEY:
Availability of NO_2 past equimolar $NO:NO_2$ reaction

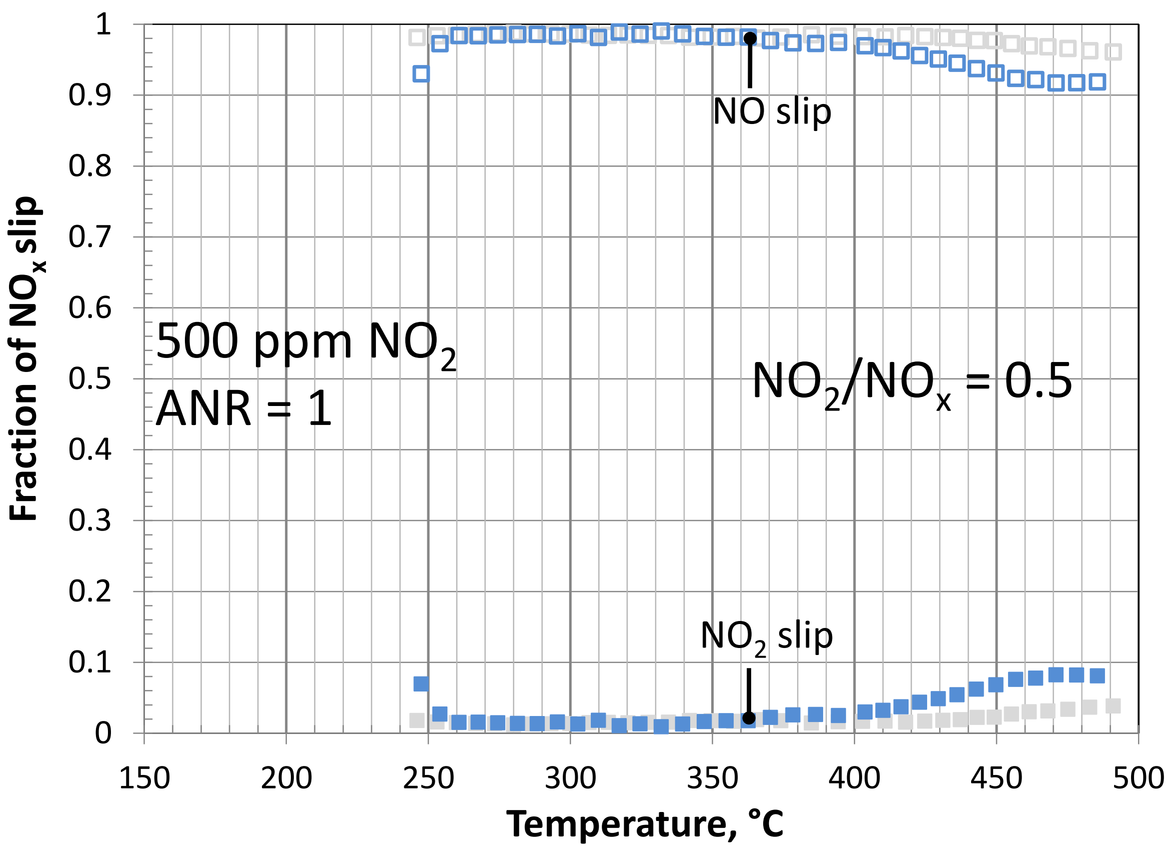
NO_x SLIP

- Separating NO_2 fraction
  - NO_2 constant, varying total NO_x



NO_x SLIP

- Separating NO_2 fraction
  - NO_2 constant, varying total NO_x

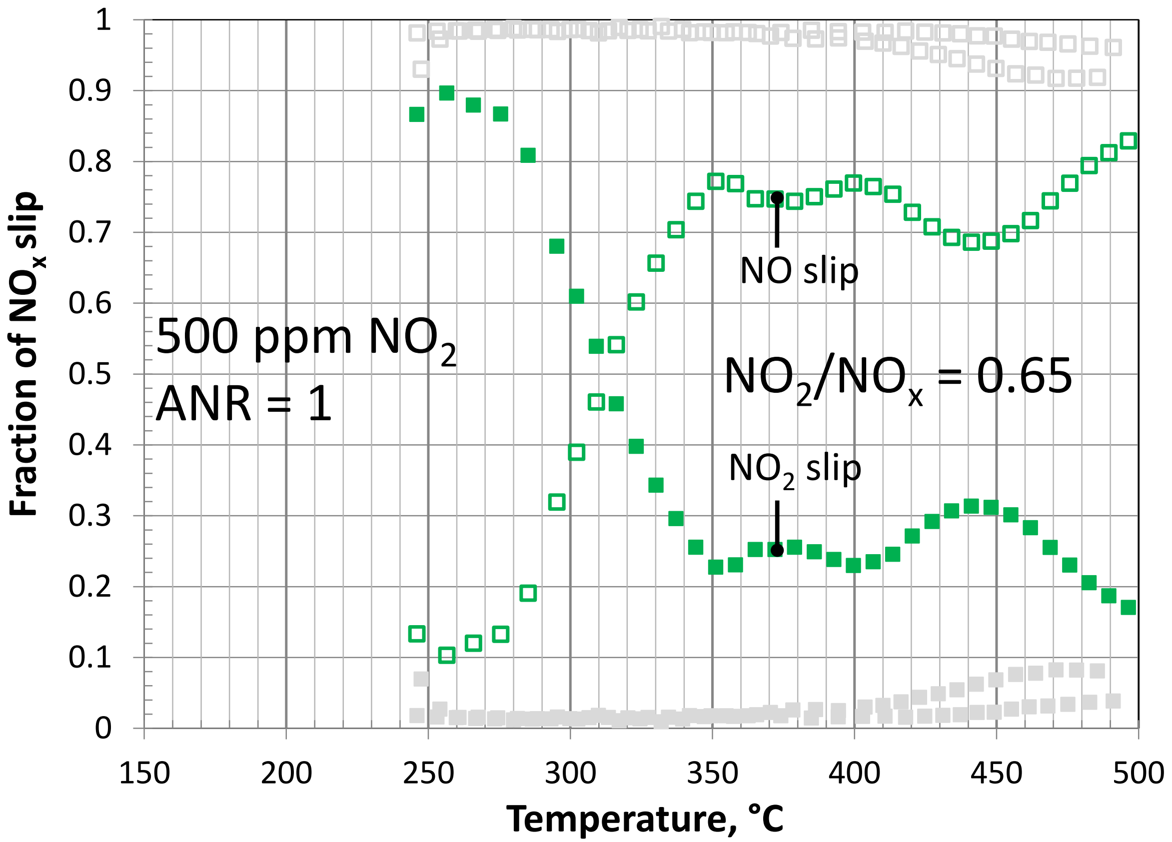


NO_2/NO_x 0.33 → 0.5 Extremely similar NO & NO_2 fraction of NO_X slip

Thus similar oxidation behavior

NO_x SLIP

- Separating NO_2 fraction
  - NO_2 constant, varying total NO_x

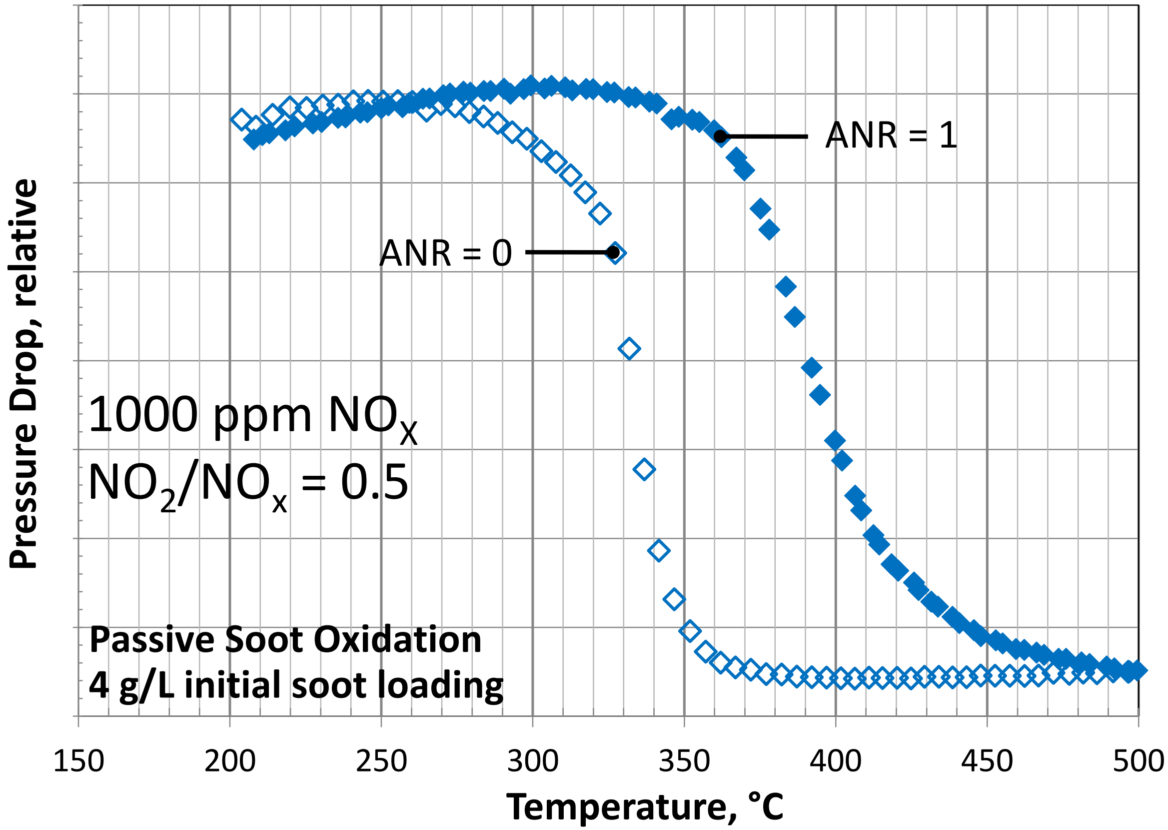


NO_2/NO_x 0.5 → 0.65 Increased NO_2 fraction of NO_X slip

Demonstrates NO_2 availability and subsequent key role in passive oxidation

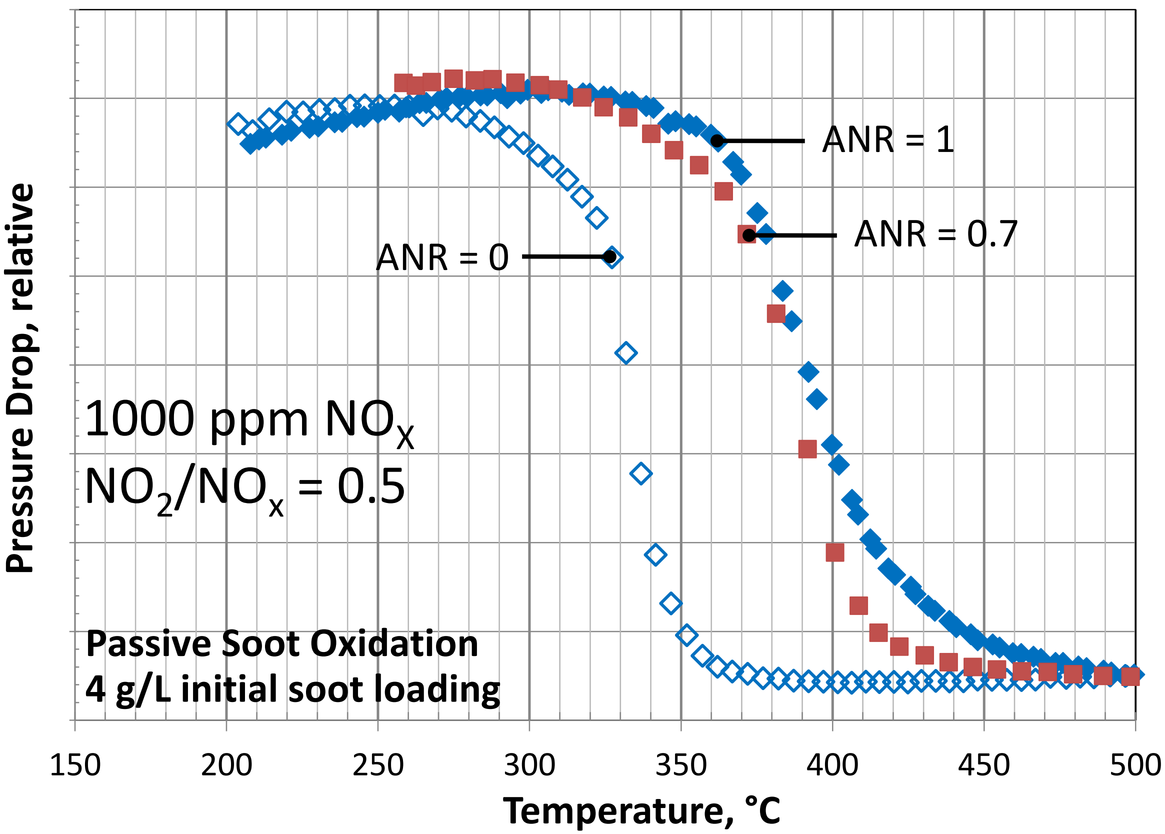
NH_3/NO_x RATIO

- Effect of decreased NH_3/NO_x ratio at NO_2/NO_x = 0.5



NH_3/NO_x RATIO

- Effect of decreased NH_3/NO_x ratio at NO_2/NO_x = 0.5



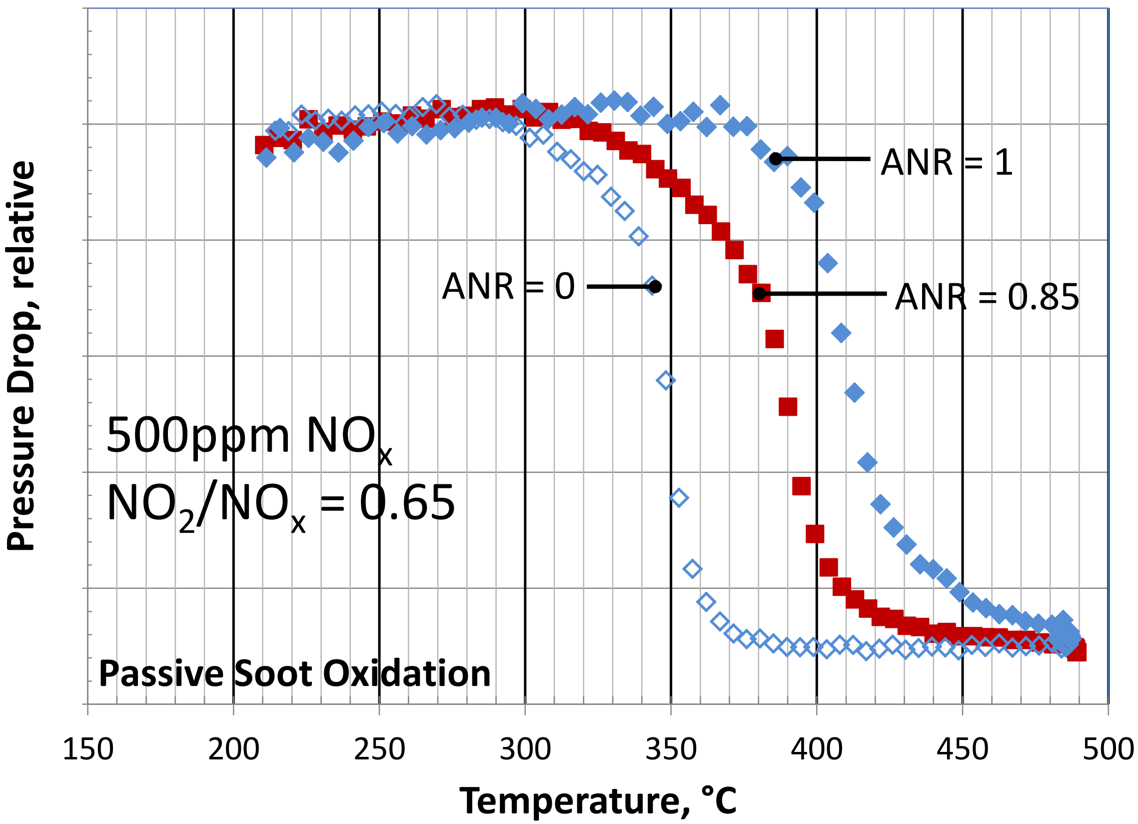
At NO_2/NO_x = 0.5

Soot oxidation affected little by decreased ANR

(supported by modeling and NO_2 concentration profile)

NH_3/NO_x RATIO

- Effect of decreased NH_3/NO_x ratio at NO_2/NO_x = 0.65



At NO_2/NO_x > 0.5

Decreased ANR facilitates greater soot oxidation

KEY:
NO_2 availability

SUMMARY DPF-SCR INTEGRATION

- Facilitating passive soot oxidation
  - **Reaction competition**: passive soot oxidation vs. SCR
  - KEY: NO_2 balance in the system, with the primary driver being the fast SCR reaction (equimolar NO & NO_2 consumption)
- Modeling can help guide us to develop an understanding of proper reactive and thermal management of SCRF
- Implementation & control – Truck & engine OEMs
  - Thermal management
  - DOC specification
  - etc.

ACKNOWLEDGEMENTS

- Work funded through DOE's Vehicle Technologies Program
- BASF – Heavy Duty Systems Development Group
- Corning
- Dr. Maruthi Devarakonda (formerly PNNL)
  - SCR kinetic model development

Pacific Northwest
NATIONAL LABORATORY