Cummins-ORNL\FEERC Emissions CRADA: NO_x Control & Measurement Technology for Heavy-Duty Diesel Engines

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Project ID: ACE032

2013 DOE Vehicle Technologies Program
Annual Merit Review
May16, 2013, Arlington, Virginia

U.S. DOE Program Management Team:
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Overview

Timeline

- New SOW start: Sept. 2012
- Current end date: Sept. 2015
- ~13% Complete

Budget

- 1:1 DOE:Cummins cost share
- DOE Funding:
  - FY2012: $450k
  - FY2013: $400k

Barriers

- *Emissions controls*
  - Catalyst fundamentals,
  - Reactions & mechanistic insights
  - Catalyst models (design tools & imbedded)
  - Control strategies & OBD
- Combustion Efficiency
  - Shift emissions tradeoff to fuel efficiency
- *Durability*
  - Enhanced durability via knowledge-based controls
- *Cost*
  - Lower catalyst & sensor costs
  - Lower development costs

Partners

- **ORNL & Cummins Inc.**
- Several informal collaborators

Objectives & Relevance

Elucidate Practical & Basic Catalyst Nature

for enabling improved Modeling, Design & Control

Objectives

- Develop diagnostics to advance applied & basic catalyst insights
- Understand parameters controlling distributed NH_3 storage
- Model distributed steady state SCR performance

Relevance – Detailed Catalyst Insights impact:

- Design models
- Control strategies & models
- NH_3 dosing control
- Required engineering margins (engine-efficiency vs. -emissions tradeoffs)
- System capital & operation costs

Milestones

✓**2012 Milestones:**

- Improve instrumental methods for transient analysis of catalyst state
  - Instantaneous NH_3 coverage & loading rate, instantaneous conversion

2013 Milestone (on target for Sept. 2013 completion):

- Assess distributed performance of degreened & field-aged commercial 2010 Cummins SCR catalyst samples with focus on mechanistic understandings
- Extend steady state distributed SCR model
  - Include transient & inhibition behavior
- Demonstrate & characterize NH_3 & Cu-oxidation-state sensor

Global Approach for Improving Energy Security

Develop & apply advanced diagnostics for catalyst characterization to improve: catalyst models, design, state assessment & *controls for fuel-efficient engine systems*

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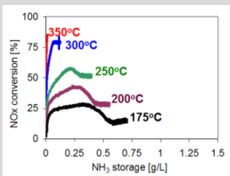
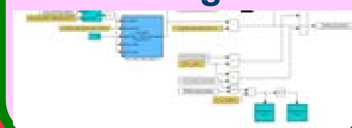
Catalyst Functional Behavior



Control & OBD Strategies



Proprietary Models
- For development
- For OBD

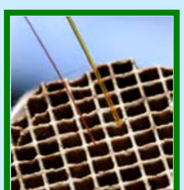
Clean,
Fuel-Efficient,
Durable
Engines in the Marketplace

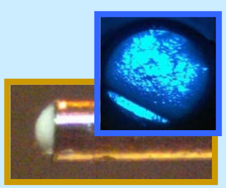
Cummins 2007 6.7L ISB

- ***Focus***
- ***Goals***
- ***Strategy***
- ***Analysis***

ORNL

Diagnostics & Method Development





Catalyst Insights
- Reaction network
- Mechanisms
- Catalyst state & control measures

Improve Models
- With collaborators
- Kinetic parameters
- Use models to study catalysis

Detailed Approach for 2013 Objectives

Spatiotemporal Intra-Catalyst Characterization

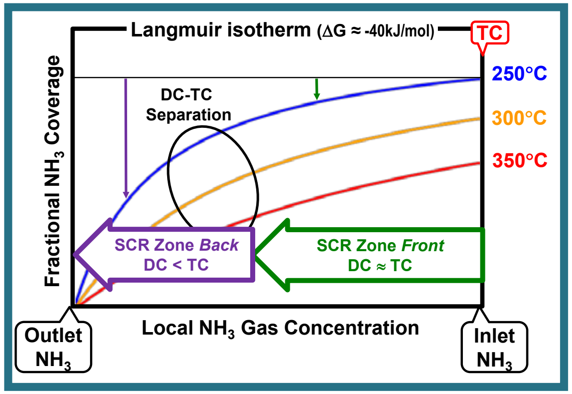
to Enhance Performance, Control, Cost & Durability

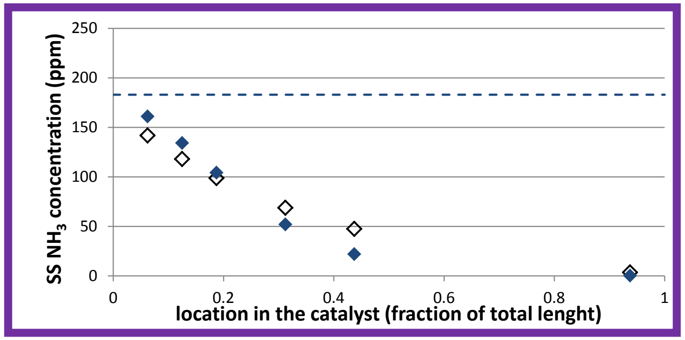
- Cummins-ORNL CRADA Team identifies catalyst-performance barrier
  - Distributed NH_3 capacity is not well understood & impacts performance
- Develop procedures to measure intra-SCR distributed NH_3 capacity
- Apply diagnostics to characterize distributed SCR performance
  - NH_3 capacity, SCR, parasitic NH_3 oxidation, NO & NH_3 oxidation
- Correlate distributed NH_3 capacity with other performance parameters
  - Compare insights with SpaciFTIR results from other DOE project
- Model distributed SCR behavior in collaboration with Chalmers partners
  - Based on AVL Boost
  - Determine kinetic parameters from SpaciMS data
  - Precompetitive model of distributed steady state SCR performance
- Incorporate insights into Cummins' proprietary models
- Enable clean, fuel-efficient engine-catalyst systems

Technical Progress: *Summary*

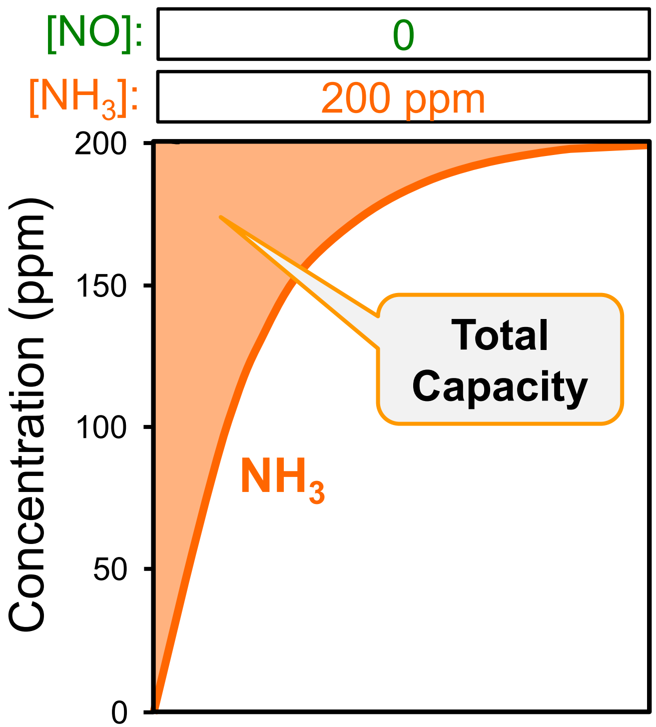
- **Nature of Distributed NH_3 Capacity *(New Insights)***
  - Correlating with distributed SCR conversion
  - on Model Cu-Beta Zeolite catalyst
  - on Commercial 2010 Cummins SAPO 34 catalyst
  - Control by Adsorption Isotherm

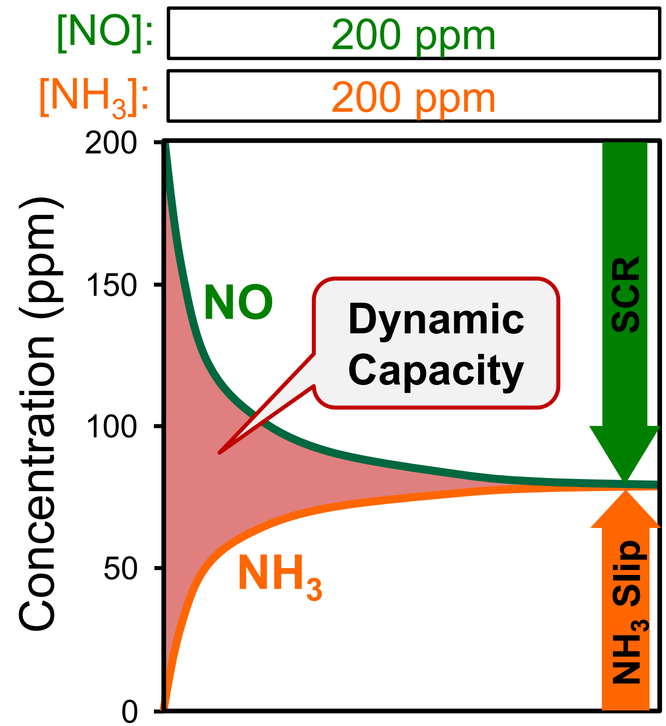
- **Modeling Distributed Steady State SCR Performance**
  - Determining kinetic parameters from SpaciMS data
  - Precompetitive AVL Boost distributed SCR model





Standard Protocols Resolve SCR Reaction Parameters





NH_3 Saturation

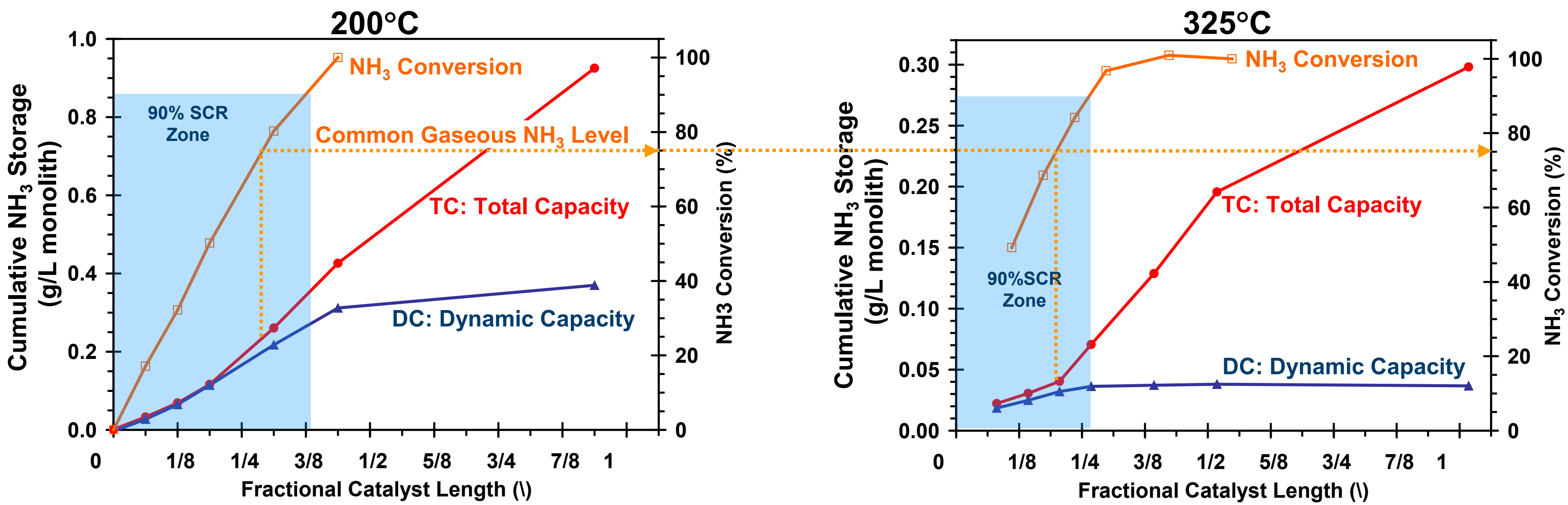
- ***Total NH_3 Capacity (TC)***
- Coverage at inlet conditions
  - Maximum NH_3 at inlet conditions
  - i.e., inlet NH_3 concentration & Temp.

SCR Conditions

- SS Conversion & NH_3 slip
- ***Dynamic NH_3 Capacity (DC)***
- ***DC: fraction of TC used for SCR***
- Unused Capacity (UC) = TC-DC

We will focus on: ***Total & Dynamic NH_3 Capacity***

NH_3 Coverage Distribution Imposed by Gas-Phase NH_3 Distribution

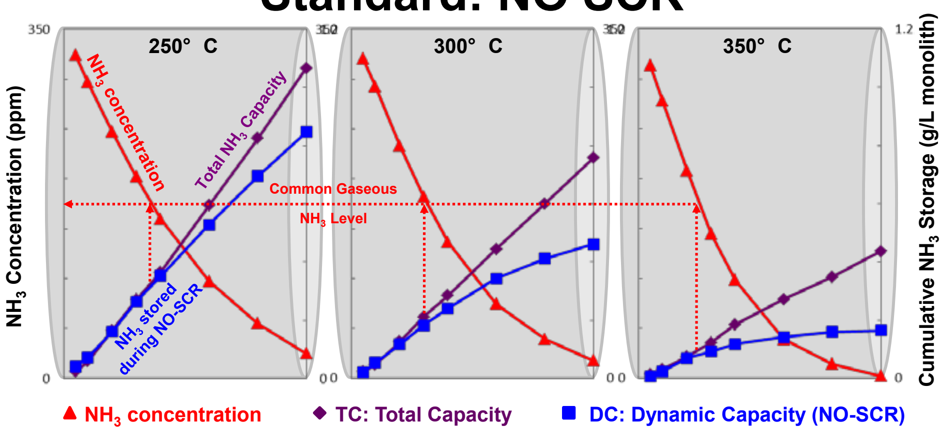


- Cu-Beta Zeolite catalyst, Standard SCR
- SCR zone shifts to catalyst front at higher temperatures
  - high NH_3 concentrations exist deeper into catalyst at lower temperature
- High NH_3 coverage at catalyst front where gas-phase NH_3 is high
  - Dynamic = Total capacity in high NH_3 concentration front section
- Dynamic-Total separation occurs at a *common NH_3 level* (ca. 50ppm NH_3)
- NH_3 coverage distribution changes with temperature
  - but Dynamic-Total capacity separation imposed by local gas-phase NH_3
  - & gas-phase NH_3 distribution is imposed by SCR conversion distribution

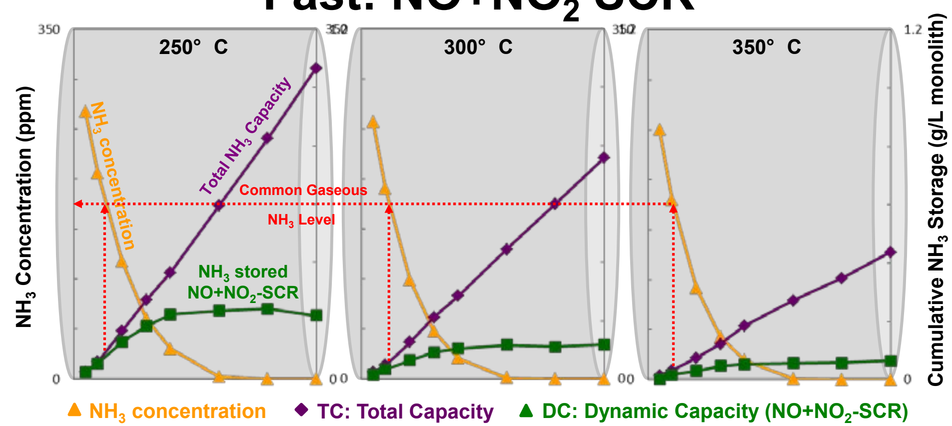
Cu-SAPO-34 Catalyst Shows Similar NH_3 Coverage Behavior

- Comparing CRADA insights to commercial catalyst behavior
  - Very different Model Cu-Beta-Zeolite & Commercial Cu-SAPO-34 catalysts
  - Validate & expand applicability of CRADA findings
- Dynamic = Total capacity above *same NH_3 level* for all conditions!
  - Separation at ~175ppm NH_3 for commercial catalyst (vs. ~50ppm for Cu-Beta-Z)
  - A case where Standard & Fast SCR are similar!
  - NH_3 coverage equilibrium reactions much faster than even Fast SCR
- **Local gas-phase NH_3 & Adsorption Isotherm control local NH_3 coverage**
  - SCR imposes gas-phase NH_3 distribution & local NH_3 concentration
  - Local gas-phase NH_3 & adsorption isotherm dictate local NH_3 coverage
  - NH_3 coverage distribution specified by gas-phase NH_3 distribution & isotherm

Standard: NO SCR

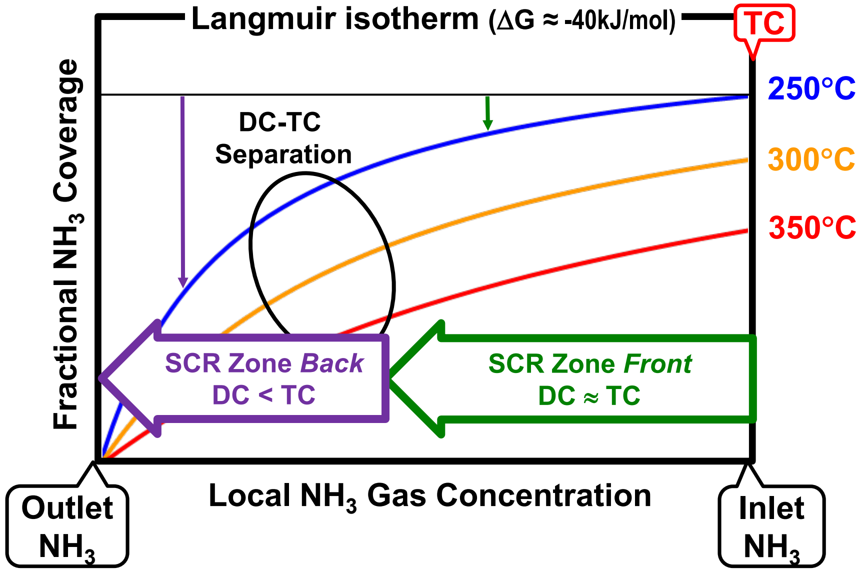


Fast: $NO+NO_2$ SCR



SpaciFTIR data from Michigan Tech DOE Project

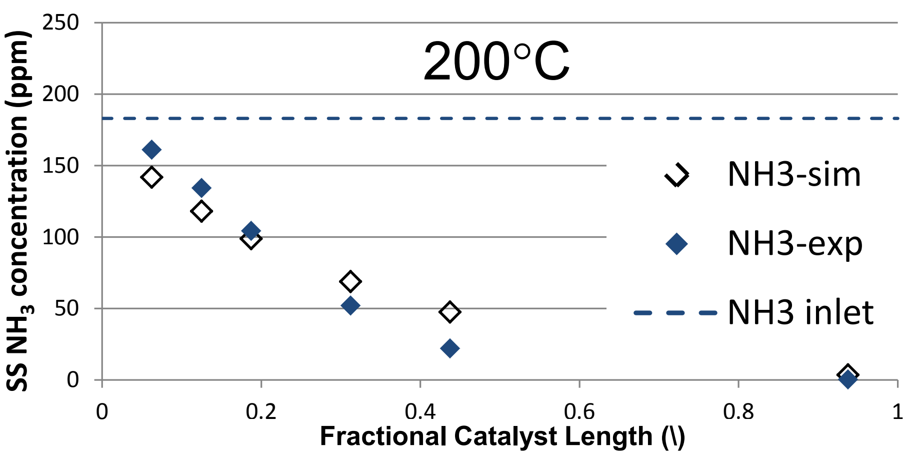
Isotherm & Gas-Phase NH_3 Distribution Set NH_3 Coverage Distribution

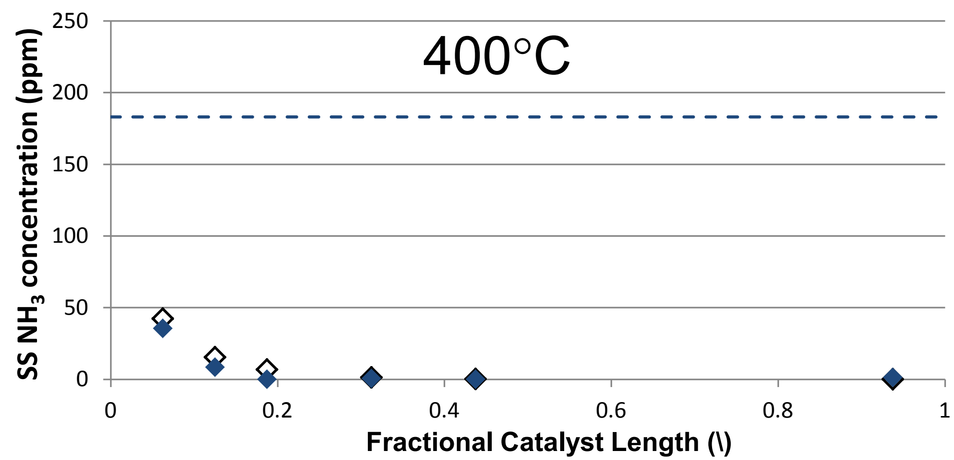


- Adsorption isotherm indicates equilibrium-coverage variation with NH_3
  - Total capacity measured at inlet NH_3, and decreases at higher temperatures
- Coverage variation is relatively flat in high-NH_3 region
  - practically: Dynamic ≈ Total capacity in this region
- Dynamic & Total capacity should separate around the isotherm knee
- SCR reduces the gas-phase NH_3 concentration along the catalyst length
  - lower local coverage equilibrium, Dynamic < Total capacity
- Specific SCR reaction does not change the isotherm
  - only changes where these zones occur spatially within the catalyst
- Adsorption isotherm shape varies with catalyst formulation
  - E.g., different NH_3 site types, coverage dependence,..

Intra-Catalyst Measurements Enable Calculation of Kinetic Parameters under Realistic Operating Conditions

- Based on KCK Cu-Beta-Zeolite catalyst & Standard SCR
- Kinetic parameters determined from steady state Intra-SCR SpaciMS data
  - NO oxidation, NH_3 oxidation, NH_3 Standard SCR (published in Coelho thesis)
  - Further demonstrates rich nature of intra-catalyst distributed (SpaciX) analysis
  - ***Enables determining kinetic parameters under realistic conditions***
  - Avoids unrealistic temperatures &/or space velocity where chemistry may differ
- AVL BOOST model in good agreement with experimental measurements
  - Distributed NO & NH_3 oxidation, & SCR
  - Kinetic & equilibrium controlled temperature regimes
  - Zero Parasitic Oxidation despite significant neat NH_3 oxidation



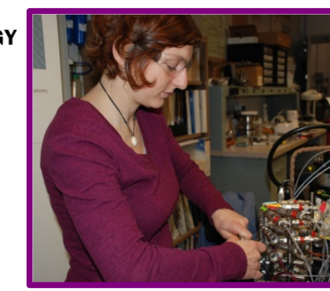


Modeling performed at Chalmers KCK in Louise Olsson Group
Filipa Coelho: Erasmus Programme MS Student

Collaborations & Coordination

- **Cummins**
  - CRADA Partner, Neal Currier (Co-PI)
- **Chalmers (Prof. Olsson)**
  - SCR measurements, kinetic analysis & modeling (Xavier Auvray & Filipa Coelho)
- **Michigan Tech. University (Prof. Parker)**
  - SpaciFTIR analysis of Cummins 2010 SCR catalyst (Josh Pihl)
- **Politecnico di Milano (Profs. Tronconi & Nova)**
  - Precompetitive study of selected SCR mechanisms
  - Prof.s Tronconi & Nova to ORNL Oct. 15, 2012
  - PoliMi PhD student working at ORNL Oct.-March, 2012 (Maria Pia Ruggeri)

- **CLEERS (ACE022, Wednesday 2:15pm)**
  - Diagnostics, analysis & modeling coordination
- **Institute of Chemical Technology, Prague (Prof. Marek & Dr. Kočí)**
  - Precompetitive study of LNT N_2O chemistry (with CLEERS)
  - KONTAKT II Grant from Czech Republic Government
  - Dr. Kočí working at ORNL April 16-20, 2012
  - ICTP PhD student working at ORNL Oct.-Dec., 2012 (Šárka Bártová)



- **Dissemination via Publications & Presentations**
  - 1 Archival Journal Publication & 12 Presentations

Future Work

2013 Work:

- Measure distributed chemistry of commercial SCR
  - degreened & field-aged 2010 Cummins SCR samples
  - Standard & Fast SCR; 200, 300 & 400°C
- Extend steady state distributed SCR model (w/ Chalmers)
  - Include transient & inhibition behavior
- Investigate mechanistic aspects of selected SCR reactions (w/ PoliMi)
- Continue collaborations with CLEERS, PoliMi, ICT Prague & Chalmers
- Demonstrate & characterize NH_3 & Cu-oxidation-state sensor

2014 Work:

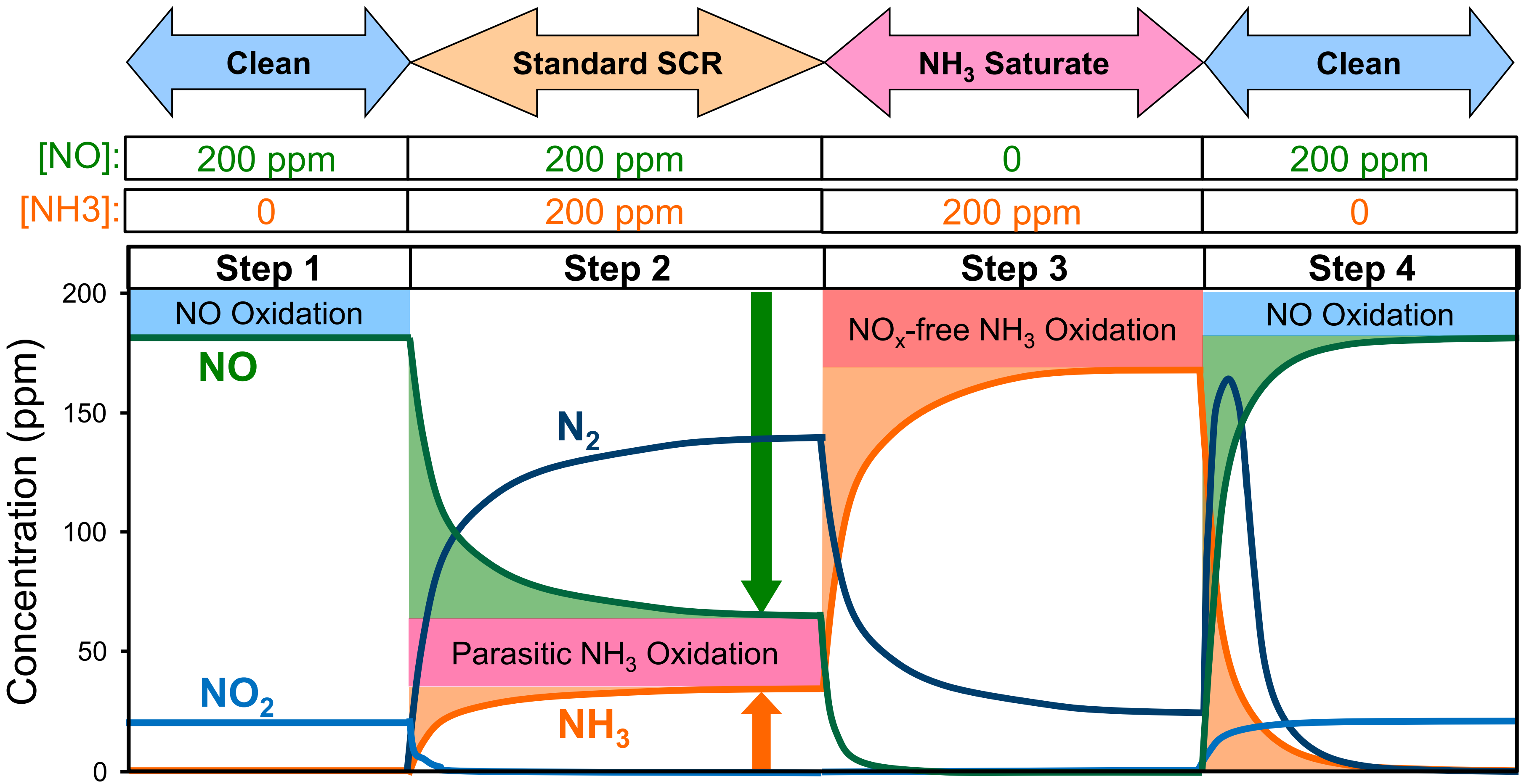
- Measurements to further understand commercial SCR performance
  - Alternate, incremental and various methods for ageing
  - Focus on insights for improved modeling, design and control
- Exercise SCR model to understand selected inhibition nature

Summary

- **Relevance**
  - CRADA work enables improved catalyst knowledge, models, design & control
  - This reduces catalyst system costs & required engine-efficiency tradeoffs
  - This in turn enables improved fuel economy
- **Approach**
  - Develop & apply diagnostics to characterize catalyst nature
  - Analyze data to understand mechanistic details of how the catalyst functions
  - Develop improved catalyst models based on improved catalyst knowledge
- **Technical Accomplishments**
  - New insights regarding parameters controlling distributed NH3 coverage
  - SpaciX data allows determining kinetic parameters under realistic operating conditions
  - Steady state distributed SCR model accurately predicts catalyst performance
- **Collaborations**
  - Numerous university collaborations resulting in presentations, publications and advances
  - Coordination & collaboration with other DOE projects to maximize benefit
- **Future Work**
  - Analysis & tuning of EGR mixing model – identify mixing and model-data difference origins
  - EGR Probe Improvements : interference identification & probe-to-probe variations
  - Diagnostic identification & development for addressing next-generation efficiency barriers

Technical Back-Up Slides

Cummins 4-Step Protocol Resolves Reaction Parameters



- Step1: NO oxidation
- Step2: SS NO_x & NH_3 conversions, Parasitic NH_3 oxidation, Dynamic NH_3 capacity
- Step3: NO_x-free NH_3 oxidation, Unused NH_3 capacity
- Step4: NO oxidation, Total NH_3 capacity

Total = Dynamic + Unused