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

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U.S. DEPARTMENT OF ENERGY
Cummins
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Overview

Timeline

- Start: FY1998
- Major Revisions: 2001, 03, 06, 10
- Current term: 2010-’12 revision
- Current end date: Sept. 2012
- ~80% Complete

Budget

- 1:1 DOE:Cummins cost share
- DOE Funding:
  - FY2010: $400k
  - FY2011: $450k
  - FY2012: $450k

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.**
- Chalmers Univ. of Technology
- Politecnico di Milano

Objectives & Relevance

- **Quantify & correlate transient SCR performance distributions**
- **Improved methods & tools for enhanced analysis**

Enabling & Applications for:

- Better understanding of how catalyst operating & mechanistic insights
- Improved SS & dynamic catalyst simulations
- Better development tools
- Methods & ideas for improved control (OBD) & catalyst-state assessment
- Better vehicles for consumers:
  - ***Higher Efficiency:*** *lower engineering margins via better design & control*
  - ***Lower Emissions:*** *better design tools, models, controls & OBD*
  - ***Improved Durability:*** *advanced controls for extended catalyst lifetime*
  - ***Lower Cost:*** *Analysis-led design, fewer & lower-$ sensors, urea utilization*

Milestones

2011 Milestone:

- ✓ Dynamic analysis of SCR-catalyst performance
  - NH_3 capacity distributions

2012 Milestones (on target for Sept. 2012 completion):

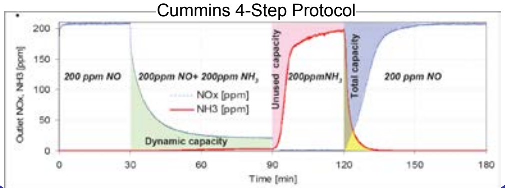
- Improve instrumental methods for transient analysis of catalyst state
  - Instantaneous NH_3 coverage & loading rate, instantaneous conversion
- Characterize spatiotemporal performance of Cummins Commercial SCR catalyst (SAPO-34)

Approach *for addressing SCR Control Challenges*

ORNL

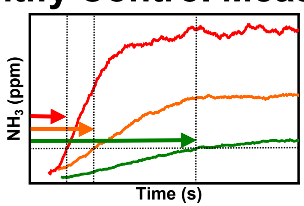
Catalyst Knowledge

Evaluate static & dynamic catalyst nature



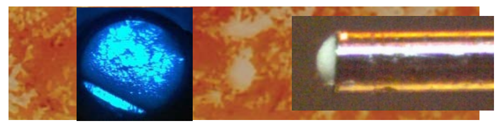
Understand chemical & spatiotemporal relationships

Identify Control Measures



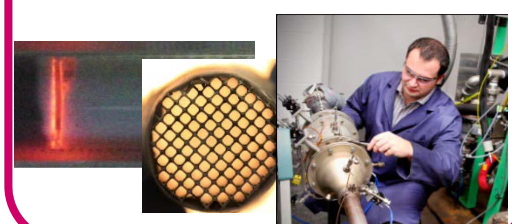
Diagnostic Tools

Develop diagnostics



Prioritize high-potential diagnostics

Bench & engine evaluation



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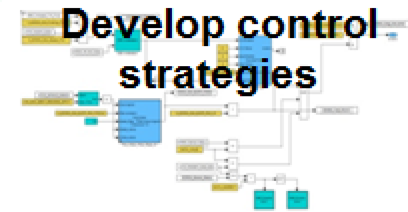
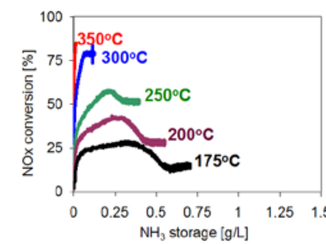
System Integration

Develop control strategies



Develop OBD strategies

Elucidate catalyst functional behavior



Improve models

Understanding + Diagnostics for Real-Time Catalyst Control

Improved Fuel Economy, emissions & catalyst durability

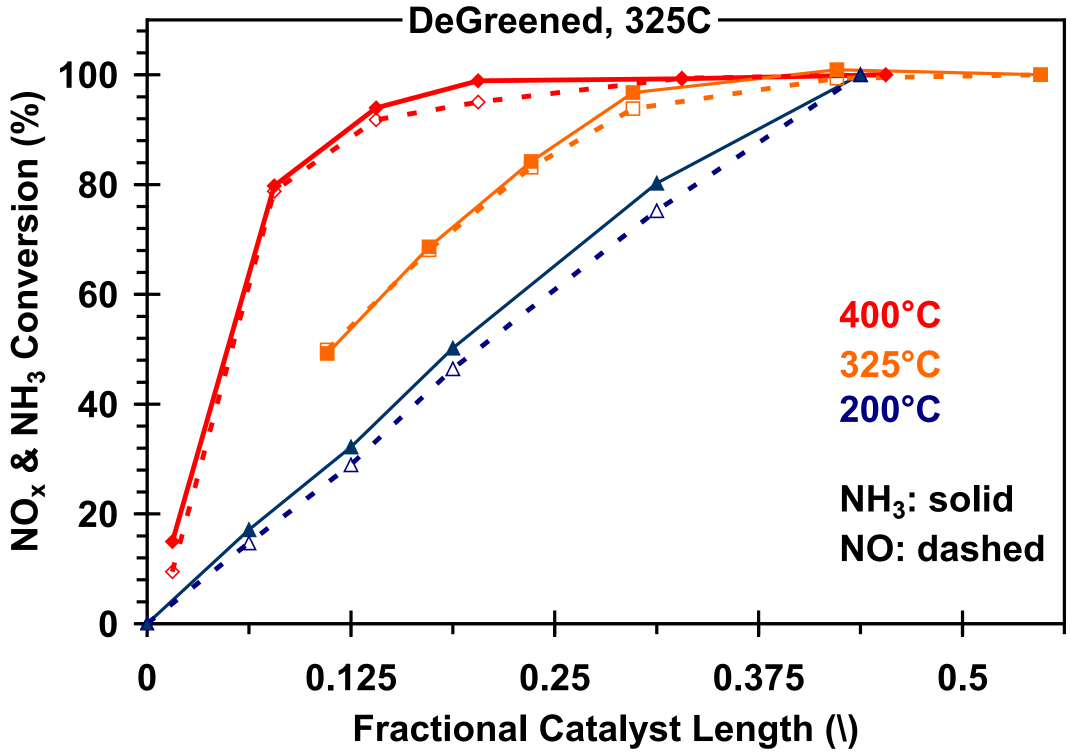
Improve models & designs

Technical Progress: *Summary*

- **Temperature impact on SCR performance**
  - SCR Zone
  - Parasitic NH_3 Oxidation

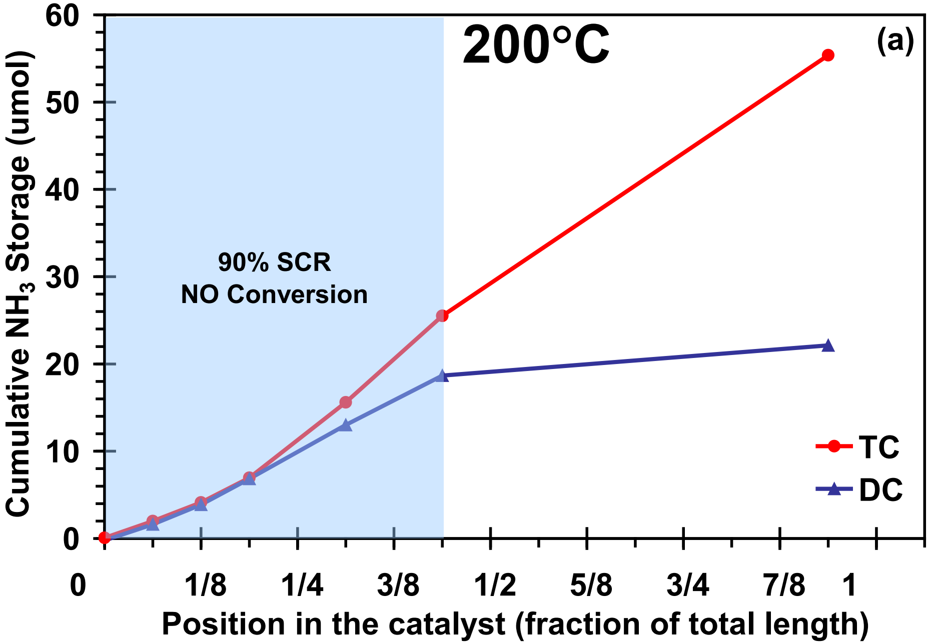
- **NH_3 Capacity Distributions** ***(New Insights!)***
  - Correlation w/ SCR zone
  - Control implications
- **Hydrothermal Ageing**
  - Correlations w/ DeGreened results
  - Mechanistic implications
- **Dynamic & SS NH_3 Inhibition** ***(New Insight for Cu Zeolite catalyst!)***
  - Location of Dynamic Inhibition
  - Mechanistic implications

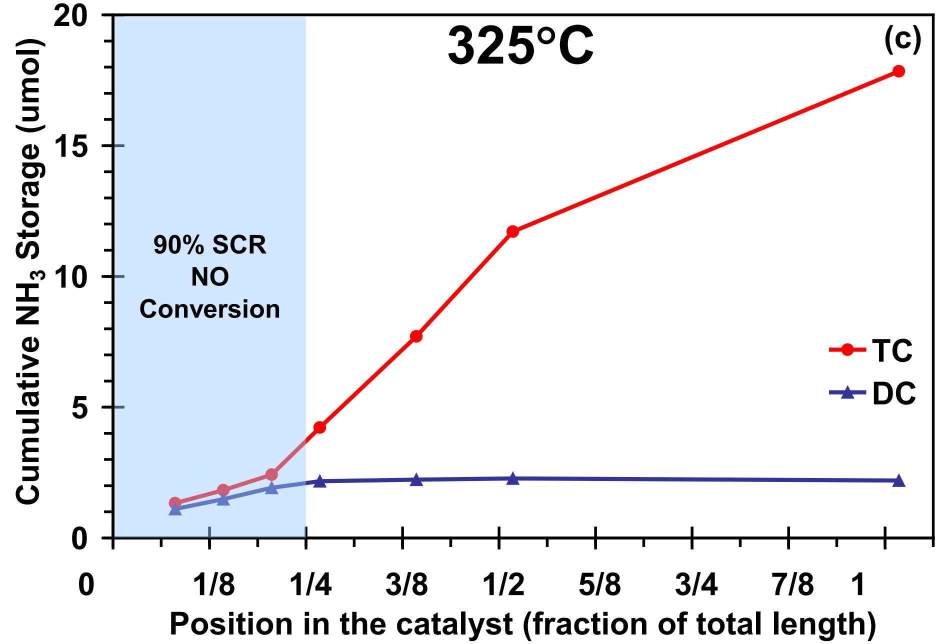
Technical Progress: *Temperature-Induced SCR Shifts*



- SCR zone shifts to catalyst front w/ increasing temperature
  - Major internal variations despite same 100% integral conversion
  - High NH_3 levels survive deeper into catalyst at lower T
- Negligible Parasitic NH_3 Oxidation
  - Despite significant NO_x-free NH_3 oxidation
  - i.e., SCR rate greater than O_2 + NH_3 rate

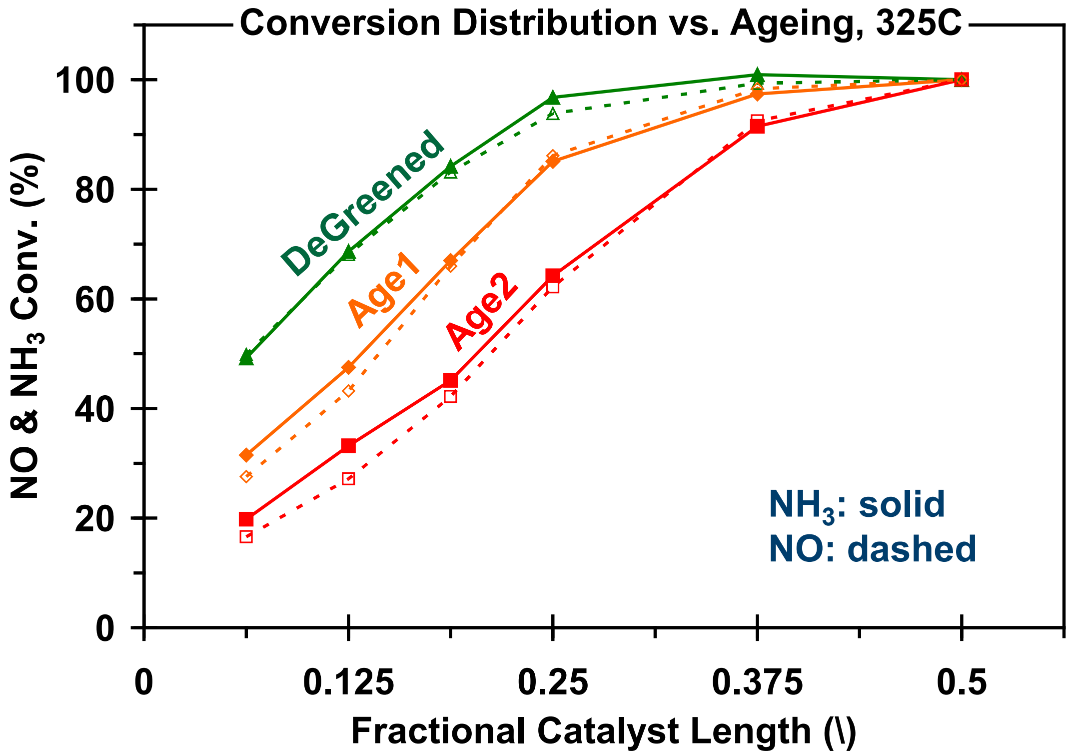
Technical Progress: *100% NH_3 Coverage in SCR Zone*





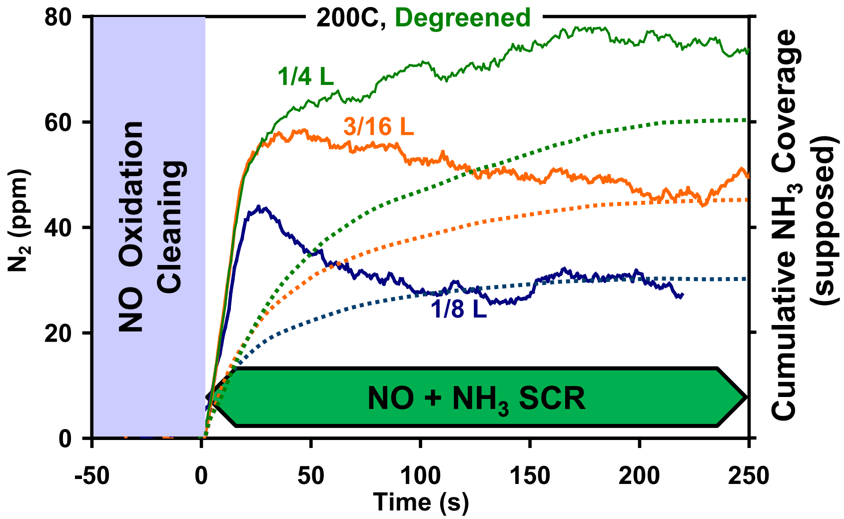
- Various components to NH_3 capacity
  - Dynamic (DC): capacity used in SCR
  - Unused (UC) and Total (TC) capacity
  - TC = DC + UC
- ***DC = TC in SCR zone***
  - Saturated surface NH_3 in SCR zone
  - Implies UC=0 in SCR zone
  - Corroborated by UC measurements
- DC plateaus after SCR zone
  - Because NH_3 is fully consumed
- DC & UC indicate catalyst use
  - DC/TC: fraction used for SCR
  - UC/TC: unused fraction of catalyst
  - ***Can use for effluent analysis & catalyst control!***

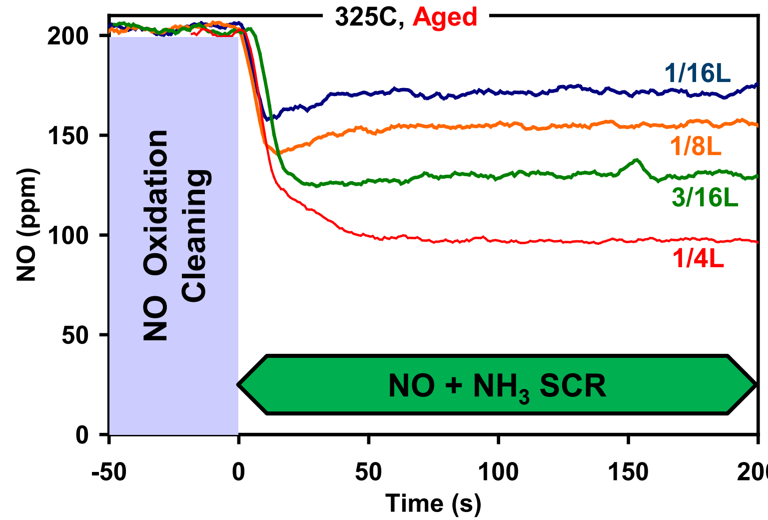
Technical Progress: *Hydrothermal Ageing Spreads SCR*



- Same integral 100% conversion
- Negligible Parasitic NH_3 oxidation
- TC decreases w/ Hydrothermal Ageing
- Similar NH_3 capacity observation
  - ***DC=TC in SCR zone***
- Slower SCR w/ ageing
  - More catalyst required
  - Consistent w/ active site loss
  - ***Generally follows TC degradation***
  - ***Suggests SCR dominated by available NH_3 coverage***

Technical Progress: *Dynamic Inhibition when NH_3 is High*





- Dynamic inhibition indicates threshold NH_3 coverage for inhibition onset
  - Conversion inflection indicates SCR slowing w/ continued NH_3 coverage buildup
  - NH_3 coverage continues to grow beyond inflection point
  - Occurs when coverage buildup is fast
    - i.e., when $NH_{3\ (gas)}$ concentration is high
    - Observable when at these points (usually within the catalyst)
- Can get to SS inhibited condition w/o passing through dynamic
  - Because low [NO] & slow (low) NH_3 coverage buildup
- Important for catalyst model & controls development
- Need improved temporal resolution of analytical methods

Collaborations & Coordination

- **Cummins**
  - CRADA Partner, Neal Currier (Co-PI)
- **Prof. Louise Olsson, Chalmers**
  - SCR measurements & analysis (Xavier Auvray)
  - Modeling steady state distributed SCR performance (Filipa Coelho)
- **Prof. Enrico Tronconi & Isabella Nova Politecnico di Milano**
  - Mechanistic investigation of selected SCR reactions
  - Plan for 6-month ORNL visit in CY2012 (Maria Pia Ruggeri)
- **CLEERS**
  - Diagnostics, analysis & modeling coordination
- **Prof Milos Marek & Dr. Petr Kočí, Prague Institute of Chemical Technology**
  - LNT modeling N_2O chemistry
  - KONTAKT II Grant from Czech Republic Government
  - Petr to ORNL April 17-20
- **Dissemination via Publications, Presentations and Patents**
  - 10 Presentations & 1 Major Award in 2011

Future Work

2012 Work:

- Model instrument response for improved transient analysis
- Characterize spatiotemporal performance of Cummins commercial catalyst
  - NH_3 capacity utilization, Parasitic oxidation, inhibition, transient analysis
- Transient analysis of model & commercial catalyst
  - Evolution & instantaneous SCR conversion, NH_3 coverage (w/ Chalmers)
- Modeling steady state SCR conversion distributions (w/ Chalmers)
- Investigate mechanistic aspects of selected SCR reactions
  - Experimental & numerical, reported to CLEERS (w/ Politecnico di Milano)

2013 Work:

- Impact of conditions on spatiotemporal SCR performance
  - NH_3:NO_x, NO:NO_2, HC
- Extend SS distributed SCR model to include transient performance
- Demonstrate diagnostics for SCR-state characterization
- Correlate control relationships w/ performance parameters
  - Identify strategies for SCR-catalyst control & diagnostics

Summary

- CRADA approach effectively addresses major DOE & Cummins goals
  - Insights for better SCR understanding, models & control
  - Advanced diagnostics to elucidate the same
  - Enabling improved SCR ***efficiency, cost and durability***
- Analytical methods improved to allow transient analysis (DC, TC & UC)
  - Further improvements planned for 2012
- New CRADA insights improve understanding of SCR performance & control
  - NH_3 coverage is saturated over SCR zone
    - DC & UC indicate portion of the catalyst Used & Unused for SCR
  - Dynamic NH_3 inhibition occurs at the catalyst front
    - Due to high $NH_{3\ (gas)}$ causing fast NH_3 coverage buildup rate
- Leveraging collaborations to strengthen CRADA & enhance value
  - Modeling distributed steady state SCR performance w/ Chalmers
  - Studying SCR reaction mechanisms w/ Politecnico di Milano ***(cf. 2011 Review feedback)***
  - Improving analytical methods w/ CLEERS
- Future work focuses on:
  - Commercial Cummins SCR catalyst
  - Better transient analysis to elucidate dynamic performance of realistic drive cycles
  - Modeling transient SCR performance
  - Insights & diagnostics to demonstrate and enable advanced control strategies