SwRI Proposal No. 03-83490
Submitted April 2018

A Proposal for
AC²AT-II

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

A Consortium of SwRI

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EXECUTIVE SUMMARY

SwRI is proud to propose a four-year Cooperative Research program entitled "Advanced Catalyst and Aftertreatment Technologies-II", also known as "AC^2AT-II". This four-year cooperative joint industry program will be a continuation of the previous four years of SwRI's successful AC^2AT program, which focuses on aftertreatment simulation tools and catalyst and emissions control technologies for advanced internal combustion engines. The program provides an avenue for research in catalyst and aftertreatment systems for advanced combustion technologies that enable improved fuel efficiency while meeting stringent criteria pollutant regulations. The proposed program supplements work being performed globally to develop new engine and combustion technologies to achieve the newly enacted greenhouse gas emissions and fuel economy standards.

The overall goal of the AC^2AT-II consortium is to enable the development of cost-effective solutions for future engine systems by identifying and addressing the opportunities and challenges for integration of catalysts and aftertreatment systems to engines with advanced combustion technologies. The proposed consortium will include clients representing catalyst formulators, substrate and component manufacturers, emission control system integrators, engine and vehicle manufacturers, and simulation software providers. The focus of the program will be to develop the tools and technologies necessary for the synergistic application of catalysts to advanced engine technologies. This consortium will provide a collaborative environment for the fundamental evaluation of advanced combustion engine emissions and novel catalyst technologies.

The proposed four-year program incorporates projects focused in four distinct areas:

- Development of aftertreatment simulation tools
- Low temperature catalyst design
- Advanced aftertreatment system integration
- Catalyzed urea water solution (UWS)

The program will be managed by SwRI with direction and oversight provided by a Program Advisory Committee (PAC), consisting of one representative from each of the member companies. The PAC members are encouraged to provide input at any time, and regular monthly conference calls will be organized by SwRI, to aid in this process. In addition, SwRI will organize meetings of the PAC on regular four-month intervals to summarize results, plan test execution, and vote for future research efforts. SwRI will also maintain a secure website where the members can log in to access and download the regular monthly progress reports and special progress reports, as they are completed by the SwRI Project Team. The annual cost for the four-year program is $95,000 per year for OEMs and suppliers. The program will commence on 16 November 2018 or when twelve members have agreed to participate, and end on 15 November 2022 or four years after the start date.

INTRODUCTION

SwRI has a strong history of leading cutting edge, industry focused engine research consortia. The longest running consortium led by SwRI is the Clean High Efficiency Diesel Engine (CHEDE-VII) consortium. This consortium focuses on compression-ignited combustion engines, and is in its 25th year.

The HEDGE (High Efficiency Dilute Gasoline Engine) Consortium was begun in 2005. With the advent of new, lower emissions levels (fuel-neutral Tier III, Euro 6d, feasibility of an ultra-low NO_X standard for US HD, and others), the additional cost of lean aftertreatment devices and their associated efficiency penalties were eroding some of the advantages that diesel engines have typically enjoyed in the area of fuel efficiency. Similar to CHEDE-VII, the focus of HEDGE-IV is on combustion and engine related technologies and there are no tasks focused on emissions control system development.

The AC^2AT consortium began in November 2014 and was designed to address the challenges and opportunities associated with the integration of catalysts and aftertreatment systems on the advanced combustion engines being developed as part of the CHEDE-VII and HEDGE-III consortia, in addition to other novel combustion concepts which are being developed by outside parties. Another major focus of AC^2AT was the development of simulation tools to predict urea deposit formation within exhaust systems. The success of the cooperative research and milestones achieved in emissions technology are the driving force for the continuation of this consortium.

The proposed goals for the AC^2AT-II consortium, as outlined in Table 1, stems from increased global demands for cleaner emissions, various industry aftertreatment applications, collaborative contributions and input from current and potential AC^2AT participants, new government regulations, and SwRI's drive to be the leader in developing new and innovative technologies that lead to clean and efficient emissions systems for the industry.

Table 1: Goals of AC^2AT-II Consortium

- Develop aftertreatment system simulation tools that accurately simulate full aftertreatment system performance
- Define the requirements for emissions control from advanced combustion engines
    - Identify synergistic aftertreatment technologies for emissions control
    - Quantify impact of alternative combustion modes on state-of-the-art emission control technologies
- Propose and evaluate novel catalytic solutions for emissions control from advanced combustion engines
- Improve fuel efficiency of stoichiometric engines by 5% through thermo-chemical waste heat recuperating using catalytic devices
- Develop further understanding of aftertreatment technology which will improve the application and integration of emission control systems
- Determine the feasibility and optimization of catalyzed UWS to enable low temperature dosing while minimizing the risk of deposit formation
- Propose and evaluate novel methodologies to promote low temperature decomposition of UWS

AC^{2}AT-II

AC^{2}AT-II will develop the tools and technologies required for the synergistic application of catalysts to advanced internal combustion engines. This includes the development of advanced aftertreatment system simulation tools and implementing advanced aftertreatment strategies for low temperature operation. There also exist some opportunities on advanced engine platforms to utilize catalysts outside of the exhaust system to reduce fuel consumption and/or reduce emissions while utilizing otherwise wasted thermal energy.

Objectives

The objective of the AC^{2}AT-II consortium is to continue to evaluate the integration of catalysts and aftertreatment technologies into compression-ignited and spark-ignited engine systems. A portion of the proposed work is intended to further our understanding of current state-of-the-art emission control systems, while other projects are focused on evaluating new uses of catalytic devices to improve engine efficiency through thermo-chemical waste heat recuperation. One of the primary focuses of the AC^{2}AT-II consortium is to develop simulation tools to improve the analysis led design of emission control systems with the purpose of streamlining the design and integration process. Another area of potential work will examine the feasibility and optimization of catalyzed UWS to enable low temperature dosing while minimizing the risk of deposit formation. The AC^{2}AT-II program will be used as a means for member companies to jointly examine high risk / high reward technologies they might not consider due to resource constraints if a member company had to evaluate the technology on its own.

Specific Goals

The goals for the AC^{2}AT-II consortium will be finalized during the final AC^{2}AT PAC meeting in November 2018. However, the preliminary goals proposed above in Table 1 were based on input from discussions with current and potential PAC members. In addition, each project will have separate, more detailed goals that are aligned with the overall consortium goals. Since the AC^{2}AT-II consortium is a continuously evolving research program, the goals of the consortium will be modified on an infrequent basis as the results from the program and funding levels dictate.

Work Scope

The work scope of the AC^{2}AT-II consortium will be based on the tasks required to meet the goals outlined in Table 1. Where available, SwRI will utilize existing engine and burner based test stands at SwRI's facility in San Antonio. If an existing engine platform is not available for the focused project task, SwRI will install the desired engine platform to execute the task. To maintain flexibility in meeting the program goals and encourage continual innovation, SwRI and the AC^{2}AT-II PAC will re-visit the work scope for each platform and the program on a regular basis. The intention of SwRI is to create a work plan to meet the goals described in Table 2, while being flexible and dynamic enough to react to new developments. After the commencement of the program, SwRI will poll the PAC members for their interest in the topics that are presented below in Table 2. A description of each task will be made available on the AC^{2}AT-II website and member companies will be asked to read the description and rank order the proposed topics in order of interest. The final project list, with priority and budget allocations, will be selected by the PAC at the kickoff meeting and reviewed and adjusted on a regular basis. The final level of effort and task priority will be determined by the program budget and the desires of the PAC members.

Table 2: Potential Projects for AC^{2}AT Consortium

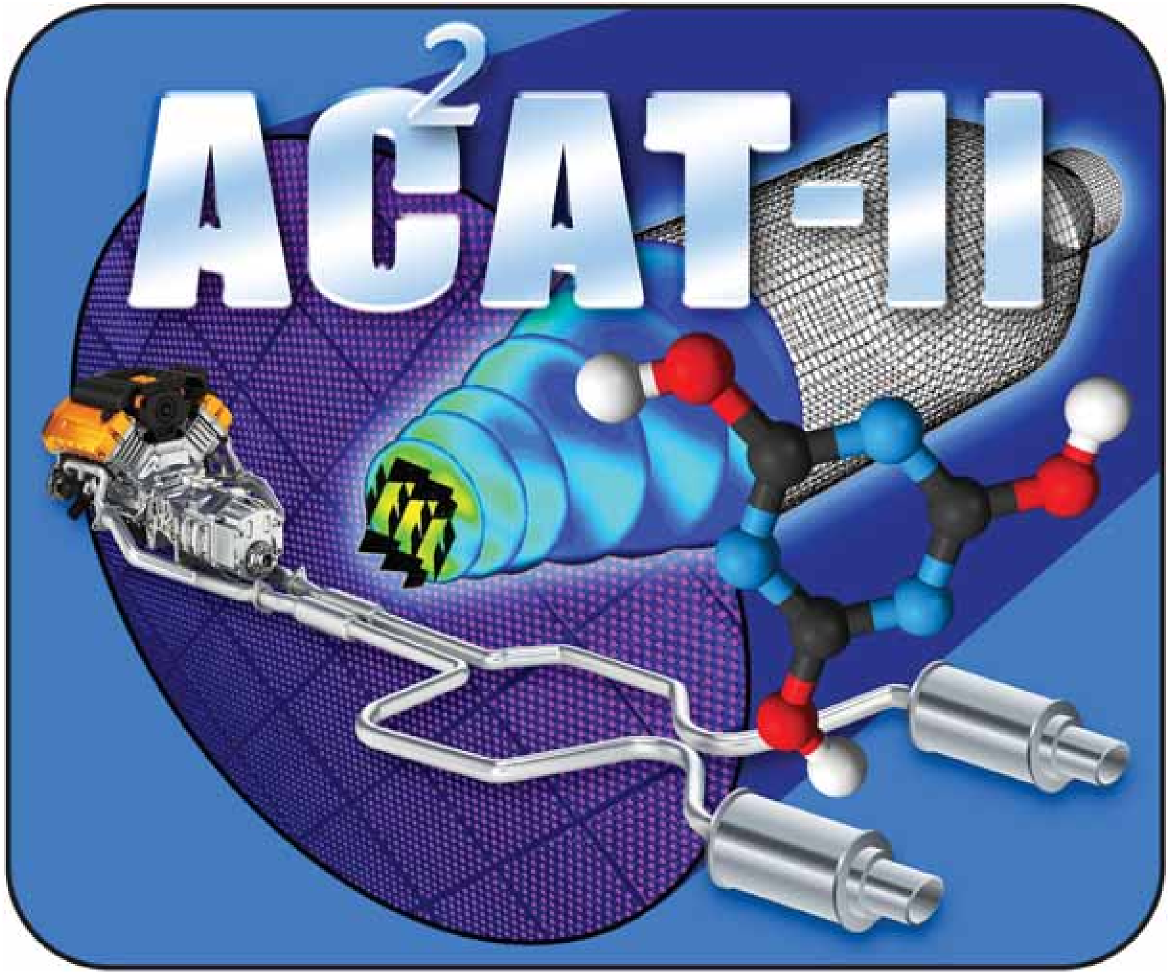
TASK NUMBER	TASK
1	Coupled 3-D CFD – chemical kinetics simulation tool for aftertreatment performance evaluation
2	Effects of catalyzed UWS on system performance, including decomposition and NO_X reduction
3	Chemical waste heat recovery (steam reformation) for spark-ignited, stoichiometric engine
4	Mixed metal oxide catalyzed SCRF for simultaneous NO_X conversion and soot oxidation
5	Application of advanced aftertreatment strategies for lean-burn SI engines
6	Zeolite design for DOC, HC trap, NO_X adsorber, and/or SCR
7	Application of HC-SCR for low temperature combustion regimes
8	Passive NO_X storage for cold start NO_X emission reduction
9	Production of gaseous NH_3 from liquid UWS to enable low temperature dosing
10	High efficiency thermal management for improved cold-start emissions performance
11	Heat storage devices for conventional and plug-in electric hybrid applications

Program Price

The consortium program is a four-year annual renewal Cooperative Research Program. The yearly price for the AC^{2}AT-II consortium is $95,000 per year for original equipment manufacturers and suppliers. The program is scheduled to begin on November 16, 2018 and will continue for four years after the start date.

APPENDIX A

Promotional Material of AC^2AT_II

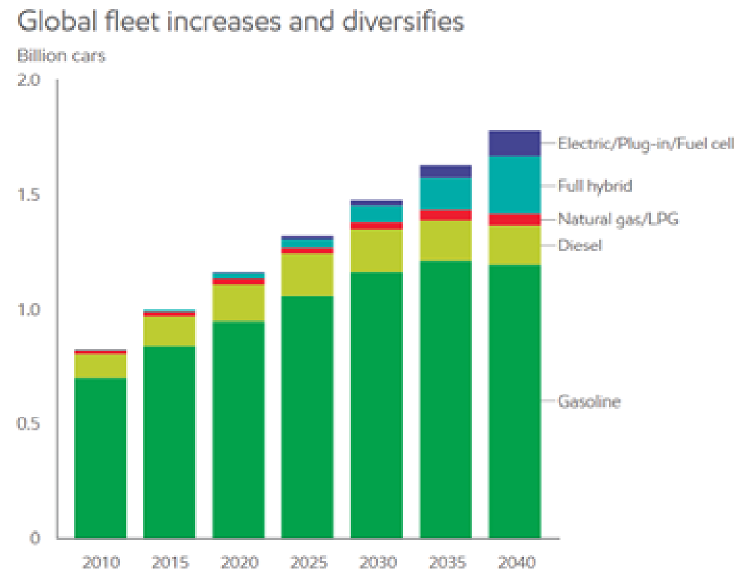


- AC²AT - II: Advanced Combustion Catalyst and Aftertreatment Technologies - II

Future Market for Light Duty Vehicles

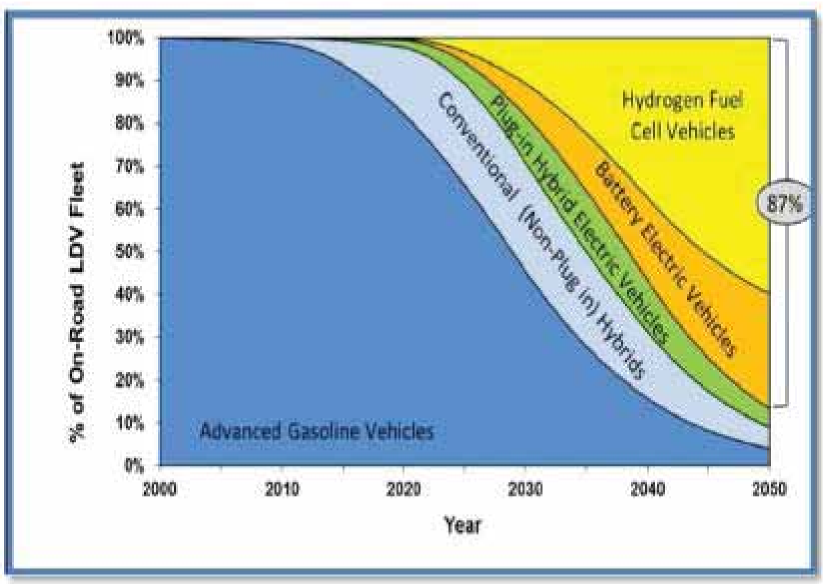
ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Global Light Duty Fleet is Projected to Expand by 80 Percent Over the Next 25 Years
- Gasoline Will Remain Dominant Fossil Fuel, Though Diesel Market Will Also Grow



Exxon Mobil Energy Outlook 2017

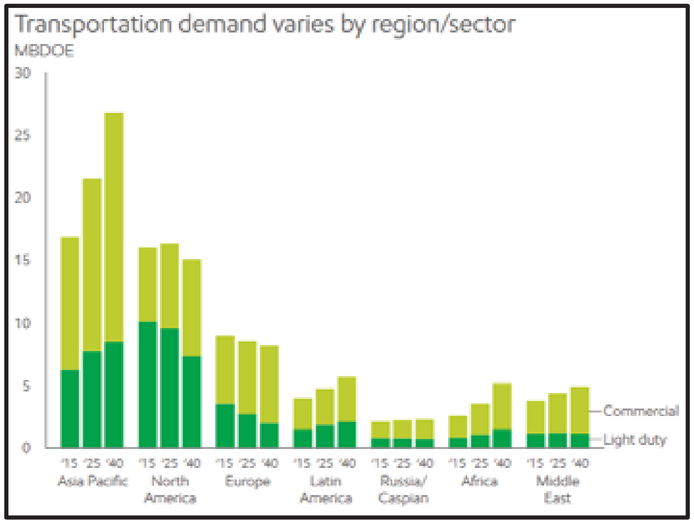
Ayala, ARB, CRC Emissions 2015

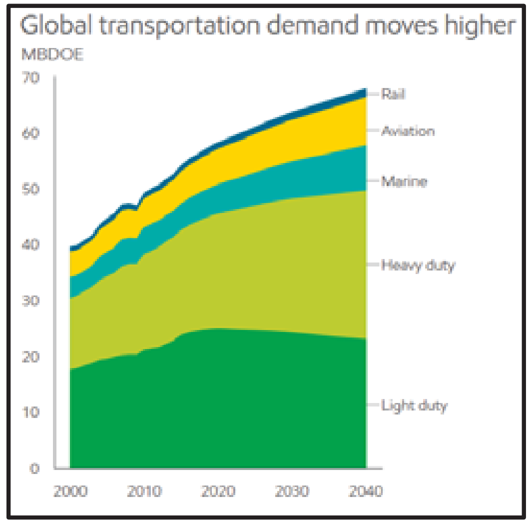


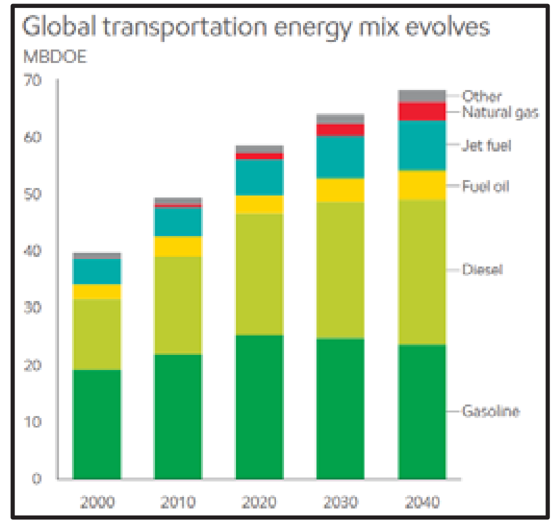
- Due to More Stringent Regulation, CARB Vision is Very Different From Global Perspective
- CARB Expects a Market Dominated by Alternative Technologies in 2050

Future Market for Heavy Duty Vehicles

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES







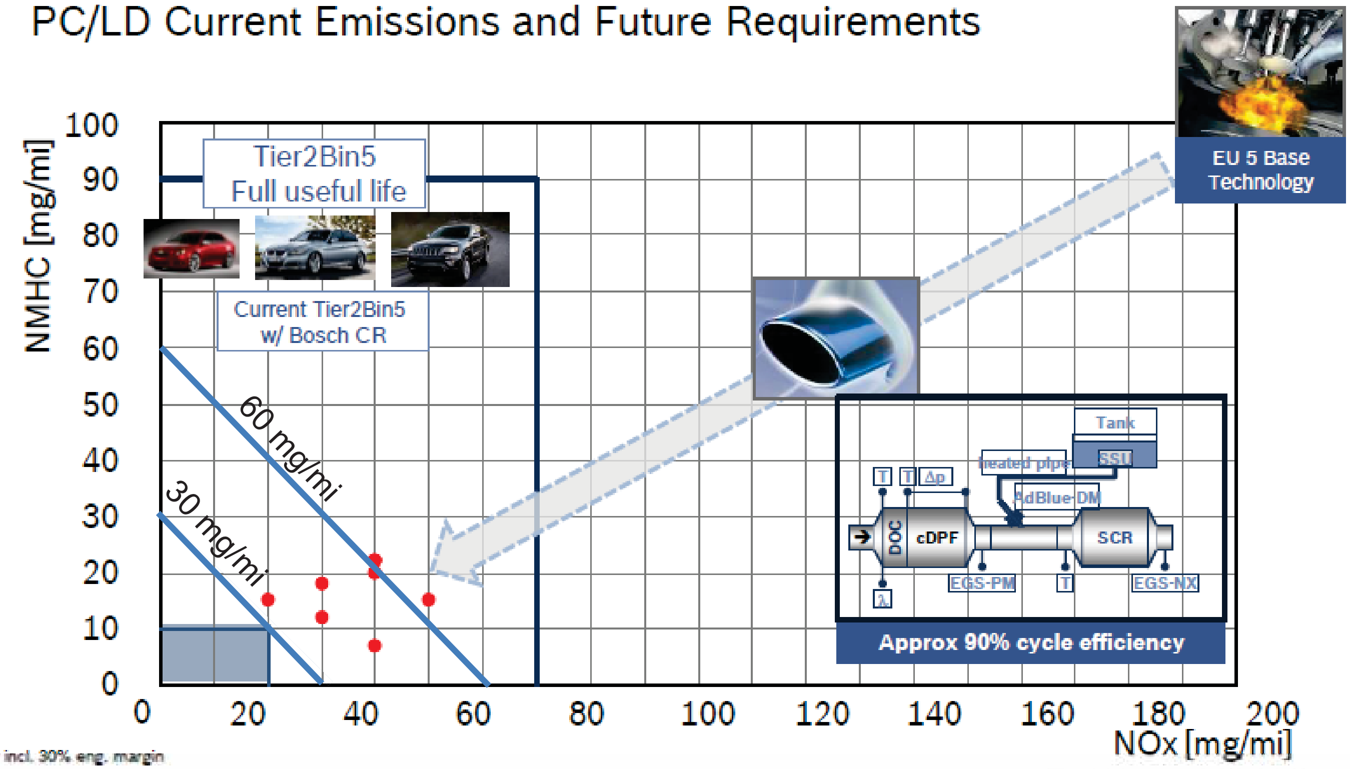
Exxon Mobil Energy Outlook 2017

- All Regions Project an Increased Demand in Commercial Transportation Energy as Economic Growth Stimulates Demand for Trucking, Aviation, Marine and Rail
- Growth of About 25 Percent is Projected in Global Transportation Energy Demand from 2015 - 2040
- Heavy Duty Growth is the Largest by Volume
- The High Duty Cycle of Commercial Transportation Demands Diesel as a Primary Fuel
- Diesel Will Remain Dominant Fuel Over the Next 25 Years

EPA Tier 3 Requires 90% NMHC+NO_X Reductions from LDD

- Tier 3 NMHC+NO_X = 30 mg/mi
  - May require an average deNO_X of 95 percent over the test cycle (up from the current 90 percent)

PC/LD Current Emissions and Future Requirements



Bosch SAE Congress 2016

* incl. 30% eng. margin

Challenges with Cold-Start NO_X During RDE

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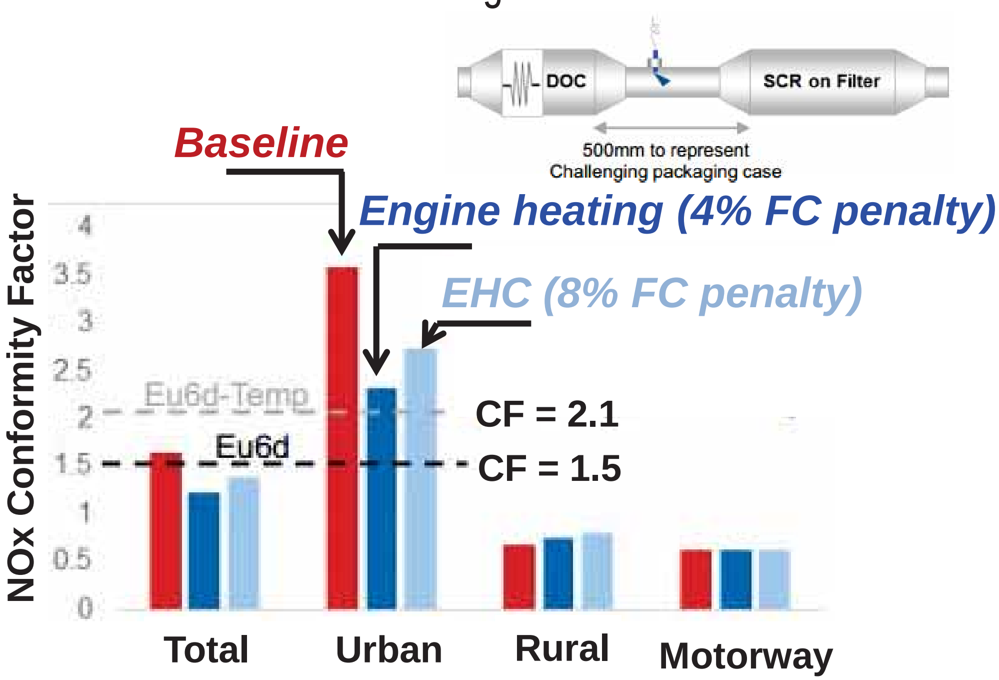
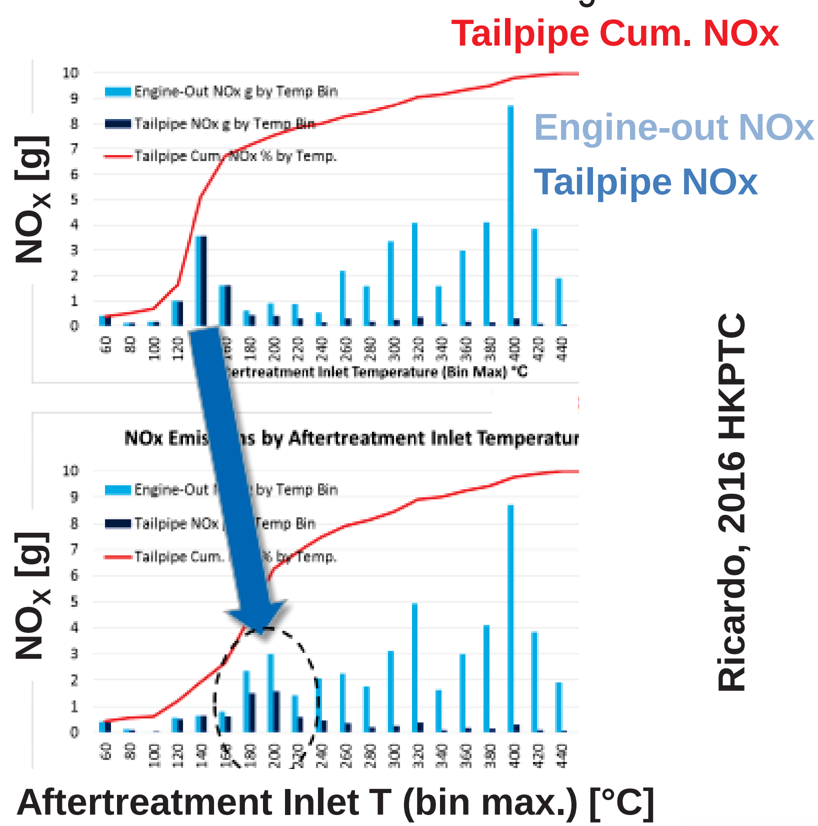
- Active Thermal Management is a Viable Solution, but it Comes with a Fuel Penalty

Urban NO_X exceeds limits despite active thermal management



Testing completed on Ricardo "RC130" congested-city cycle for challenging low exhaust T conditions

Urea dosing & NO_X conversion initiated earlier w/ thermal management



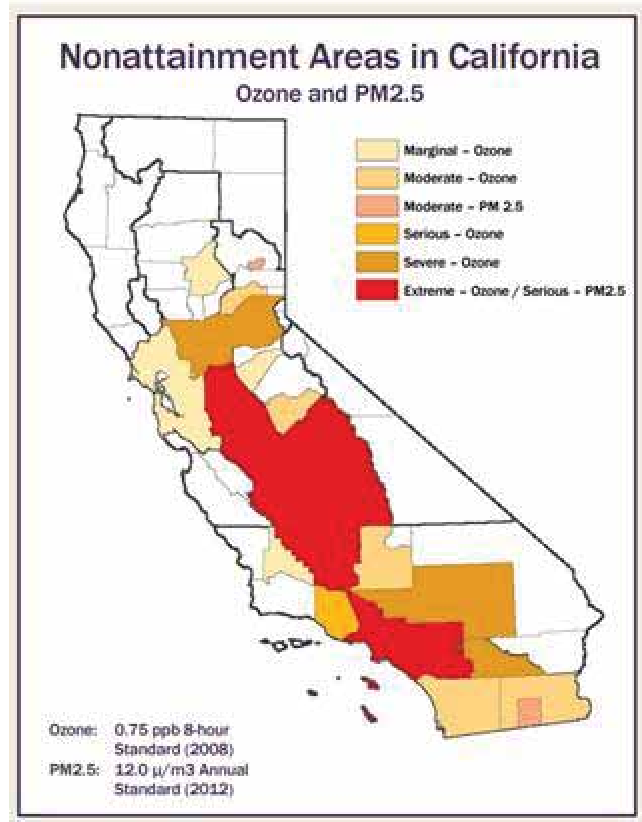
Ricardo, 2016 HKPTC

POWERTRAIN ENGINEERING

CARB Pushing for 90% Reduction in NO_X for HDD

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- 2010 Emission Standards for HD Engines Have Established a Limit for NO_x Emissions of 0.20 g/bhp-hr, a 90% Reduction From the Previous Emission Standards
- However, it is Projected That the Upcoming National Ambient Air Quality Standards (NAAQS) Requirements for Ambient PM and Ozone will not be Achieved in California Without Further Significant Reductions in NO_X
- CARB is Funding a Research Program to Explore the Feasibility of Significantly Reducing NO_X Below the 2010 Standard

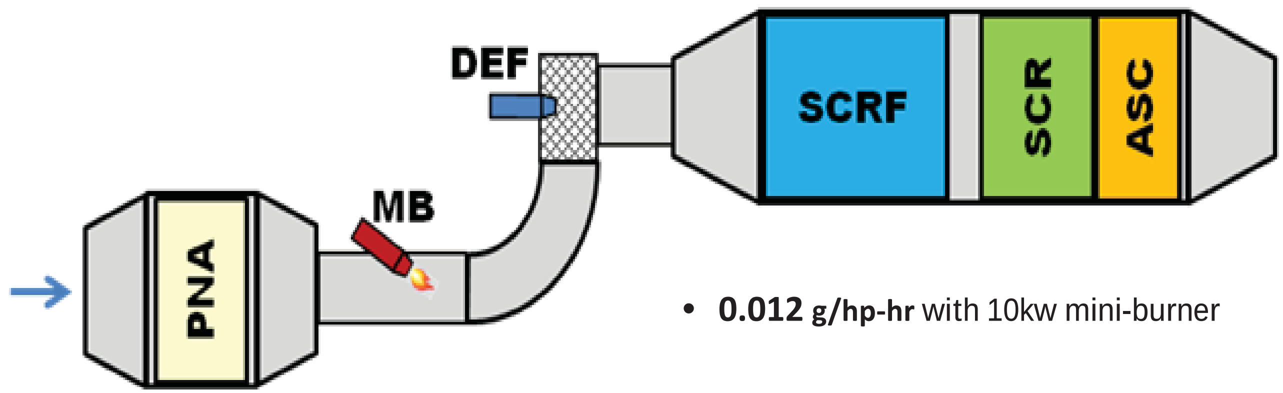


arb.ca.gov/msprog/hd

SwRI Led CARB Low NO_X Program

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Development Target was to Demonstrate 90% Reduction from Current HD NO_X Standards (0.02 g/bhp-hr)
  - 0.012 g/bhp-hr was demonstrated on a complex aftertreatment system
  - Improvements could be made to design a more cost and fuel efficient system



- **0.012 g/hp-hr** with 10kw mini-burner

Synergistic Approach to Engine System R&D

Overview of AC²AT - II

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- **Charter:** Develop tools and technologies for the synergistic application of catalysts to advanced internal combustion engines

- **Program Details:**
  - 4 year program
  - Multi-client consortium
  - Pre-competitive research
  - Vision is 5-10 years in the future

- **Research Areas:**
  - Development of Aftertreatment System Simulation Tools
  - Low Temperature Catalyst Design
  - Advanced System Integration
  - Catalyzed UWS

- **Technology Transfer:**
  - Members receive royalty free license to newly developed IP

- **Annual Membership:**
  - USD 95,000

AC^2AT - II Structure

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

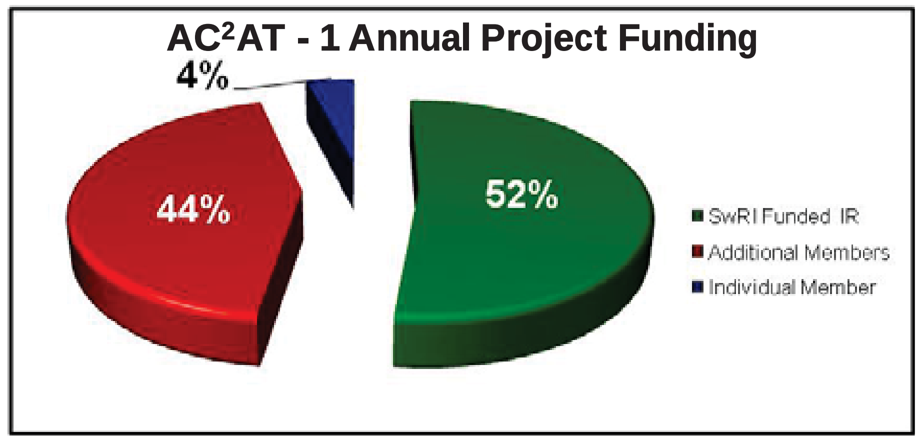
- **SwRI Cooperative Research Program**
  - Not a catalyst or emission control system development program
  - **Focused on pre-competitive technologies and fundamental evaluation**
    - REQUIRED as part of National Cooperative Research Act of 1984
  - Goal is to further our understanding of catalysts and emission control systems to improve fuel efficiency and reduce emissions
- **Structure:**
  - SwRI Responsibilities
    - Manage budget
    - Manage Technical tasks
    - Develop new concepts and IP
  - PAC Responsibilities
    - Select technical tasks
    - Provide input on results
    - Provide guidance for future programs

Value Proposition

- To Provide Collaborative Environment for Fundamental Evaluation and Application of Novel Catalyst Technologies
  - Collaborative, non-competitive research focus enables multiplication of research funds

25 Members

12 Members



AC²AT – I Annual Project Funding: $2,377,500

- >25x each member's investment of $95,000

AC²AT – I Members

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

Scope of AC^{2}AT - II

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

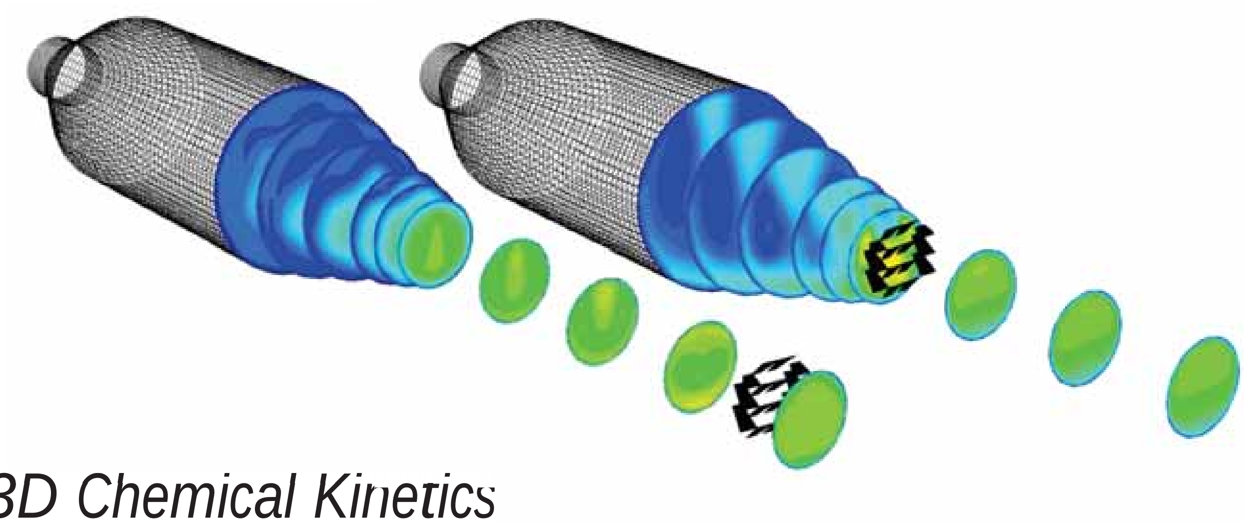
- AC2AT - II
  - Simulation
  - Low Temperature Catalyst Design
  - Advanced System Integration
  - Catalyzed UWS

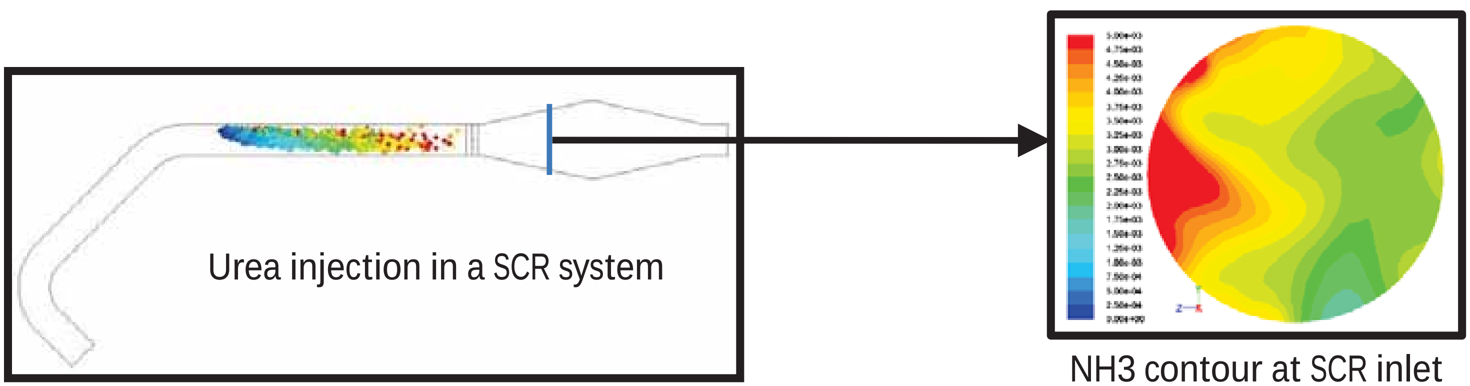
Simulation: System Performance

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Catalyst Dynamics
- Flow Distribution
- Reductant Delivery
  - Mixing
  - Decomposition
- Thermal
- *3D CFD Coupled to 3D Chemical Kinetics*

Flow visualization :





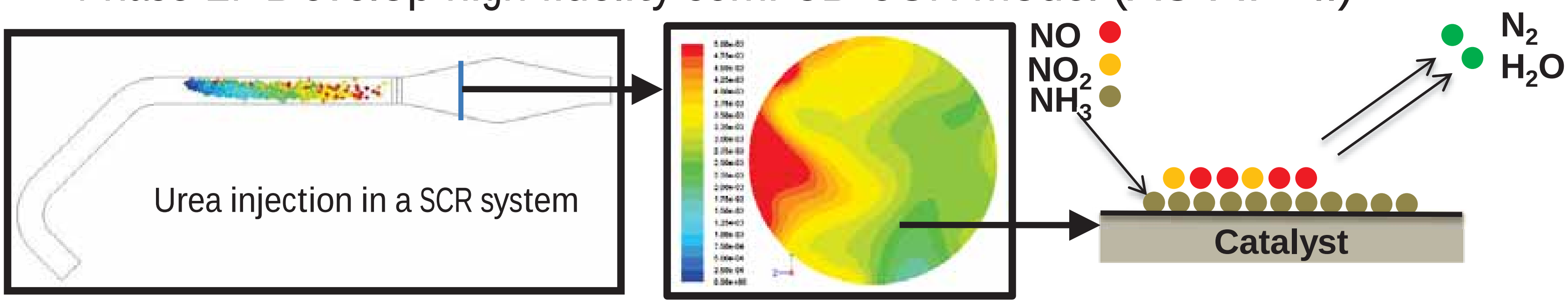
NH3 contour at SCR inlet

SwRI, SAE 2013-01-1757

Model Based SCR Development

- Project Objective: Develop Full Predictive 3D Urea-SCR Aftertreatment System Model
  - Phase 1: Develop predictive model for urea deposit formation (AC^{2}AT)

  - Phase 2: Develop high fidelity semi-3D SCR model (AC^{2}AT - II)



NH_3 contour at SCR inlet

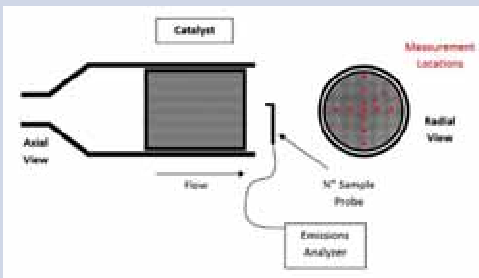
  - *Phase 3: Incorporate ash and soot loading impact to enable 3D SCR-F simulation capability (AC^{2}AT - II)*

Phase 2 Overview (AC²AT - II)

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

<table>
<tr><th>PHASE 2</th><th>Mixing Uniformity</th><th>1-D SCR Kinetic Modeling</th><th>SCR Catalyst Model Integration</th></tr>
<tr><td>Test Bench</td><td>

➢ Radial Sampling of NH_3 Downstream of SCR



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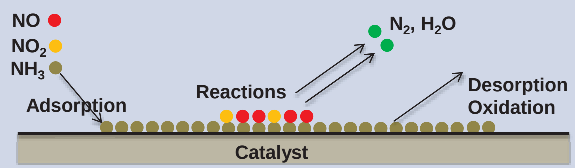
➢ Reactor Bench Testing (USGR) of SCR Performance



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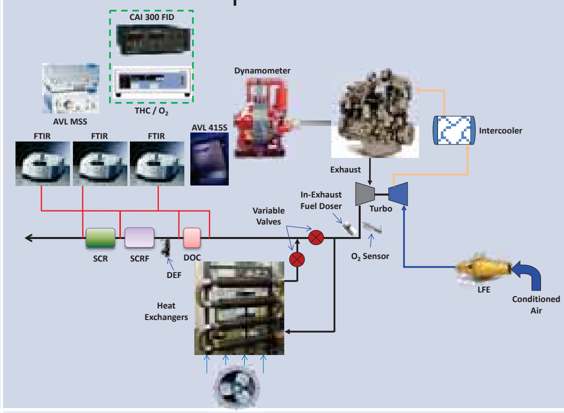
➢ SCR System Performance Evaluation with Varied Inputs



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<tr><td>Model Based Simulation</td><td>

➢ Tune Model Mixing Performance

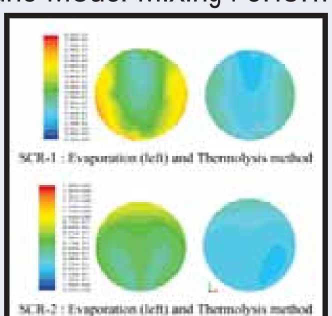

Figure 12. Contour of ANR at SCR inlet

Source: SAE 2013-01-1575, Abidin et. al

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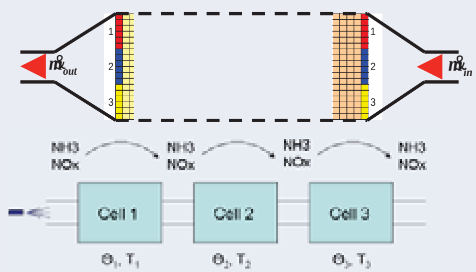
➢ Tune Individuals Cells Within Model



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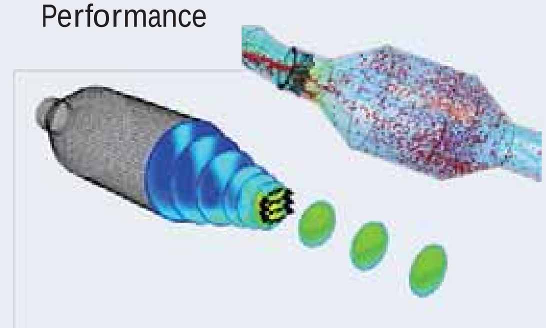
➢ Combine Urea and SCR Catalyst Models for Evaluation of Total System Performance



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AC²AT-II

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

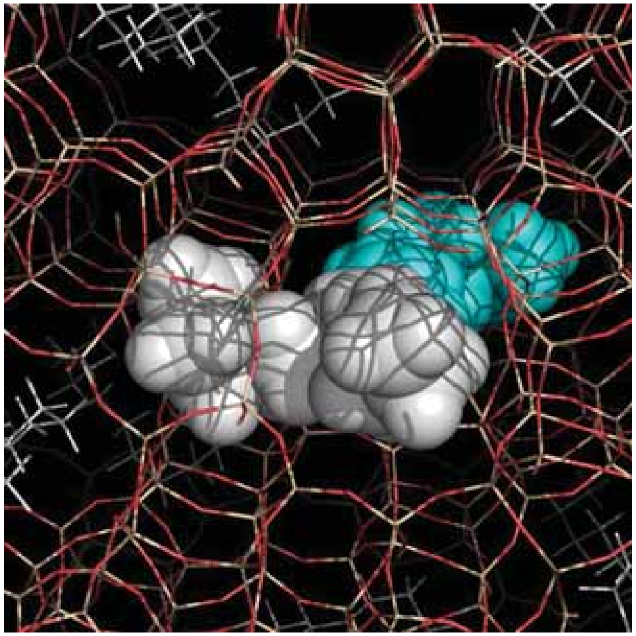
A Consortium of SwRI

Advanced SI Strategies

Molecular Catalytic Simulations via Rhodium™

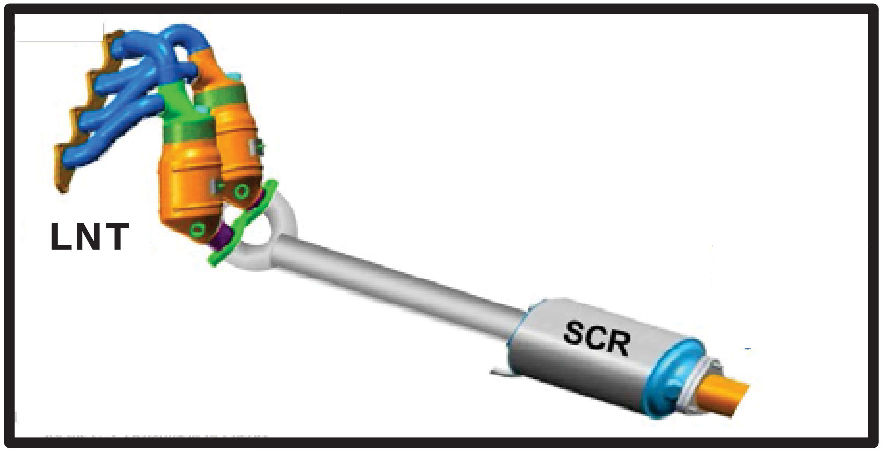
ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Explore Kinetic Modeling Capabilities of Rhodium
  - Predict performance of zeolite catalysts in adsorption and desorption of HC
  - Select a series of zeolites widely used in automotive industry based on literature
- Conduct HC Storage Simulations on selected Zeolites
- Wash Coat Catalyst Cores with the Best Zeolite Candidates
- Evaluate HC trapping efficiency via Universal Synthetic Gas Reactor (USGR®) system



Advanced SI AT Strategies

- Lean NO_X Trap With Underfloor SCR Enables Lean Operation With Increased NO_X Conversion And Reduced Fuel Consumption
- LNT Must Be Formulated For Selective Formation Of NH_3
- NH_3 Is Stored On SCR During Rich Operation
- SCR Catalyst Must Be Robust to HC Fouling/Poisoning During Rich Operation
- During Lean Operation, NO_X is Reduced Via NH_3 Stored On SCR



Adapted From ORNL, DEER 2012

- SCR Catalyst Must Be Cool Enough To Effectively Store NH_3 During Rich Cycling
- GM And ORNL Developed Similar Technology Using TWC + SCR, But LNT + SCR On The D-EGR Application Is Expected To Provide Further Improvements In Fuel Consumption

Emerging GPF / TWC-F Technologies

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

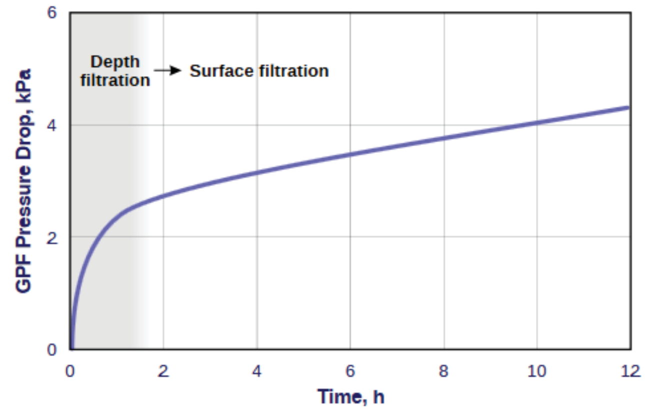
- Mature Wall Flow Filters Used on Conventional Diesel Applications Cannot be Simply Applied to GDI:
  - Soot levels
    - GDI soot (by mass) are ~10x lower than diesel
    - GDI soot is emitted mainly during cold start
  - O_2 / Temperature Levels
    - Gasoline has ↑ temperatures but ↓ O_2
    - Diesel has ↓ temperatures but ↑ O_2
  - Soot cake
    - Little or no soot cake on GPF
    - Soot cake provides the 99%+ filtration in DPF
  - Ash deposition profiles
    - For LD applications, ash generally forms a plug at end of DPF channel
    - Ash deposits / penetrates into walls of GPF in addition to forming plugs
  - Controls
    - DPF controls are based on dP vs soot load
    - dP control strategy does not work well for GPF
  - Substrate Material
    - Cordierite is preferred for GPF
    - LD / MD DPFs are usually not cordierite

Impact of Soot & Ash on GPF / TWC-F Functionality

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

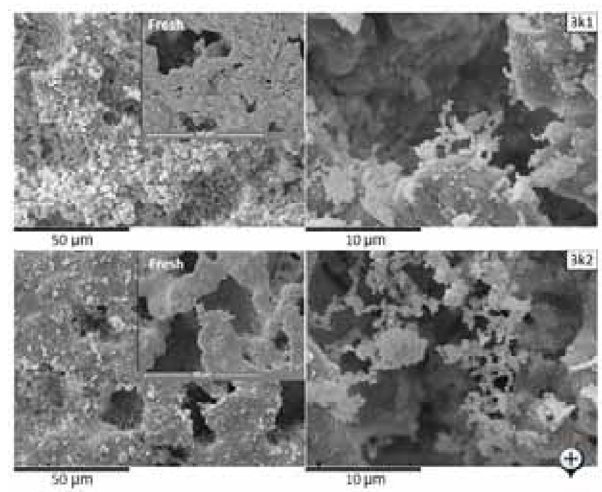
- The GPF / TWC-F Technology is Still in its Infancy, With Very Limited Applications in Production Utilizing this Component
  - Long-term durability, including soot and ash deposition mechanisms, are still not completely understood

- Durability Requirements are Becoming Increasingly Stringent, Therefore Soot and Ash Effects Within the GPF / TWC-F are of Great Concern
  - Increased tailpipe emissions
  - Increased exhaust backpressure = *fuel penalty*
  - Impact on filtration efficiency



Soot loading of a clean GPF on the Mercedes S500 M278 engine
Soot loading: exhaust gas flow 200 kg/h, GPF inlet temperature 450°C
ΔP measurement: gas flow 650 kg/h, temperature 750°C

Lanzerath, 2017 Internationales Stuttgarter Symposium



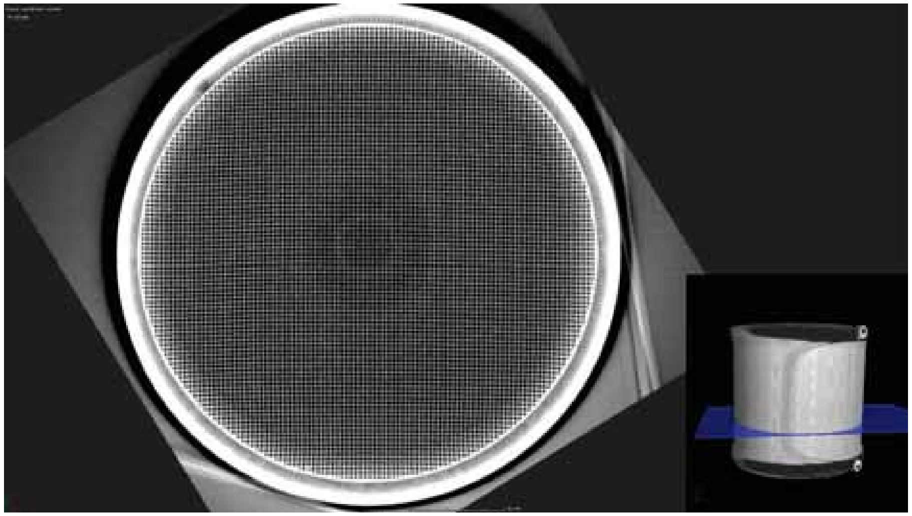
Ash Particles Bridging GPF Pores

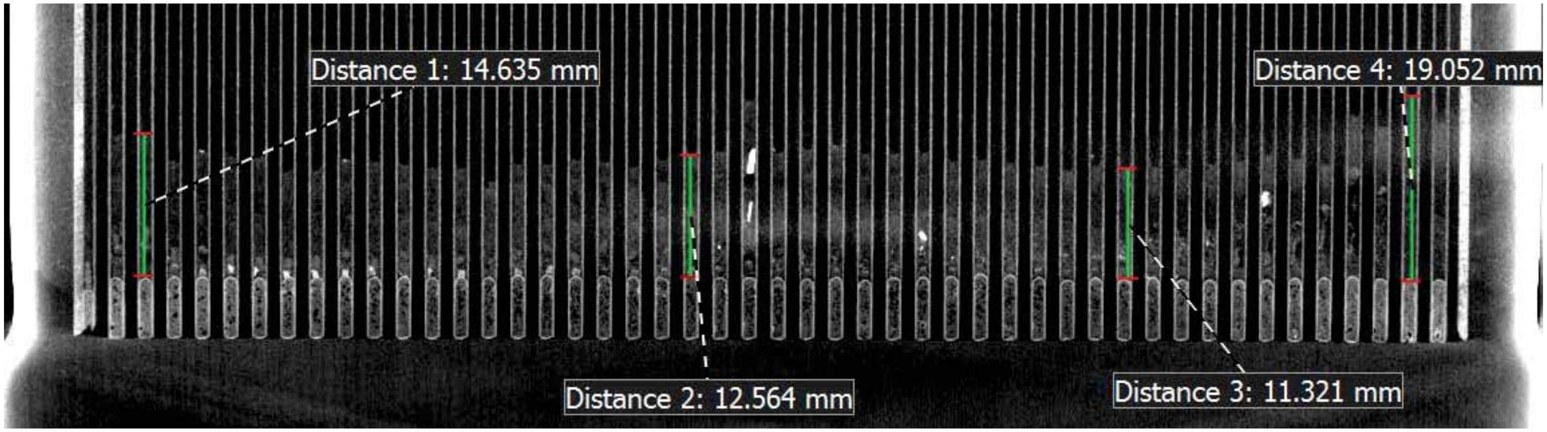
Ford Motor Company SAE 2017-01-0930

Impact of Ash on TWC-F Functionality

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

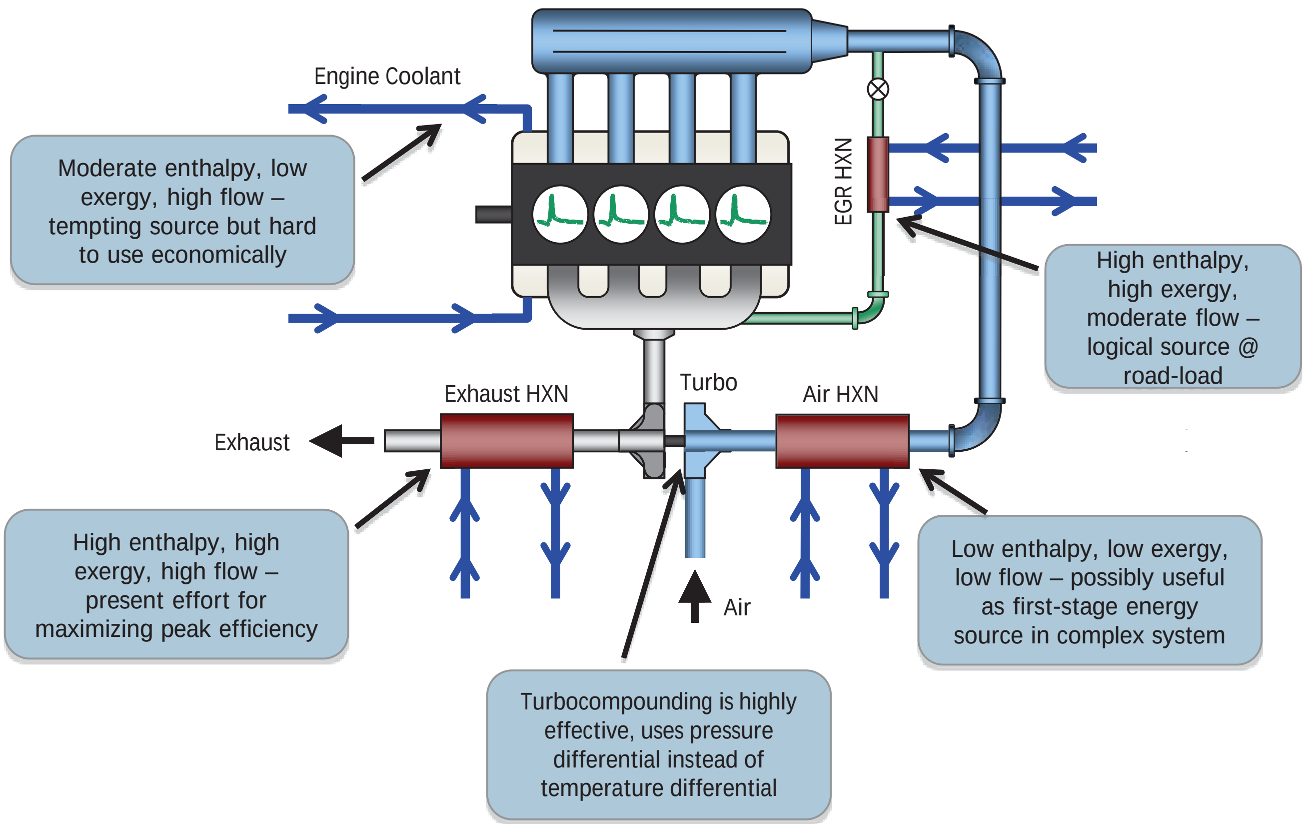
- CT-Scan can be Used to Correlate Ash Deposition Profiles Based on the Accelerated Ash Loading & Regeneration Methods





Catalytic Waste Heat Recovery Opportunities

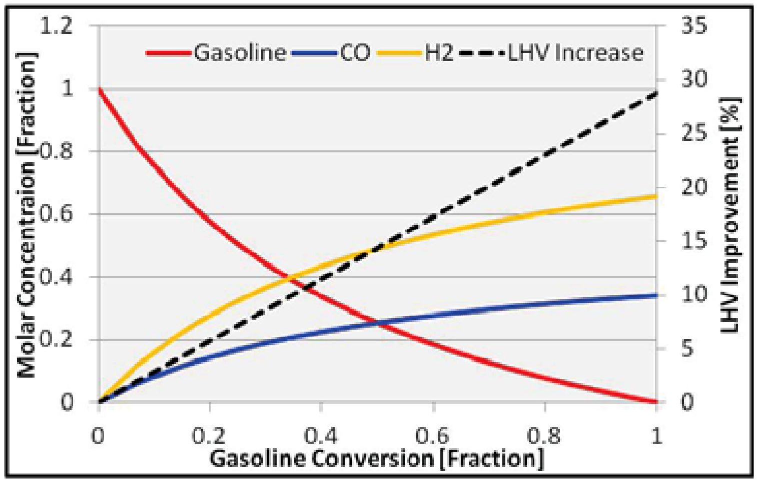
ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

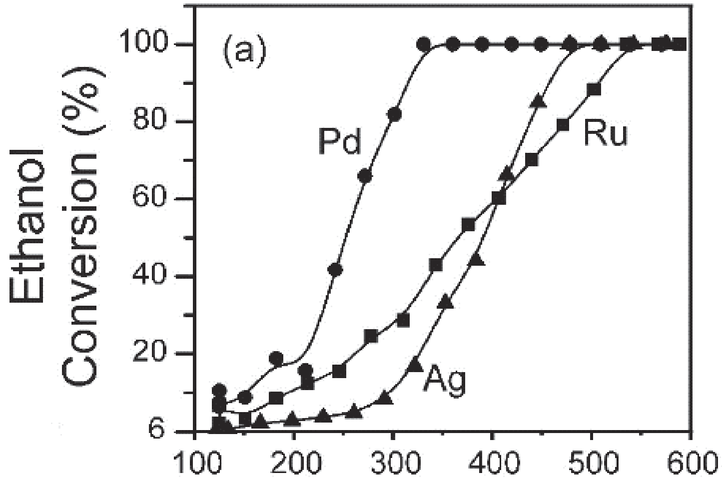


Waste Heat Recovery Through Steam Reforming

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- $C_xH_y + xH_2O \leftrightarrow xCO + (x+y/2)H_2$
  - Endothermic reaction converts thermal to chemical energy
  - 29% increase in LHV of gasoline
- Relevant in NH_3 Production



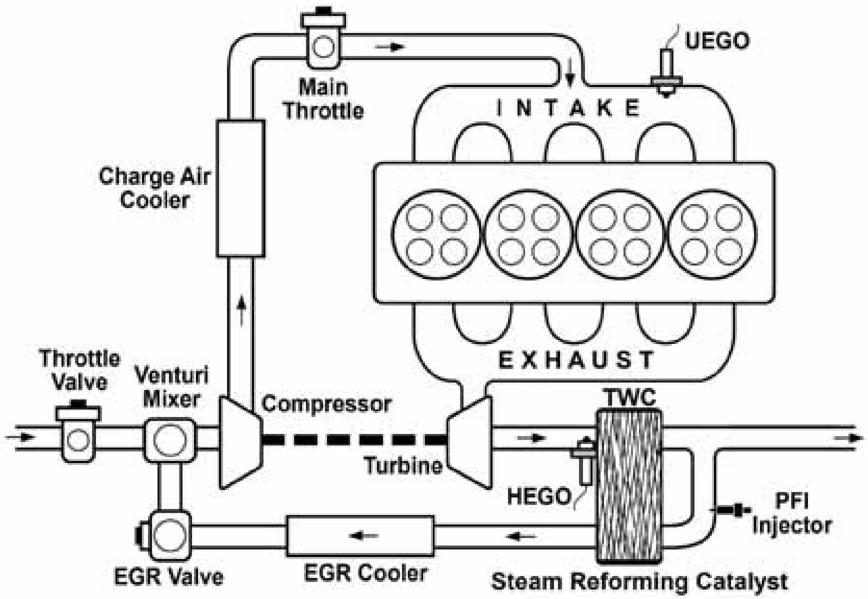


- Requires High Temperatures 350 °C to 600 °C
- Ni is a Common Catalyst but Pd, Ag and Ru are Also Promising
- Challenges are Catalyst Coking and Thermal Management

Waste Heat Recovery Through Steam Reforming

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Catalyzed Heat Exchanger Transfers Heat from the Exhaust Stream to Reformation Catalyst
  - TWC on exhaust side provides added thermal energy
- Water Sourced from Combustion Products in EGR Stream
- HC Introduced by PFI
- Newly produced CO and H_2 circulate back to Engine
  - Increase in Chemical Energy
  - Increase in Combustion Efficiency



AC^{2}AT-II

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

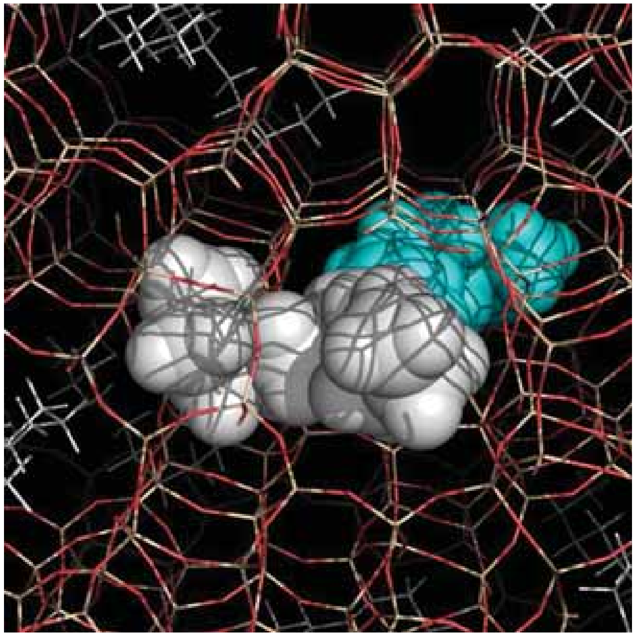
A Consortium of SwRI

Advanced CI Strategies

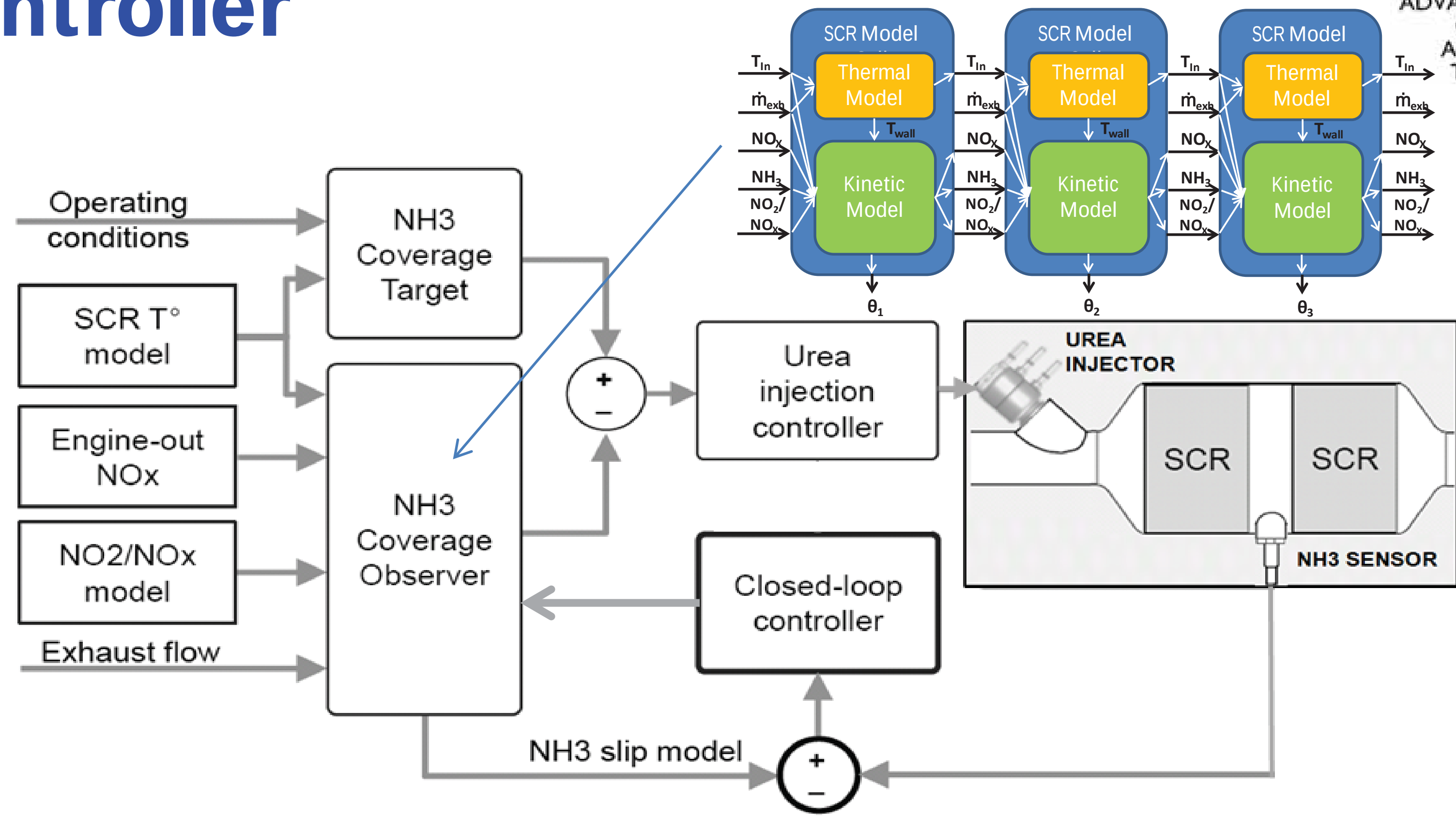
Expanding Kinetic Modeling with Rhodium™

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Expand Rhodium™ Application to LNT and NH_3-SCR Reactions
  - Optimize zeolite cage structures to maximize NH_3 storage and minimize sulfur adsorbtion



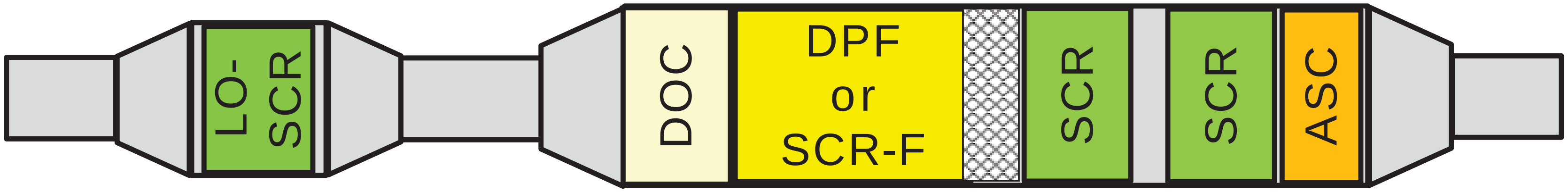
Universal Model-Based SCR Dosing Controller



- Model Based Controls Provide an Opportunity for Improved Accuracy and Precision
- Instead of Targeting a Level of NO_X or NH_3 Slip, Model Based Controls Target a Specified NH_3 Coverage Level
- Overall Model Accuracy can be Increased or Decreased Depending on Feedback Observers

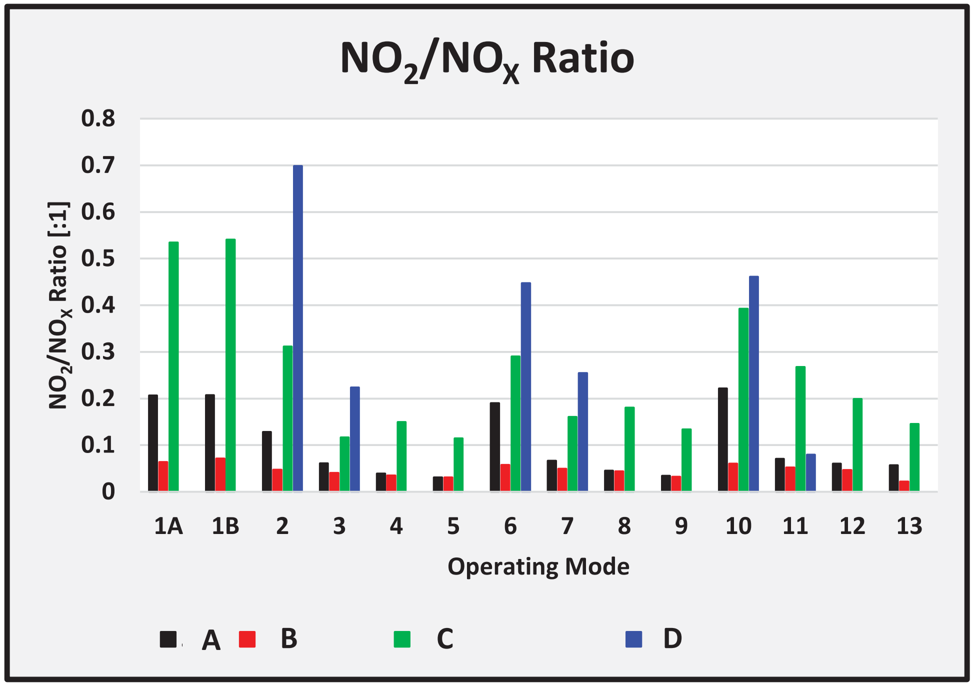
Alternative Low NO_X AT Configurations

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

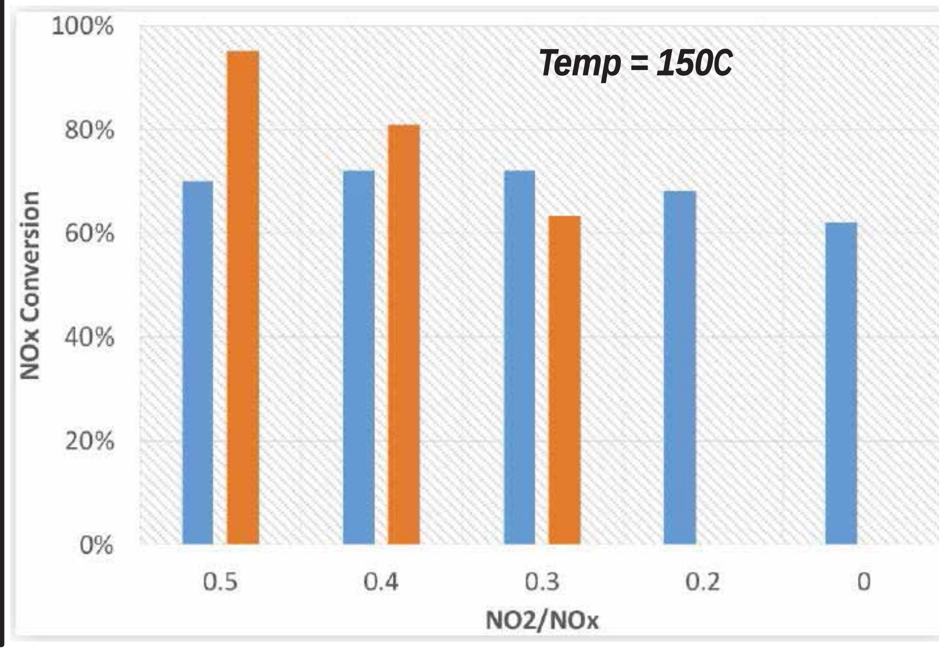


- Stage 1 ARB Low NO_X System Utilized Several Novel Technologies (PNA, mini burner, and SCR-F) Due to the Low Exhaust Gas Temperature of the Demonstration Engine
- Less Complex AT Systems May be Possible on “More Typical” GHG2017 Type Engines
- With Increased Exhaust Gas Temperature, it May be Possible to Replace the PNA and Mini-Burner Components with a “Light-Off” SCR Component Close-Coupled to the Engine

Engine Outlet NO_2/NO_X Can be Manipulated to Improve LT-SCR



Cummins, SAE 2018-01-0341

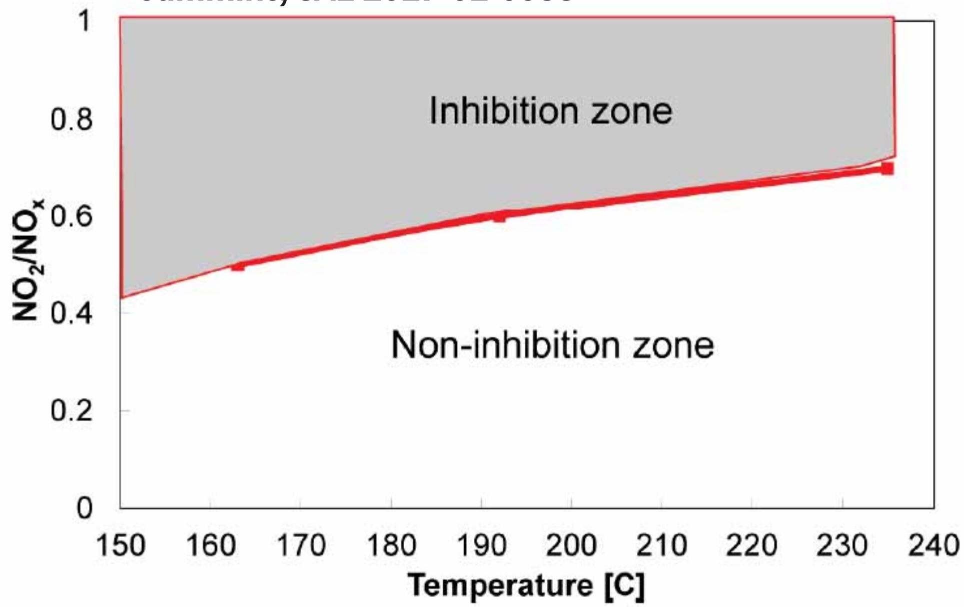


- Engine Outlet NO_2/NO_X is Highly Dependent on Combustion Recipe and Engine Operating Conditions
- Controlling NO_2/NO_X to Ideal "Fast" SCR Conditions Can Yield Significant Reductions in Tailpipe NO_X Emissions
  - TP NO_X can be reduced by as much as 90% at 150C at ideal NO_2/NO_X ratios

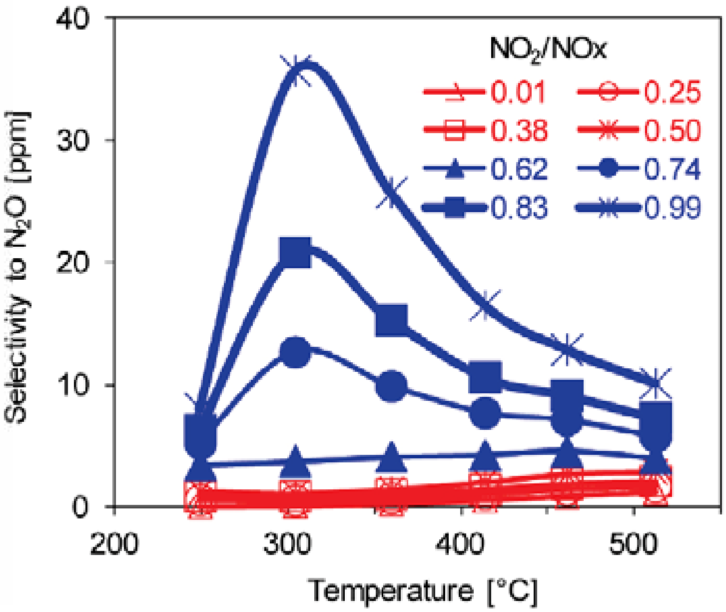
Catalyst Design and Engineering Controls Minimize NH_4NO_3

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

Cummins, SAE 2017-01-0953



Cummins, SAE 2012-01-1085



- Several Important Considerations Must be Taken Into Account if Relying on NO_2/NO_X Manipulation for Low Temperature NO_X Conversion
- High NO_2/NO_X Ratios Can Lead to the Formation of Ammonium Nitrate (NH_4NO_3) at Low Temperature Conditions
- At Moderate Exhaust Gas Temperatures High NO_2/NO_X Can Lead to Significant N_2O Production on the SCR Catalyst

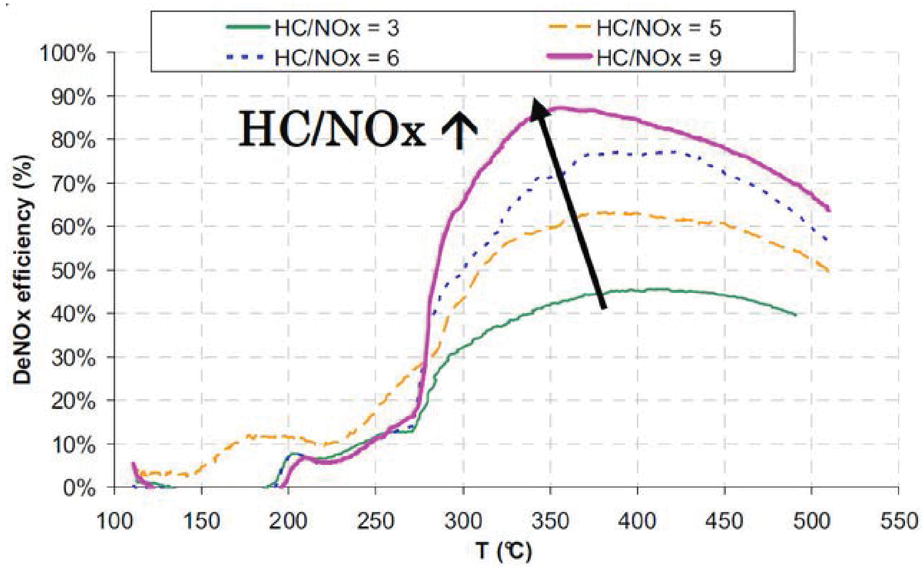
HC-SCR for Lean Burn NO_X Reduction

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Although Urea-SCR is Widely Recognized as a Promising Technology for its NO_X Reduction Efficiency Under Lean Burn Conditions, There are Drawbacks to the Technology:
  - Need for external reductant (urea)
  - Deposit formation
  - NH_3 Slip
  - Solution freezing
  - Urea injection system and space requirements

- HC are Considered an Alternative Reductant for SCR Due to the Ease of HC Production on an Engine
  - H_2 has been shown to effectively reduce NO_X at temperatures below 200°C *
  - LT combustion strategies that produce HC emissions (i.e. RCCI) may benefit from this technology

HC-SCR on Silver-Based Catalyst

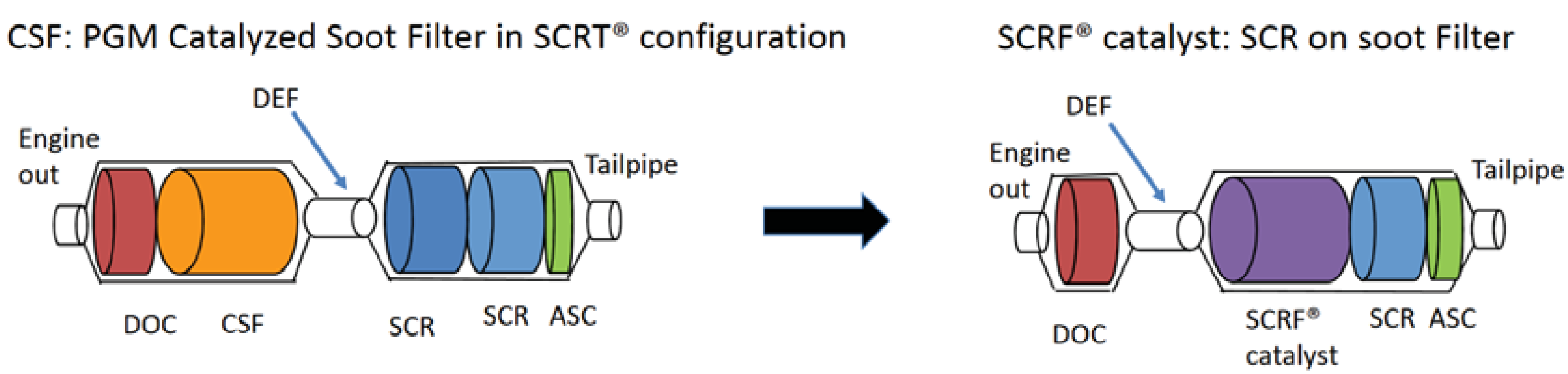


SAE 2011-01-2092

* Long Z. M., Li J. H. and Woo S. I., "Recent advances in the selective catalytic reduction of NOx by hydrogen in the presence of oxygen" Energy & Environmental Science 10, pp.8799-8814 (2012)

Opportunities for Soot Oxidation on Conventional SCRF

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES



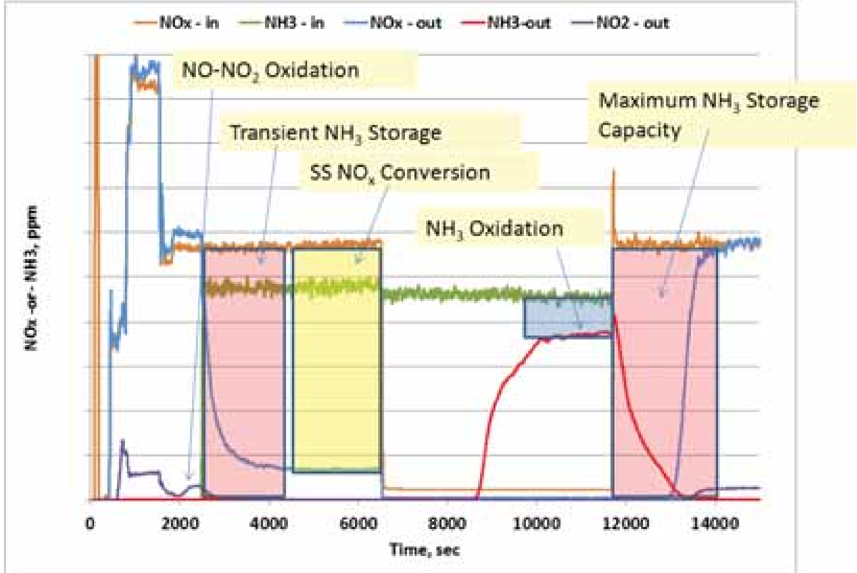
Johnson Matthey, CLEERS 2016

- CSF has Higher Soot Oxidation Efficiency At Temperatures >270 °C when Compared to SCRF
  - Competition for NO_2 due to fast SCR reaction
- Active Regeneration (i.e. >550 °C) Strategies Yield Higher Soot Oxidation Rates for the CSF than the SCRF
  - NO_2/NO_X at the DOC outlet is low due to HC inhibition
  - DOC outlet NO_2 is consumed by SCR fast reaction in SCRF

Mixed Metal Oxide Catalyzed SCRF

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Evaluate the Potential Use of a Mixed Metal Oxide Catalyzed SCRF for Simultaneous NO_X Conversion and Soot Oxidation
- Evaluate the Impact of Ash on SCR Functionality
- Use SwRI's USGR System to Evaluate the Function Specific Performance of SCRF Ash Loaded Cores
- The Cummins Developed Four Step Protocol Can be Utilized to Quantify the Functional Performance of the SCRF Component, Including:
  - NO oxidation, parasitic NH_3 oxidation, NH_3 oxidation in oxygen, NO_X conversion, transient NH_3 storage, and total NH_3 storage
- Additional Testing can be Conducted to Evaluate the Impact of Temperature, Space Velocity, and ANR

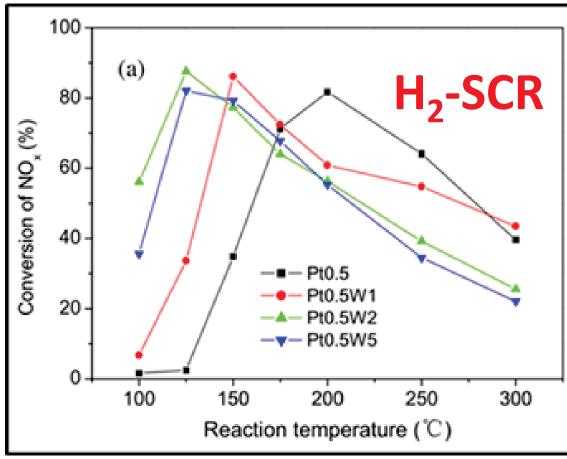


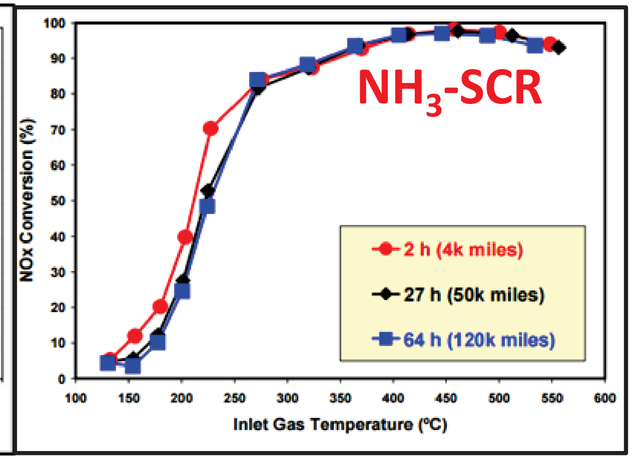
H_2-NH_3 SCR System Can Significantly Expand High deNO_X

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

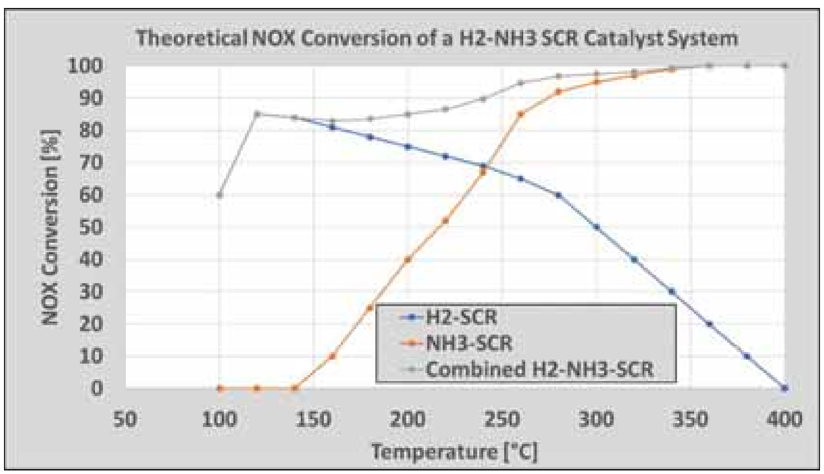
- NH_3-SCR and H_2-SCR Are Highly Effective Towards NO_x Reduction, but at Two Different Temperature Regimes
- H_2-SCR is Most Effective Between 75-200°C and NH_3-SCR at Temperatures >200°C

App. Cat. B, 2010, 94, 254-262





SAE 2007-01-1575



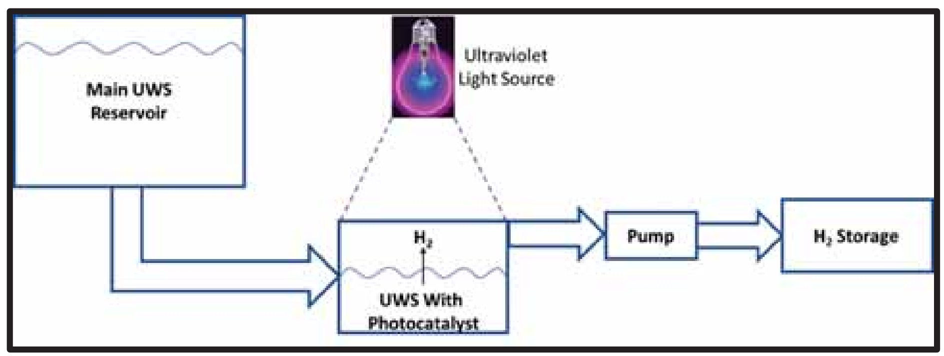
- Typical NH_3-SCR Catalysts are Zeolite or Vanadia Based, While H_2-SCR Catalysts are Noble Metal Based
- Development of a H_2-NH_3 SCR System may Provide a Means for NO_x Reduction Across an Extended Temperature Window, Particularly at Temperatures < 200 °C

Production of H_2 From Urea-Water Solution

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- By Necessity, SCR-Equipped Vehicles Carry Urea-Water Solution (UWS) for NO_X Abatement
- The UWS may Potentially be Utilized For Hydrogen Production On-Board the Vehicle Using Two Different Methods
  1. Electrolysis of urea present in the UWS
     - The required potential is much less than electrolysis of water for H_2 production (0.37 vs. 1.23 V)
  2. Photocatalytic decomposition of urea using the appropriate catalyst and light source

Electrolytic Cell Developed by Ohio University

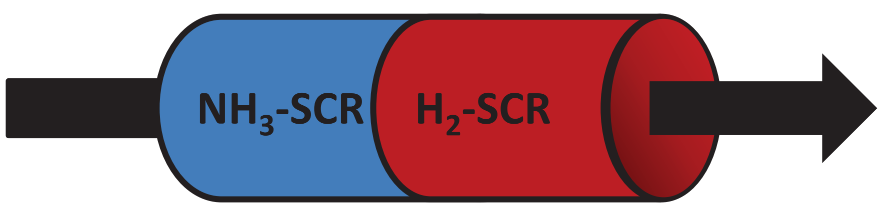


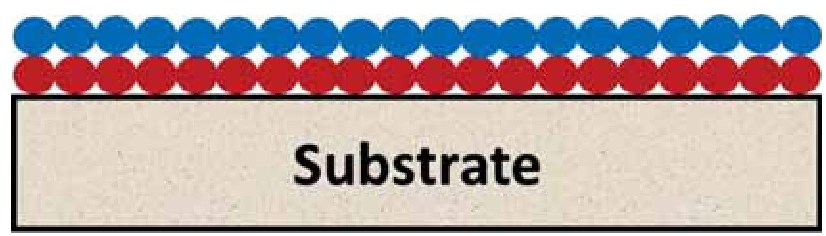
Potential System for Photocatalytic Decomposition of Urea

Smart Catalyst Coating Techniques Can Optimize Performance

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Due to the PGM Components Utilized for H_2-SCR, NH_3 Oxidation (to NO and/or N_2O) is of Concern
- Several Catalyst Coating Strategies Have Been Conceived for Development of a Dual H_2-NH_3 SCR System
  - Zone coating (H_2-SCR followed by NH_3-SCR or vice versa)
  - Layered coating (NH_3-SCR on top of H_2-SCR or vice versa)

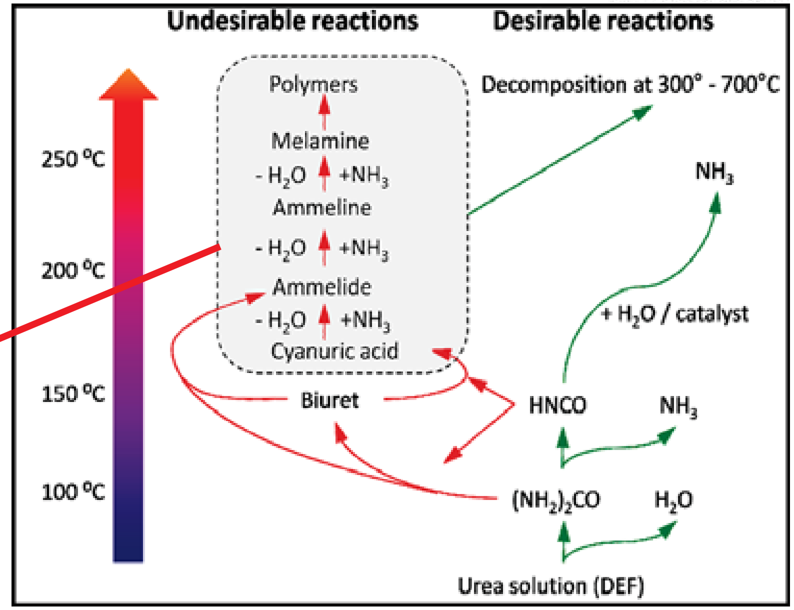




Catalyzed DEF (Cat-DEF™) Can Promote Low Temperature Activity

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Other Conventional NH_3-SCR Catalyst may be Combined with New Techniques for NH_3 Generation from DEF to Improve Low Temperature NO_X Conversion
- Ideally, Urea in Urea-Water Solution (UWS) Undergoes Thermolysis and Hydrolysis Reactions to Form NH_3 and CO_2



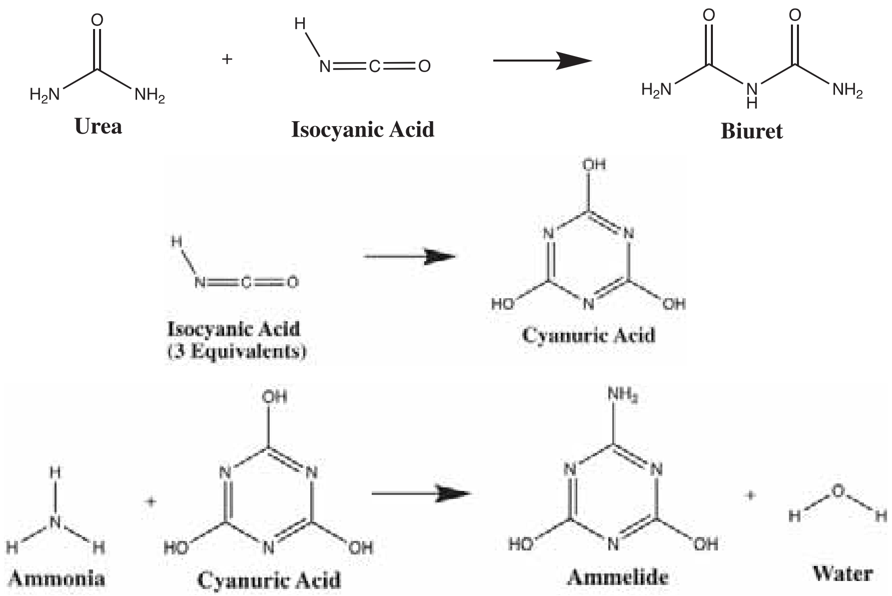
SAE 2009-01-2780

- However, HNCO May Participate in Undesirable Reactions That Lead to the Formation of Other Molecular Species
- SwRI Has Developed Novel Strategy for Catalyzing Diesel Exhaust Fluid to Promote Low Temperature NH_3 Generation

Deposit Formation in SCR Systems

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

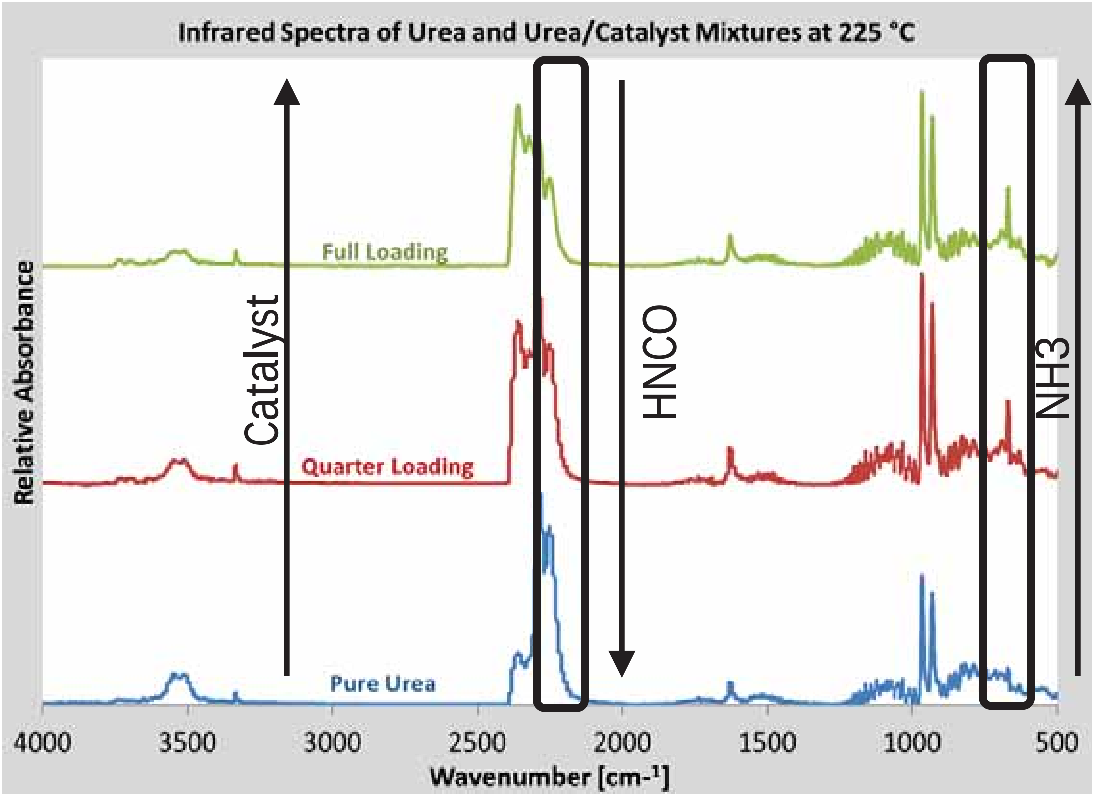
- One Significant Limitation of SCR Systems is Deposit Formation as a Result of Incomplete Urea Decomposition
- SCR Systems Require Periodic High-Temperature Regenerations to Remove Deposits



- When Isocyanic Acid Undergoes Reactions Other Than Hydrolysis, Deposit Formation Commences
- Urea-Derived Deposits Consist of Various Molecular Species Such as Biuret, Cyanuric Acid, and Ammelide Among Others

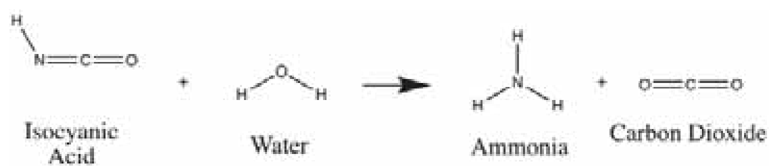
TGA-FTIR Data Show Increased NH_3 Yield with Catalyzed DEF

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES



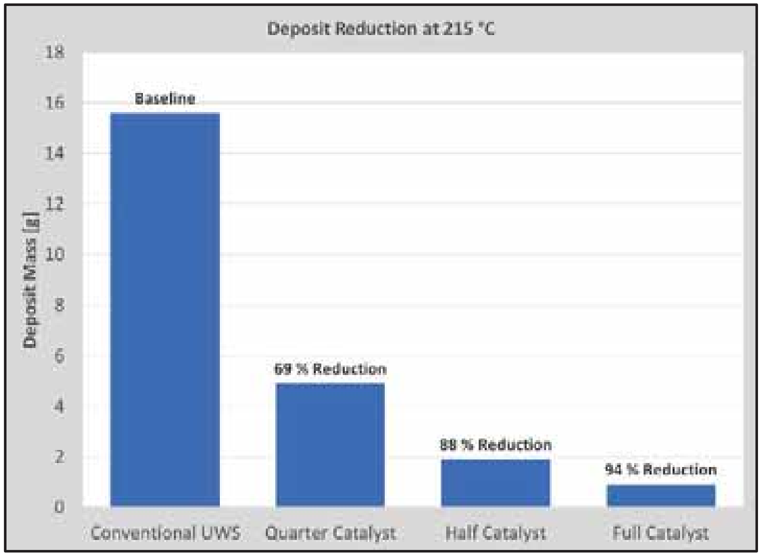
- Pure Urea and Urea/Catalyst Mixtures Were Heated Using TGA and Off-Gasses Were Analyzed Via FTIR
- Pure Urea Only Partially Decomposed as Indicated by Emission of HNCO
- Addition of Catalyst Increased the Concentration of CO_2 and NH_3, and Reduced the HNCO Concentration

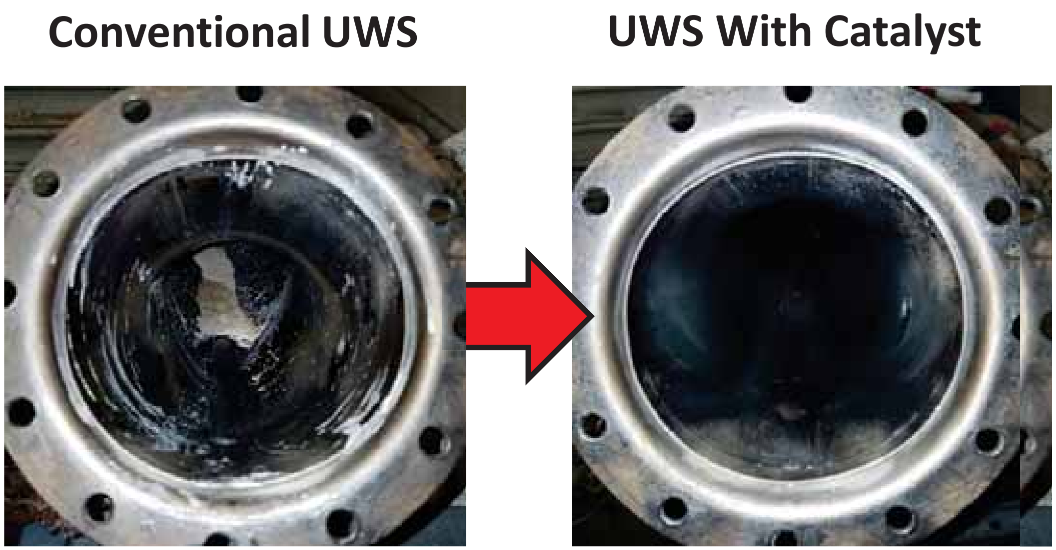
- This Result is a Strong Indication That the Incorporated Catalyst is Indeed Catalyzing Hydrolysis of Isocyanic Acid



In Addition to Increasing NH_3 Yield, Cat-DEF Reduces Deposits

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES





- The Hydrolysis Catalyst was Added to UWS at Three Separate Concentrations and the Mass of Deposits was Measured
- Addition of the Hydrolysis Catalyst Reduced Deposits by up to 94%

Gas Temperature [°C]	UWS Flow Rate [kg/hr]	Exhaust Flow Rate [kg/hr]	Duration [min]
215	0.92	660	60

Catalyzed Urea Water Solution Proof-of-Concept

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

Conventional UWS

Catalyzed UWS;
86 % Deposit Reduction

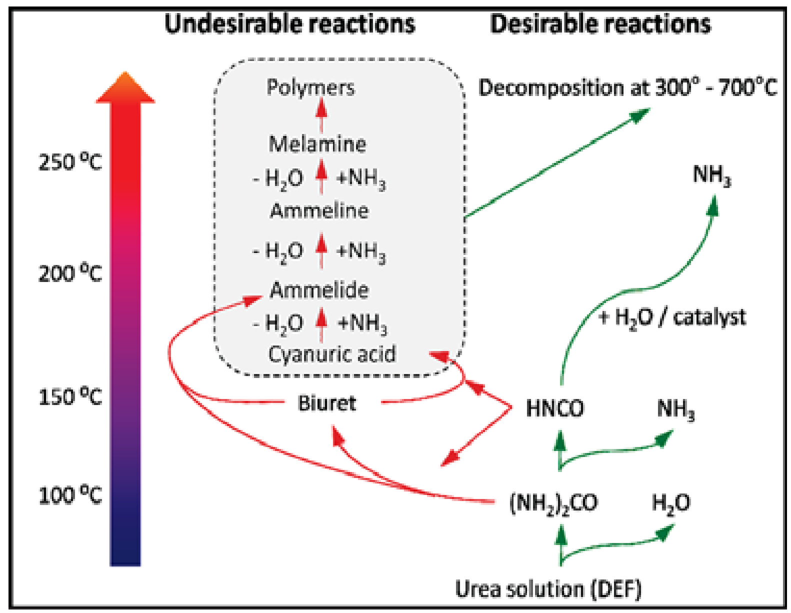
Conventional UWS with Surfactant;
81 % Deposit Reduction

Catalyzed UWS with Surfactant;
98 % Deposit Reduction

Identifying Effects of Catalyzed UWS on System Performance

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- NO_X Reduction Efficiency
- Urea Decomposition
- Particulate Emissions and Composition
- Inclusion of Surfactants to Extend Lower End Temperature Range for Dosing
- Any Impact on Soot Oxidation for SCRF



SAE 2009-01-2780

Modeling Long Term Aging Affects of Conventional Diesel Aftertreatment

ACAT-II ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Durability Requirements for by LD and HD Applications are Expected to Increase Beyond Current Standards
  - Deactivation mechanisms are well known (i.e. thermal and chemical), however further optimizations are needed to ensure long term durability
  - SwRI can leverage DAAAC coupled with field supplied parts and operational data to understand deterioration mechanisms in a lab setting
  - Core reactor experiments (USGR) and other post-mortem analytical techniques can be used to identify root causes of deterioration
  - Forensics can assist with designing impervious materials that will improve long-term durability

DAAAC Diesel Aftertreatment Accelerated Aging Cycles

Potential AC²AT – II Projects

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

1. Coupled 3-D CFD – chemical kinetics simulation tool for aftertreatment performance evaluation
2. Effects of catalyzed UWS on system performance, including decomposition and NO_X reduction
3. Application H_2-NH_3 SCR for extended low temperature operation
4. Modeling long term aging affects of conventional diesel aftertreatment
5. Chemical waste heat recovery (steam reformation) for spark-ignited, stoichiometric engine
6. Mixed metal oxide catalyzed SCRF for simultaneous NO_X conversion and soot oxidation
7. Impact of soot and ash on GPF / TWC-F functionality
8. Application of advanced aftertreatment strategies for lean-burn SI engines
9. Zeolite design for DOC, HC trap, NO_X adsorber, and/or SCR
10. Application of HC-SCR for low temperature combustion regimes
11. Passive NO_X storage for cold start NO_X emission reduction
12. Production of gaseous NH_3 from liquid UWS to enable low temperature dosing
13. High efficiency thermal management for improved cold-start emissions performance
14. Heat storage devices for conventional and plug-in electric hybrid applications

Example Deliverables, IP, and Novel Capabilities

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

- Members of AC^2AT – I Received Several Items:
  - User defined function that is compatible with commercial CFD packages for prediction of urea deposits
  - Lean burn gasoline LNT+SCR demonstration (supported by a SwRI internal research program)
  - Detailed emissions characterizations for 8 different engine platforms
  - Patent rights and detailed information on catalyzed diesel exhaust fluid
  - GPF accelerated ash loading demonstration (supported by a SwRI internal research program)
  - Impact of ash and soot on SCRF performance
  - Low temperature improvement of SCRF over conventional SCR
  - Low temperature catalyst performance inhibitors
  - Using an internally developed simulation tool (Rhodium) to predict HC storage of various Zeolite structures
  - Non-intrusive IR Thermography of urea mixer surfaces
  - *In-Situ* urea deposit imaging

SwRI AC^{2}AT – II Consortium

ADVANCED COMBUSTION CATALYST AND AFTERTREATMENT TECHNOLOGIES

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