Update on Modeling for Effective Diesel Engine Aftertreatment Implementation - Master Plan, Status and Critical Needs

B. Bolton, X. Fan, N. Hakim, K. Sisken, H. Zhang

Detroit Diesel Corporation, DaimlerChrysler Powersystems

An integrated diesel engine-aftertreatment-vehicle system is extremely complex with numerous interacting variables and an unlimited number of control options. An experimental approach to develop an optimized viable system is tedious, if at all possible. Sophisticated component, subsystem and integrated simulation tools offer an excellent option of a virtual lab approach to the development of such a complex system. A viable and robust diesel engine aftertreatment system can thus be developed within optimum time and resources when this virtual simulation is integrated with selective hardware-based testing.

Detroit Diesel has developed an effective virtual lab integrated system package. A multi-level common platform embodies 0-, 1- and multi-dimensional models of selected components and subsystems. Different models can be coupled or integrated, and simulated tests can be carried out in order to define optimum control parameters or to predict system response. This paper will present the technology development master plan, update technical status of the simulation fidelity and outline critical needs that impact simulation tool development and serious application.

DaimlerChrysler
DaimlerChrysler Powersystems

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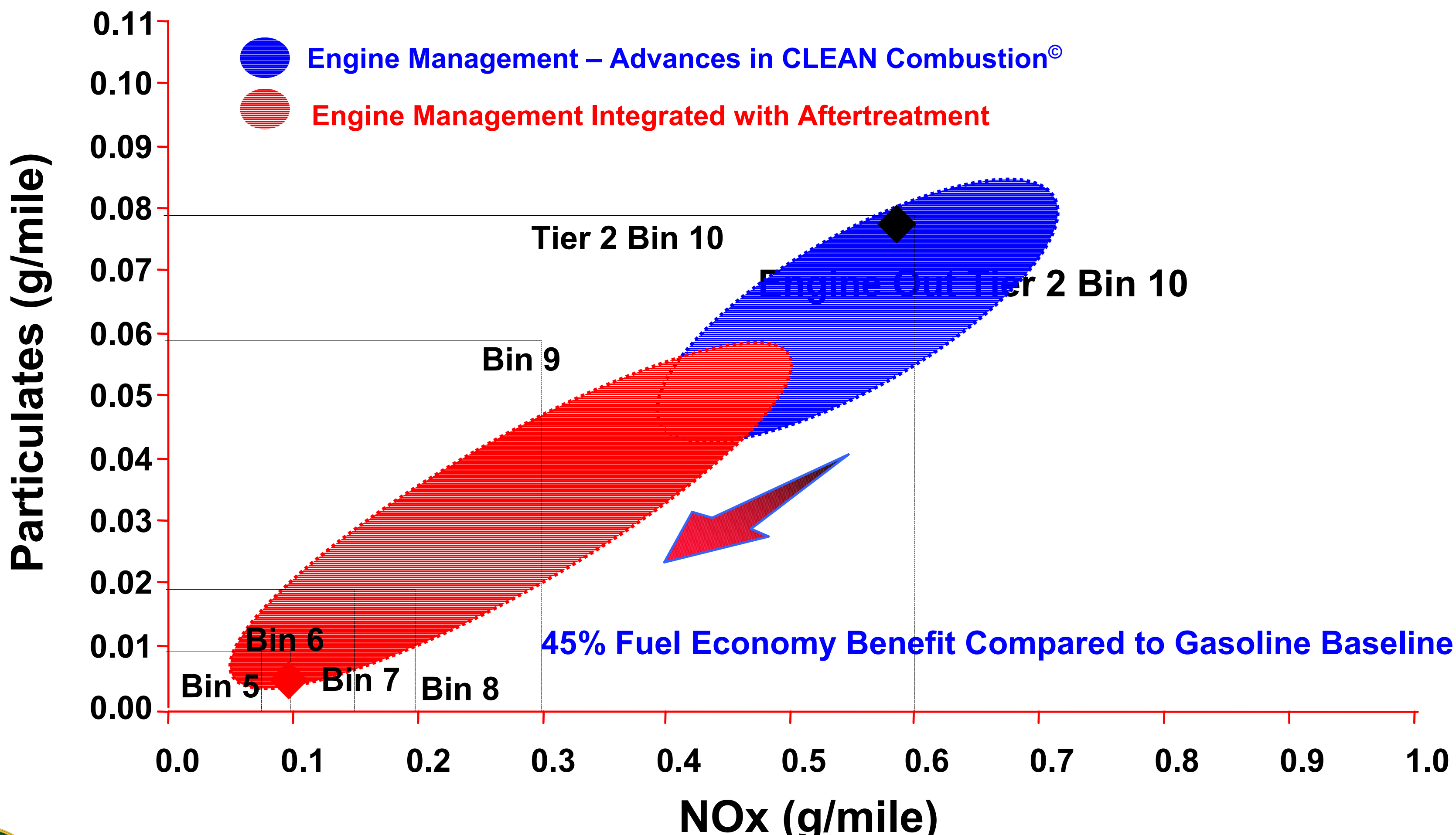
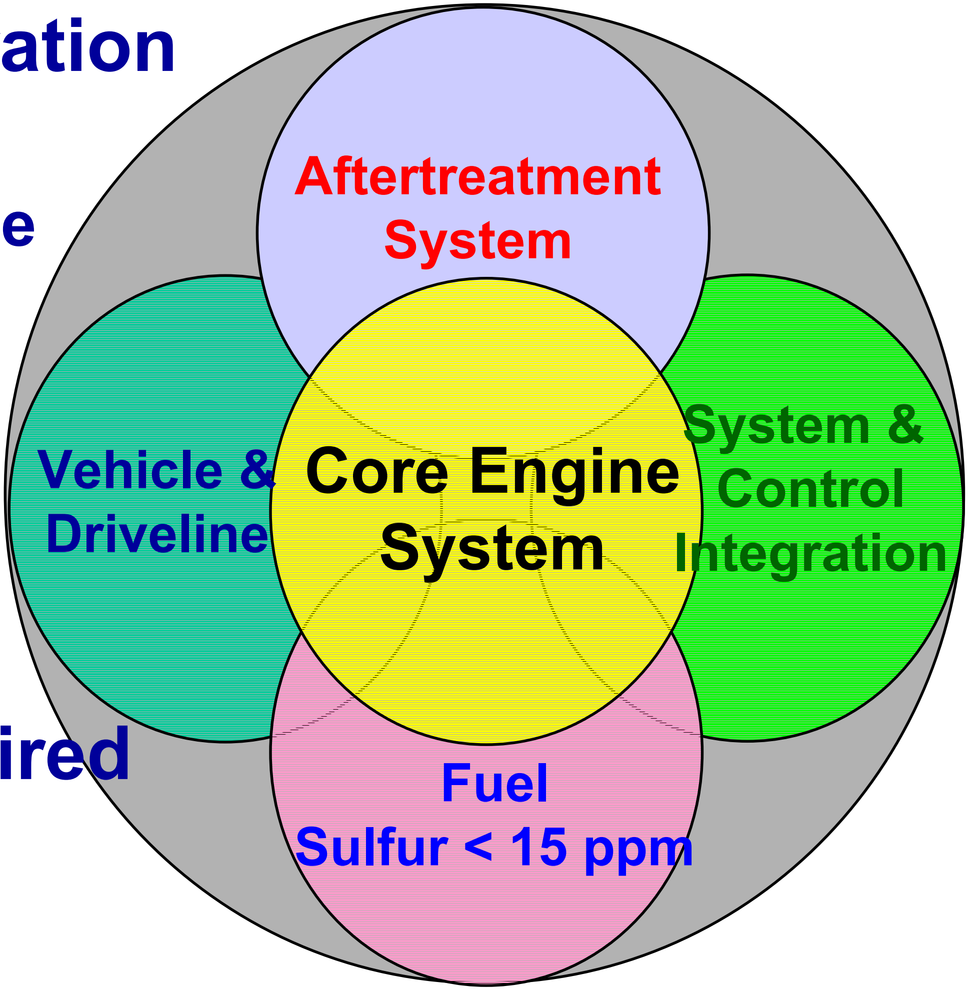
Light Truck Platform



Development Strategy

- Engine/Vehicle Integration is the Key
  - A.T. Price Performance
  - A.T. Useful Life
  - Drivability
  - Vehicle Operational Efficiency
  - System Complexity
- Modeling Tools Required
  - Controls – System Integration - Design



DDC's Tool Box Description

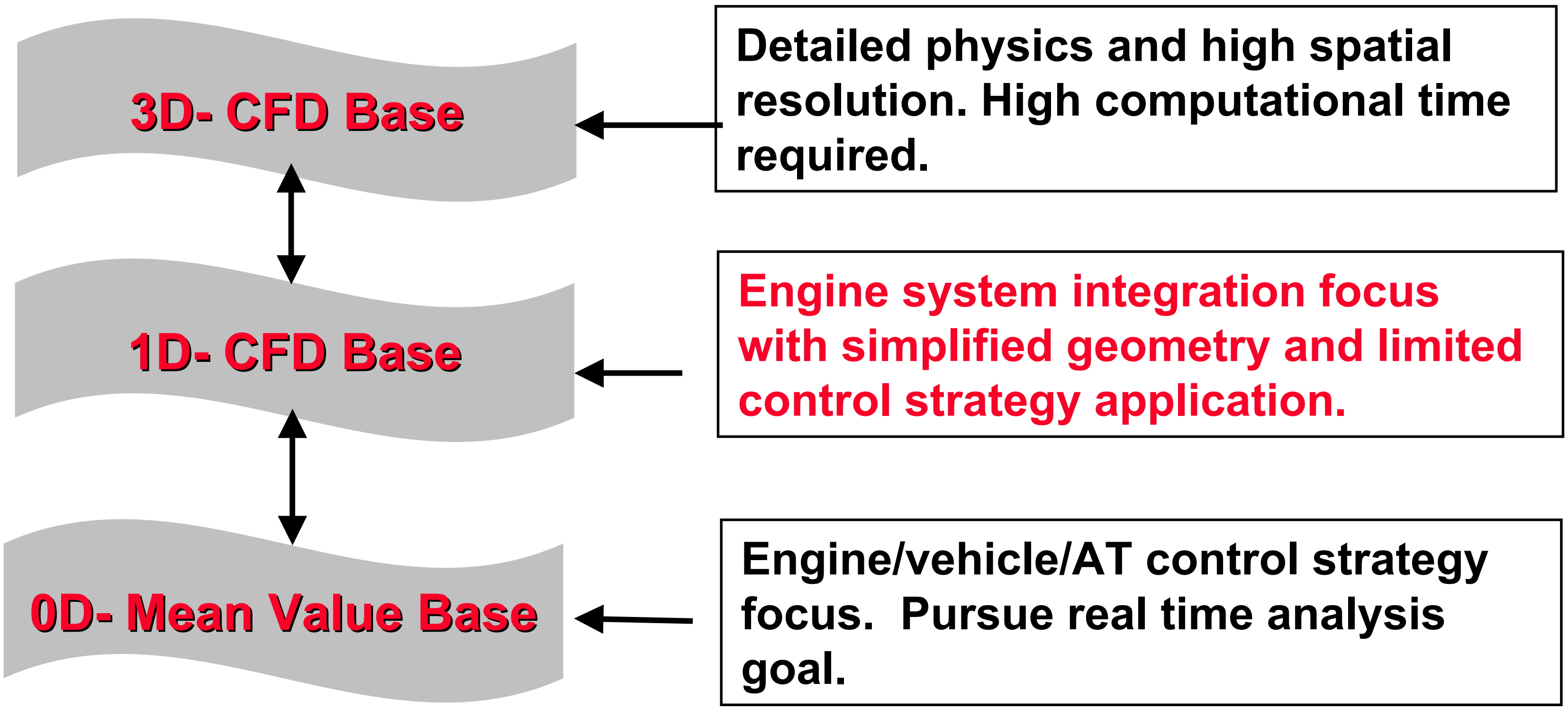
- Engine
  - Mapped Data
  - Mean Value (MV) Model
  - Cycle Simulation
  - Multi-Dimensional Models
- Vehicle Model
  - Simple
  - Complex
- A.T. Models
  - DPF
  - SCR
  - LNT
  - DOC

Aftertreatment Model Philosophy

- Plug & Play
  - Simulink and Fortran Based Models
  - Common Framework
  - Can Be Combined Freely
- Variable Resolution - Adaptable
  - Prime Path A.T. Models are 1D
  - 0D and 3D Also Developed
- Common Framework
  - Sub-Models for
    - » Flow
    - » Chemical Kinetics
    - » Thermal Modeling
    - » Storage

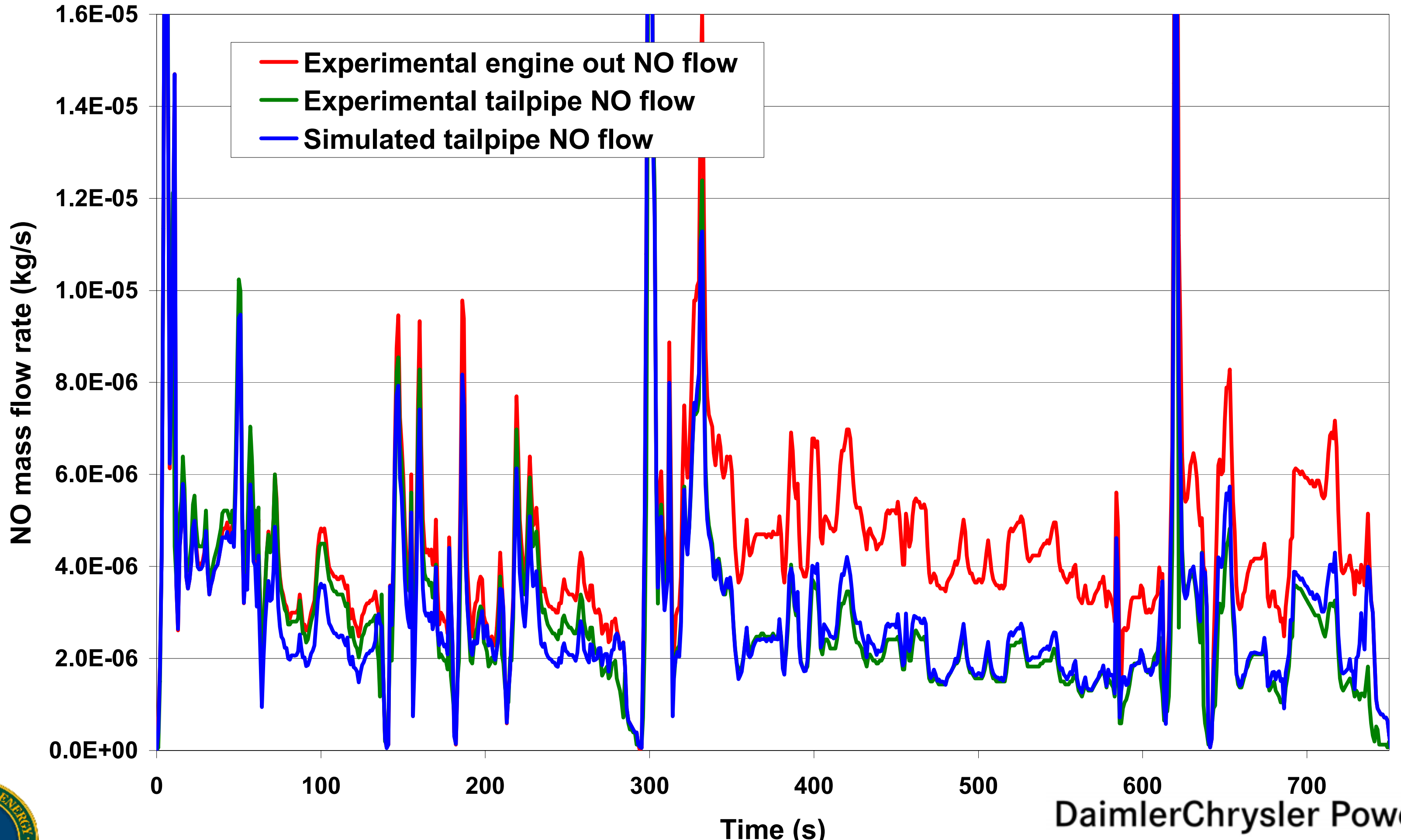
Aftertreatment Virtual Lab Technical Path

"Three-Layer" Development Strategy



1-D SCR Model Calibration
Transient Vehicle Test

Model NOx Prediction Within 5% of Measured Data Over Transient Event



SCR Modeling

1-D CFD Based with Macro-Kinetics

- 1-D CFD Based with Macro-Kinetics
  - Lumped NO and NO_2 reactions with NH_3
  - Reaction Rate Using Langmuir-Hinshelwood Model

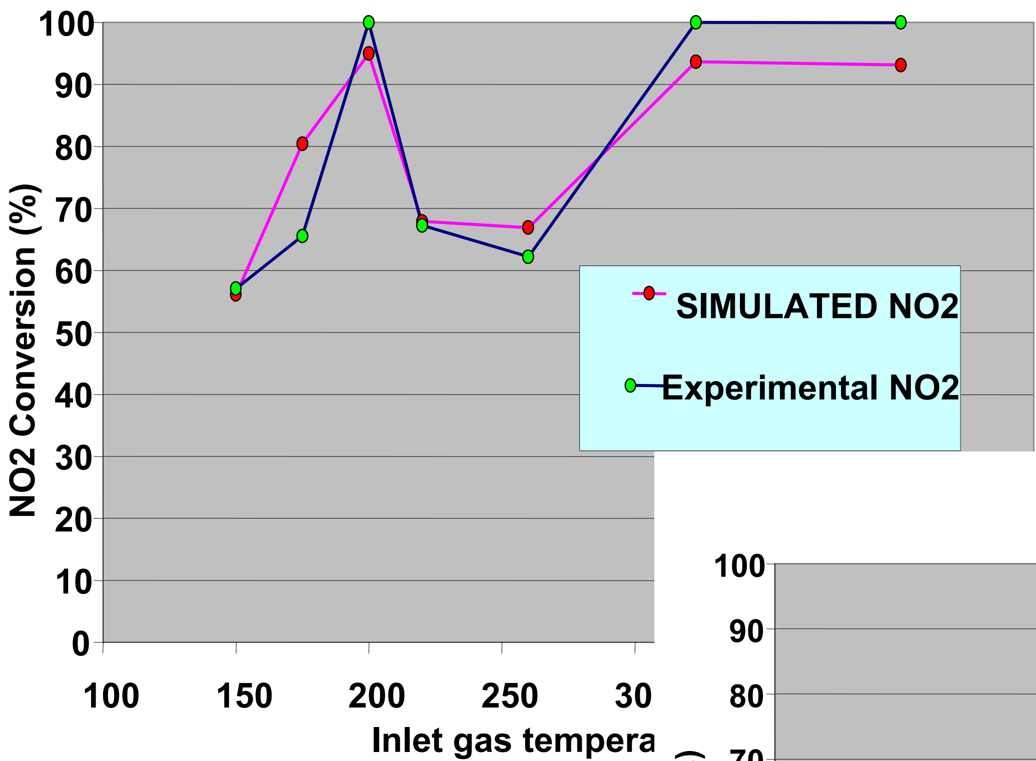
$$R = k\,[A]\,[B] / D_1 D_2 D_3$$

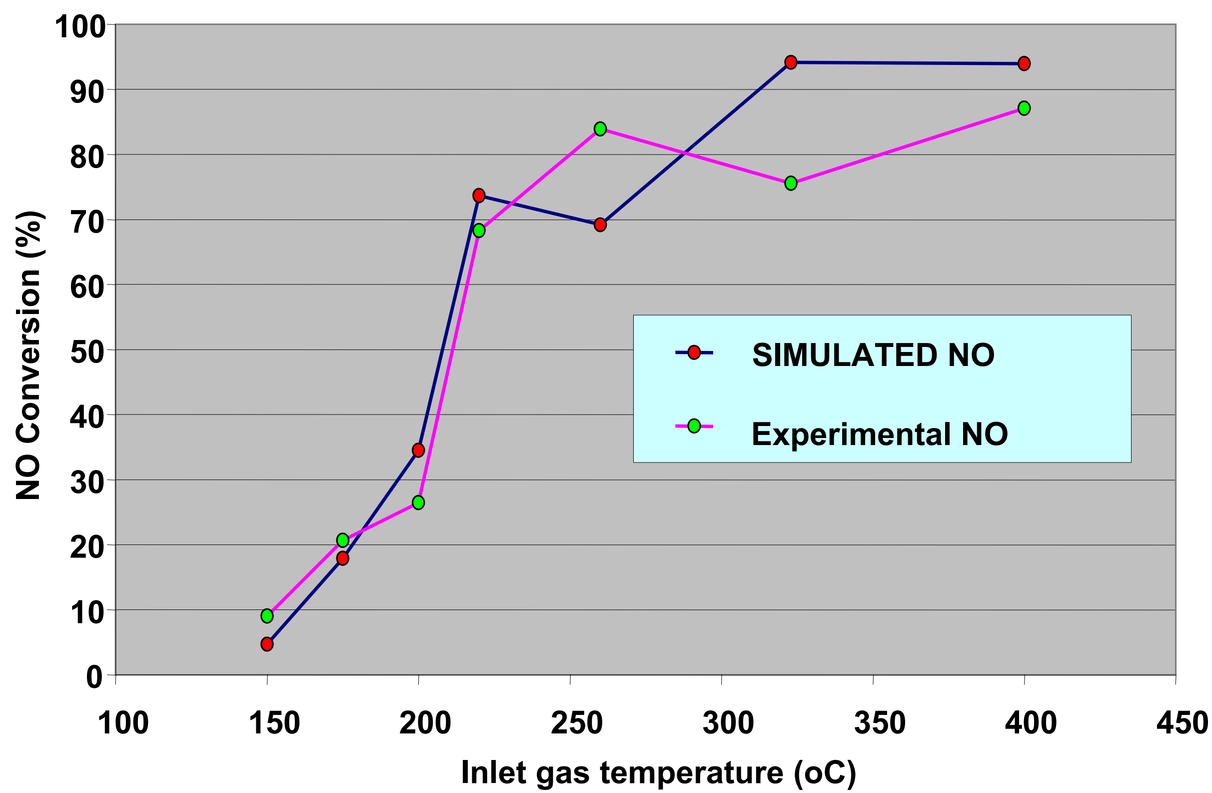
k: Arrhenius kinetic term

D: inhibition terms

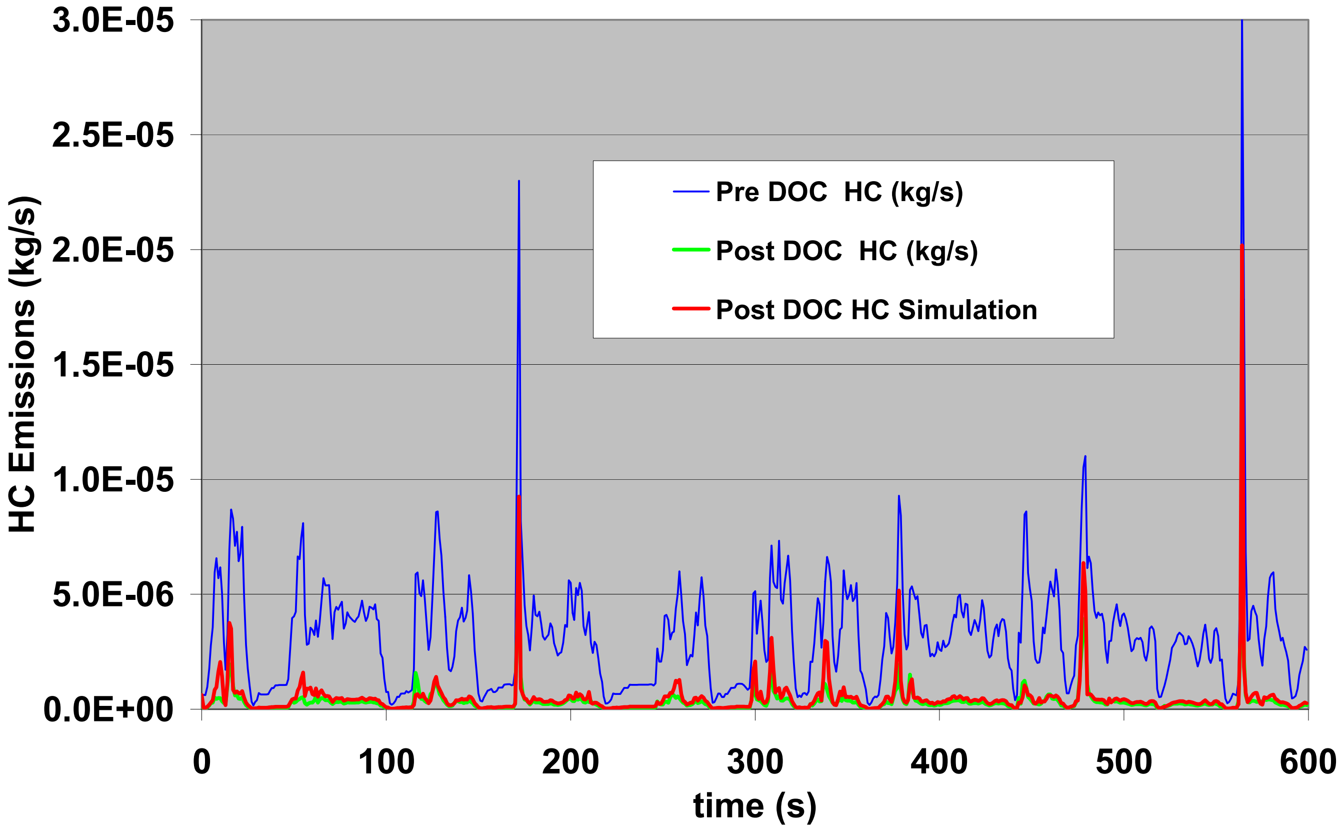
- 1-D Resolution in Axial (Flow) Direction
  - Urea/ammonia and exhaust gas radial distribution in catalyst not accounted for
- Models Largely Empirical
- Can Be Potentially Integrated with Micro-Kinetics

SCR Model Performance

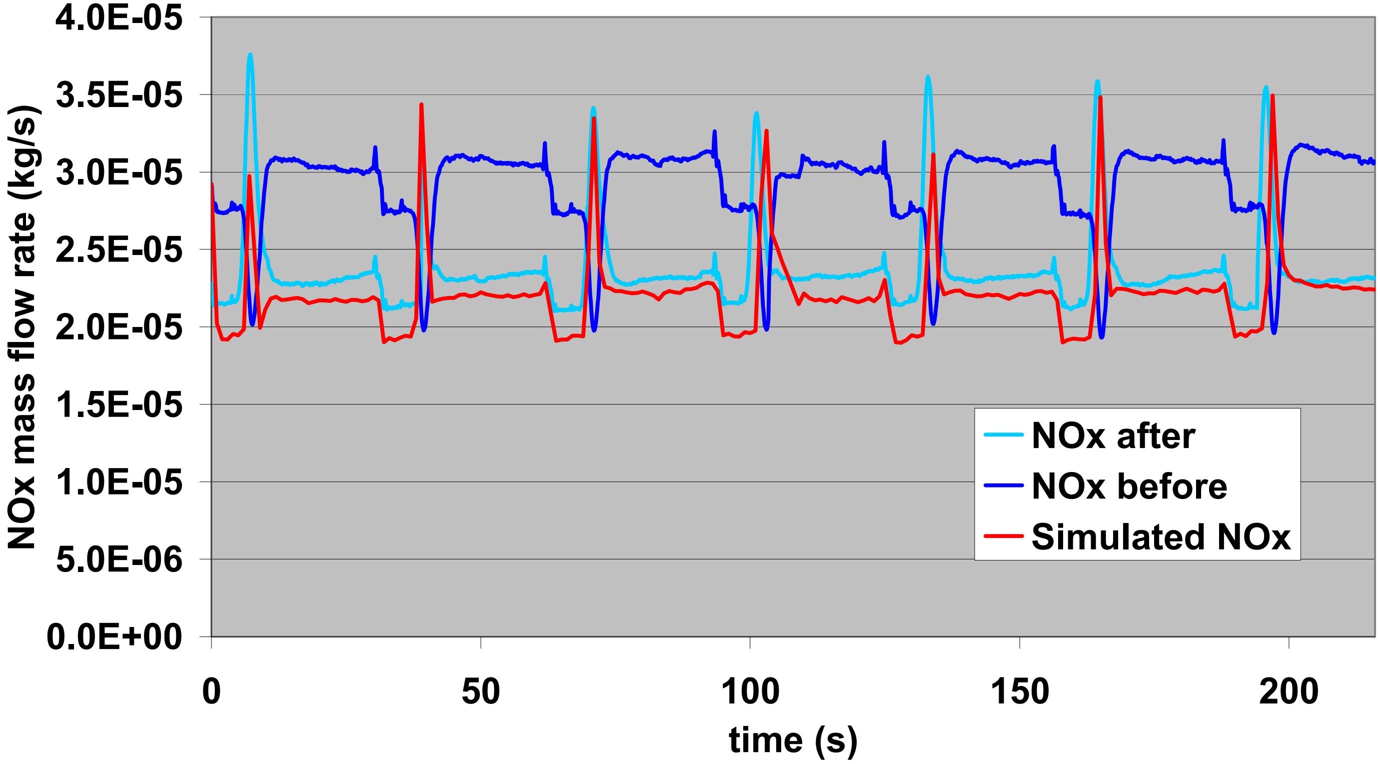




Transient Validations for DOC



Transient Validations for LNT



SCR Modeling
3-D CFD Based with Micro-Kinetics

- 3-D CFD Based with Micro-Kinetics
  - Detailed Reaction Steps
  - Reaction rate using Arrhenius term

$$k = A\, T^{\beta}\, EXP\,(-E/RT)$$

  - Kinetics data availability is a major hurdle
  - Quality of kinetics data and solver technology impact model predictability
- 3-D Resolution Using "Representative Channel" Methodology
  - Can also integrate with urea injection and conversion

Detailed NO Reactions Steps on Vanadium SCR Catalyst

1. NH_3 ADSORPTION ON ACID SITES

   $NH_3 + V^{5+}–OH \rightarrow V–ONH_4$

   $V–ONH_4 \rightarrow NH_3 + V^{5+}–OH$

2. ACTIVATION OF SURFACE NH_3 WITH REDOX SITES

   $V–ONH_4 + V = O \rightarrow V–ONH_3–V^{4+}–OH$

   $V–ONH_3 – V^{4+}–OH \rightarrow V–ONH_4 + V=O$

3. NO REMOVAL STEP

   $NO + V–ONH_3 –V^{4+}–OH \rightarrow N_2 + H_2O + V^{5+}–OH + V^{4+}–OH$

4. REMOVAL OF SURFACE OH TO FORM H_2O

   $2V^{4+}–OH \rightarrow H_2O + V^{3+} + V=O$

   $H_2O + V^{3+} + V = O \rightarrow 2V^{4+}–OH$

5. REOXIDATION OF CATALYST BY O_2

   $O_2 + 2V^{3+} \rightarrow 2V=O$

6. H_2O ADSORPTION ON ACID SITES

   $H_2O + V^{5+}–OH \rightarrow V^{5+}–OH_3O$

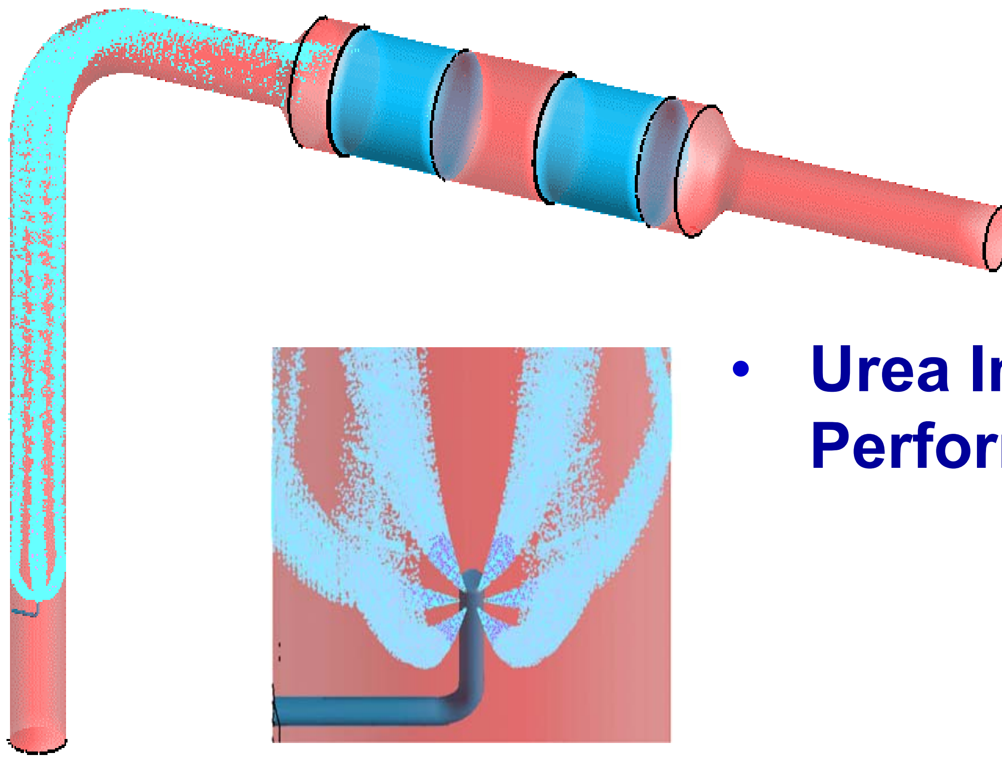
   $V^{5+}–OH_3O \rightarrow H_2O + V^5$

Urea Injection and Conversion to NH_3

Coupled 3D Flow Effects, Mixing and Kinetics

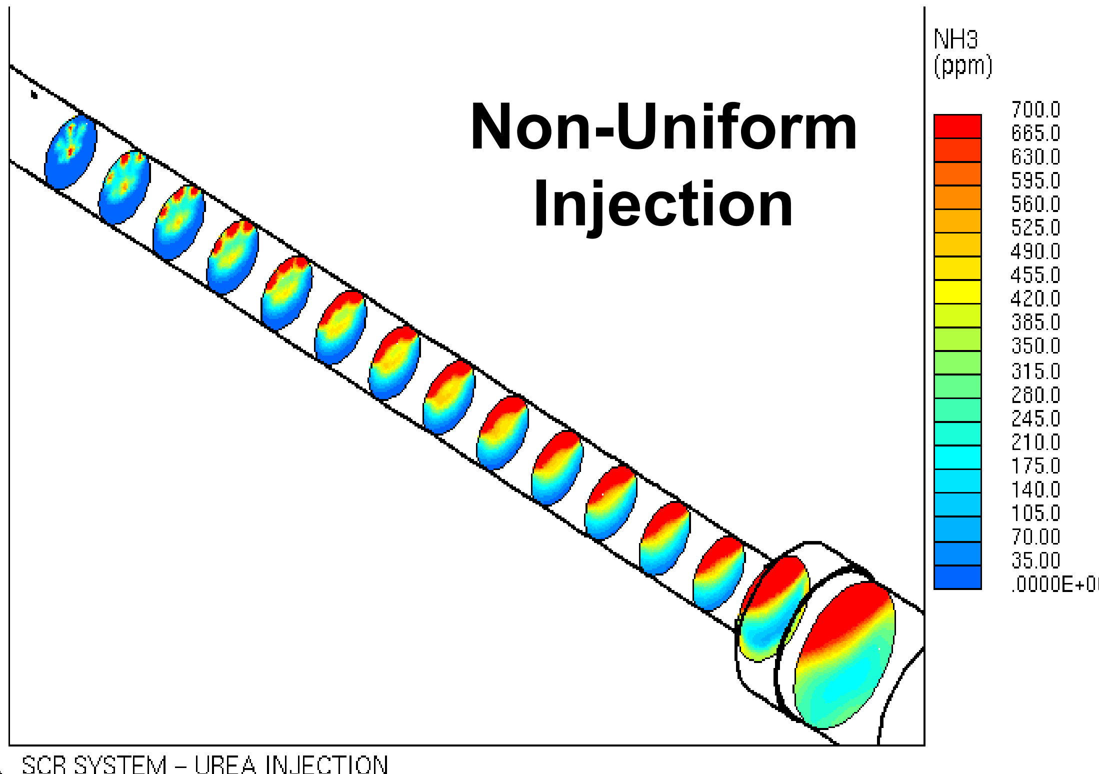
THERMOLYSIS: $(NH_2)_2CO \rightarrow NH_3 + HNCO$

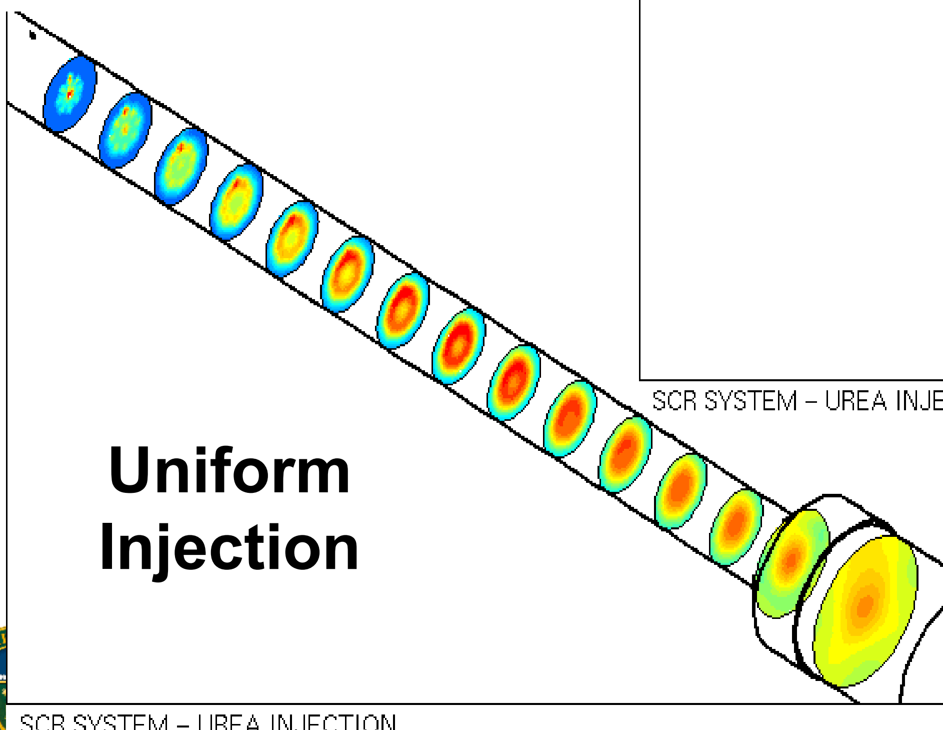
HYDROLYSIS: $HNCO + H_2O \rightarrow NH_3 + CO_2$



- **Urea Injection Performance**

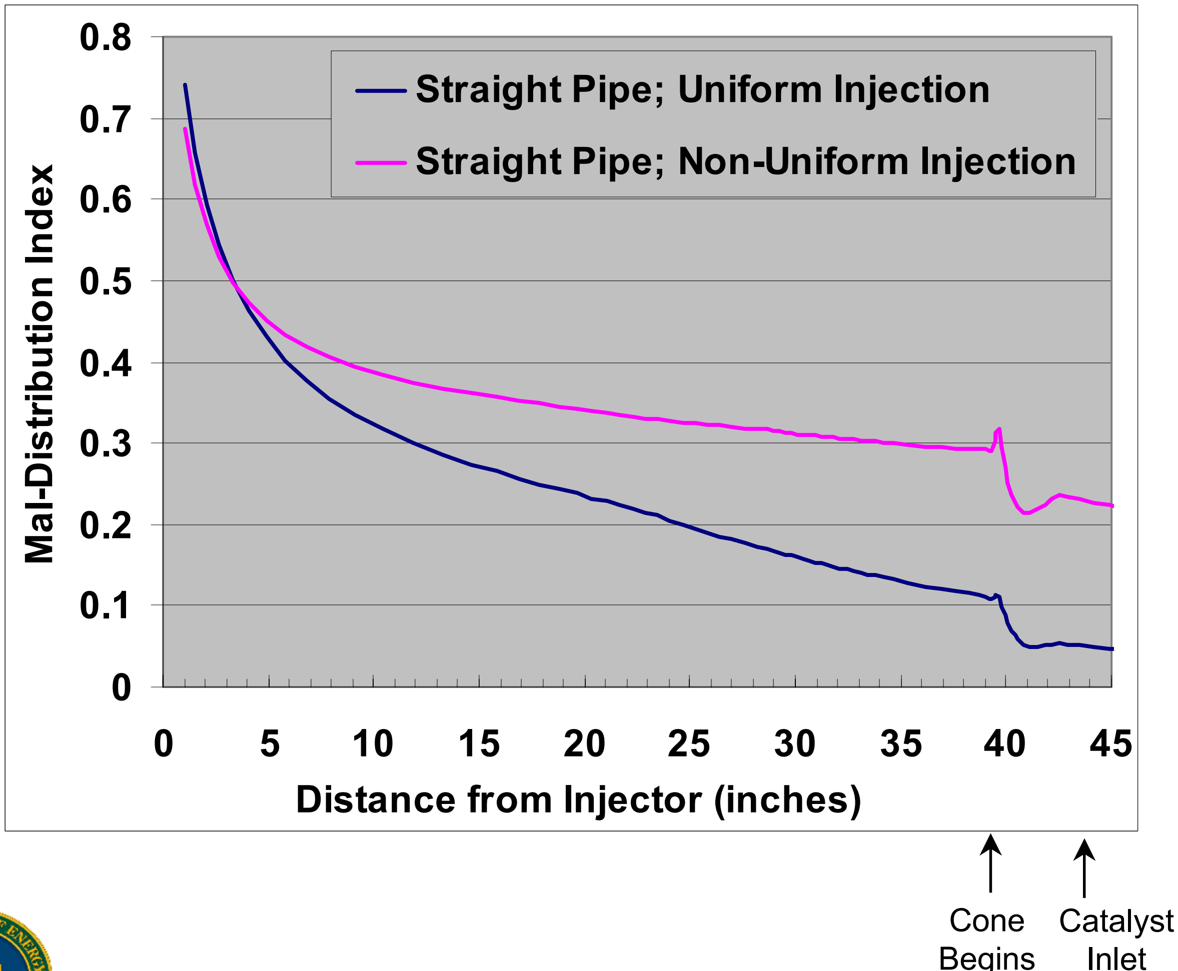
NH3 Distribution





Mal-Distribution Index

Require Mixer, very uniform Spray or very Long Distance

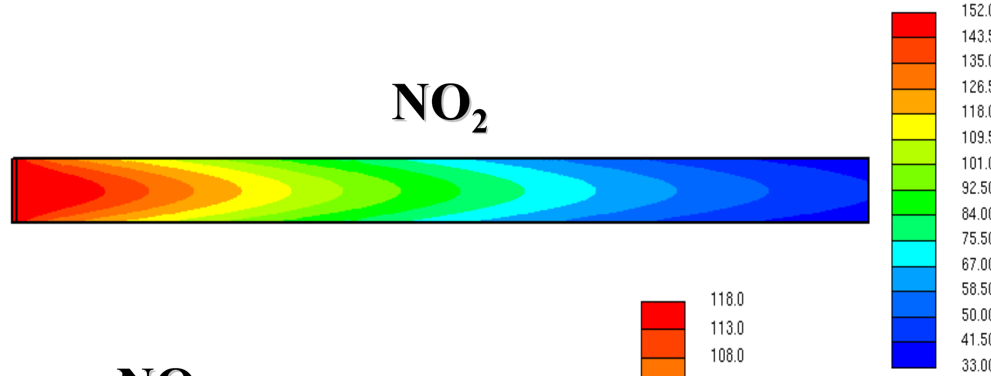


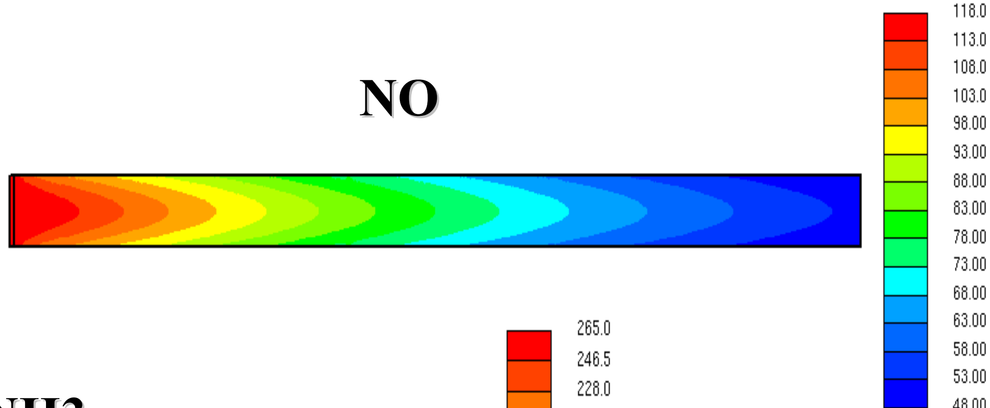
Definition:

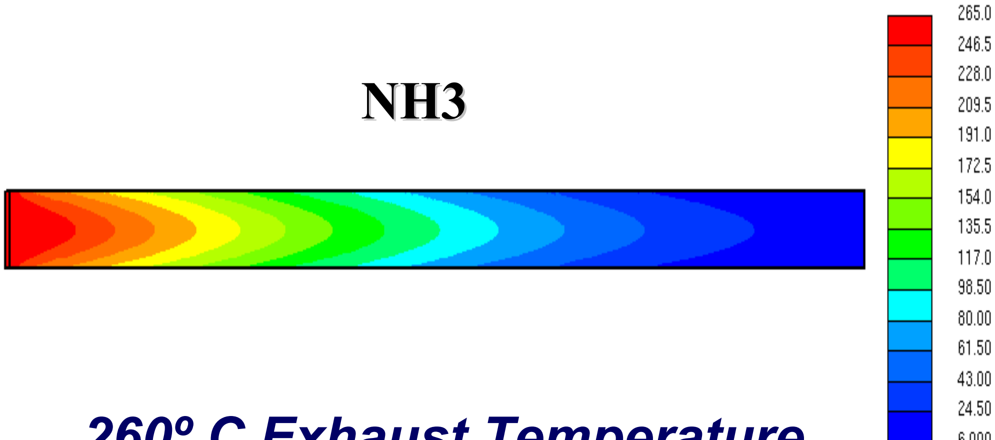
$$\varphi = \frac{1}{2N}\sum_{i=1}^{N}\left|\frac{\alpha_i}{\alpha_{avg}} - 1\right|$$

φ = 0: Homogenous

SCR Channel CFD & CHEMKIN Model Results



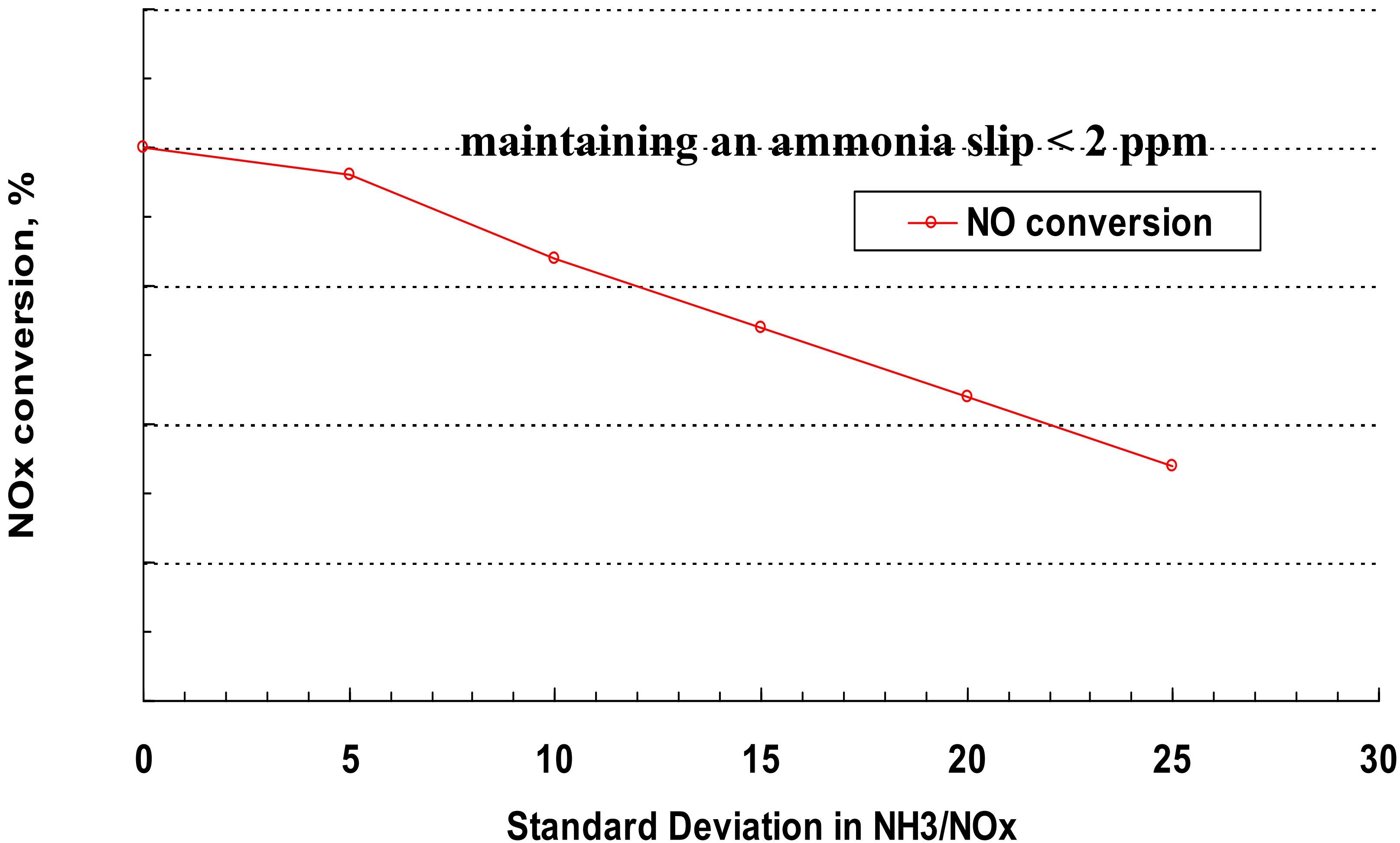




Single Channel Results (Channel not drawn to scale)

260º C Exhaust Temperature

SCR Performance Sensitivity to NH_3 Distribution



SCR Modeling Needs

Framework Exists – Fundamental Data Needed

- SCR Kinetic Data
  - Chemical Reaction Steps
    - Gas Phase and Surface Reactions
    - Micro-Kinetics or Detailed Steps
    - Lumped/Reduced Reaction Steps
  - Reaction Rate Models and Data
    - Detailed Data for Model Validation
    - Improved Model Predictability
  - NH_3 Storage and Release
    - Physical and/or Chemical Mechanisms
    - Storage/Release Models and Kinetic Data
  - Urea to Ammonia Conversion
    - Thermolysis Kinetics
    - Hydrolysis without Catalyst

Summary

- **Modeling Framework Has Been Created**
- **Catalyst Formulations Continue To Evolve & Improve**
- **<u>More/Better Kinetic Data Is Required</u>**
  - **This "Void" Will Exist For Some Time**
  - **Industry, Catalyst Suppliers, National Laboratories, and Universities Can Work Together To Fill This Pre-Competitive Void**

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