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

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Detroit Diesel Corporation
Light Truck Platform

Engine Management – Advances in CLEAN Combustion©
Engine Management Integrated with Aftertreatment

45% Fuel Economy Benefit Compared to Gasoline Baseline
• 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

3D- CFD Base
- Detailed physics and high spatial resolution. High computational time required.

1D- CFD Base
- Engine system integration focus with simplified geometry and limited control strategy application.

0D- Mean Value Base
- Engine/vehicle/AT control strategy focus. Pursue real time analysis goal.
1-D SCR Model Calibration
Transient Vehicle Test

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

- Experimental engine out NO flow
- Experimental tailpipe NO flow
- Simulated tailpipe NO flow
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
    \[ R = \frac{k [A] [B]}{D_1D_2D_3} \]
    \[ k: \text{Arrhenius kinetic term} \]
    \[ D: \text{inhibition terms} \]

- 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
    \[ k = A \ T^\beta \ \text{EXP} (-E/RT) \]
  - 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. **NH₃ ADSORPTION ON ACID SITES**
   \[ \text{NH}_3 + \text{V}^{5+} \cdot \text{OH} \rightarrow \text{V} \cdot \text{ONH}_4 \]
   \[ \text{V} \cdot \text{ONH}_4 \rightarrow \text{NH}_3 + \text{V}^{5+} \cdot \text{OH} \]

2. **ACTIVATION OF SURFACE NH₃ WITH REDOX SITES**
   \[ \text{V} \cdot \text{ONH}_4 + \text{V} = \text{O} \rightarrow \text{V} \cdot \text{ONH}_3 \cdot \text{V}^{4+} \cdot \text{OH} \]
   \[ \text{V} \cdot \text{ONH}_3 \cdot \text{V}^{4+} \cdot \text{OH} \rightarrow \text{V} \cdot \text{ONH}_4 + \text{V} = \text{O} \]

3. **NO REMOVAL STEP**
   \[ \text{NO} + \text{V} \cdot \text{ONH}_3 \cdot \text{V}^{4+} \cdot \text{OH} \rightarrow \text{N}_2 + \text{H}_2\text{O} + \text{V}^{5+} \cdot \text{OH} + \text{V}^{4+} \cdot \text{OH} \]

4. **REMOVAL OF SURFACE OH TO FORM H₂O**
   \[ 2\text{V}^{4+} \cdot \text{OH} \rightarrow \text{H}_2\text{O} + \text{V}^{3+} + \text{V} = \text{O} \]
   \[ \text{H}_2\text{O} + \text{V}^{3+} + \text{V} = \text{O} \rightarrow 2\text{V}^{4+} \cdot \text{OH} \]

5. **REOXIDATION OF CATALYST BY O₂**
   \[ \text{O}_2 + 2\text{V}^{3+} \rightarrow 2\text{V} = \text{O} \]

6. **H₂O ADSORPTION ON ACID SITES**
   \[ \text{H}_2\text{O} + \text{V}^{5+} \cdot \text{OH} \rightarrow \text{V}^{5+} \cdot \text{OH}_3\text{O} \]
   \[ \text{V}^{5+} \cdot \text{OH}_3\text{O} \rightarrow \text{H}_2\text{O} + \text{V}^{5} \]
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

Uniform Injection

Non-Uniform Injection
**Mal-Distribution Index**

**Require Mixer, very uniform Spray or very Long Distance**

\[
\phi = \frac{1}{2N} \sum_{i=1}^{N} \left| \frac{\alpha_i}{\alpha_{avg}} - 1 \right|
\]

**Definition:**

\(\phi = 0: \text{Homogenous}\)

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**Graph Description:**
- **Straight Pipe; Uniform Injection**
- **Straight Pipe; Non-Uniform Injection**

**Axes:**
- **Y-axis:** Mal-Distribution Index
- **X-axis:** Distance from Injector (inches)

**Legend:**
- **Cone Begins**
- **Catalyst Inlet**
SCR Channel CFD & CHEMKIN Model Results

**NO₂**

**NO**

**NH₃**

**Single Channel Results**
*(Channel not drawn to scale)*

260° C Exhaust Temperature
SCR Performance Sensitivity to NH₃ Distribution

maintaining an ammonia slip < 2 ppm

NOx conversion, %

Standard Deviation in NH₃/NOx
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
  - NH₃ 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

• More/Better Kinetic Data Is Required
  – 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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