



#### Simulation approaches to predict Transient performance of Aftertreatment systems

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#### Acronyms

- 1. Aftertreatment System (ATS)
- 2. Diesel Oxidation Catalyst (DOC)
- 3. Diesel particulate Filter (DPF)
- 4. Selective Catalytic Reduction (SCR)
- 5. Ammonia Oxidation Catalyst (AMOX)
- 6. Ammonia to  $NO_X$  Ratio (ANR)
- 7. Computational Fluid Dynamics (CFD)
- 8. Diesel Exhaust Fluid (DEF or AdBlue)
- 9. Particulate Matter (PM)

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### **Aftertreatment solutions**

#### **CORE TECHNOLOGIES**



### Agenda

- 1. Introduction
- 2. 3D CFD+1D AVL BOOST Coupling Overview
- 3. 3D CFD+1D AVL BOOST Coupling Approach: PDF Method
- 4. Case Study : Conversion Efficiency
- 5. Application: Sensor Accuracy Modeling Process and Automation
- 6. Case Study : Sensor Accuracy
- 7. Application: System Level Modeling In Closed Loop
- 8. Case Study: System Level Modeling
- 9. Summary and Conclusion

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#### Introduction

- 1. Aftertreatment system cleans exhaust gases.
- 2. DPF: collects and oxidizes the soot.
- 3. DOC: aids in hydrocarbon oxidation process.
- 4. DEF is injected into the hot exhaust stream in the Decomposition Reactor.
- 5. SCR: converts  $NO_x$  and urea mixture into harmless nitrogen gas (N<sub>2</sub>) and water vapor (H<sub>2</sub>O).





Fig: Cut section of Cummins After treatment system

https://www.youtube.com/watch?v=NvLj6e7JdUo

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Fig: Cummins After treatment system

# 3D+1D coupling overview and scope of the study

- 1. Steady state 3D CFD:
  - 1. ANR special distribution prediction.
  - 2. Not feasible running transient cycles.
  - 3. Tools: ANSYS Fluent, Converge CFD
- 2. 1D kinetic models:
  - 1. Real time prediction of transient SCR performance.
  - 2. Can not capture the effect of non-axial non-uniformities.
  - 3. Tool: AVL BOOST
- 3. 3D+1D coupling methods:
  - 1. Predict transient SCR system performance, taking the effect of ANR non-uniformity into account.
  - 2. Non-uniform storage on the catalyst due to non-uniform ANR distribution is also considered.

**Scope :** Product development and modification by using 3D-1D coupling process developed in Cummins Emission Solutions (CES)







Fig: ANR contour at SCR inlet



Fig: Transfer function

# **3D CFD+1D AVL BOOST coupling overview**



- 1. Pressure drop
- 2. DEF decomposition Uniformity Index





3. Interpolation

- 3D+1D coupling application
- Steady state and Transient NO<sub>X</sub> conversion efficiency
- 2. NH<sub>3</sub> slip
- 3. Sensor accuracy
- 4. Design modification to meet emission performance
- 5. Catalyst size modification to meet emission performance





Fig: NH3 slip

Fig: Outlet species distribution

### **3D+1D Coupling approach: PDF Method**

- 1. Empirical PDF was used to fit the ANR data and then discretized into bins. Average ANR for each bin calculated and fed into BOOST for parallel simulations.
- 2. Can be used for both steady-state and transient simulations.
- 3. Data fitting and averaging results in a loss of fidelity.



Ref: Kalyankar, A., Munnannur, A., and Liu, Z., "Predictive Modeling of Impact of ANR Non-Uniformity on Transient SCR System DeNOx Performance," SAE Technical Paper 2015-01-1055

### **Case study: Conversion efficiency**



- 1. Mass flux and temp at inlet boundary defined as a global parameter and this input is provided through explorer.
- 2. NH3 ppm is calculated using ANR factors and provided as input.



- 1. Mass flux and temp at inlet boundary provided as constant input.
- 2. DEF dosing is calculated using ANR controller, formula is provided in the calculator.



 $NO_{x}$  conversion efficiency (%)



- 1. Based on the availability of data, the user can select the method of modeling ATS.
- 2. With both methods, results accuracy is good.
- 3. The above shown results are with the method 2 and there is a good correlation found with test data. (less than 10%)

### Sensor accuracy modeling process



#### **Applications:**

- 1. Accuracy of sensor reading
- 2. Best position to place sensor
- 3. Geometrical changes required to meet sensor accuracy
- 4. Design changes for cost reduction



AVL supports modeling catalyst reactions. The entire analysis process is automated by using state of the art tools.

#### **Case Study: Sensor accuracy**

#### **Problem statement/ Objective:**

- Reposition sensor to accurately predict the species in the exhaust gas.
- 2. Provide a cost-reduced solution that meets the requirement.

Accuracy Error(%) = 
$$100x = \frac{(NOx_{sensor} - NOx_{Ref})}{NOx_{Ref}}$$

Concept	Sensor location	Sensor accuracy error (normalized)	
		Analysis	Test
Baseline	А	1.1	1.05
Concept1	В	0.19	0.16
	А	0.70	0.81
	С	1.05	1.11

Test results replication

Ref: Kalyankar, A., Munnannur, A., and Liu, Z., "CFD Modeling of Tailpipe NOx Sensor Accuracy" SAE



Fig: ATS architecture

#### Analysis Sensor accuracy error (normalized) Clocking Concept Test Point 1 Test Point 2 Test Point 3 Concept1 -1.26 -0.08 1.43 В **Concept1** Optimised 5.67 -1.42 0.52 Concept1 -0.36 -4.20 0.10 Α **Concept1** Optimised 0.07 -0.15 -3.01 Concept1 -6.82 1.88 0.08 С **Concept1** Optimised 0.79 0.35 -2.10

#### Optimized concept1 which works for all clocking of sensor

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#### System level modeling in closed loop



Fig: Schematic of system model

Fig: 1D kinetic model setup

- 1. 1D kinetic model is created as per ATS architecture and calibrated for temperature and pressure drop.
- 2. Controller, sensors, and other components like doser are modeled in a closed loop architecture.
- 3. Application:
  - 1. Virtual rigs for programs to validate system
  - 2. Cycle emissions (NOx)
  - 3. Thermal management interaction
  - 4. Fuel economy
  - 5. Failed part analysis
  - 6. System robustness

#### **Thermal calibration of model**



DOC out, DPF out, and SCR in all temperatures are following test trends and the difference is very minimal. "© 2020 Cummins Inc. All rights Reserved."

### Case study: System level modeling

**Objective:** The goal is to replicate emission performance test virtually for ATS





- 1. The results shown here are without considering the 3D+1D coupling approach.
- 2. Implementing the 3D+1D approach to system level model is complex, the approach is ready but needs some tuning.
- 3. We have seen a good correlation with test results with scope for further improvement.

### **Summary and Conclusion**

- 1. Lack of integrated framework resulted in lot of testing iterations at system & subsystem level.
- 2. The system modeling framework is developed including interactions of subsystems like doser, mixer, SCR & NOx sensor in the Aftertreatment system (ATS). The developed framework predicts the mixer effectiveness, optimized tailpipe NOx sensor location & ATS system out emissions predictions across 100 steady state data points (95 % accuracy in comparison with Test cell data)
- 3. System modeling is used in many ways in the ATS modeling like:
  - 1. Catalyst selection
  - 2. Emission performance analysis
  - 3. Design changes
  - 4. Cost reduction
  - 5. Digital Twin

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