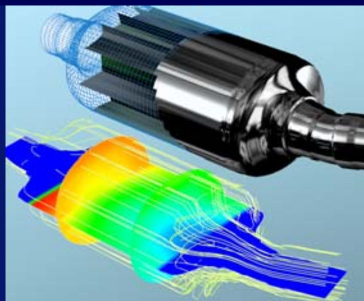
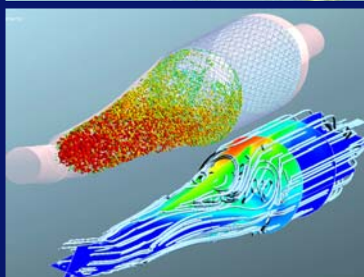
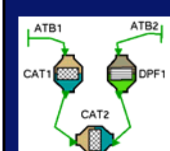


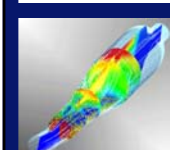


Simulation and Optimization of DPF and SCR Systems

Roland Wanker
Johann C. Wurzenberger

Contents





- Introduction
  - Model Status
  - Model Integration
  - Model Application
- Aftertreatment Simulation Workflow
- Simulation Examples
  - SCR System Optimization
  - DPF System Optimization
- Summary

Aftertreatment Simulation Strategy, I

Variety in:

- **Concepts for Emission Control Systems**
  - Diesel
  - Gasoline, ...
- **Components**
  - Catalysts
  - DPFs
  - Urea/Diesel Injection, ...
- **Targets for Optimization**
  - Uniformity of Flow, Concentrations
  - Completeness of DPF Regeneration
  - Cycle Emissions
  - Heat-Up
  - ECU Calibration, ...

Need for:

Integration of Models

into a Variety of Simulation Tools

Pre-Defined Models

Ready-to Use Chemistry for Catalysts and DPFs

Flexibility of Models

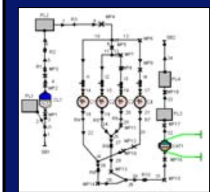
to Define any Reaction Model According to Customer Specific Needs

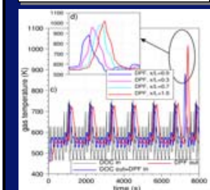
Aftertreatment Simulation Strategy, II

Integration	▪ BOOST 1D Aftertreatment ▪ CRUISE (using BOOST 1D as dll) ▪ BOOST 1D s-function in Matlab/Simulink ▪ FIRE 2D/3D **Identical physical and chemical models**
Application	▪ Diesel Oxidation Catalyst (DOC) ▪ Diesel Particulate Filter (DPF, CSF) ▪ Selective Catalytic Reduction (SCR) ▪ Three Way Catalyst **Dedicated kinetic models for each specific application**
Flexibility	▪ Use BOOST 1D Aftertreatment as Platform ▪ User Coding Interface allows 100% Access to all Features **Customer's proprietary kinetic models**

Model Integration, I

AVL





- **BOOST 1D Aftertreatment**
  - 1D, fast, robust
  - Pre-defined reaction models available
  - Connected to iSIGHT for parameter identification

➔ Component and system level simulations and optimization

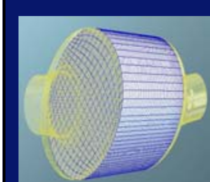
➔ Analysis of reaction chemistry

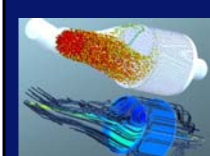
➔ Prediction of mode emissions

➔ Starting point for any aftertreatment simulation activity

Model Integration, II

AVL





- **FIRE 2D/3D Aftertreatment**
  - 3D, very detailed
  - Pre-defined reaction models available
  - Pre-calibrated model from BOOST can be used

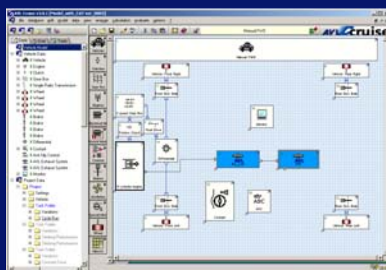
➨ Uniformity optimization
(e.g. of species, temperature or mass flow)

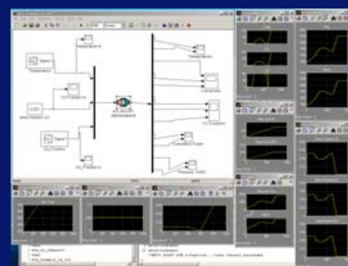
➨ System optimization
(e.g. spray, homogeneous reactions, DOC, SCR, DPF)

➨ CFD - FEM coupling
(e.g. thermal stress during regeneration of a DPF)

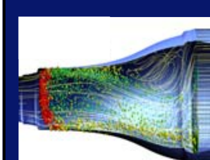
Model Integration, III

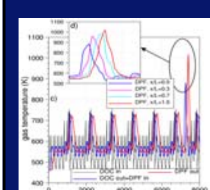
- **CRUISE Aftertreatment**
  - Pre-calibrated model from BOOST can be used
  - ➨ Investigate influence of different vehicles on catalyst and DPF performance (and vice-versa)
- **Matlab/Simulink s-Function**
  - ➔ BOOST 1D aftertreatment connects to the whole world of MATLAB/SIMULINK





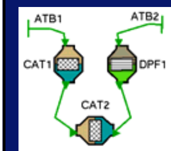
Application, Optimization Targets

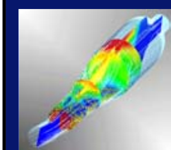


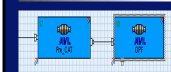


- **Catalyst**
  - DOC (TWC): Heat-Up during Cold Start
  - DOC (TWC): Flow Distribution, and Mode Emissions
  - DOC: NO <--> NO2 Conversion
  - SCR: System Configuration (HSO, ...)
  - SCR: Injection of Urea, Evaporation and Mixing
- **DPF**
  - Loading: Soot Distribution and Pressure Drop
  - Regeneration: Duration, Completeness and Thermal Stresses
- **Exhaust System**
  - Losses to Ambient
  - Heat-Up of Pipes, Insulation Material, ...

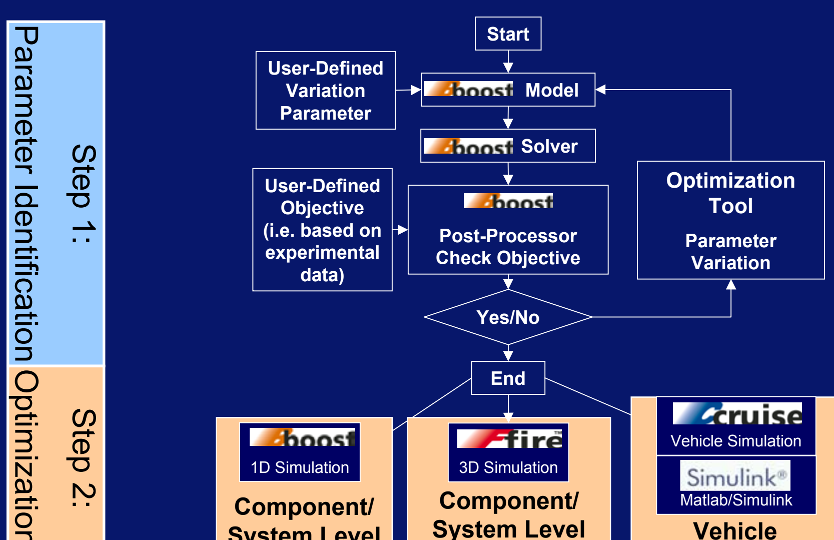
Contents







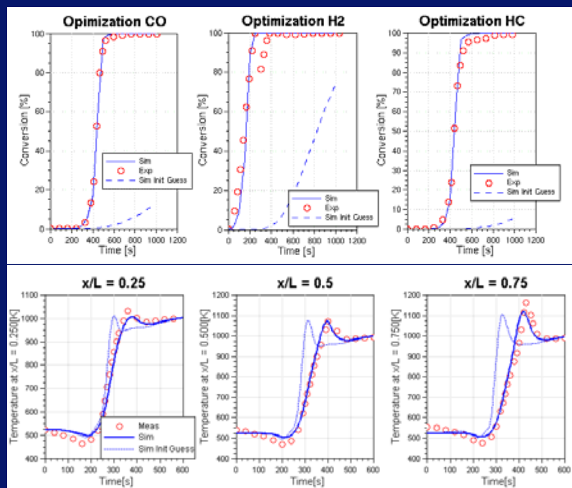
Aftertreatment Workflow Concept



Step 1, Parameter Identification

AVL

Comparison of Experimental Data with Guessed and Tuned Kinetic Parameters



Oxi-cat Light-off

840 BOOST Runs in iSIGHT v7.1

DPF Regeneration

100 BOOST Runs in iSIGHT v7.1

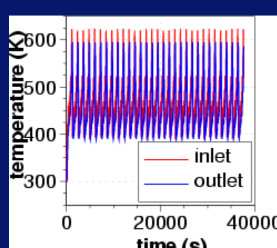
Step 2, System Optimization

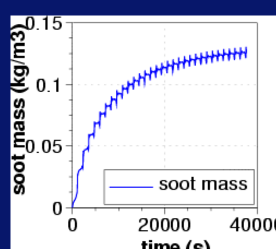
AVL

boost

CRT-System,

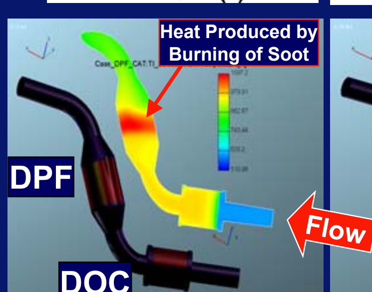
30 NEDCs

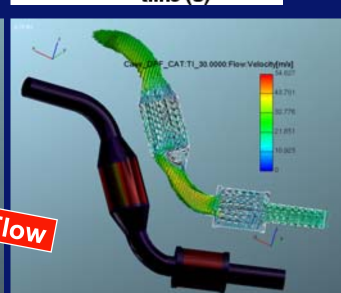




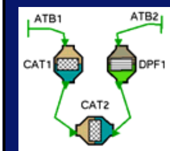
fire

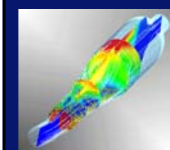
Exhaust Gas Line
DOC and DPF

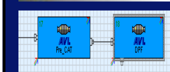




Headline







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V-HSO System

- Pre (Vor)-Catalyst
- Hydrolysis, SCR and Oxidation Catalyst

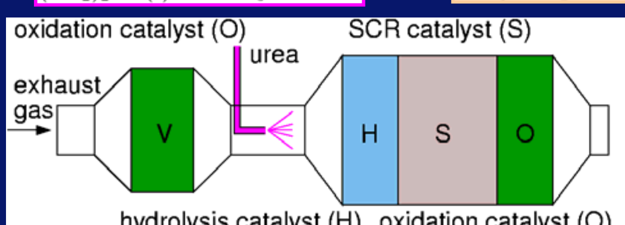
$$NH_3 + S \xrightarrow{k_6} NH_3(S)$$
$$NH_3(S) \xrightarrow{k_7} NH_3 + S$$

$$4NH_3 + 4NO + O_2 \xrightarrow{k_1, k_8} 4N_2 + 6H_2O$$
$$4NH_3 + 2NO + 2NO_2 \xrightarrow{k_2} 4N_2 + 6H_2O$$
$$8NH_3 + 6NO_2 \xrightarrow{k_3} 7N_2 + 12H_2O$$

$$(NH_2)_2CO(aq) \longrightarrow (NH_2)_2CO(s) + 7.1H_2O(g)$$

$$(NH_2)_2CO(s) \xrightarrow{k_{hom}} NH_3 + HCNO$$

$$4NH_3 + 3O_2 \xrightarrow{k_4, k_9} 2N_2 + 6H_2O$$



$$2NO + O_2 \longleftrightarrow 2NO_2$$

$$HCNO + H_2O \xrightarrow{k_5} NH_3 + CO_2$$

$$4NH_3 + 3O_2 \xrightarrow{k_4, k_9} 2N_2 + 6H_2O$$

V-HSO System

SAE-2005-01-0948: (Wurzenberger and Wanker, AVL)

- steady-state kinetic model validation
- transient kinetic model validation
- component level simulation
- system level simulation

SAE-2006-01-0643: (Birkhold et al., BOSCH)

- urea spray model validation
- wallfilm model validation
- evaporation and thermolysis reaction model validation

Rate Equations

▪ Steady-State, Eley-Rideal

Hydrolysis Section

$$\dot{r}_5 = \mathrm{K}_5^0 \cdot \exp\left(\frac{-\mathrm{E}_5}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{HCNO}} \cdot c^{\mathrm{L}}_{\mathrm{H_2O}}$$

SCR Section

$$\dot{r} = \mathrm{K}_1 \cdot \exp\left(\frac{-\mathrm{E}_1}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NO}} \cdot \frac{\mathrm{K}_2 \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}{1 + \mathrm{K}_2 \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}$$

$$\dot{r} = \mathrm{K}_1 \cdot \exp\left(\frac{-\mathrm{E}_1}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NO}} \cdot c^{\mathrm{L}}_{\mathrm{NO_2}} \cdot \frac{\mathrm{K}_2 \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}{1 + \mathrm{K}_2 \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}$$

$$\dot{r} = \mathrm{K}_1 \cdot \exp\left(\frac{-\mathrm{E}_1}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NO_2}} \cdot \frac{\mathrm{K}_2 \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}{1 + \mathrm{K3} \cdot \exp\left(\frac{-\mathrm{E}_2}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}}$$

$$\dot{r}_4 = \mathrm{K}_4^0 \cdot \exp\left(\frac{-\mathrm{E}_4}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}$$

Oxidation Section

$$\dot{r}_4 = \mathrm{K}_4^0 \cdot \exp\left(\frac{-\mathrm{E}_4}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}$$

▪ Transient, Temkin-Type

Hydrolysis Section

$$\dot{r}_5 = \mathrm{K}_5^0 \cdot \exp\left(\frac{-\mathrm{E}_5}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{HCNO}} \cdot c^{\mathrm{L}}_{\mathrm{H_2O}}$$

SCR Section

$$\dot{r}_6 = \mathrm{K}_6^0 \cdot \exp\left(\frac{-\mathrm{E}_6}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}} \cdot [1 - Z_{\mathrm{NH_3}}(\mathrm{S})]$$

$$\dot{r}_7 = \mathrm{K}_7^0 \cdot \exp\left\{\frac{-\mathrm{E}_7 \cdot [1 - \epsilon \cdot Z_{\mathrm{NH_3}}(\mathrm{S})]}{T_s}\right\} \cdot Z_{\mathrm{NH_3}}(\mathrm{S})$$

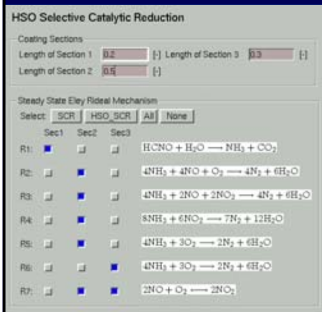
$$\dot{r}_8 = \mathrm{K}_8^0 \cdot \exp\left(\frac{-\mathrm{E}_8}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NO}} \cdot Z^*_{\mathrm{NH_3}}(\mathrm{S}) \cdot \left\{1 - \exp\left[\frac{Z_{\mathrm{NH_3}}(\mathrm{S})}{Z^*_{\mathrm{NH_3}}(\mathrm{S})}\right]\right\}$$

$$\dot{r}_9 = \mathrm{K}_9^0 \cdot \exp\left(\frac{-\mathrm{E}_9}{T_s}\right) \cdot Z_{\mathrm{NH_3}}(\mathrm{S})$$

Oxidation Section

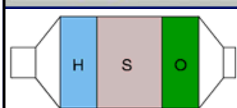
$$\dot{r}_4 = \mathrm{K}_4^0 \cdot \exp\left(\frac{-\mathrm{E}_4}{T_s}\right) \cdot c^{\mathrm{L}}_{\mathrm{NH_3}}$$

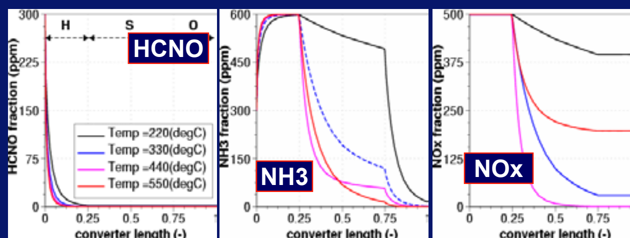
SCR, Pre-Defined Kinetic Models, “Steady”



HSO SCR Catalyst, Steady-Approach

- 3 Different Reaction Sections
- 1 Hydrolysis Reaction for HCNO
- 3 SCR Reactions of Eley-Rideal Type
- 2 Oxidation Reactions for NH3
- 1 Reversible Oxidation Reaction for NO



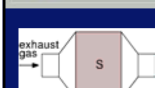


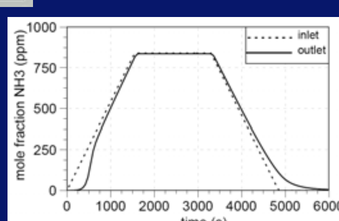
SAE 2005-01-0948,
Wurzenberger, Wanker

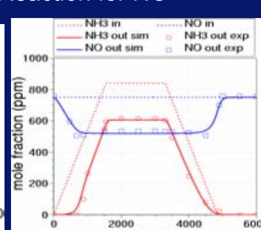
SCR, Pre-Defined Kinetic Models “Transient”

HSO SCR Catalyst, Transient Approach

- 3 Different Reaction Sections
- 1 Hydrolysis Reaction for HCNO
- 2 Adsorption/Desorption Reactions for NH3
- 3 Transient SCR Reactions
- 2 Oxidation Reactions for NH3 (transient/steady)
- 1 Reversible Oxidation Reaction for NO



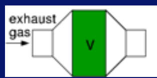




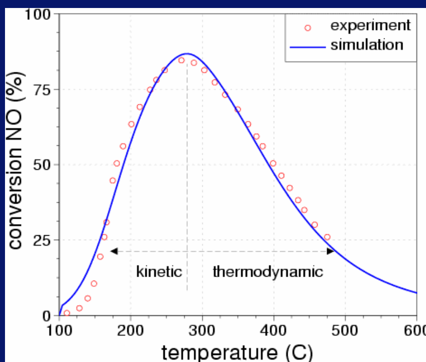
SAE 2005-01-0948, Wurzenberger, Wanker   Catalysis Today (60), 2000, Nova et al.

SCR, Pre-Oxidation Catalyst

AVL

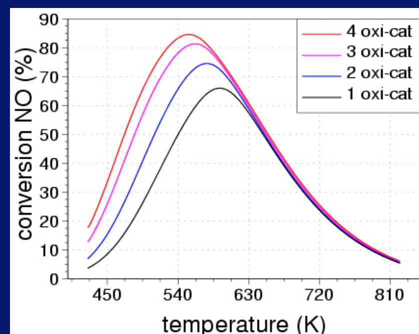


- **Light-Off, Comparison with Measurement**



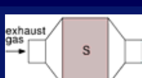
SAE-2000-01-189, Gieshoff et.al, Degussa-Hüls AG

- **Light-Off for Different Converters Sizes**



SCR, Light-Off Simulation

AVL



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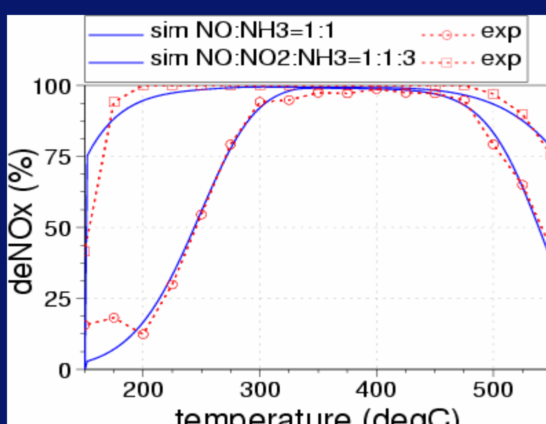
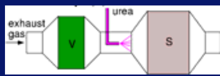
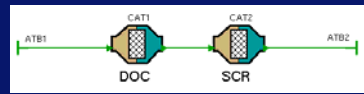


SAE-2000-01-188, Chandler et al., Johnson Matthey
SAE-2005-01-948, Wurzenberger and Wanker, AVL

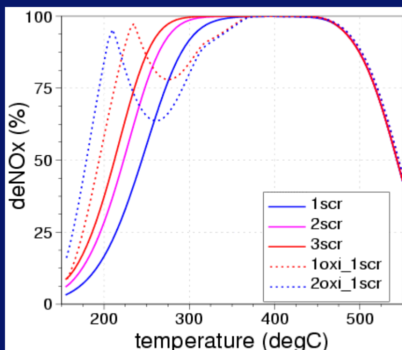
SCR, System Simulation, DOC and SCR

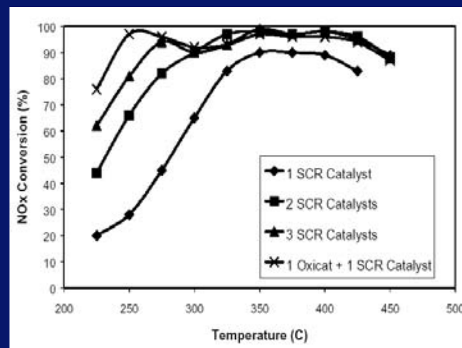
AVL





- Light-Off for Different SCR and Pre-Catalyst Sizes

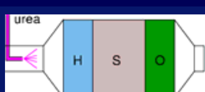


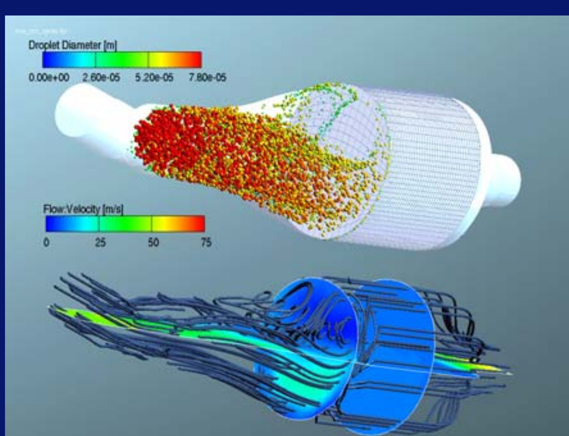


SAE-2000-01-188, Chandler et.al, Johnson Matthey

SCR, Urea Injection and 3D Flow

AVL





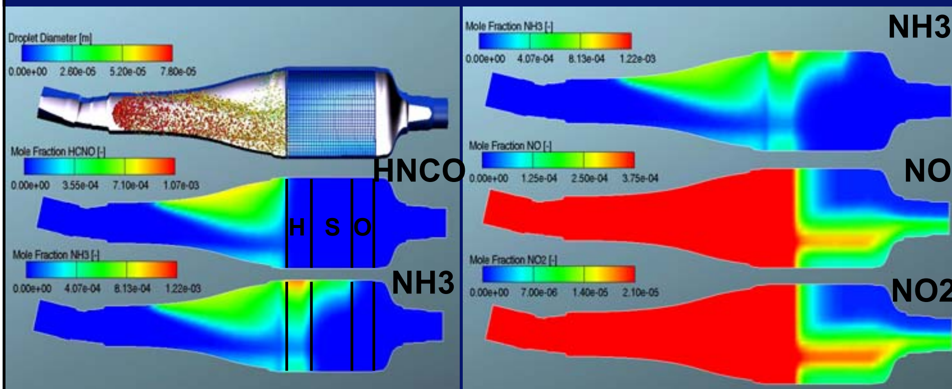
SAE-2005-01-948, Wurzenberger and Wanker, AVL

- Urea Injection
- Evaporation (Dukovicz Model)
- Homogeneous Gas Phase Reactions (Chemkin Interface)
- HSO Converter Model, with Kinetic Parameters tuned in 1D

SCR, 3D Species Distribution

AVL

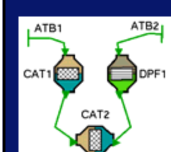
- HNCO, NH3, NO and NO2

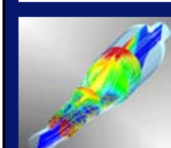


Contents

AVL

boost
fire
cruise





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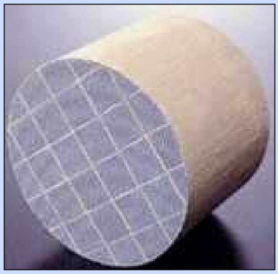
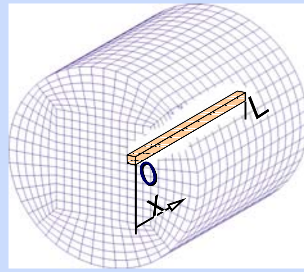
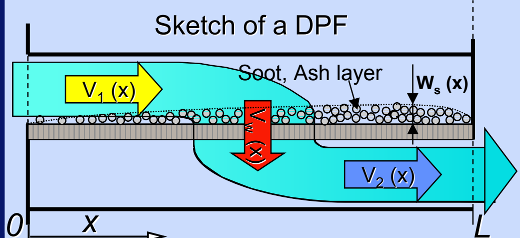
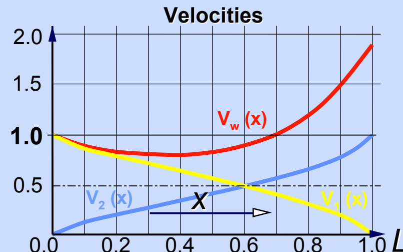
DPF Flow Model

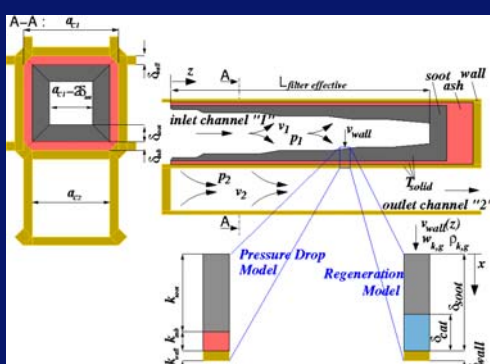








DPF Model Features



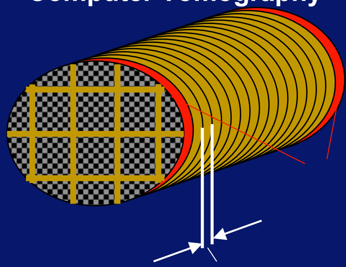
SAE 2004-01-1132, Peters et al., AVL

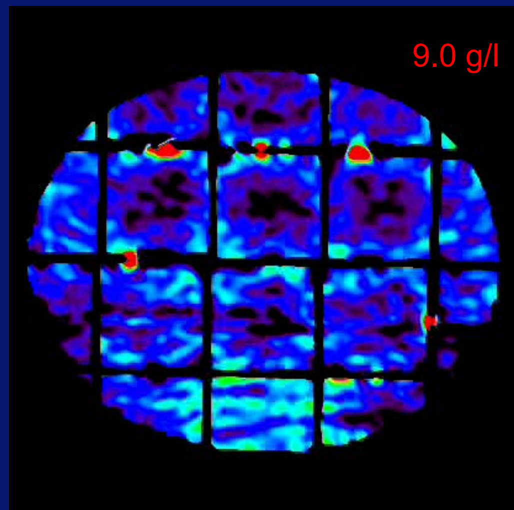
- **Geometry**
  - square channel
  - octo-square, ...
- **Material**
  - Cordierite
  - SiC
  - Dura Trap AT,...
- **Soot Filtration Model**
  - Depth Filtration
  - Cake Filtration
- **Ash Model**
- **Regeneration Model**
  - Bare Trap
  - CSF
  - Catalytic Wall Reactions

Diesel Particulate Filter
DPF Loading / Experiment

AVL

Computer Tomography

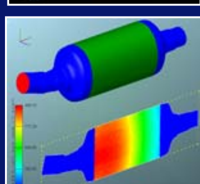


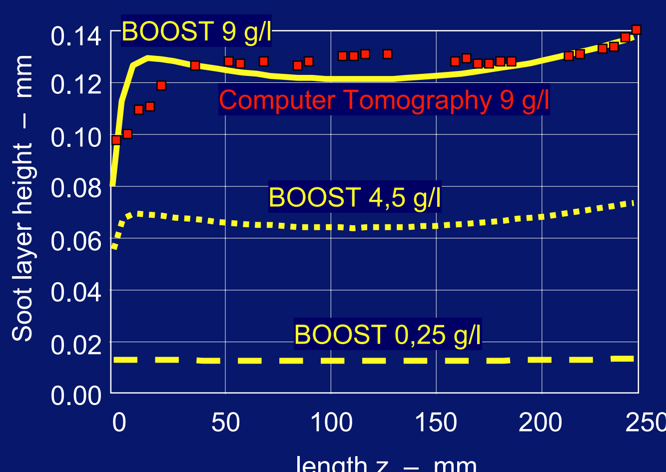


Integration of pixels in all slices: 2D plot

Diesel Particulate Filter
DPF Loading / Validation

AVL

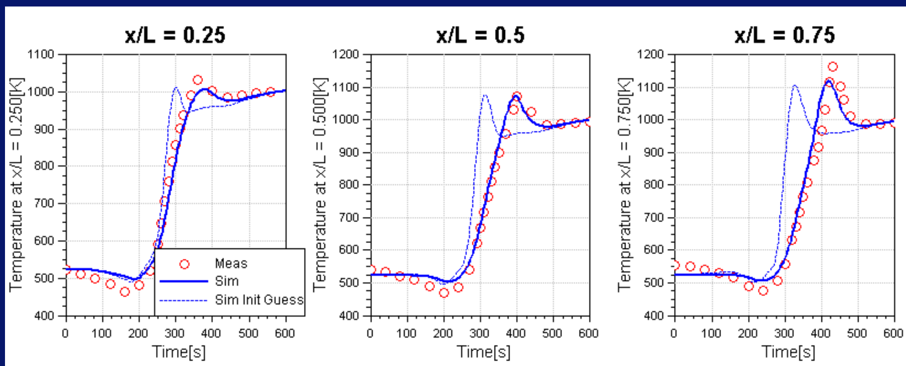




Diesel Particulate Filter
Regeneration analysis: Parameter Identification

AVL

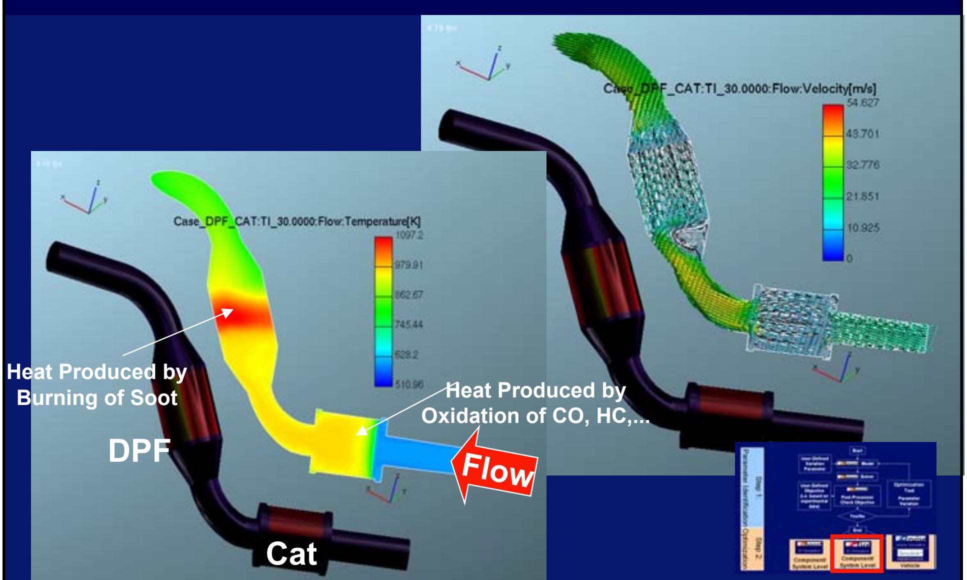
Comparison of Experimental Data With Guessed and Optimized Kinetic Parameters



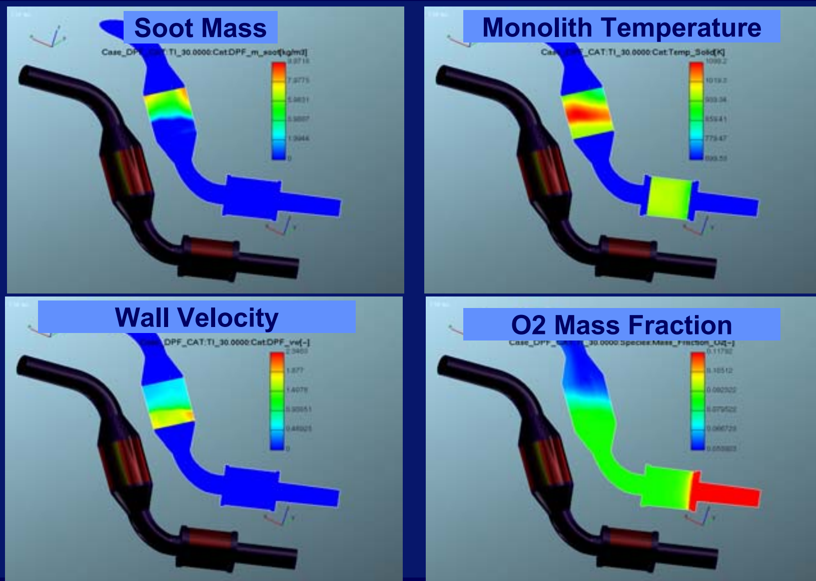
~100 1D Simulation Runs using iSIGHT v7.1

FIRE 3D: Diesel Exhaust Gas Line
DPF Regeneration (post-injection)

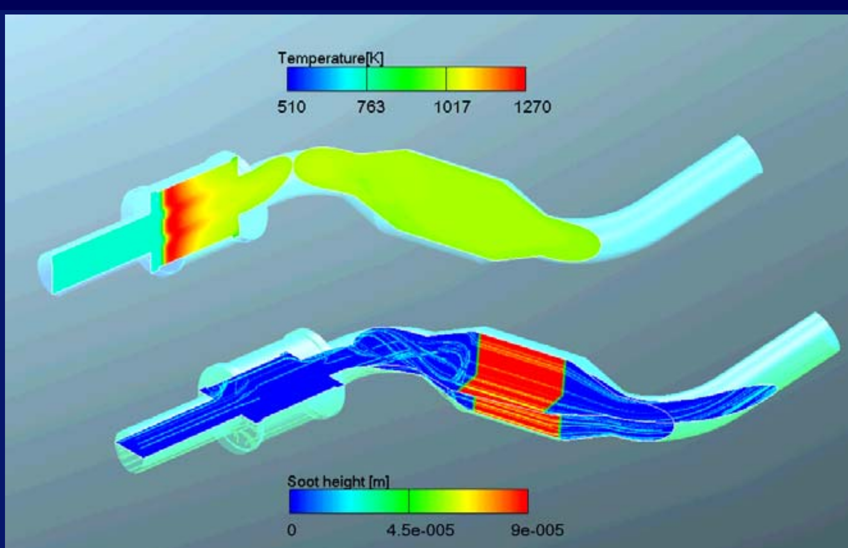
AVL



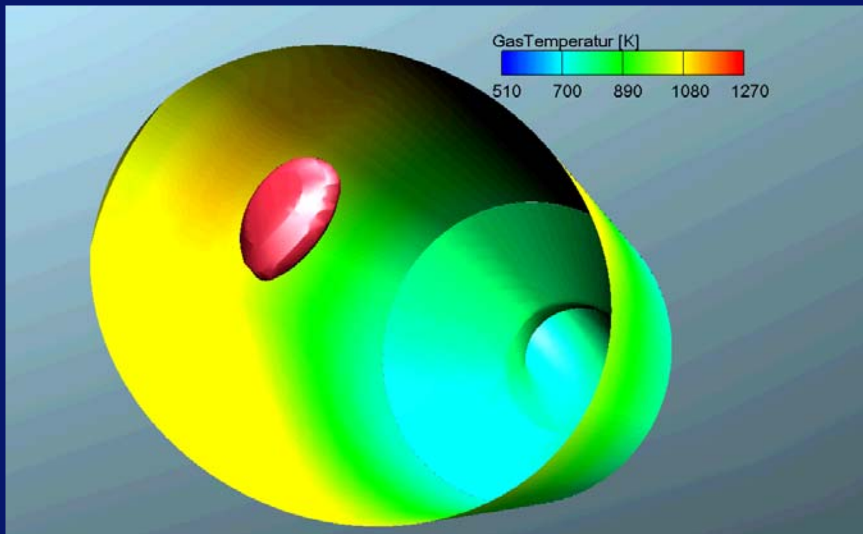
FIRE 3D: Diesel Exhaust Gas Line
DPF Regeneration (post-injection)



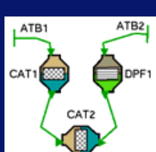
DPF Regeneration
(Movie)

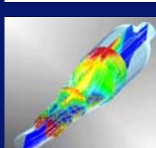


DPF Regeneration, Gas Temperature Front (Movie)



Conclusions and Outlook





- ✓ Validated models for Catalysts and DPF available
  - DOC, TWC, SCR, ...
  - DPF, CSF, ...
- ✓ Integrated Solution for Emissions Controls System Optimization
  - 1D: BOOST
  - 2D/3D: FIRE
  - Vehicle: CRUISE
  - MATLAB Interface
- Current activities
  - System level optimization
  - Integrate simulation into the development and application process