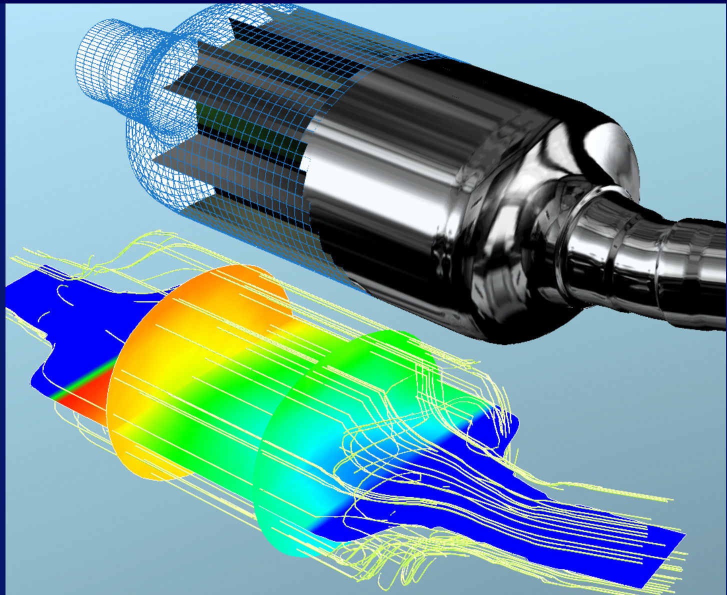
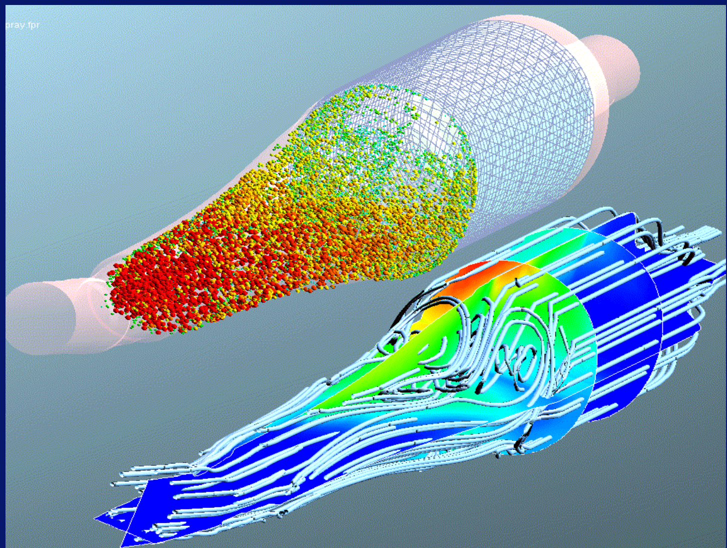
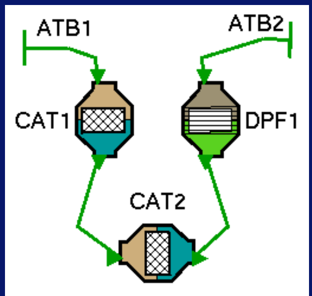


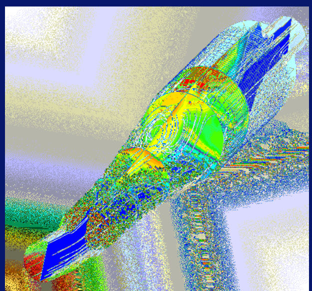


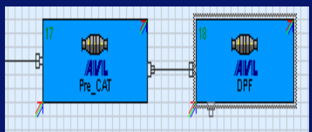
Progress in DOC, DPF and SCR Simulation

Roland Wanker
Johann C. Wurzenberger

Contents

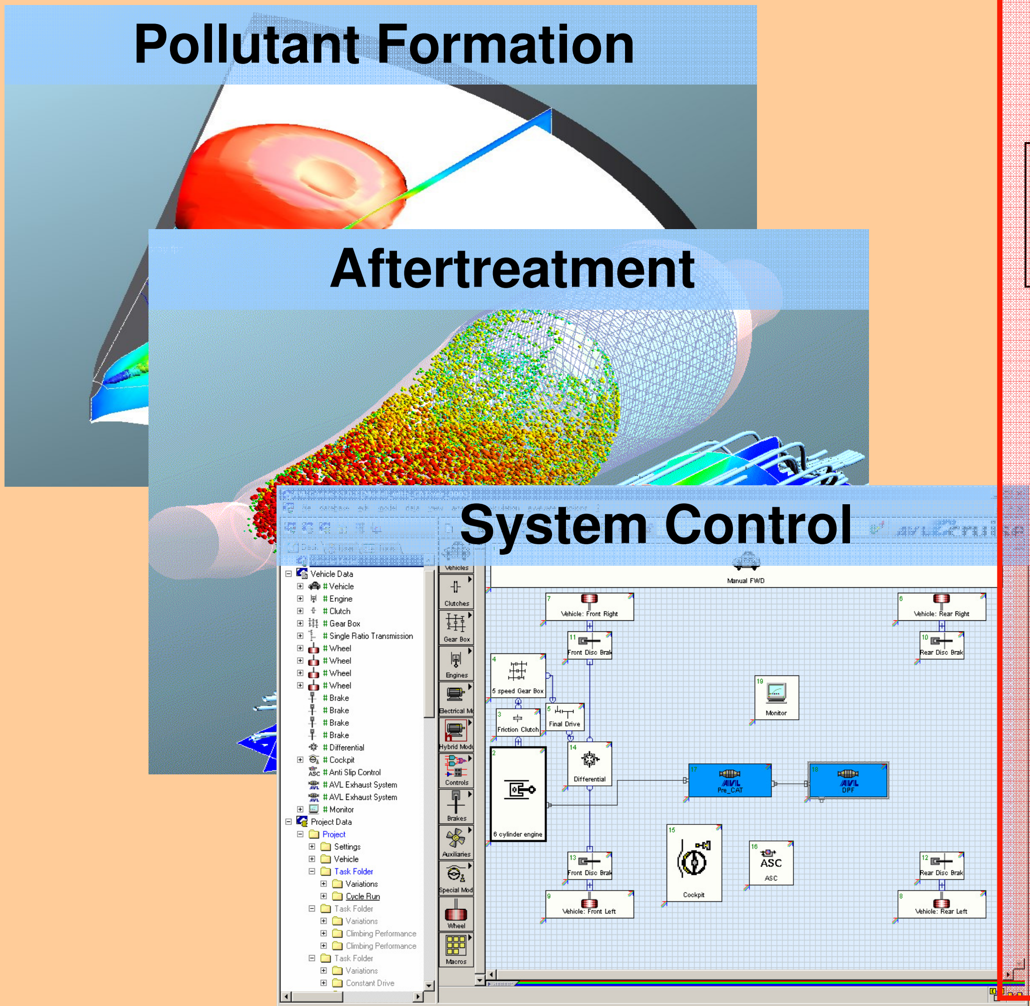


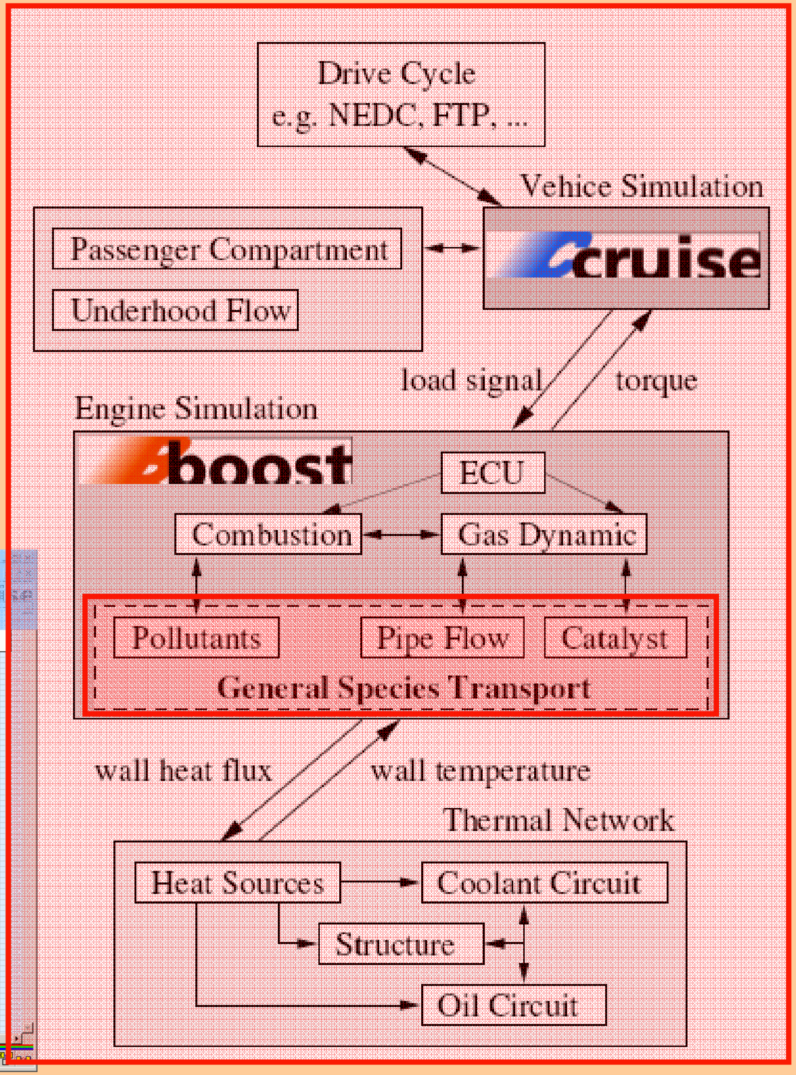




- **Aftertreatment Simulation Strategy**
- **Aftertreatment Simulation Workflow**
- **Examples**
  - **1D:** **DOC Light-Off and NEDC Cycle with HC Storage**
  - **3D:** **SCR Spray with Multi-Component Evaporation**
  - **1D/3D:** **DPF Flexible Channel Geometry and Filtration Model**
- **Summary**

- **Reduction of Diesel Engine Emission**

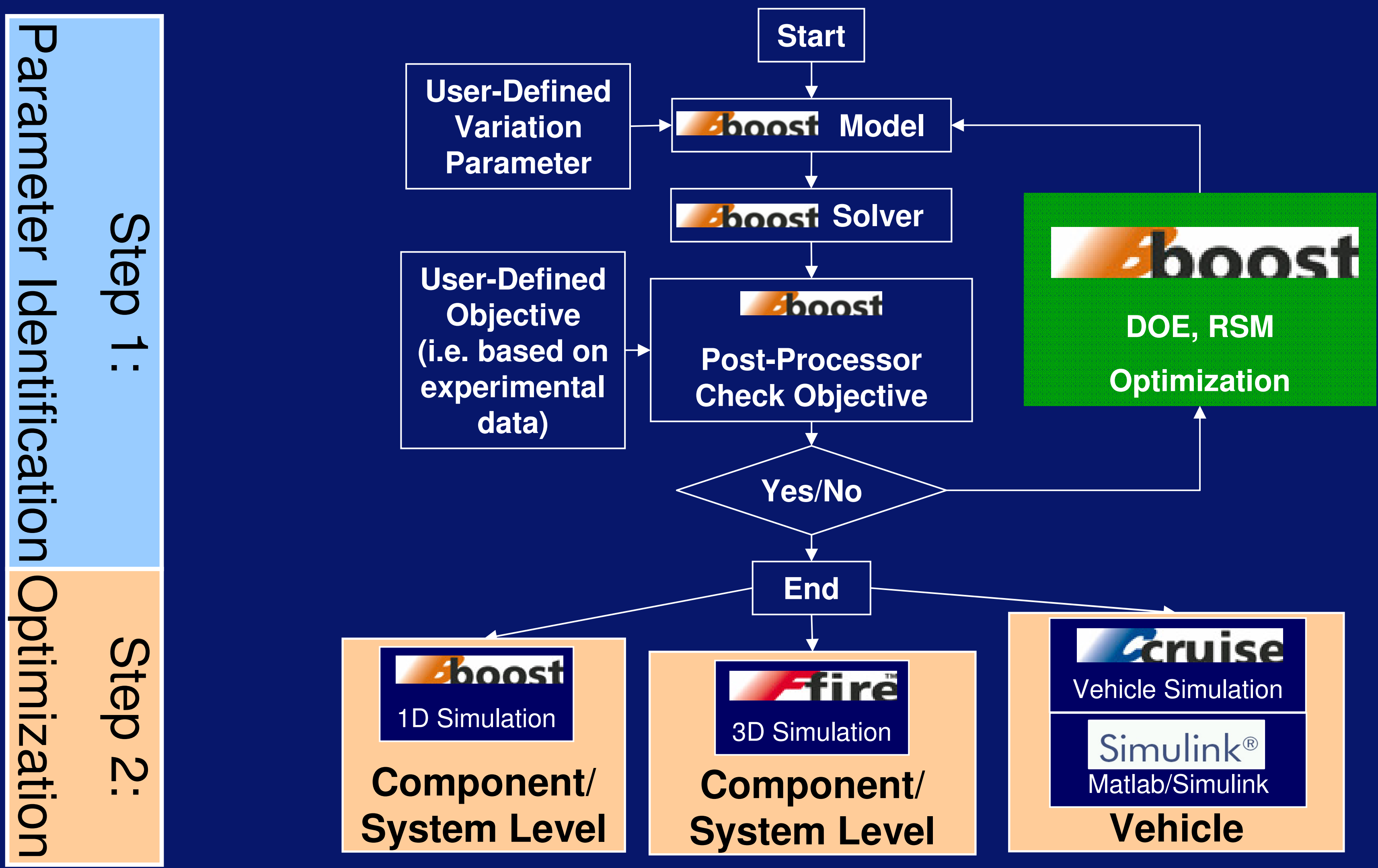




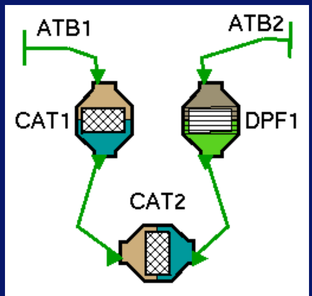
Aftertreatment Simulation Strategy, II

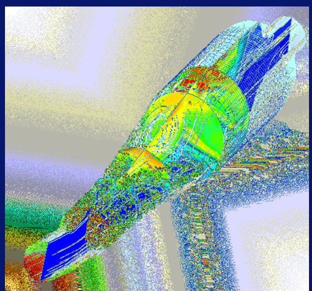
Integration	▪ **Identical Physical and Chemical Aftertreatment Models** ▪ BOOST 1D standalone ▪ BOOST 1D coupled with engine ▪ BOOST 1D coupled with engine and vehicle ▪ BOOST 1D as s-function in Matlab/Simulink ▪ FIRE 2D/3D standalone
Application	▪ **Dedicated Kinetic Models for each Specific Application** ▪ Diesel Oxidation Catalyst ▪ Diesel Particulate Filter (DPF, CSF) ▪ Selective Catalytic Reduction (SCR) ▪ NOx Trap Catalyst ▪ Three Way Catalyst
Flexibility	▪ **Customer's Proprietary Kinetic Models** ▪ Use BOOST 1D Aftertreatment as Platform ▪ User Coding Interface allows 100% Access to all Feature

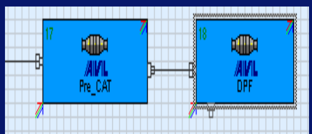
Aftertreatment Simulation Workflow



Contents







- Aftertreatment Simulation Strategy
- Aftertreatment Simulation Workflow
- Examples
  - 1D: DOC Light-Off and NEDC Cycle with HC Storage
  - 3D: SCR Spray with Multi-Component Evaporation
  - 1D/3D: DPF Flexible Channel Geometry and Filtration Model
- Summary

DOC Kinetic Model

- **AVL BOOST/FIRE pre-defined DOC kinetic model**

$$CO + {}^1\!/_2 O_2 \longrightarrow CO_2$$
$$C_3H_6 + {}^9\!/_2 O_2 \longrightarrow 3CO_2 + 3H_2O$$
$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$$
$$2NO + O_2 \longleftrightarrow 2NO_2$$

- **extended by:**

$$C_3H_6 + Me \leftrightarrow C_3H_6\,(Me)$$

$$\dot{r} = A_3 \cdot \exp\left(\frac{-A_4}{T}\right) \cdot A_{spec} \cdot (y_{HC} - y_{HC,eq})$$

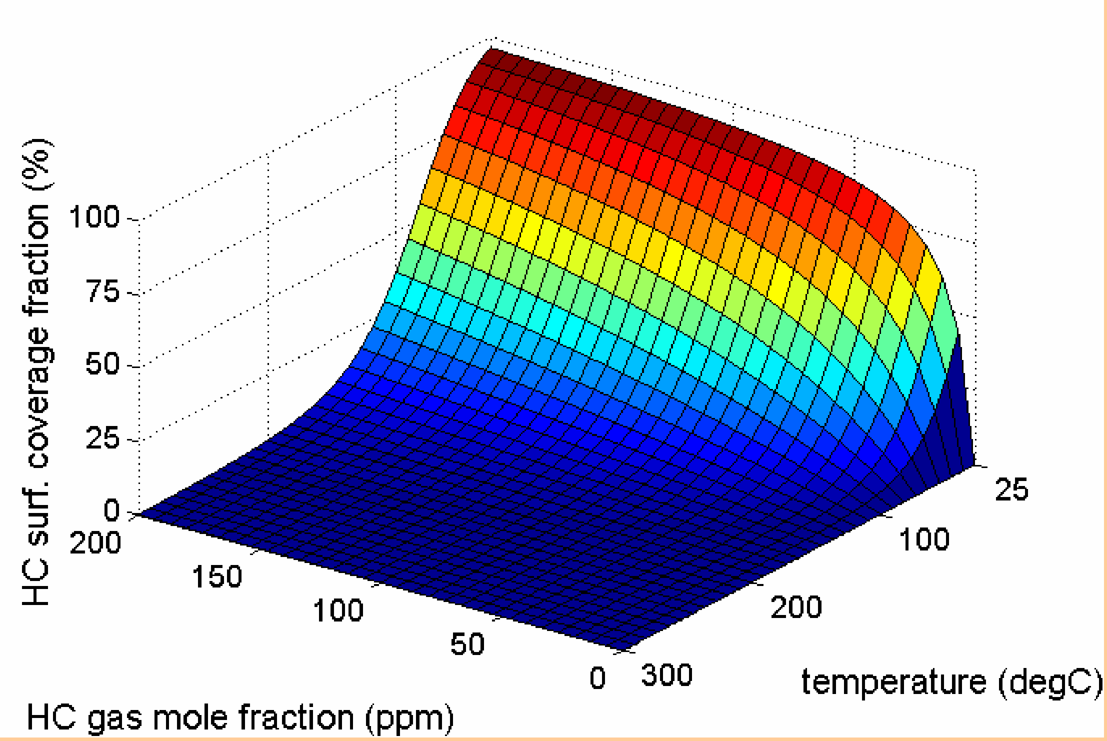
y_{HC} → **actual mole fraction**

$y_{HC,eq}$ → **equilibrium mole fraction**

DOC Kinetic Model: HC Storage

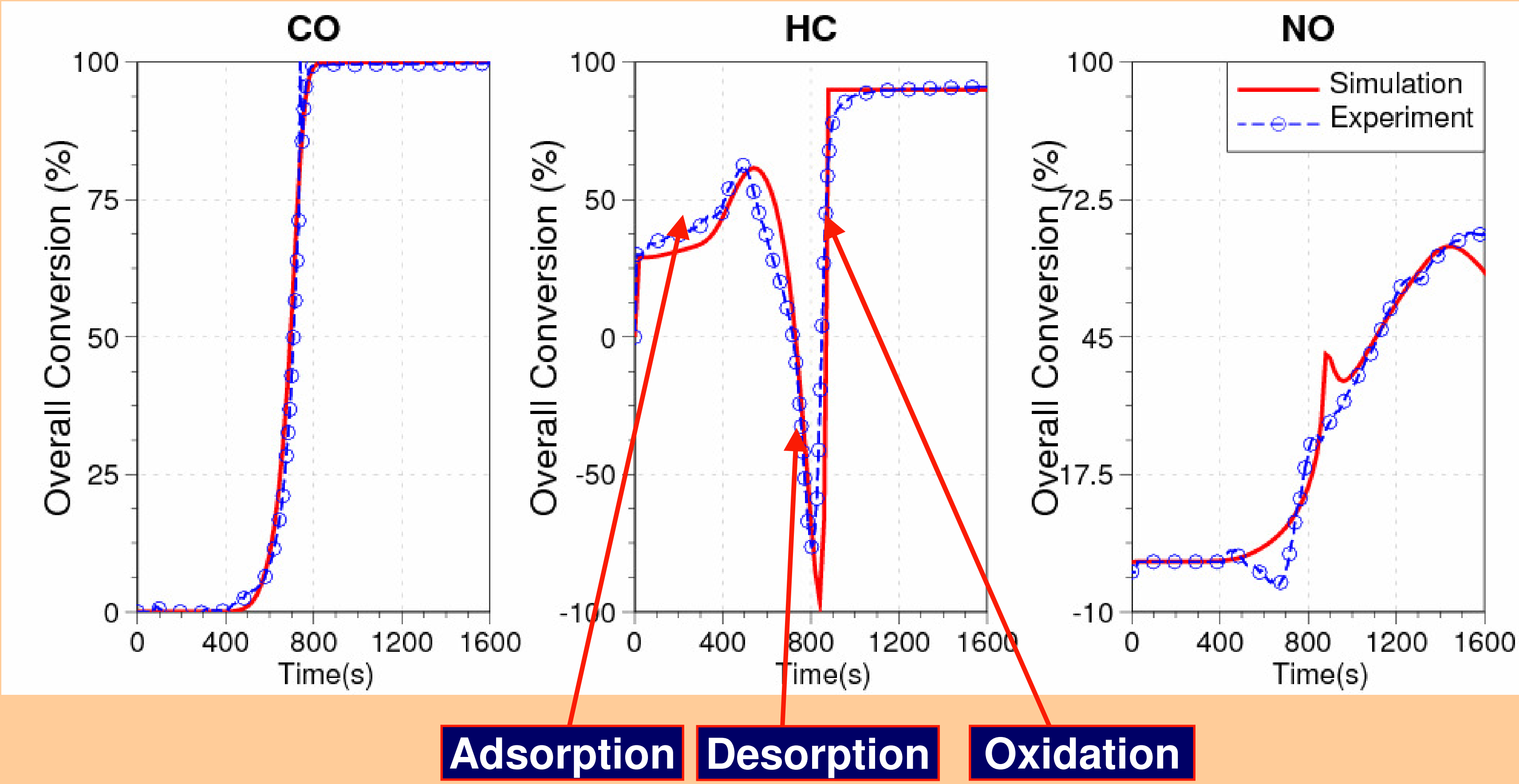
- **Langmuir Isotherm:**

$$z_{\mathrm{HC,eq}} = z_{\mathrm{HC,max}}(T) \cdot \frac{y_{\mathrm{HC,eq}}}{A_1 \cdot \exp\left(\frac{-A_2}{T}\right) + y_{\mathrm{HC,eq}}}$$



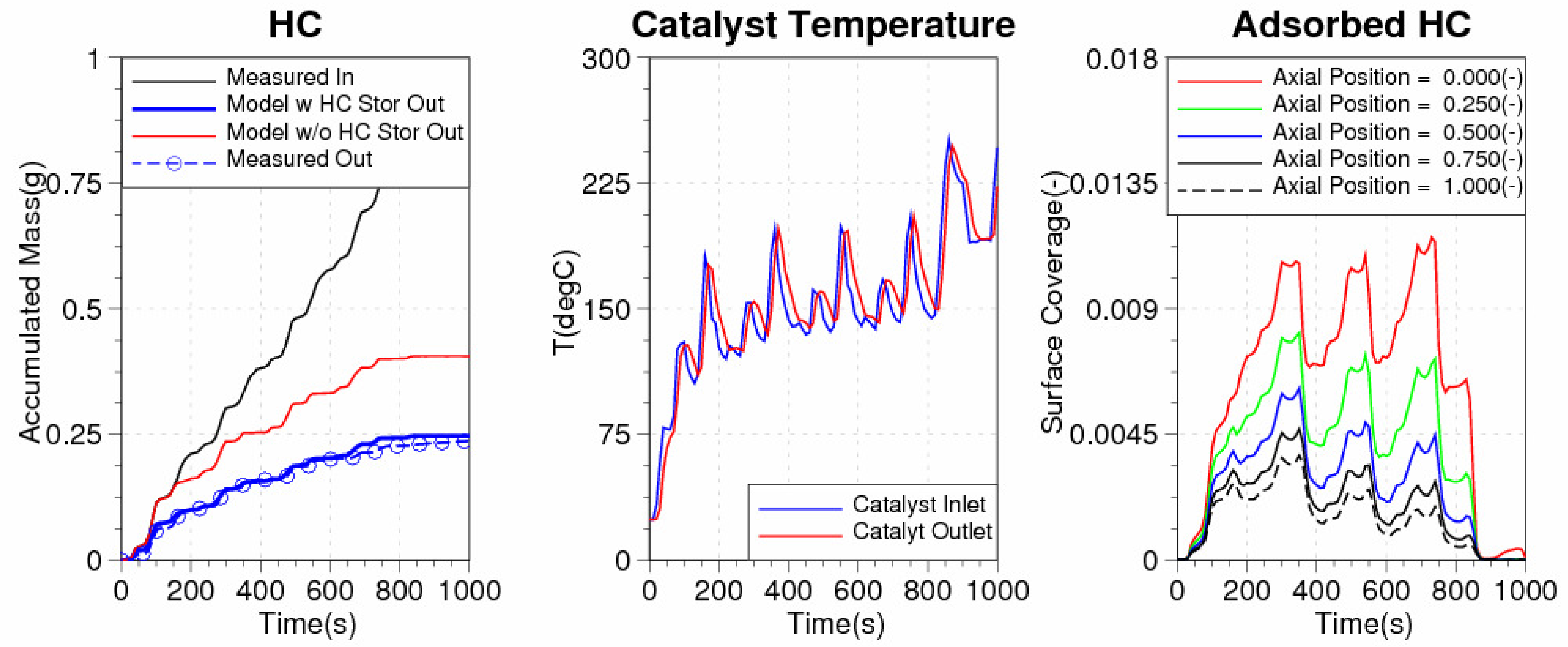
DOC: Model Parameterization using Light-Off Data

- **Parameter identification using DOE in combination with direct optimization tools**

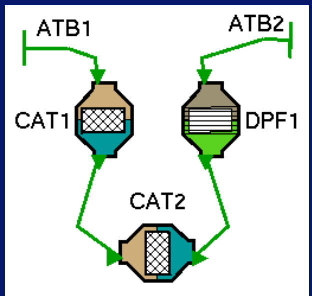


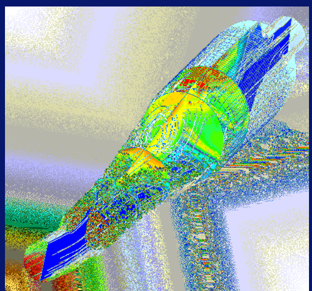
DOC: Influence of HC storage on a NEDC cycle simulation

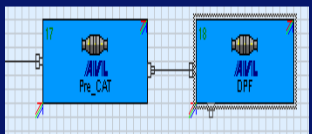
- **Passenger Car NEDC cycle test**



Contents







- Aftertreatment Simulation Strategy
- Aftertreatment Simulation Workflow
- Examples
  - 1D: DOC Light-Off and NEDC Cycle with HC Storage
  - 3D: SCR Spray with Multi-Component Evaporation
  - 1D/3D: DPF Flexible Channel Geometry and Filtration Model
- Summary

SCR, 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**

CLEERS 2006: (Masoudi, BOSCH)

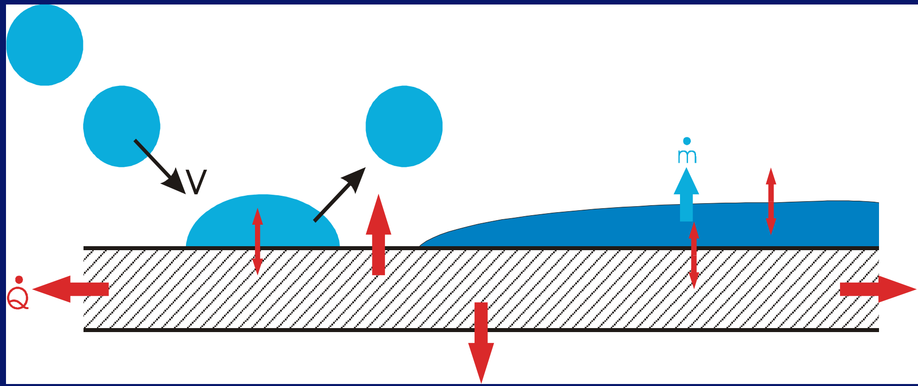
- **„BOSCH Urea Dosing Approach for Future Emissions Legislature for Light and Heavy Duty SCR Applications"**

Progress in SCR spray simulation

Advanced Simulation Technologies

Spray / gas phase:

- multi-component evaporation
- urea/water mixture properties
- thermolysis
- hydrolysis



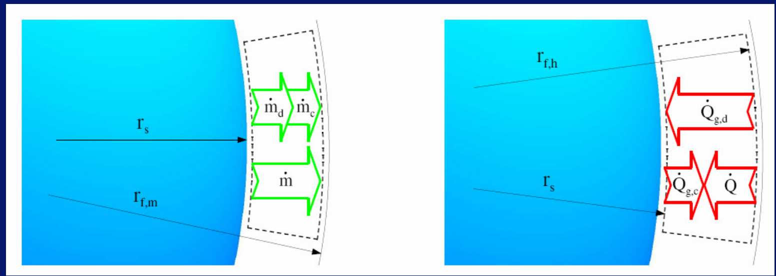
Spray wall interaction:

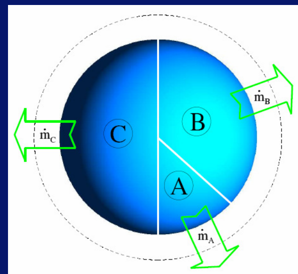
- multi-component evaporation
- heat conduction in solid walls via lateral heat conduction
- heat transfer between droplets and wall
- wall temperature dependent splashing model

Multi-component evaporation model with integrated urea thermolysis

Advanced Simulation Technologies

- Based on Abramson/Sirignano single component model with balances for mass and heat transfer in gas film around drop





$$\Rightarrow \dot{m} = 2\, r_s\, \pi\, \frac{\overline{\lambda}_f}{\mathcal{C}_{p,v}}\, Nu^*\, ln(1 + B_h)$$

$$\Rightarrow \dot{m}_i = 2\, r_s\, \pi\, \overline{\rho}_f\, \overline{D}_{ia}\, Sh_i^*\, ln(1 + B_{m,i})$$

$$\dot{m} = \sum_{i=1}^{N} \dot{m}_i$$

- Coupled equations for mass transfer and heat flux entering the drop solved with iterative procedure

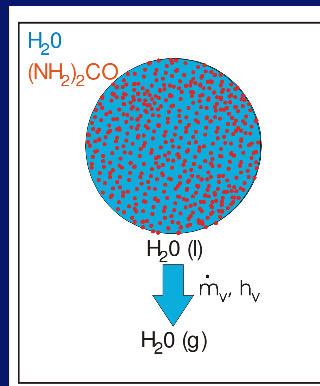
- Arrhenius approach for thermolysis: $\frac{dm_{urea}}{dt} = -\pi D_d A \cdot \exp\left(-\frac{E_a}{RT}\right)$

- Evaporation
- Thermolysis
- Hydrolysis

$$H_2O\ (l) \longrightarrow H_2O\ (g)$$

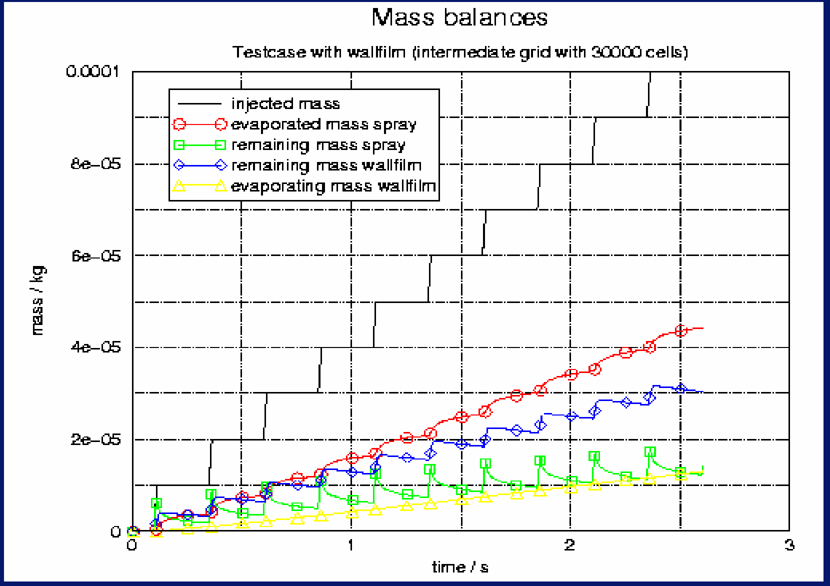
$$(NH_2)_2CO(s\ or\ l) \xrightarrow{\Delta H = +185.5 kJ/mol} NH_3\ (g) + HNCO\ (g)$$

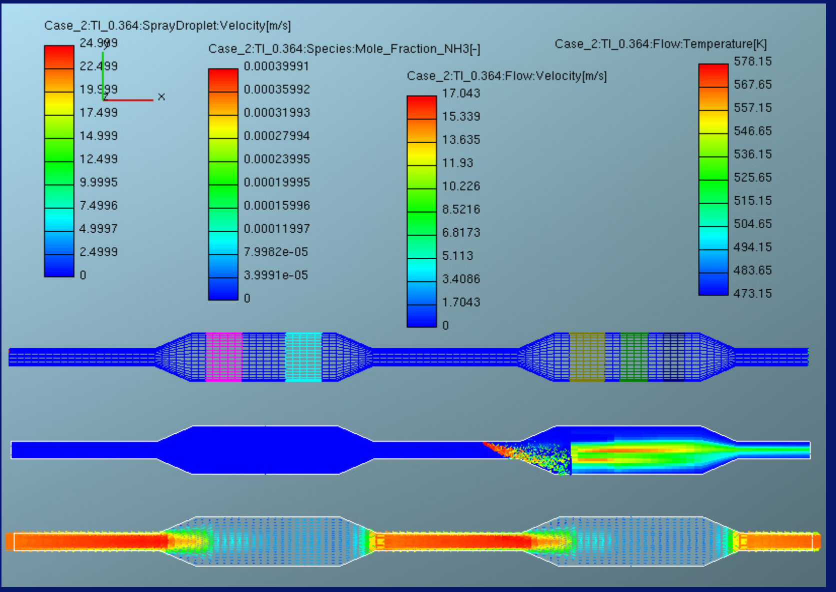
$$HCNO\ (g) + H_2O(g) \longrightarrow NH_3\ (g) + CO_2\ (g)$$

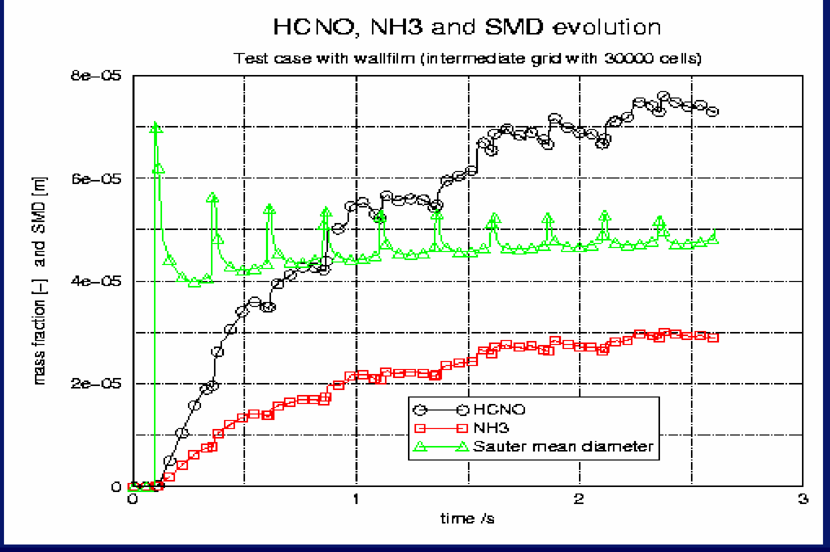


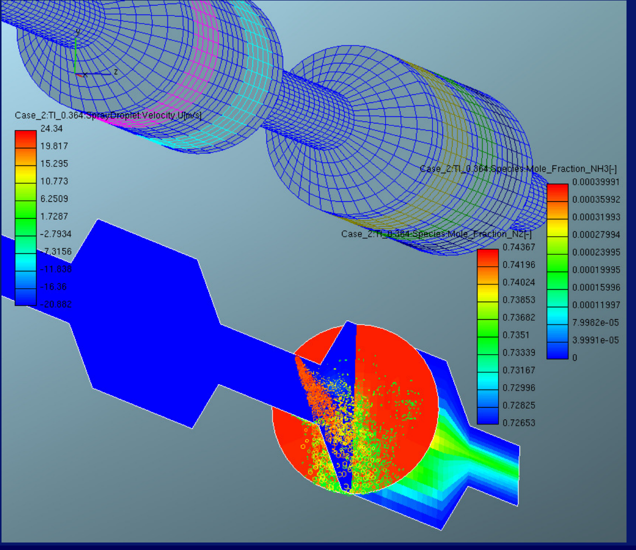
Testcase with 30000 cells (65 kg/h , 10 mg AdBlue per pulse)

AVL
Advanced Simulation Technologies

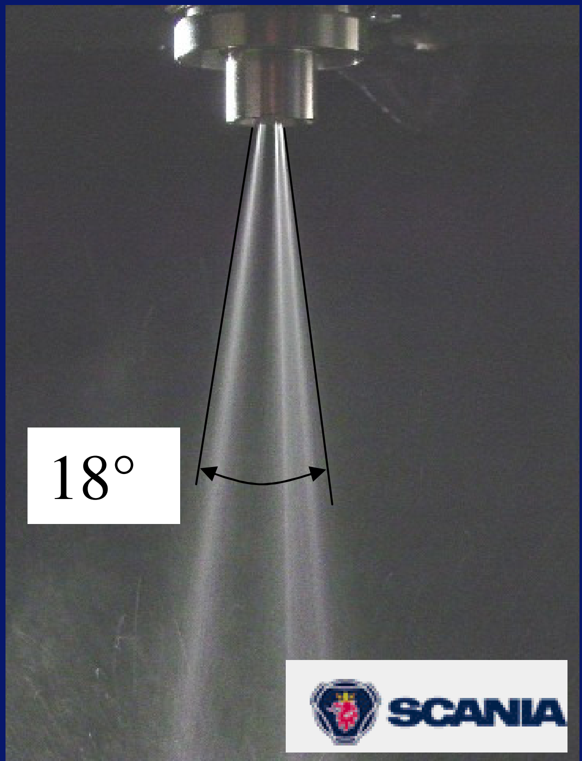


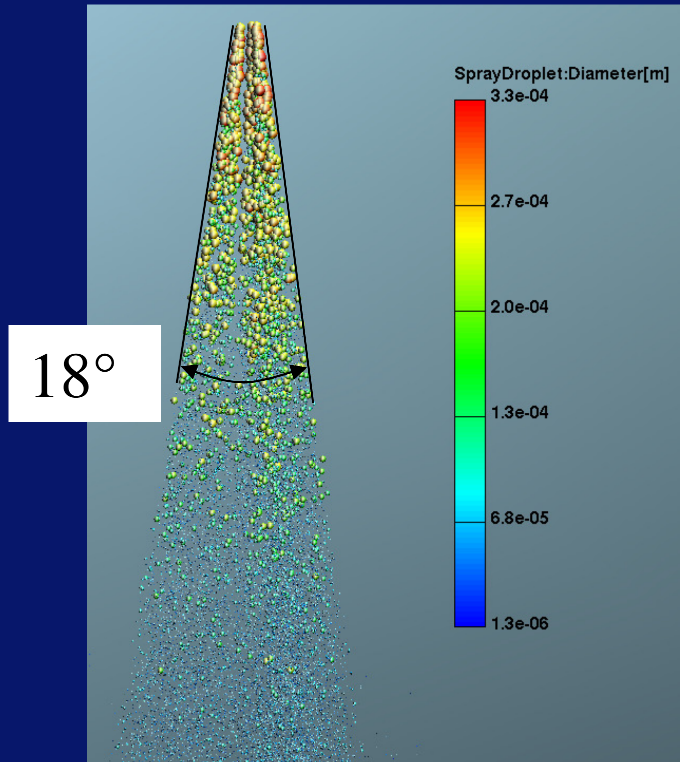






Spray Calibration



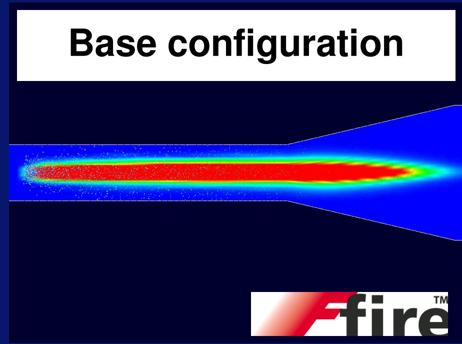


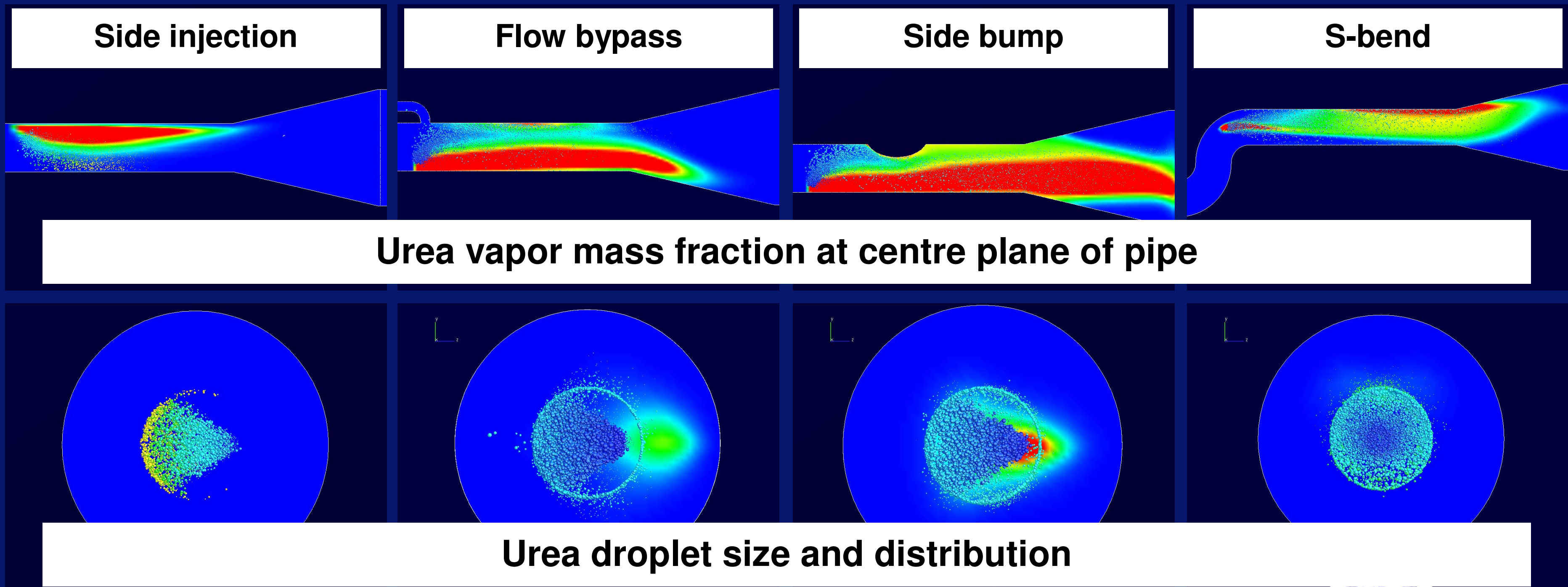
Spray Angle and Pattern is Adapted to Spray Box Measurement

Urea Distribution Study I

Investigation of urea vapor distribution during steady-state operating conditions

- Impact of different pipe/injection geometries

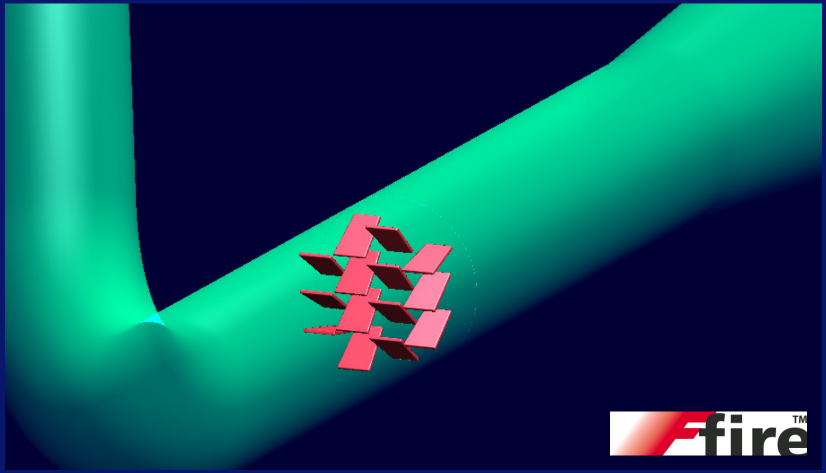


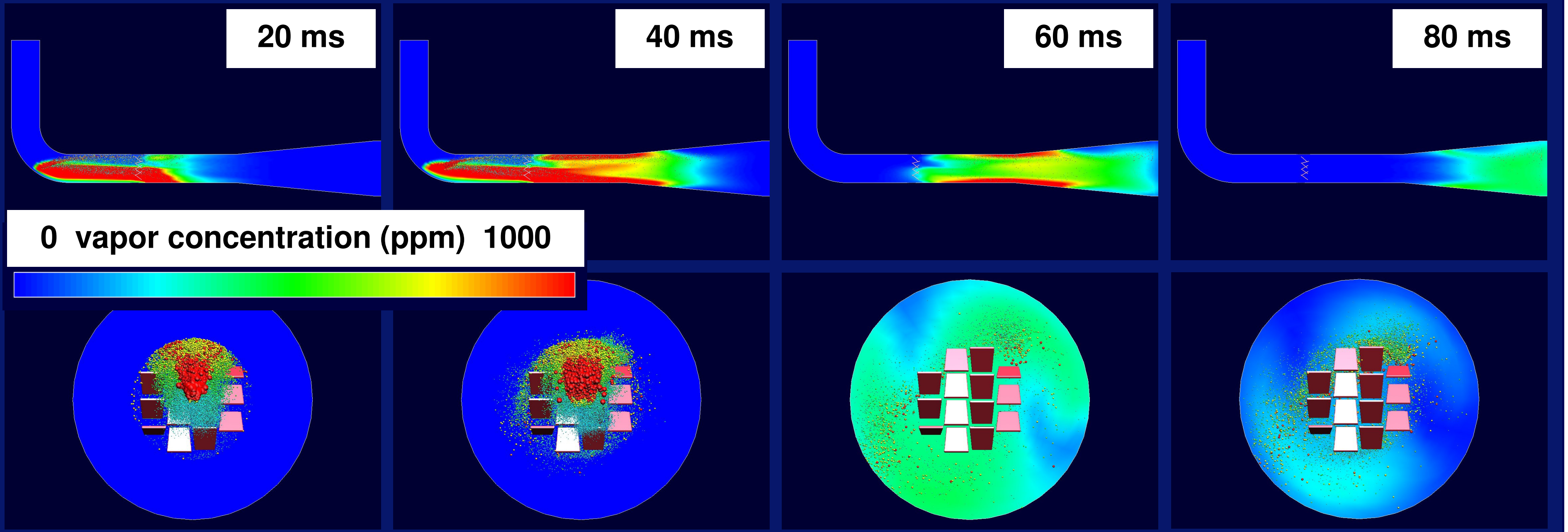


Urea Distribution Study II

Investigation of urea vapor distribution during transient injection pulse

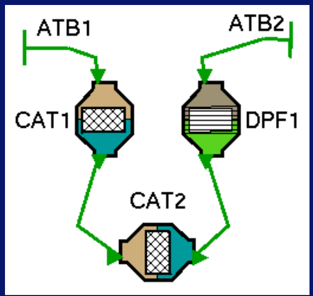
➢ Impact of mixing device

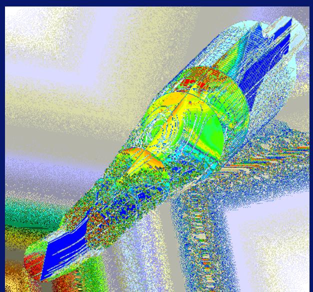


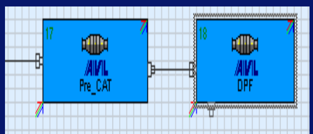


Contents

AVL

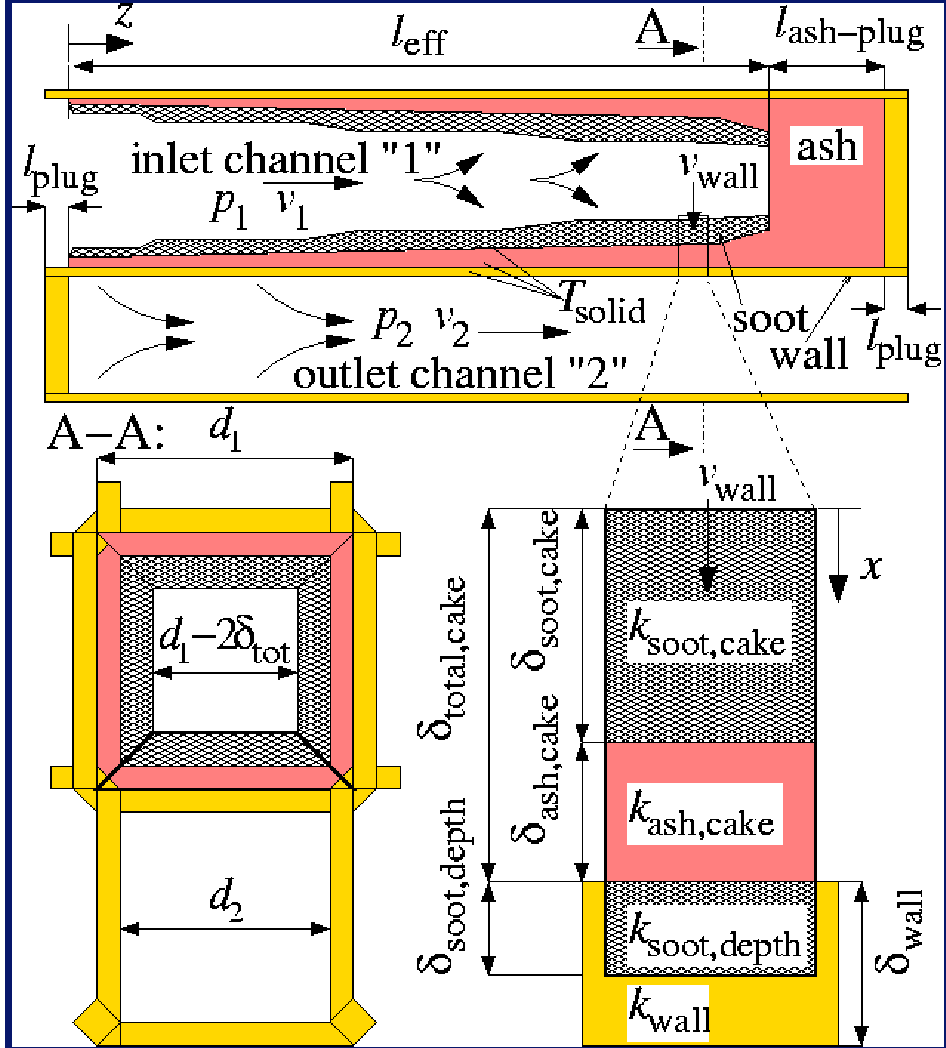






- Aftertreatment Simulation Strategy
- Aftertreatment Simulation Workflow
- Examples
  - 1D: DOC Light-Off and NEDC Cycle with HC Storage
  - 3D: SCR Spray with Multi-Component Evaporation
  - 1D/3D: DPF Flexible Channel Geometry and Filtration Model
- Summary

Generic Wall Flow DPF Model

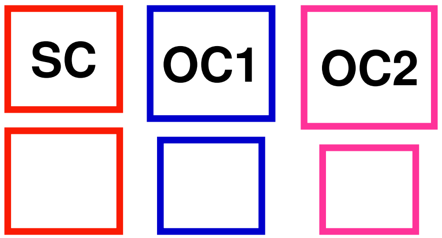


- Different Channel Diameters (Octo-Square, Asymmetric Channels, Wavy-Cells)
- Inlet/Outlet Plugs
- Ash as Layer, Plug or Combination
- Deposition as in Depth and Cake Layers

→Impact on Pressure Drop Model

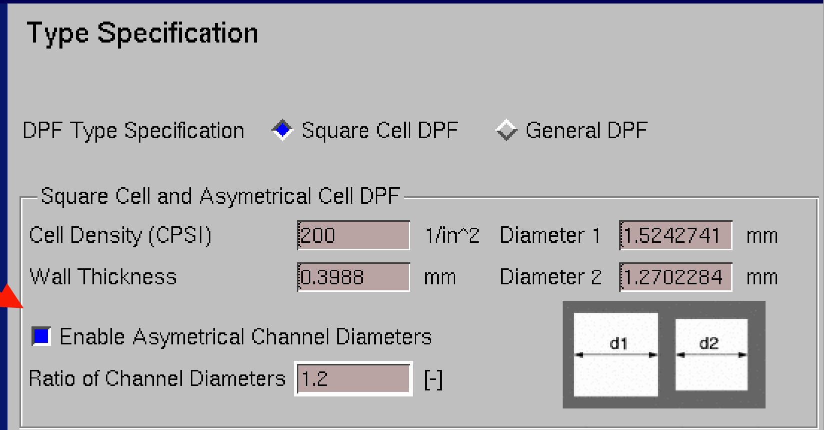
→Impact on Deposition and Regeneration Model

Loading of Asymmetric Channel Structures

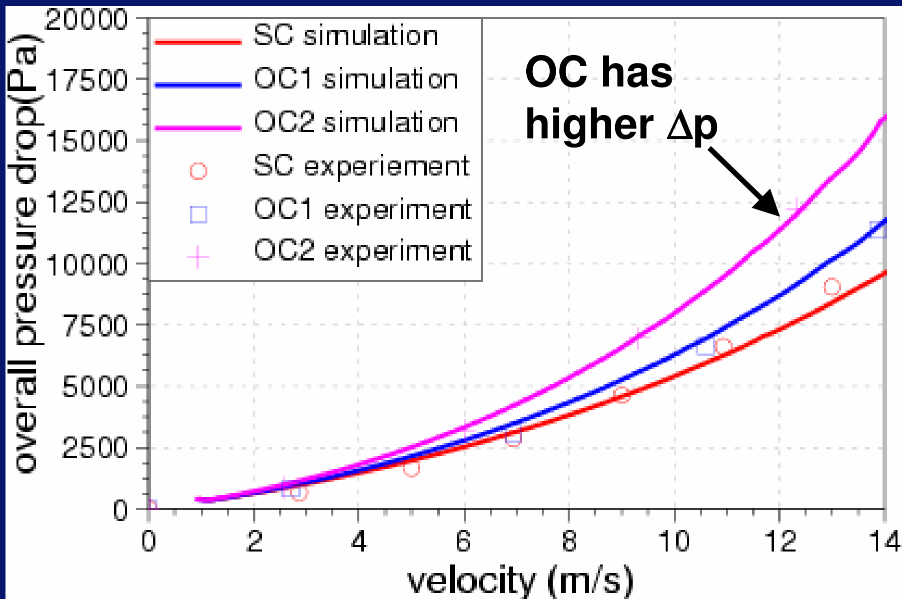


Square Cell (SC)

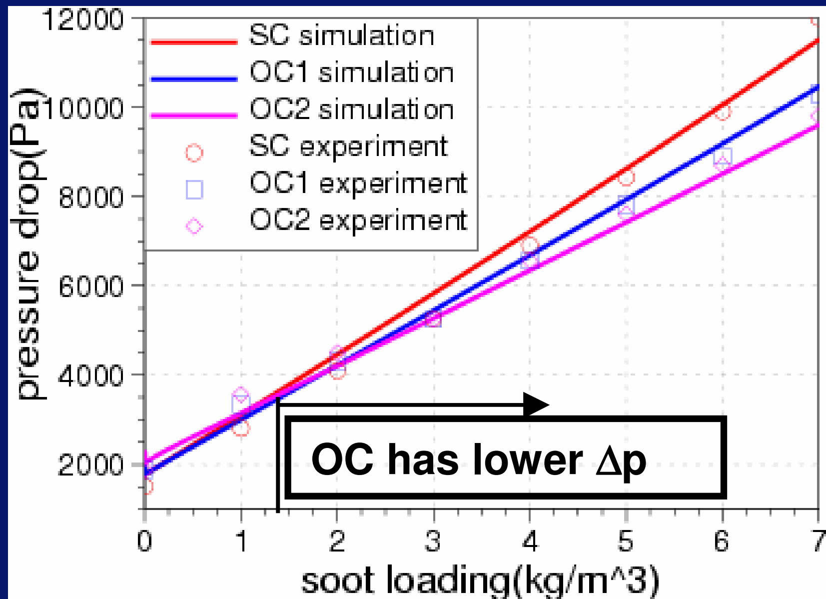
Octo-Square Cell (OC)



Pressure Drop of Empty DPF



Pressure Drop of Loaded DPF

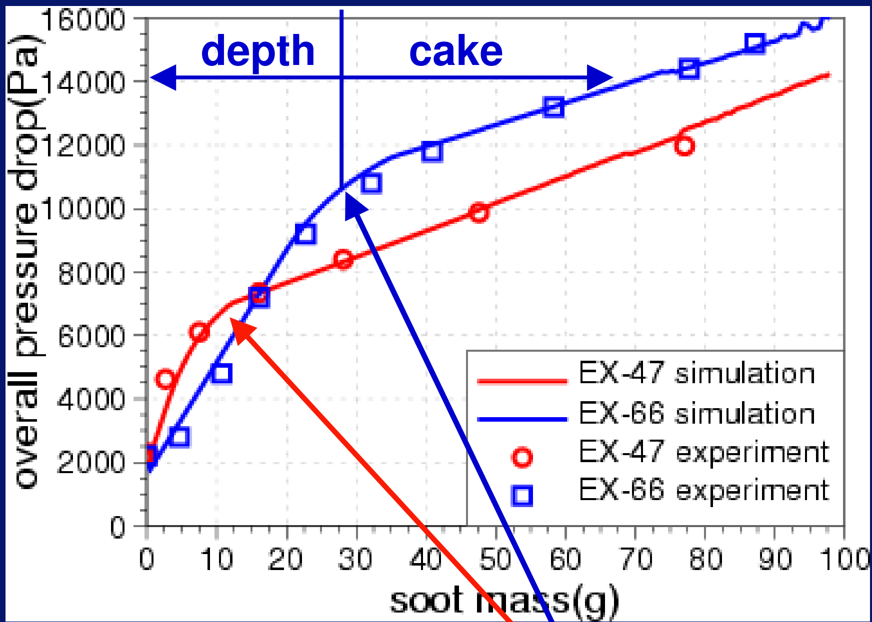


Experimental Data: SAE-2005-01-0949, Ibiden

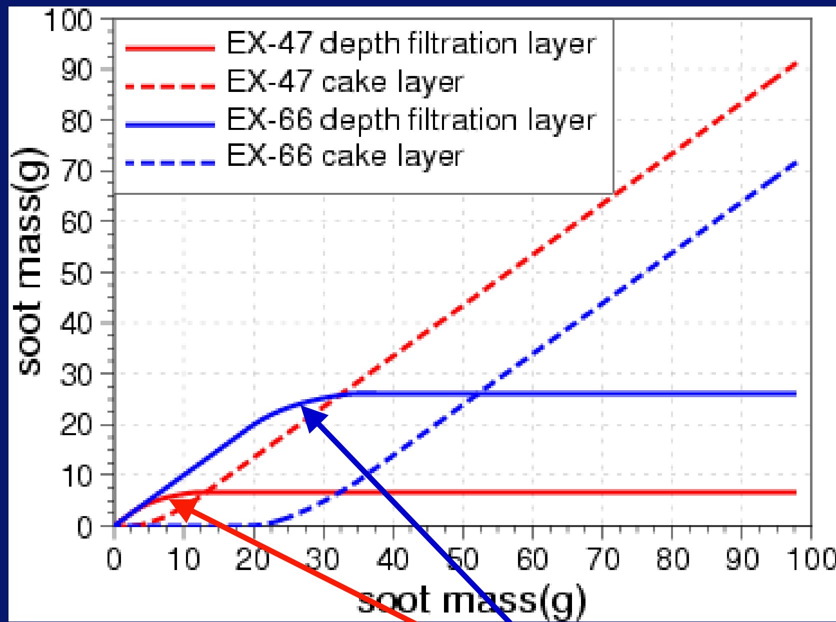
Loading and Δp due to Depth/Cake Filtration

AVL

Pressure Drop Split into Depth and Cake Portions



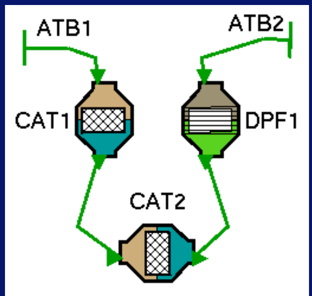
Soot Mass Split in a Depth and Cake Layer

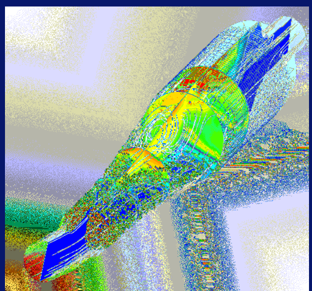


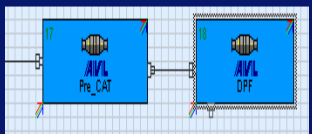
Experimental Data:
SAE-2000-01-1016,
Konstandopoulos

Transition Soot Loading is Assumed as Depth Filtration Threshold

Summary







- ✓ Catalyst and DPF Models
  - ✓ robust solvers
  - ✓ validated models for DOC, SCR, DPF,…
  - ✓ automatic parameter identification (DOE and optimization)
- ✓ Integration of Aftertreatment Simulation
  - ✓ standalone 1D and 3D
  - ✓ engine combustion and pollutant formation fully integrated with exhaust line and reactive aftertreatment devices
  - ✓ vehicle + engine + emissions (measured) linked with exhaust line and reactive aftertreatment devices