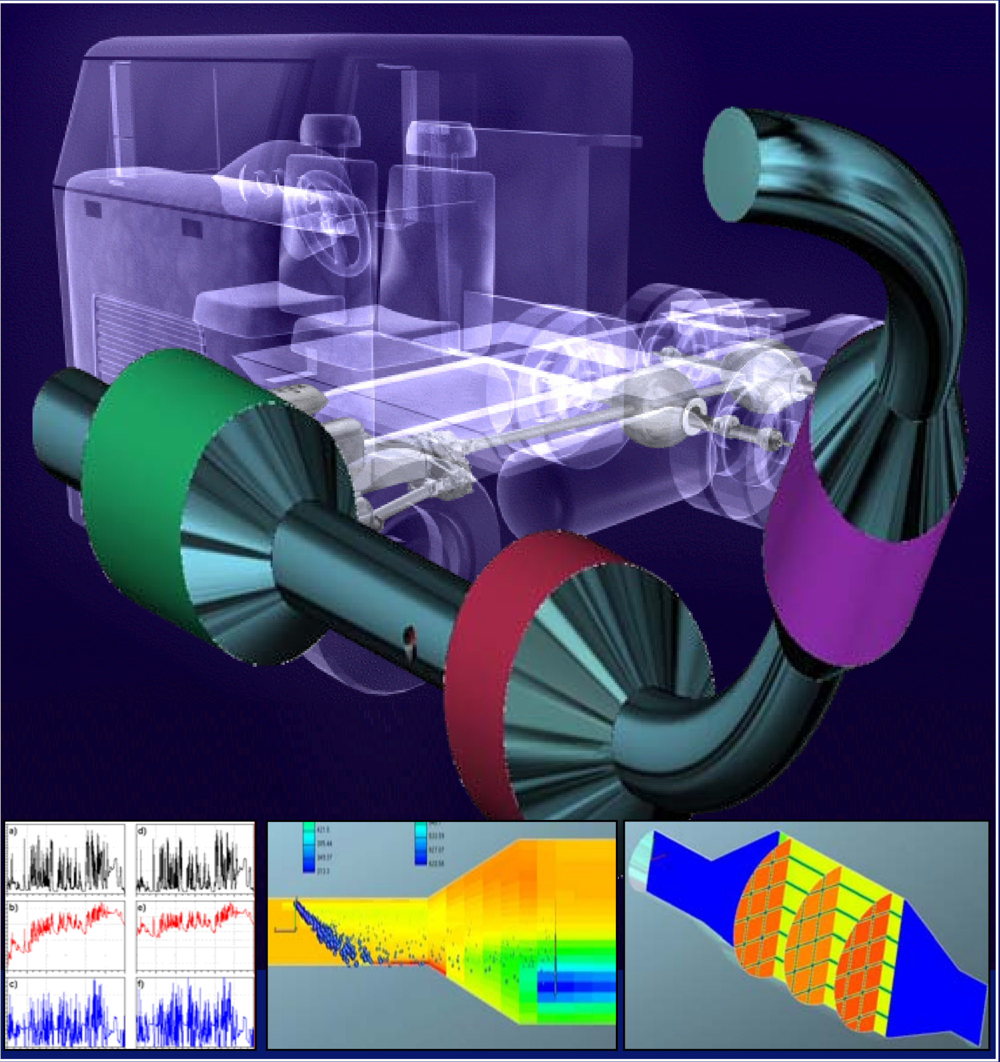
1D/3D Simulation in the Development of DeNOx Aftertreatment Systems for US 2010 Heavy Duty Applications



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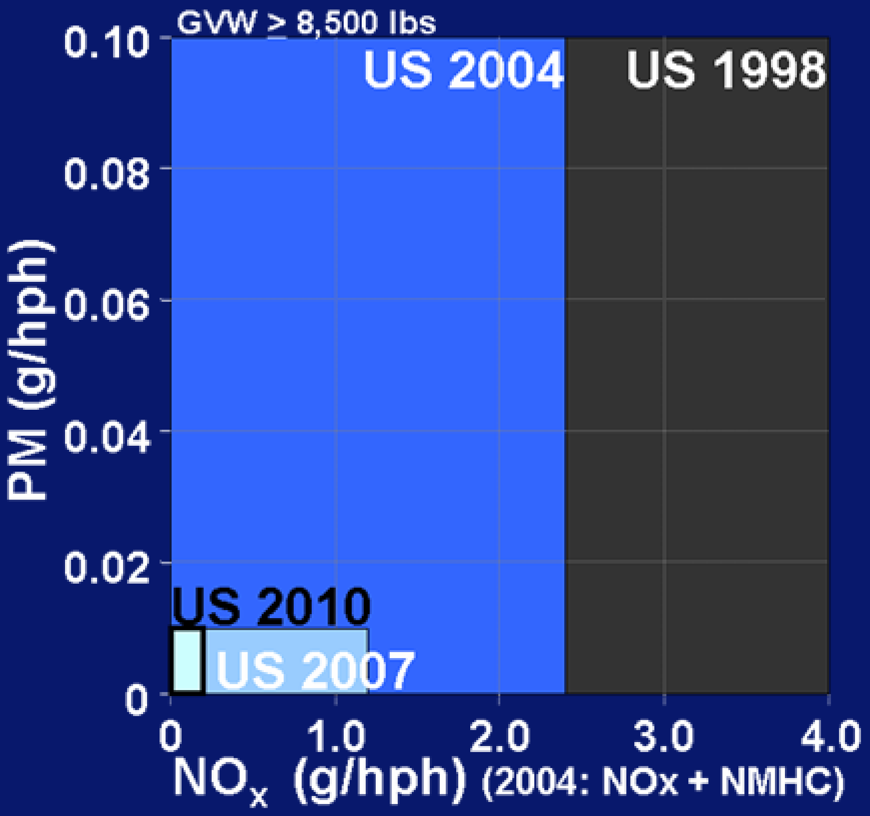
Introduction



Growing importance of exhaust aftertreatment due to emissions legislation needs more effort for

- **Component and system layout**
- **System application**

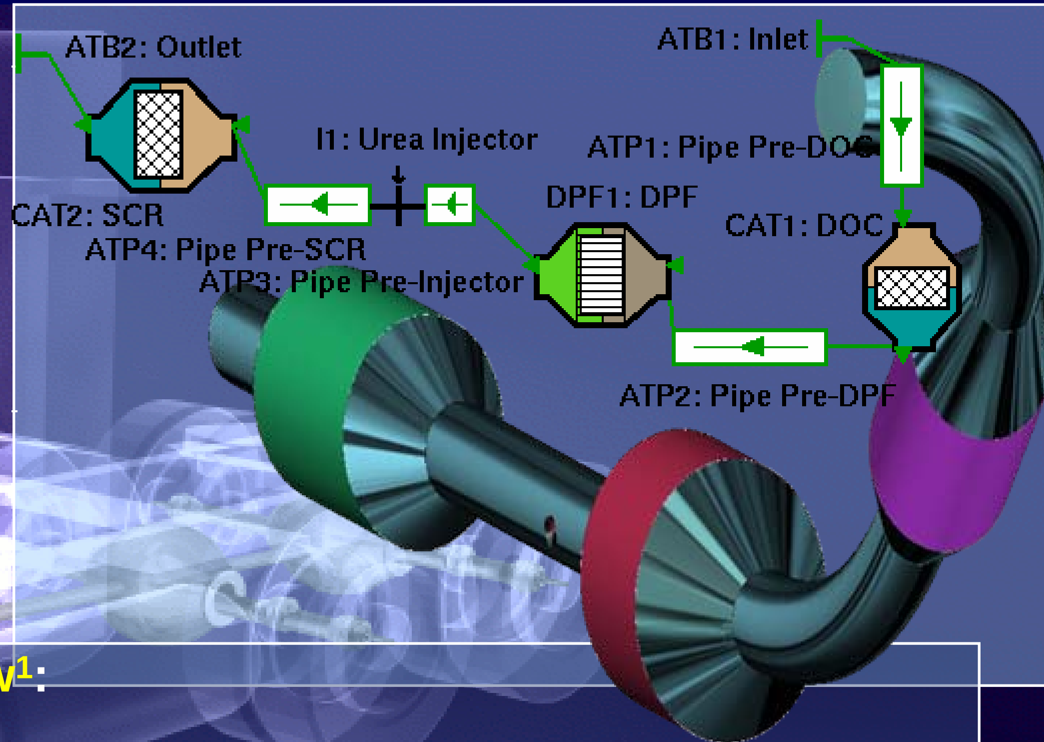
1D/3D Simulation Workflow
for efficient integration of simulation in development process using

- **1D model alibration system analysis and optimization**
- **3D detail analysis**

→ Example:

1D/3D analysis of heavy-duty exhaust system

Exhaust Gas Aftertreatment System

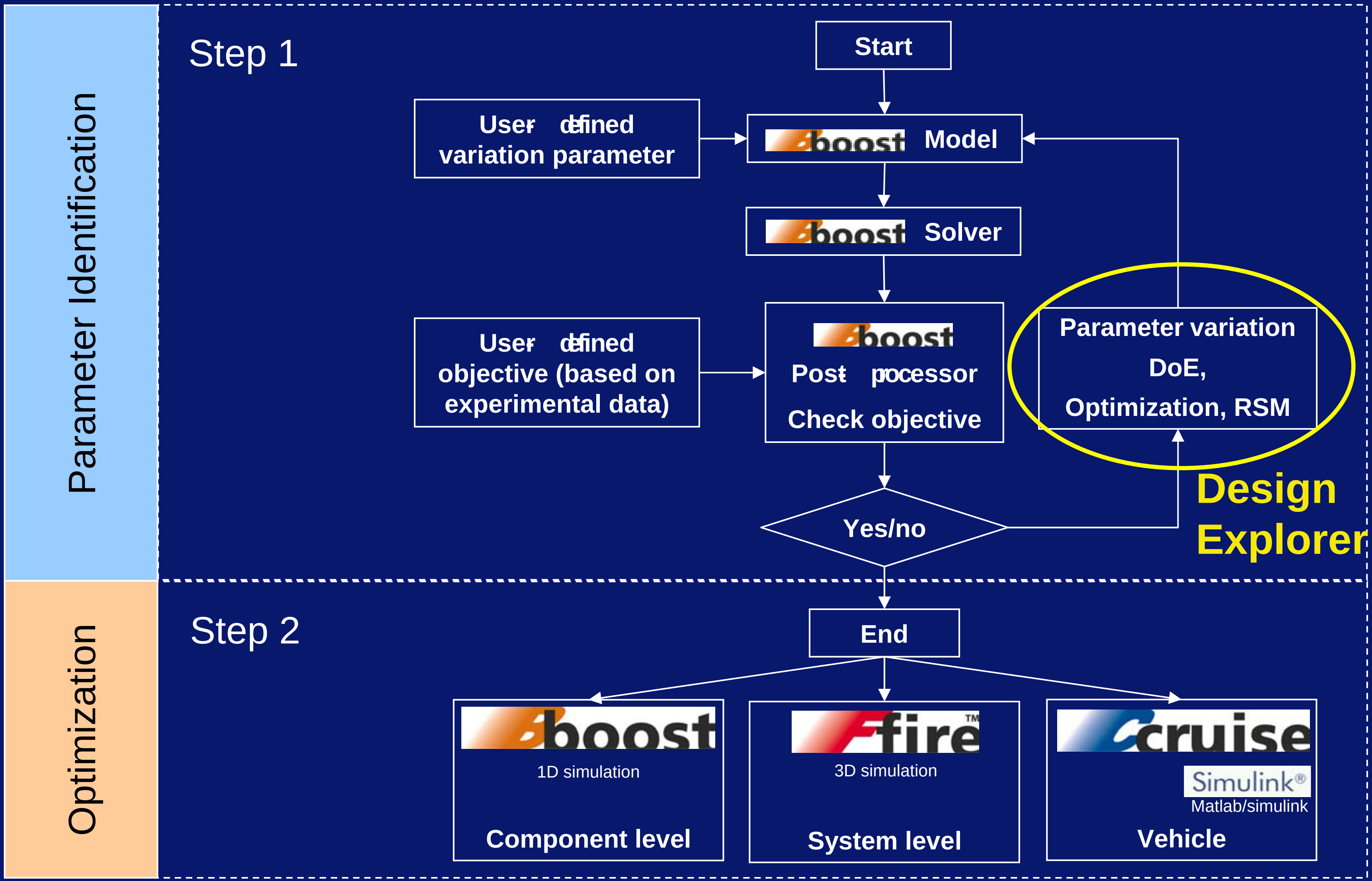


Aftertreatment Simulation Workflow[1]:

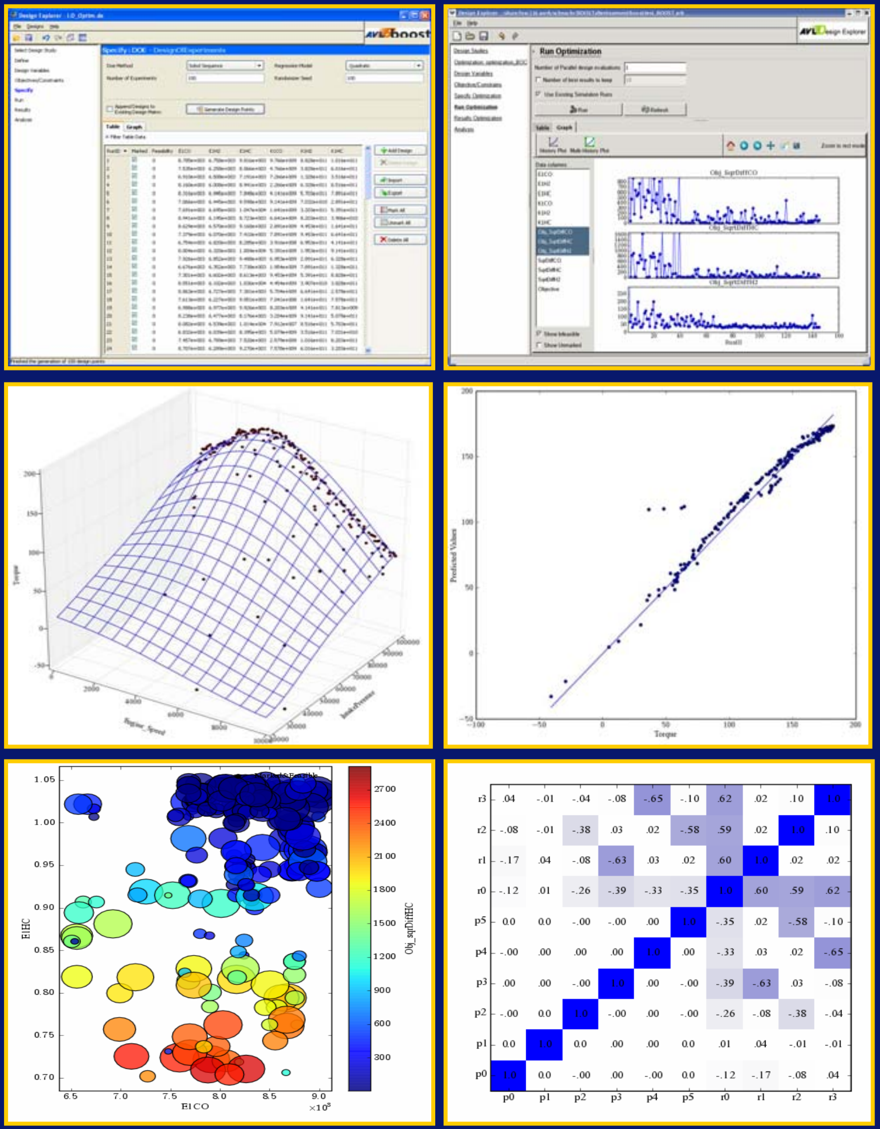
1) Calibrate individual components with experimental data in an automatic parameter optimization process (AVL Design Explorer)
2) Investigate 3D effects with FIRE
3) Build up 1D BOOST model of overall system
4) Calculate the performance of the system during drive cycle

1: see ATZ 7/8 2004

Aftertreatment Simulation Workflow



Automatic Model Calibration

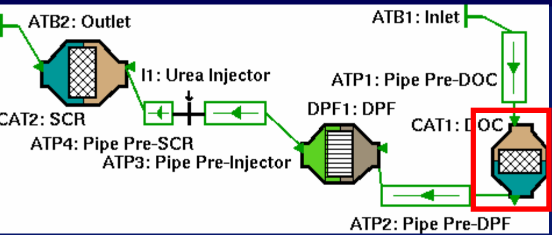


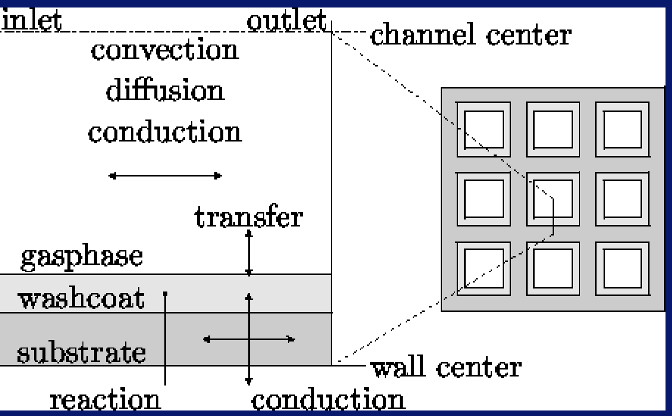
- **Design Explorer**
- **Environment for**
  - Design optimization
  - Sensitivity analysis
  - Parameter identification

Using

- **DoE** (Full Factorial Design, Sobol Sequence, Latin Hypercube Sampling, Orthogonal Arrays)
- **Optimization** (NSGA, Nelder-Mead, NLPQL,…)
- **Response Surface Methods** (NN, SVM)

DOC Model

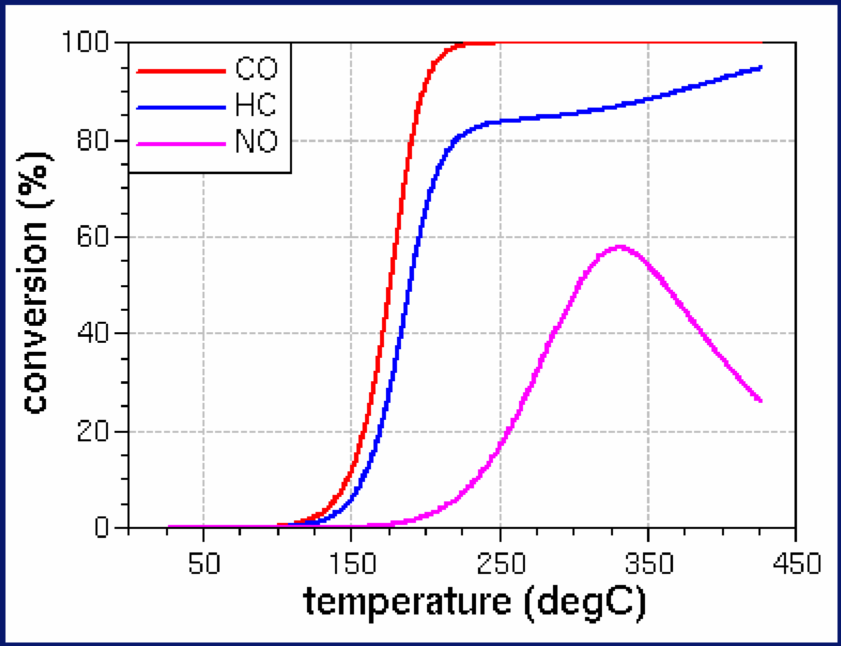




- [x] R1: $CO + {}^{1}\!/_{2}O_2 \longrightarrow CO_2$
- [x] R2: $C_3H_6 + {}^{9}\!/_{2}O_2 \longrightarrow 3CO_2 + 3H_2O$
- [ ] R3: $2CO + 2NO \longrightarrow 2CO_2 + N_2$
- [ ] R4: $H_2 + {}^{1}\!/_{2}O_2 \longrightarrow H_2O$
- [x] R5: $2NO + O_2 \longleftrightarrow 2NO_2$
- [ ] R6: $CO + H_2O \longleftrightarrow CO_2 + H_2$
- [x] R7: $C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$

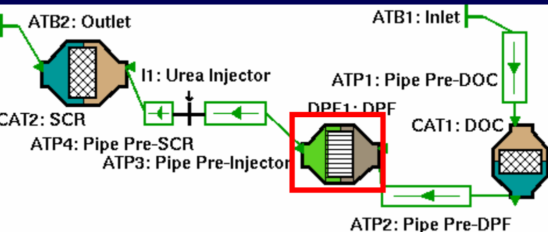
Transient 1D 2-Phase model for an arbitrary number of gas and surface species[1]

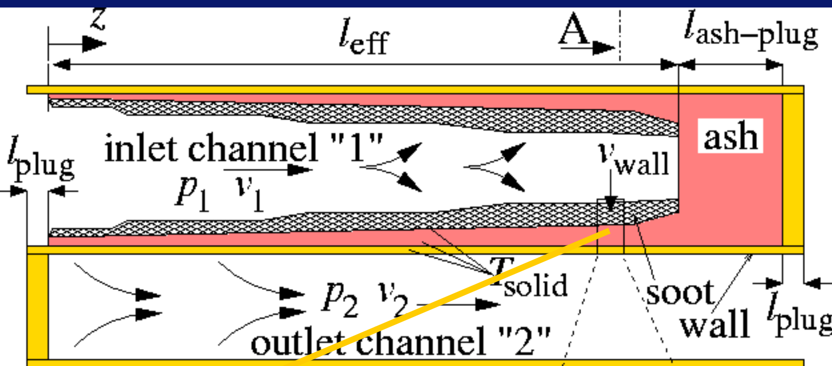
- **4 Oxidation reactions are enabled**
- **Light-off simulation shows typical behavior for CO, HC and NO**

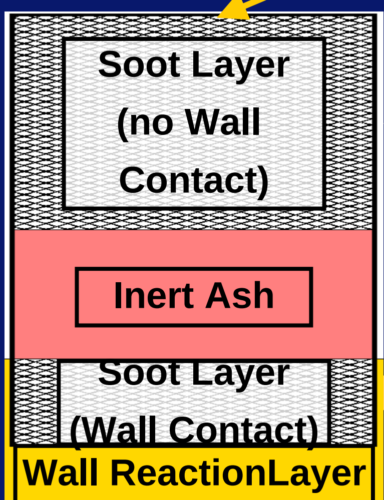


1: see SAE 2003-01-1003

DPF Model



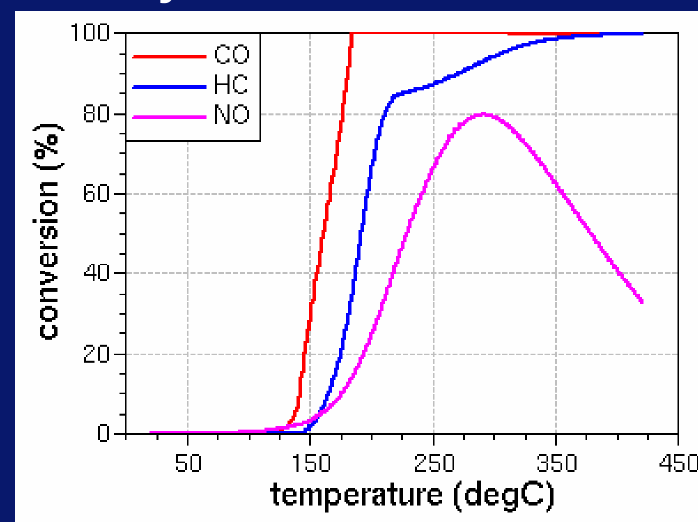




$$2C(S) + O_2 \xrightarrow{\dot r_1} 2CO$$
$$C(S) + O_2 \xrightarrow{\dot r_2} CO_2$$
$$C(S) + NO_2 \xrightarrow{\dot r_3} CO + NO$$
$$C(S) + 2NO_2 \xrightarrow{\dot r_4} CO_2 + 2NO$$
$$NO + 1/2O_2 \xleftrightarrow{\dot r_5} NO_2$$
$$CO + 1/2O_2 \xrightarrow{\dot r_6} CO_2$$
$$C_3H_6 + 9/2O_2 \xrightarrow{\dot r_7} 3CO_2 + 3H_2O$$
$$C_3H_8 + 5O_2 \xrightarrow{\dot r_8} 3CO_2 + 4H_2O$$
$$NO + 1/2O_2 \xleftrightarrow{\dot r_9} NO_2$$

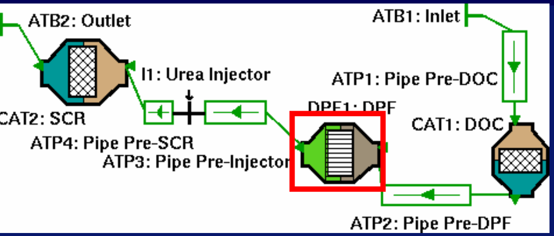
Wall flow DPF model[1]:

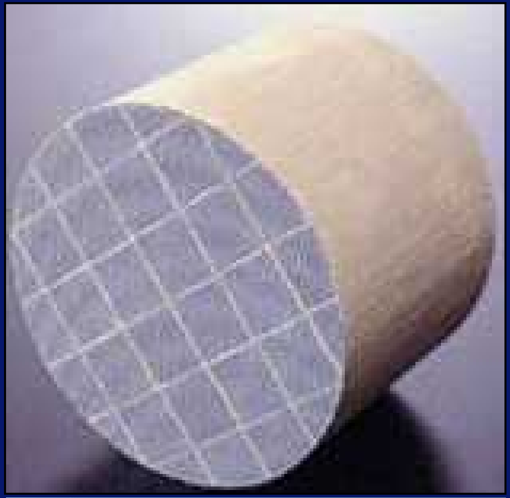
- Asymmetric channel geometries
- Ash and soot loading
- Soot depth and cake layer filtration
- Active and passive soot regeneration w/o catalytic support
- Catalytic wall reactions

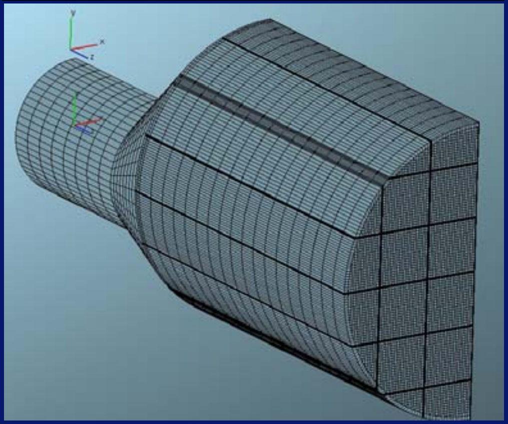


1: see SAE 2007-01-1137

SiC Filter with Segmentation



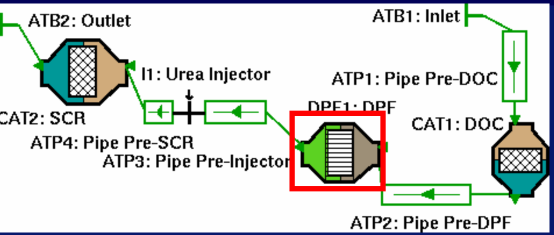




- **Gluing zones**
- **Impact on pressure drop**
  - Reduced effective flow area
  - Different number of active filtration sides near gluing zones (2/3/4 Sides)
- **Impact on regeneration**
  - Different thermal inertia
  - Different heat transfer behavior

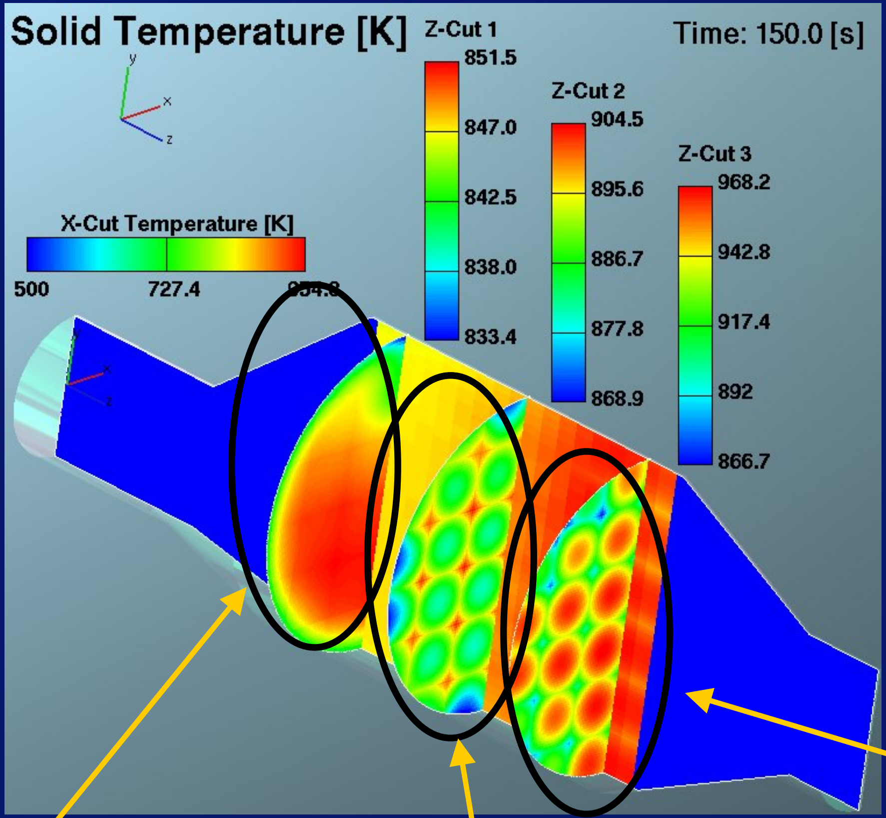
Active Regeneration of Segmented SiC DPF

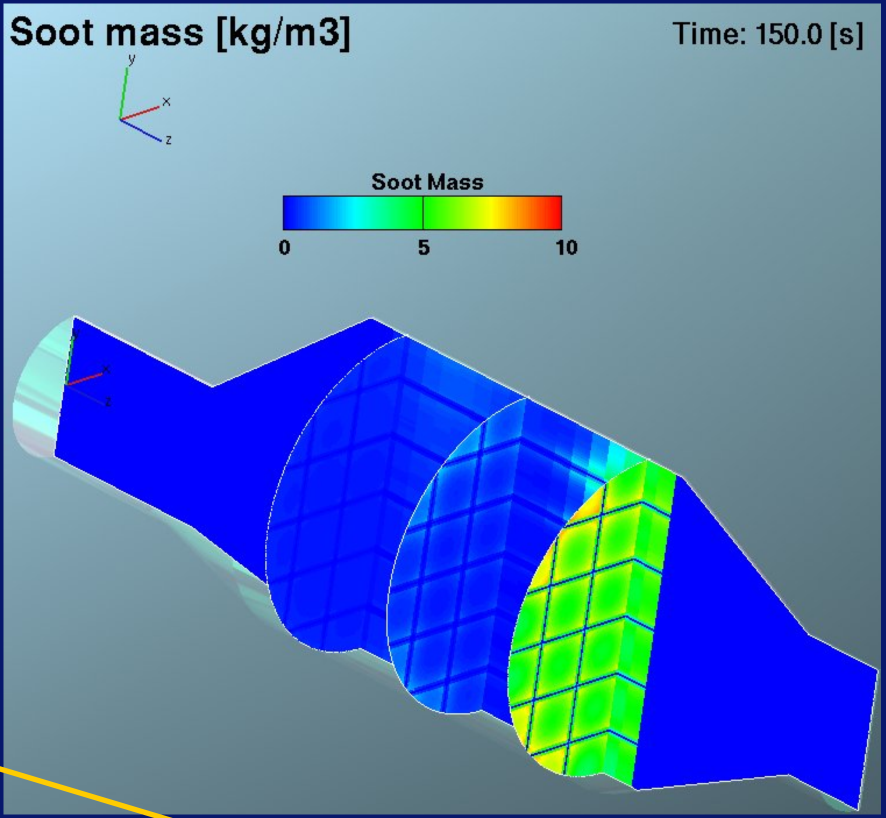
AVL



Snapshots of Movies

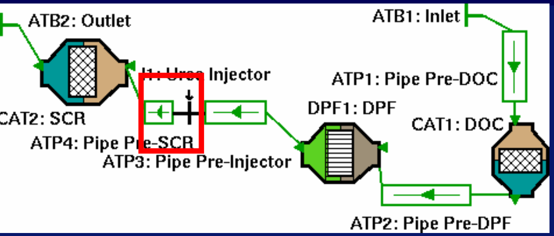
Solid temperature and soot mass at the of forced regeneration (t=150s)

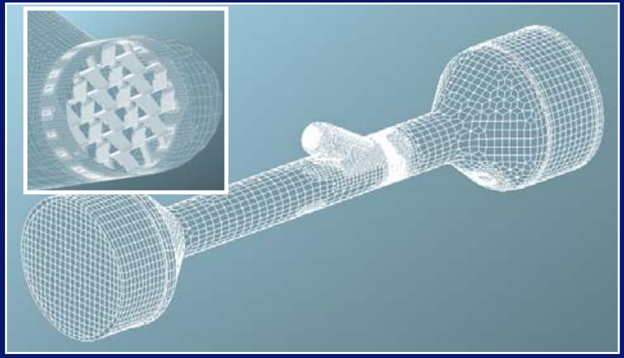


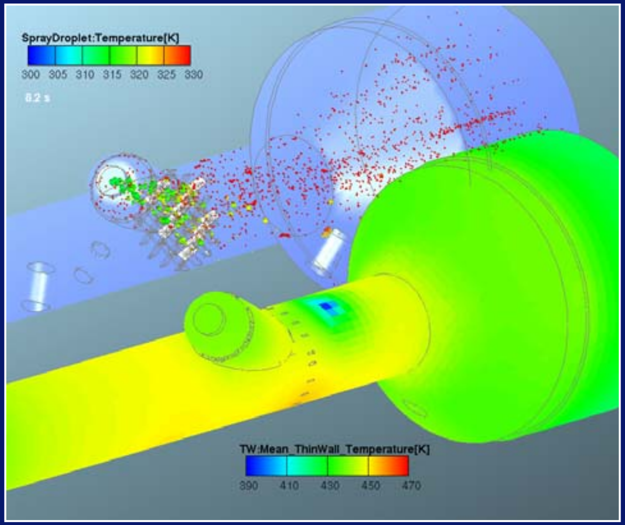


- Uniform temperature
- Gluing zones show highest temperatures
- Gluing zones show lowest temperatures

Urea Injector Model

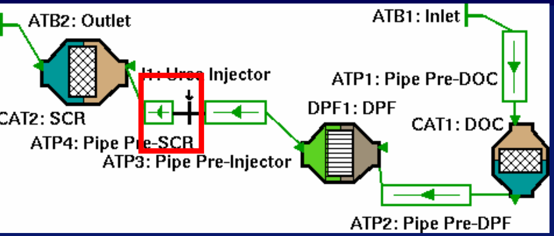




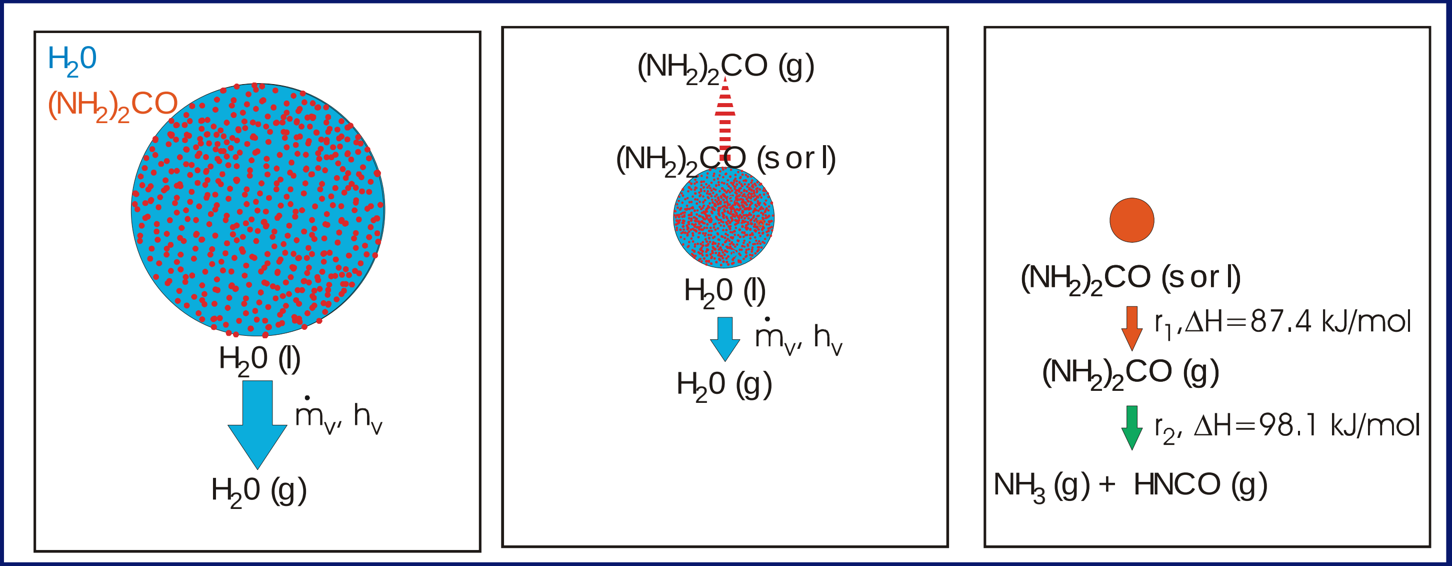


- Injection of urea-water solution
- Spray / gas interaction
  - Liquid / gaseous momentum exchange
  - Droplet / gas heat transfer
  - Water evaporation / urea thermolysis
- Spray / wall / wallfilm interaction
  - Spray impingement
  - Droplet / wall heat transfer
  - Wallfilm formation
  - Wallfilm evaporation / thermolysis
- Cooling of walls
  - Lateral heat conduction
- Hydrolysis
- Catalytic reactions

Evaporation / Thermolysis / Hydrolysis - Model



Droplet Mass transfer model

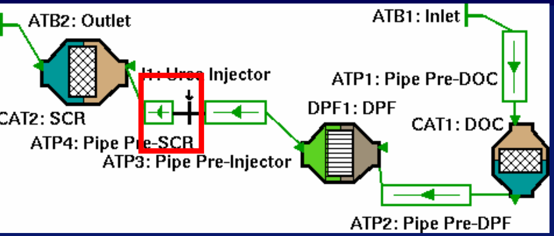


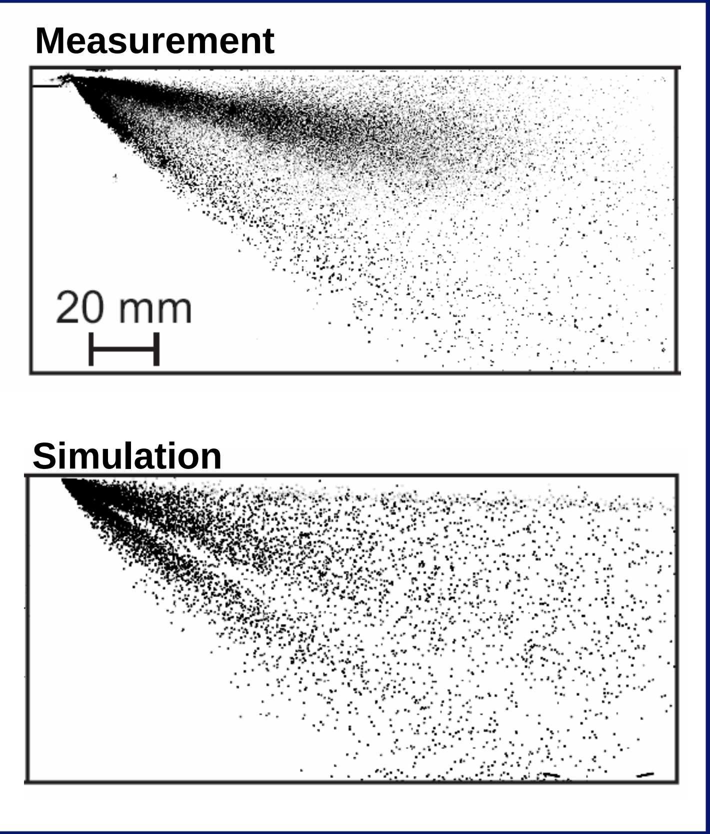
Evaporation of water: $\mathrm{H_2O\ (l) \rightarrow H_2O\ (g)}$

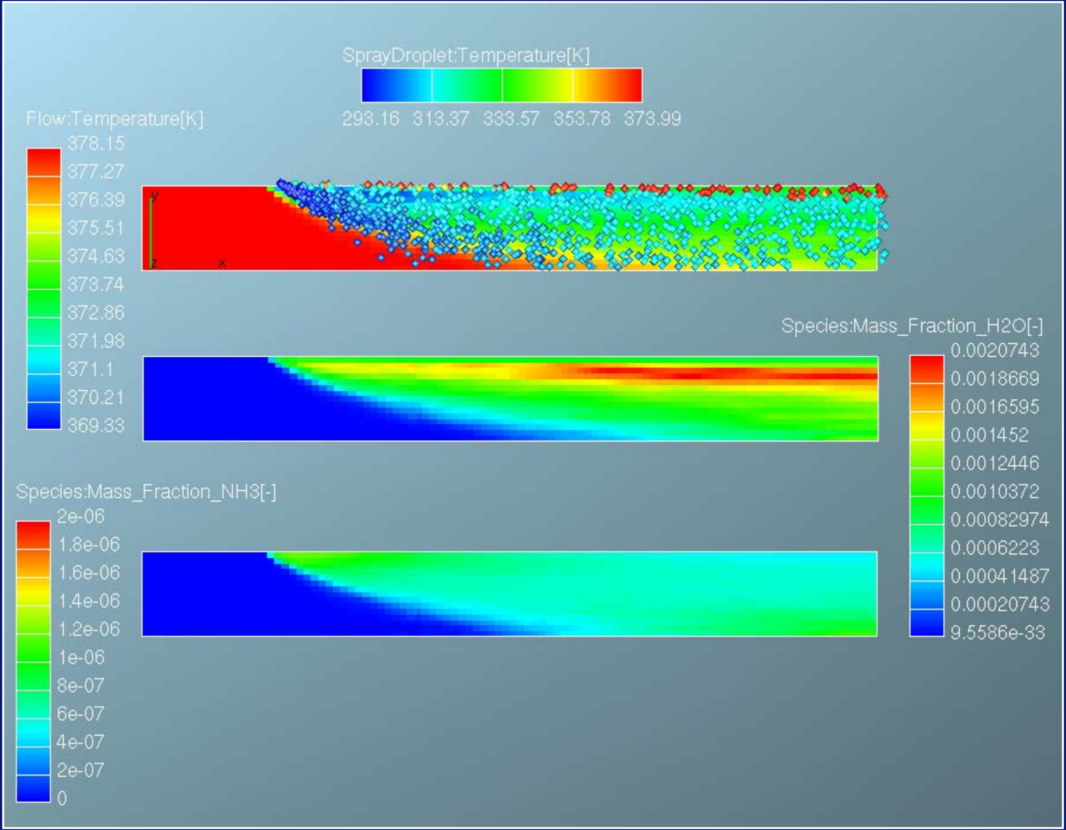
Thermolysis: $\mathrm{(NH_2)_2CO\ (s\ or\ l) \rightarrow NH_3\ (g) + HNCO\ (g)}$

Hydrolysis: $\mathrm{HNCO\ (g) + H_2O}(g) \rightarrow \mathrm{NH_3}(g) + \mathrm{CO_2}(g)$

Spray in Cross-Flow - Validation

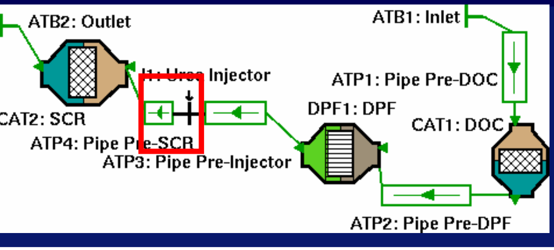


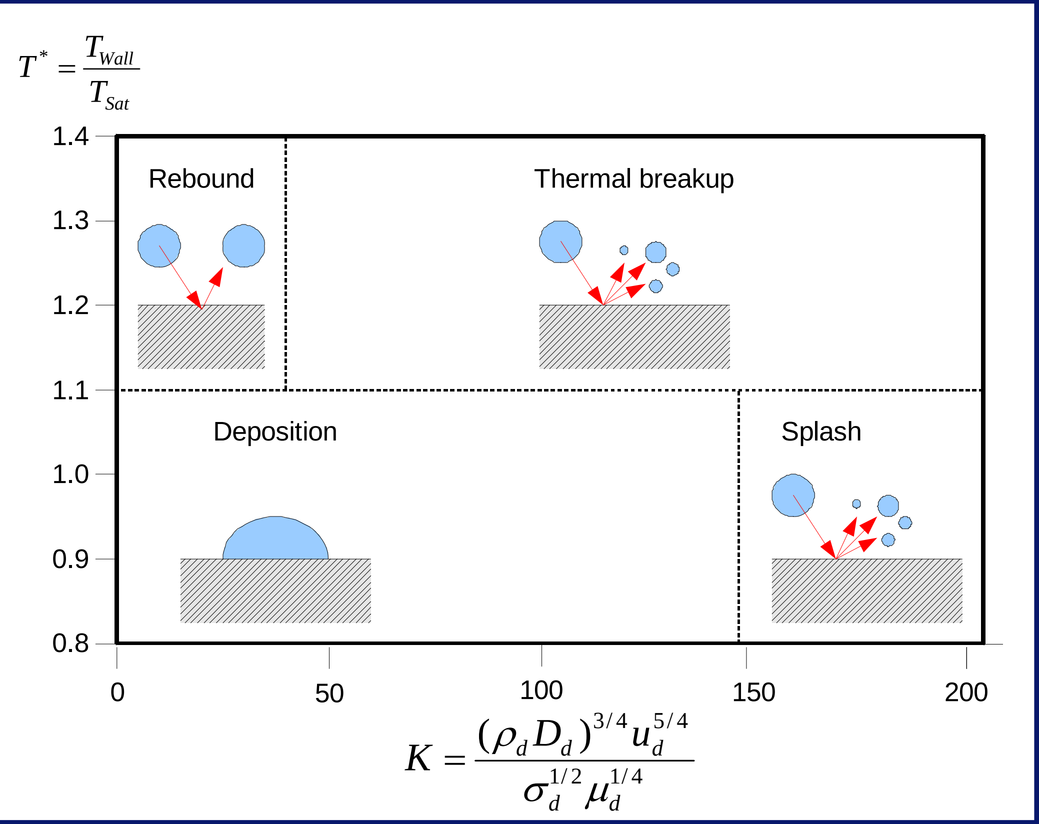




Schwarzenberg, M. Untersuchung von Spraykonzepten zur Dosierung von Harnstoff-Wasser-Lösung beim Einsatz eines SCR-Verfahrens. Diplomarbeit, RWTH Aachen, 2005

Spray Wall Interaction Model

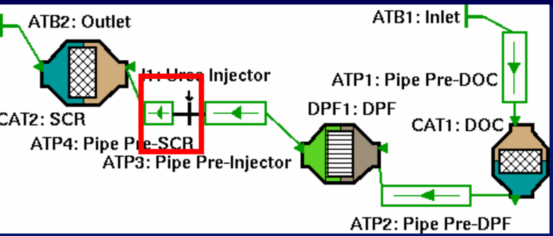




Wall Impingement depends on

- Droplet velocity
- Droplet temperature
- Wall temperature
- Droplet properties (size, viscosity,…)

Spray Wall Film Model



Sketch of Film Element

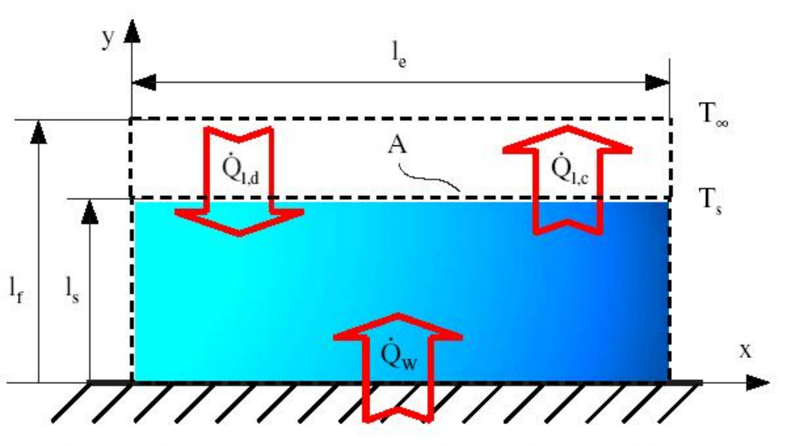
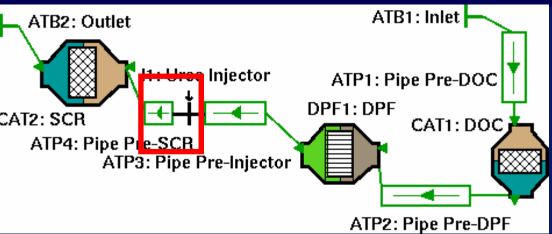


Figure A.1: Heat transfer rates and geometric quantities of a wall film cell

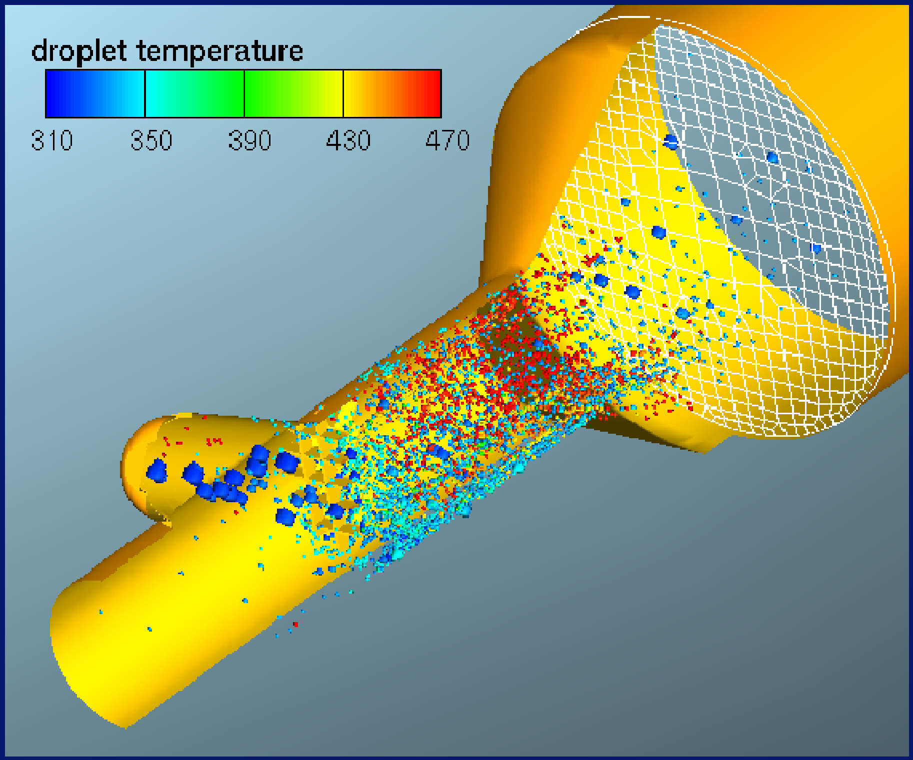
Modeled Effects:

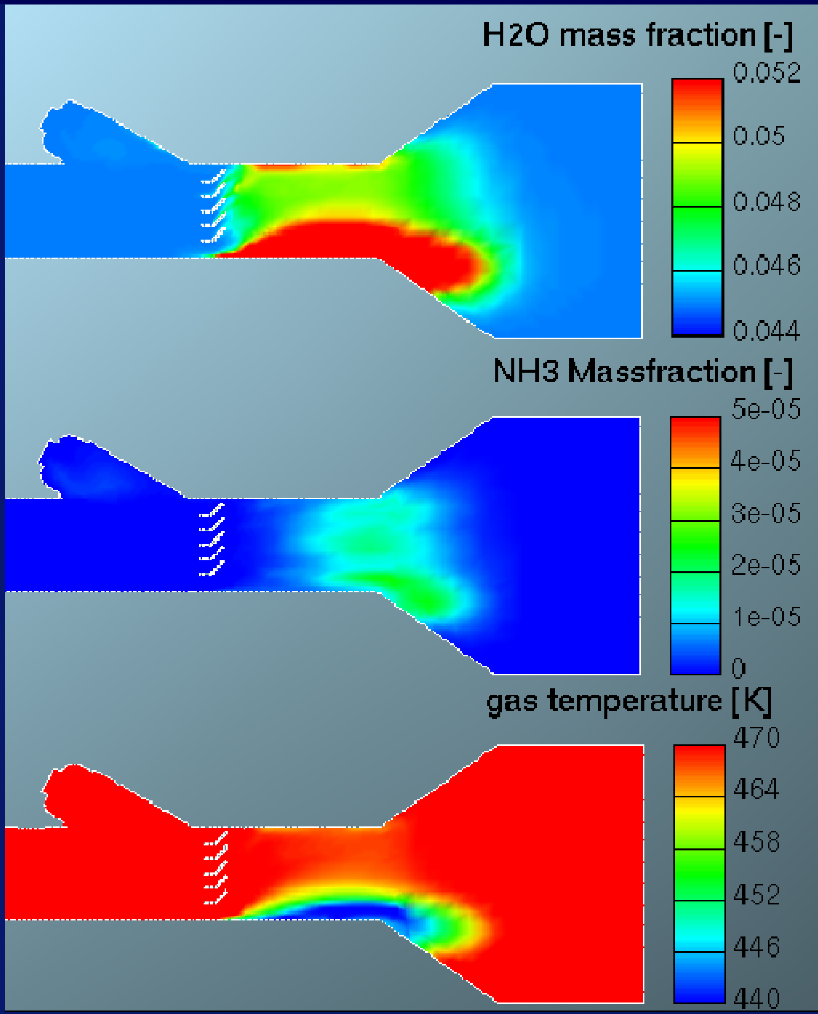
- Film formation and transport
- Temperature dependent splashing models
- Heat transfer between film, droplets and wall
- Multi-component species transport and evaporation / thermolysis

Urea-Injection and NH3 Formation



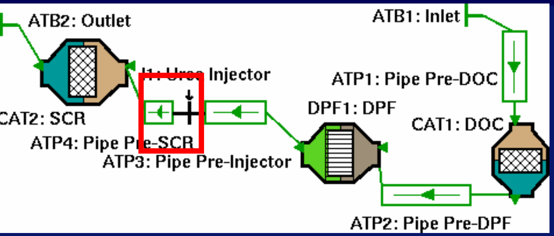
Snapshot of Movies



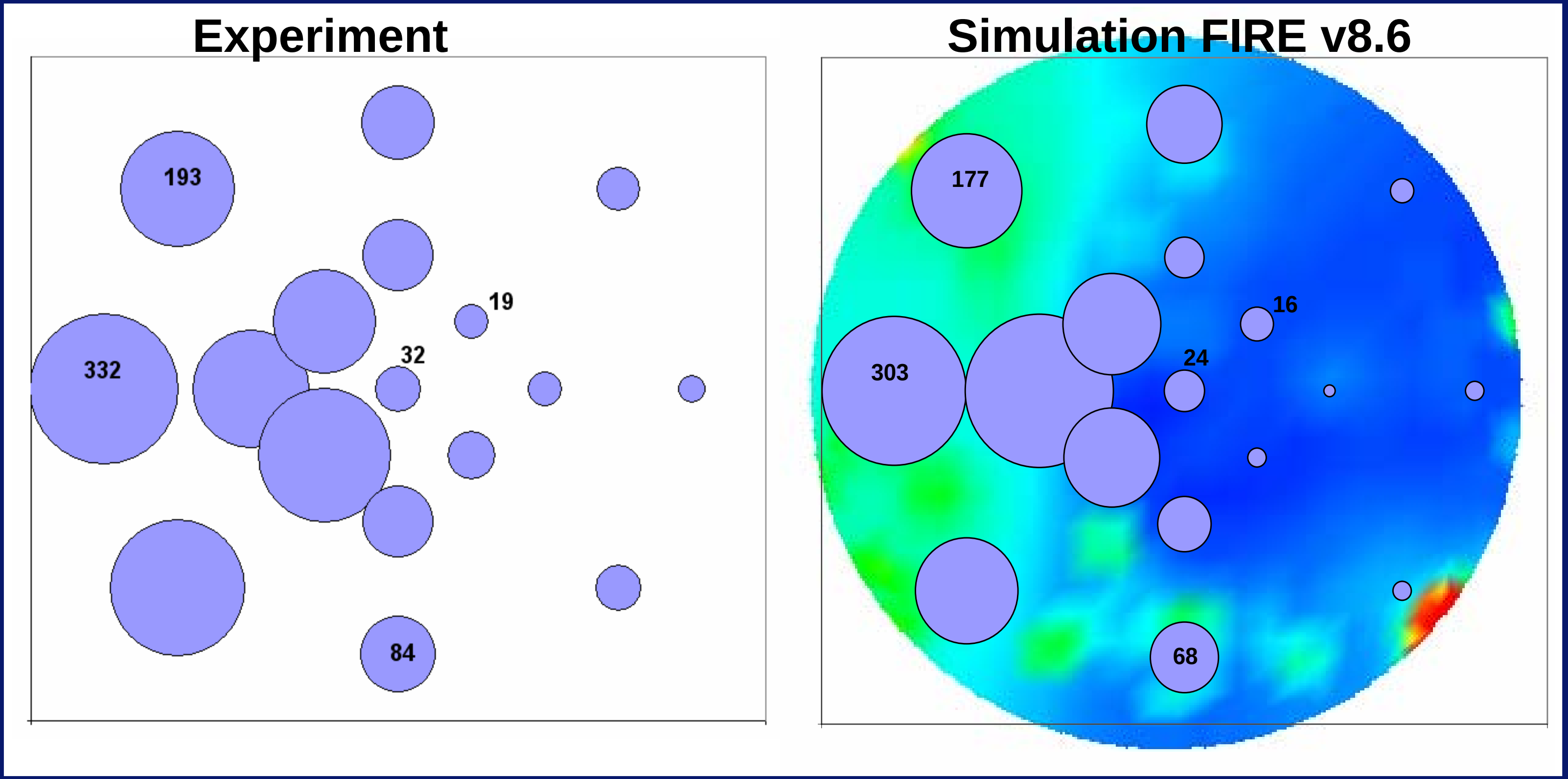


Detailed modeling of spray, evaporation, wall interaction,… is basis to predict NH3 formation and uniformity

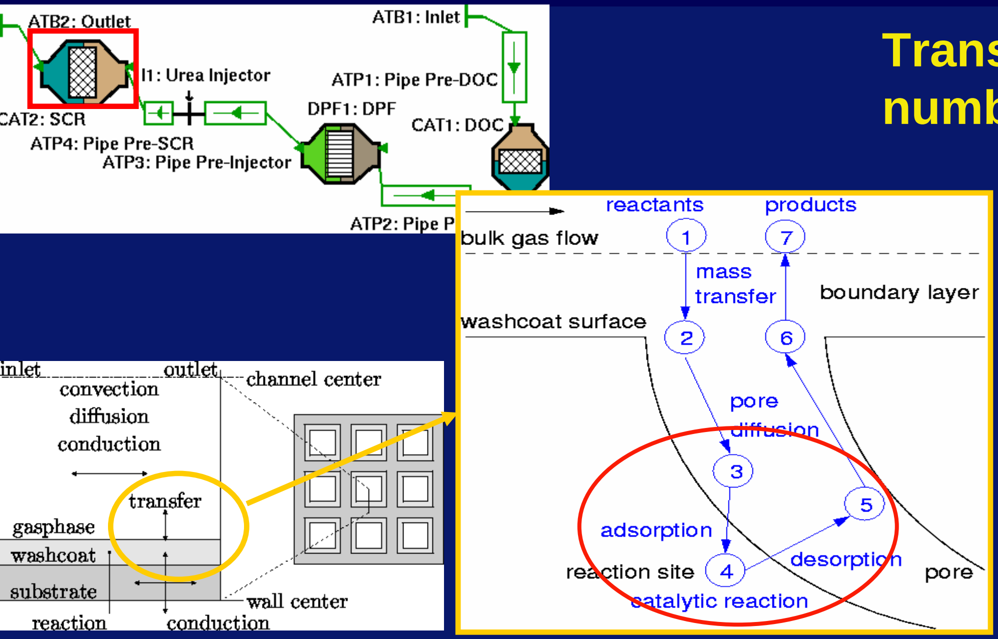
NH3 Distribution



NH3-Concentration past the hydrolysis-catalyst (ppm), application example without mixer



SCR Model



Transient SCR Mechanism

Select: SCR | HSO_SCR | All | None

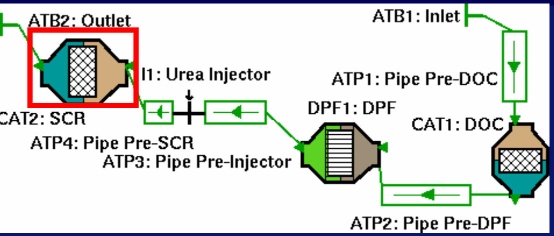
	Sec1	Sec2	Sec3	
R1:	☐	☐	☐	$HCNO + H_2O \longrightarrow NH_3 + CO_2$
R2:	■	☐	☐	$NH_3 + S \longrightarrow NH_3(S)$
R3:	■	☐	☐	$NH_3(S) \longrightarrow NH_3 + S$
R4:	☐	☐	☐	$4NH_3 + 4NO + O_2 \longrightarrow 4N_2 + 6H_2O$
R5:	■	☐	☐	$4NH_3 + 2NO + 2NO_2 \longrightarrow 4N_2 + 6H_2O$
R6:	☐	☐	☐	$8NH_3 + 6NO_2 \longrightarrow 7N_2 + 12H_2O$
R7:	☐	☐	☐	$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O$
R8:	☐	☐	☐	$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O$
R9:	■	☐	☐	$2NO + O_2 \longleftrightarrow 2NO_2$

Transient 1D 2-Phase model for an arbitrary number of gas and surface species[1]

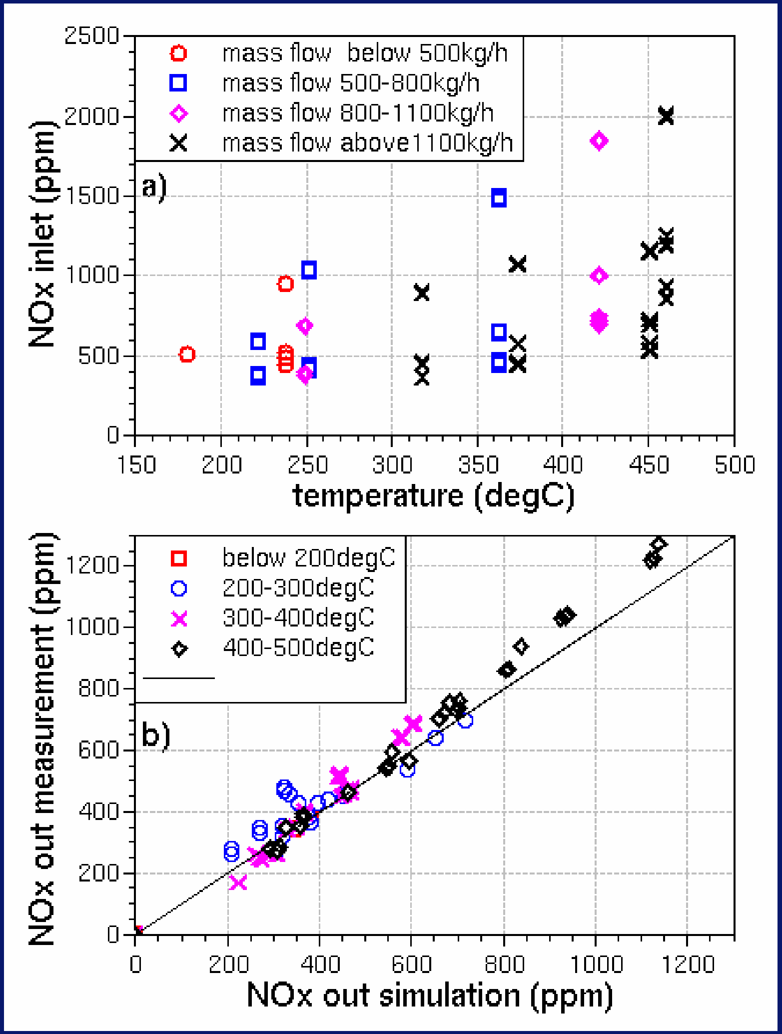
- **Storage and desorption of NH3 is explicitly taken into account**
- **The reaction model is reduced to 4 major reactions**

1: see SAE 2005-01-0948

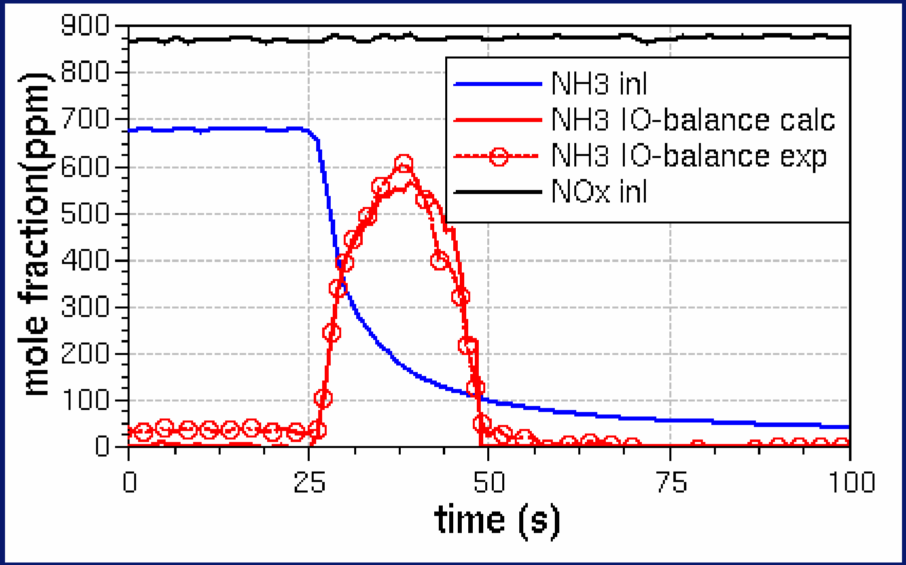
SCR, NOx-Conversion Performance



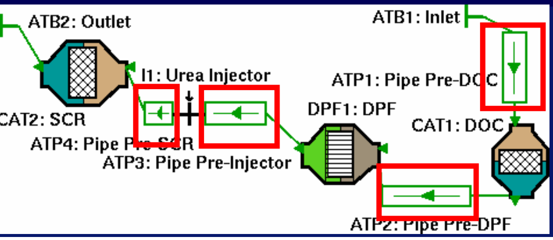
Simulation/experiment for 108 load points

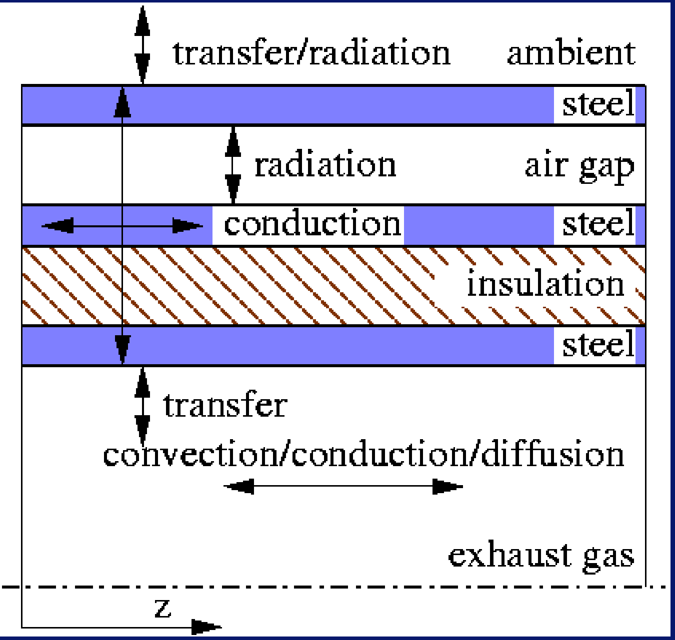


Simulation/experiment for NH3-desorption during dosing-step



Pipe Model



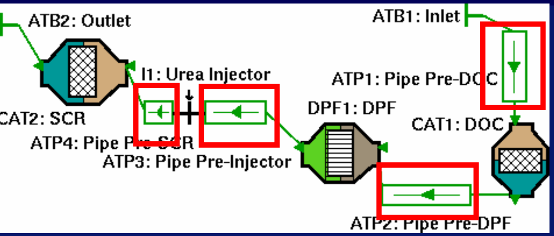


Transient 2D heat transfer model for an arbitrary number of wall layers[1]

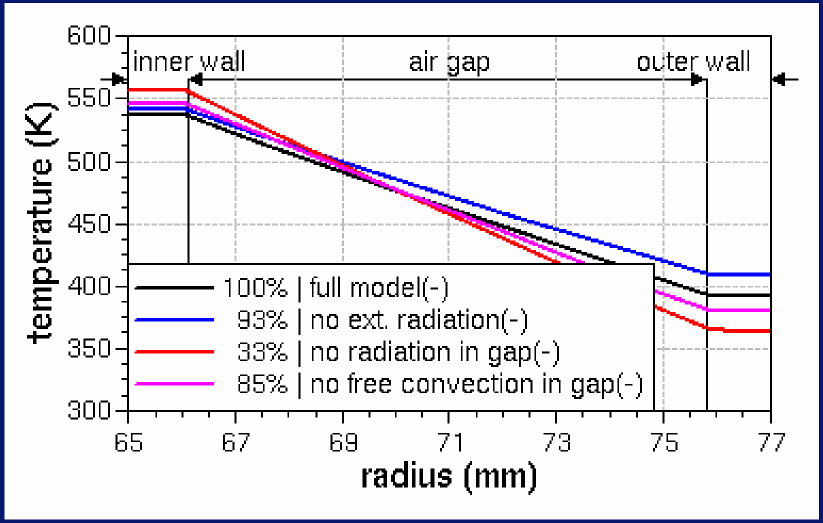
- **Main features:**
  - **Conduction in opaque layers**
  - **Radiation**
  - **Free convection in air-gaps**
  - **Free and forced convection to ambient**
  - **Temperature dependent physical properties**

1: see SAE 2008-01-0865

Pipe Wall Heat Loss Simulation

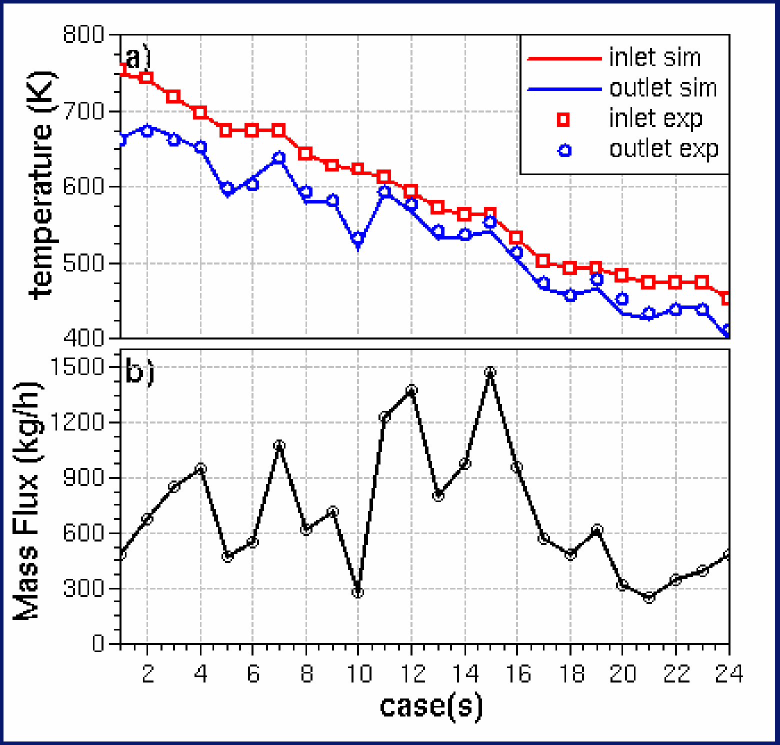


Dual wall pipe, effect study



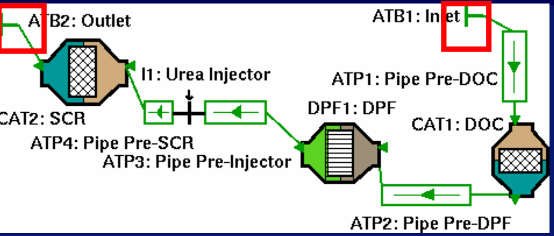
Impact of radiation in the gap is significant

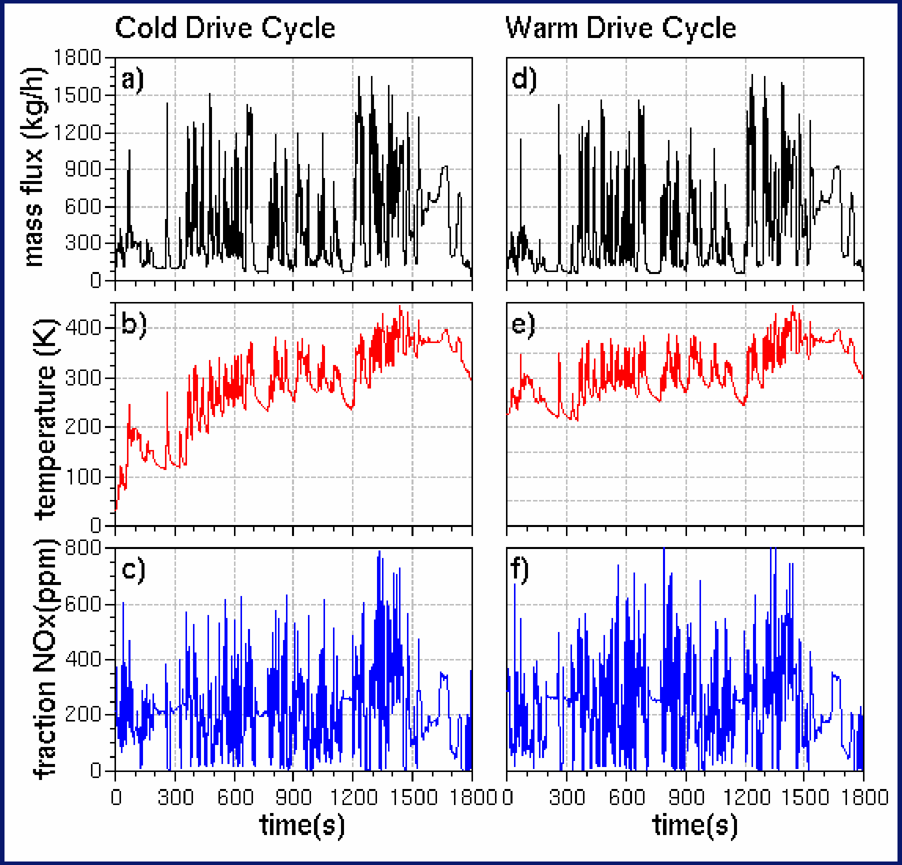
Simulation/experiment single wall pipe



Pipe outlet temperatures are well covered by the model (internal heat transfer factor was adapted)

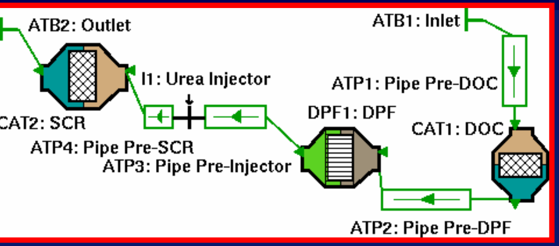
Boundary Conditions for Drive Cycle

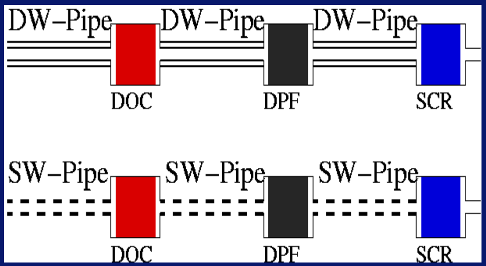




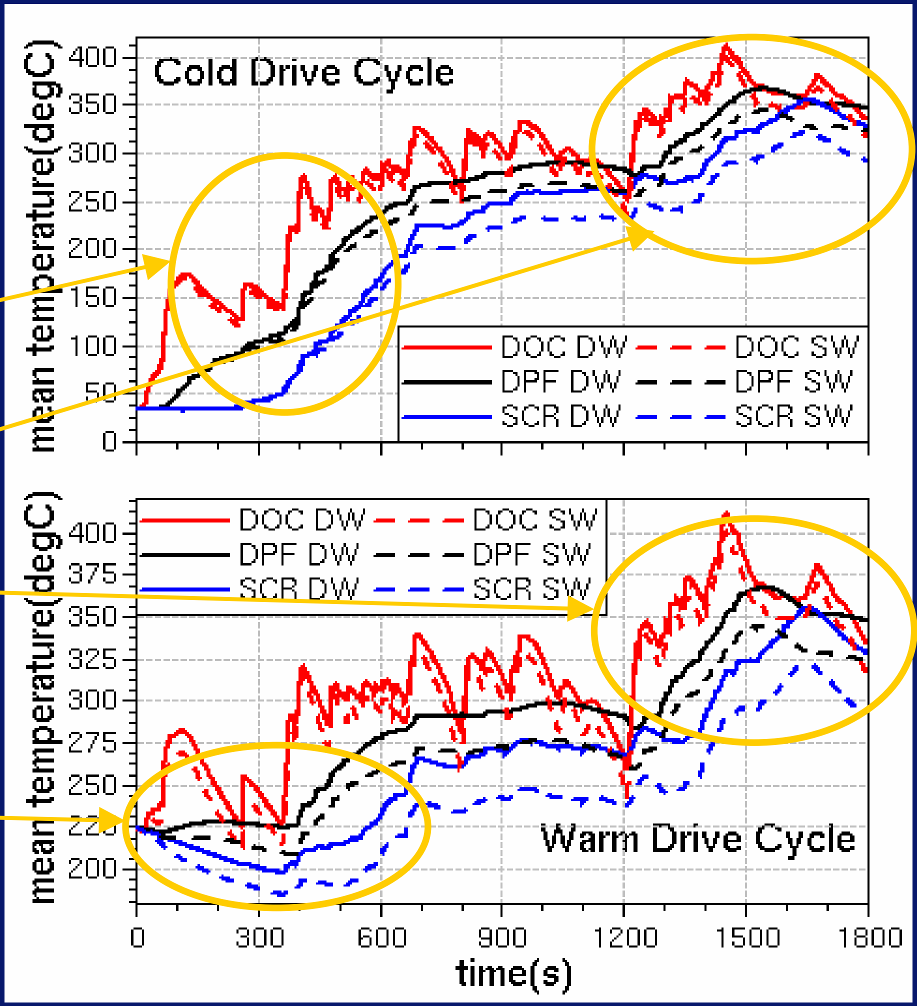
- **Inlet Conditions:**
  - **Engine Row Emissions for a WHTC given for cold and warm engine conditions**
- **Outlet Conditions:**
  - **Constant ambient back pressure**

WHTC Simulation, Pipe Insulation Study I



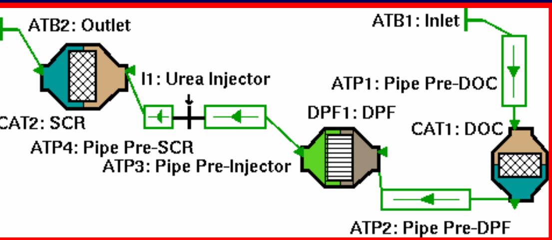


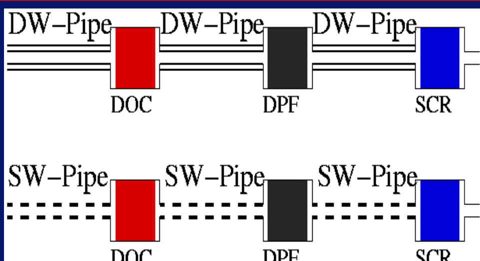
Mean DOC/DPF/SCR temperatures during cold and warm WHTC



- **Heat-up phase:**
  - **Small impact of pipe insulation**
- **High-load phase:**
  - **Dual-wall insulation shows higher temperatures**
- **Low-load phase:**
  - **Dual-wall insulation holds SCR operating temperature**

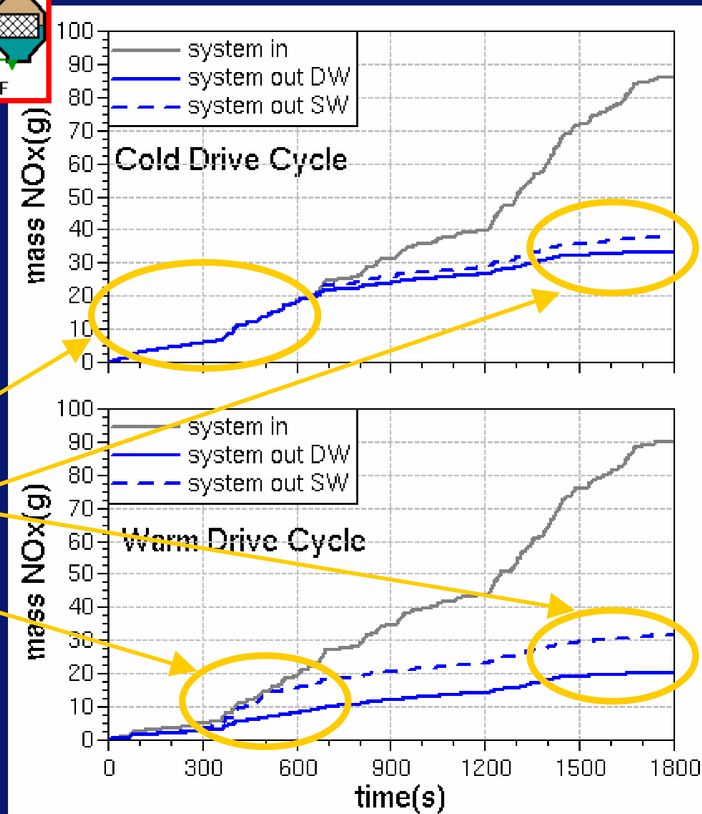
WHTC Simulation, Pipe Insulation Study II



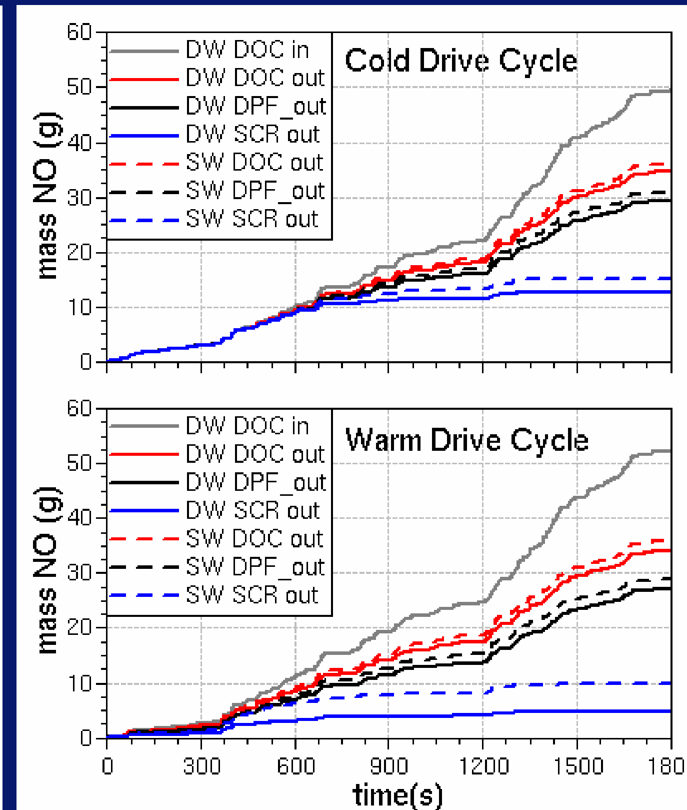


- **Heat-up phase**
- **High-load phase**
- **Low-load phase**

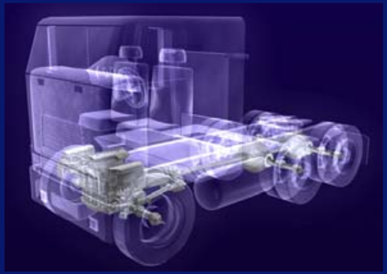
verall NOx-emissions

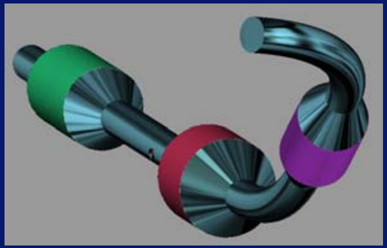


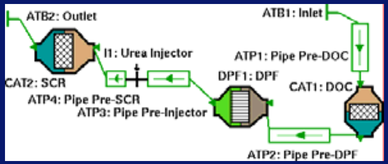
Overall NO-emissions



Summary and Conclusions







- **Demonstration of a 1D/3D aftertreatment system simulation framework by the example of a heavy-duty application**
  - **All components are pre-calibrated with experimental data**
  - **BOOST is used to investigate the overall system is investigated in 1D**
  - **FIRE is used to perform 3D detail simulations**
- **Sufficient modeling depth of all components is essential**
- **Simulation approach can be used for various system configurations**