Simulation Supporting the Exhaust Aftertreatment Development Process - 1D Concept and Control Design, 3D Detail Optimization



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# EAS Simulation

- Models and Examples
  - Flow Uniformity
  - DPF
  - DPF, Mixer
  - Urea Injector
  - SCR
  - Overall System
- Summary

# EXHAUST AFTERTREATMENT SYSTEM (EAS) SIMULATION

#### Areas addressed by 1D/3D simulation

DOC:

- Conversion behavior (CO, HC, NOx), pressure drop, flow uniformity,...

- DPF (CSF):
  - Pressure drop, spatial temperature distribution during loading and regeneration, maximum temperature control,...
- Urea Injector, Mixer:
  - Dosing control, radial NH3 distribution, impact of mixers, buildup of wallfilms,...
- SCR:
- Conversion behavior of NOx, NH3 storage,...
- Slip-Cat:
  - Conversion behavior of NH3
- System:
  - System performance for different component sizes, arrangement of components, control strategies,...









# TOOLS FOR EAS SIMULATION





# Simulation of Aftertreatment Systems with AVL-Software:

- Identical physical models (gas dynamic, thermal and chemical effects) from 1D to 3D
- Pre-defined kinetic components models
- Development platform for user-defined reaction schemes
- Parameterization of models is based on key experiments
- One single model-structure and parameterization can be used for all different tools and simulation tasks -> flexible approach
- Interface to Simulink for ECU development/calibration









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# FLOW UNIFORMITY





# Comparison of Geometries and Concepts

- Calculation of flow uniformity
- Calculation of pressure drop
- Comparison of design variants (i.e. round vs. oval inlet)
- Guidelines for sensor positioning

# **Damage Prediction**

- Durability is linked to flow conditions
- Low pressure gradients at component inlet reduce susceptibility of damage
- Uniform component usage and heatup needs to be ensured



# FLOW UNIFORMITY OPTIMZATION EXAMPLE

- Base geometry is fixed
- Fine tuning of inlet geometry to ensure satisfying flow uniformity
- Time efficient approach using
  - Parameterized geometries











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# **DPF MODEL**



# 1D DPF flow model:

- Different inlet/outlet channel sizes and shapes
- Inlet/outlet plugs
- Ash as layer, plug or combination
- Depth and cake layer deposition

# 3D DPF model:

Each axial cell raw of the 3D mesh represents one pair of DPF inlet/outlet channels



# GENERAL DPF CELL GEOMETRIES



Squared inlet channels with non-active filtration sides (i.e. near segmentation walls)







Hexagonal channels with asymmetric sides



Octagonal channels with asymmetric sides



# General DPF cell geometry model enables investigation of:

- Pressure drop during loading
- Temperatures and thermal stresses during regeneration



# DPF, PRESSURE DROP OF ASYMMETRIC CHANNELS



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# PRESSURE DROP FOR BOSCH HEXAHEX GEOMETRY



#### **Simulation Procedure**

- Permeabilities (wall, soot depth and cake layer) are tuned on measured data for a squared cell DPF
- Hexahex model applies the same permeabilities
- Hexahex shows smaller pressure drop increase













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# PM-METALIT®, CFD ANALYSIS





#### CFD analysis of PM filter device regarding to:

- Flow field (axial and radial velocity distribution)
- Radial mixing behavior of tracer gas introduced at singular point
- Transport of soot particles
- Transport of urea-water droplets
- Interaction of droplet to wall and flies
- water evaporation and urea thermolysis

# modeling

- 5 corrugated layers
- 2 flow guiding sections in axial direction
- 6 fleece layers
- periodic boundaries in radial direction
- 1.4Million computational cells

see Brück et. al ICPC 2009



# PM-METALIT®, INVESTIGATION OF TRACES GAS



Radial distribution of traces gas



~25% of the axial mass flows is exchanged in radial direction through the fleece layers

see Brück et. al ICPC 2009

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#### PM-METALIT®, UREA-WATER CONVERSION











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# UREA INJECTION, BASIC PHENOMENA







Injection of urea-water solution

# Spray / gas interaction

- Liquid / gaseous momentum exchange
- Droplet / gas heat transfer
- Water evaporation / urea thermolysis

# Spray / wall / wallfilm interaction

- Droplet / wall heat transfer
- Spray impingement
- Wallfilm formation
- Wallfilm evaporation / thermolysis

# Cooling of walls

- Lateral heat conduction
- Hydrolysis
- Catalytic reactions



# NH3 FORMATION IN HEAVY-DUTY EXHAUST SYSTEM

# **Simulation Variants**

- 1. System without mixer, injection in flow direction
- 2. System with mixer, injection downstream the mixer against flow direction

# **Comparison of**

- Wall Film mass
- Wall film thickness
- Wall film distribution
- Completeness of evaporation and thermolysis
- Flow uniformity at SCR inlet
- NH3 uniformity at SCR inlet







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# INJECTOR CHARACTERIZATION

#### **Given input data**

1. Nozzle geometry



#### 2. droplet size distribution



# **Spray Box Simulation**

- Spray angle
- Droplet distribution
- Wall impingement as function of flow field





# FLOW DISTRIBUTION, CUT PLANE THROUGH INJECTOR

 Characteristic stagnation zone around injection point of system without mixer can be observed

- Stagnation zone almost disappears for system with mixer
- High probability of wall wetting around the nozzle tip due to cross flow motions around it





#### FLOW DISTRIBUTION, OVERALL SYSTEM

- Geometry of tangential connection pipes to mixing chamber leads to significant swirl motion-> support of evaporation and thermolysis
- Mixer disturbs flow pattern but does not overcome the basic swirl motion
- Mixer causes higher pressure losses in system → impact on engine performance





#### Low load points show smaller film area compared to high load

- High load points show superior droplet break up and evaporation
- System with mixer at low load shows similar film area but smaller film mass
- System with mixer at high load shows significant film thickness in impingement region



#### NH3 DISTRIBUTION, OVERALL SYSTEM

- System without mixer shows good NH3 preparation and high NH3 uniformity at SCR catalyst inlet
- Uniformity is mainly influenced by high swirl flow in the mixing chamber
- System with mixer shows for both load points a higher amount of NH3 is released from wall film











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# **3D SCR SIMULATION**

#### **AVL Code Coupling Interface (ACCI)**

- Performs mapping between chosen faces of simulation domains
- Decouples SCR converter simulation from urea formation simulation
- Maps profiles of velocity, temperature, species, TE,... from spray simulation to SCR catalyst conversion
- Allows spreading of simulation load to different hosts via TCP/IP coupling

#### FIRE: ACCI coupling, chemical kinetics







# HYDROLYSIS AND SCR CATALYST

Radial NH3 distribution can be observed, but on a small absolute level:

- This is caused by the high urea conversion performance of the injection system
- The SCR catalyst could also reasonably be investigated with simplifying 1D models











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# **1D INJECTOR MODEL**



- Data base for pre-defined (adBlue, water, Diesel,...) and user-defined liquids
- Injection of arbitrary liquid and gas mixtures
- Pre-defined and user-defined break-up of liquids covering instantaneous evaporation and reactions (adBlue→ 2NH3+CO2+6H2O)
- User-defined build up of wall film
- Multi-component evaporation from wall film considering
  - film temperature driven evaporation pressure
  - component partial pressure in the gas phase
  - flow conditions
- Heat-transfer between wall, wall film and gas phase
- Dosing control modeling via
  - PID, Formula Interpreter elements
  - Simulink



# 1D INJECTOR MODEL, WATER/UREA DOSING





# UREA INJECTION CONTROL DURING DRIVE CYCLE



- Formula Interpreter: Sensors NO and NO2 at SCR inlet and evaluates NOx level
- PID: Sensors NH3 at SCR inlet and steers injected Urea mass flow in order to meet alpha=1

- DOC: 20lt, 400/5
- DPF: 30lt, 200/12
- SCR: 35lt, 400/7
- Pipes: 10m/100mm, dual wall





# UREA INJECTION CONTROL DURING DRIVE CYCLE











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## SUMMARY





The development of EAS is supported by an efficient and systematic simulation framework used from the early concept phase to the late calibration phase

- ID is used to
  - Calibrate reaction models
  - Perform overall system design and analysis
  - Investigate control strategies

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- 3D is used to
  - Calculate flow uniformity
  - Investigate adBlue dosing, spray and wall film
  - Investigate mixer performance
  - Predict temperature (gradients) during DPF regeneration

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