



Aftertreatment Module

The FIRE Aftertreatment Module solves demanding fluid flow, heat transfer and chemical reaction in all types of exhaust gas lines and catalytic reactors. It is fully integrated into AVL's CFD Workflow-Manager together with a number of other advanced physical models.

Introduction

More stringent emission requirements demand new approaches to the design and layout of off-gas treatment systems. The advanced concepts in this field require sophisticated simulation tools to characterize performance and help engineers integrate catalytic reactors (for reduction of gas phase pollutants) and filtration units (for reduction of solid phase pollutants) into today's vehicles.

The FIRE Aftertreatment module fulfills this requirement by offering the most advanced aftertreatment-specific physical models, unparalleled flexibility and full coupling to FIRE's renowned engine analysis capabilities.

Advanced Models

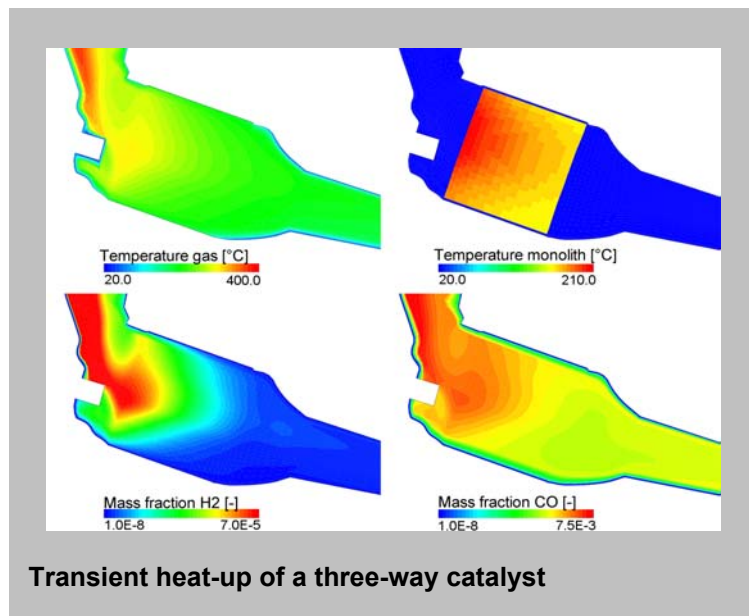
For aftertreatment applications FIRE provides the most sophisticated mathematical models available on the market today.

- The **Porosity** model (directed resistance) can be used for the analysis of flow and pressure drop (tube friction) in monolithic catalysts.
- The **General Species Transport** model allows the definition of an arbitrary number of chemical species in the gas phase. The resulting physical properties can either be defined by the user or be calculated automatically based on an extensive internal property database. Full access to user-defined thermodynamic and transport databases is provided.
- The **Aftertreatment Module** enables the user to define any number of

catalysts in the computational domain. Surface chemical species are considered in order to account for storage effects (i.e. oxygen storage in three-way catalysts).

An arbitrary number of chemical reactions is solved using a fully integrated stiff ODE solver.

- The **Thermal Behavior** of the catalyst is simulated by solving a separate enthalpy equation for the solid of the catalyst material. The equation accounts for conductive heat transfer including anisotropic thermal conductivity effects.
- The **Particle Filter model** enables the user to simulate the flow inside of a "wall flow type" particle filter. A unique filter flow model calculates the pressure drop and the velocities in the inlet and outlet channel of the particle filter as well as the corresponding wall velocity profile. It accurately accounts for non uniformly distributed soot layers as well as for the temperature variations in the filter.
 - Transient loading of the filter is simulated based on the wall velocity profile. The effect of particle migration in regions of high flow rate is considered.
 - All types of regeneration (thermal, catalytic and NO₂ assisted) are simulated using the novel local-



Transient heat-up of a three-way catalyst

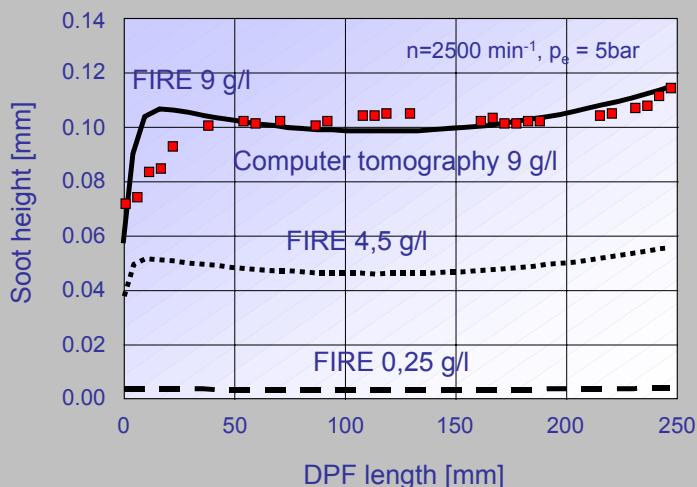
layer-discretization strategy (one or two layer approach).

- The exhaust gas line's interaction with ambient conditions is simulated using the **Thin Walls** model. It accounts for heat conduction in metallic pipes and insulation mats as well as for heat losses to the ambient (conductive and radiative).

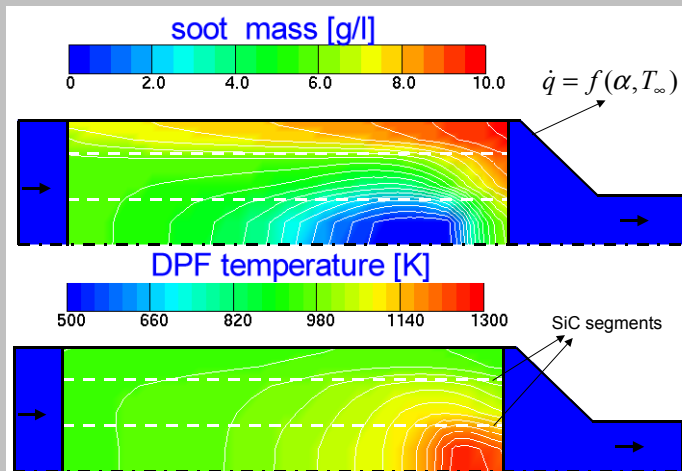
Productivity

The FIRE Aftertreatment Module is fully embedded into AVL's CFD-Workflow Manager environment. Here the pre-processing, calculation and post-processing is carried out in one Graphical User Interface, offering a consistent user environment which makes data and project management easy.

Post-processing, such as 2D results of conversions of chemical species and catalyst temperatures, can be plotted on-screen during runtime for quick analysis and design iterations. Export to ASCII and other formats is offered for further processing using 3rd party software.



Loading of a Diesel Particle Filter: Comparison with Computer Tomography Experiments



Regeneration of a Diesel Particle Filter: soot mass and temperature distribution

User Modifications

In addition to standard CFD user subroutine entry points (user defined physical properties, user defined boundary conditions, user defined initialization) the FIRE Aftertreatment module enables the user to adapt the simulation model for specific needs:

- User defined reaction rates: The user freely defines the rate laws of the specific chemical reactions. It is typically used for definition of rate laws like the Langmuir-Hinshelwood approach in standard three-way catalyst models.
- User defined heat and mass transfer: although several approaches for the calculation of heat and mass transfer in the catalysts are available by default users can define their own models here.

- User defined reaction model: here the user completely implements the calculation of source terms for the species transport and enthalpy equations. It is intended for users who already have their own reaction models available but want to use the highly flexible pre- and post-processing framework of the FIRE Aftertreatment Module.

Recent Publications

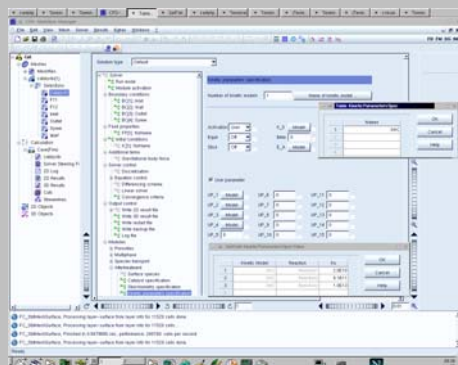
Wanker R., Granter H., Bachler G., Rabenstein G., Ennemoser A., Tatschl, M. Bollig, "New physical and chemical models for the CFD simulation of exhaust gas lines: A generic approach"; 2002-01-0066

Wanker R., Bollig M., Granter H., Tatschl R., " 3D CFD simulation of exhaust lines: A new approach to account for current and future challenges ";

JSAE 20025336

Cartus T., Diewald R., Herzog P., Strigl T., Wanker R., „Diesel Particulate System Integration – From 3D-Simulation to Production“, Wiener Motorsymposium 2002, 25.-26.4.2002, Vienna, Austria

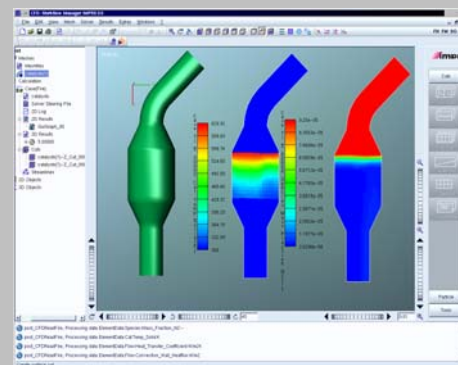
Missy, S., Thams, J., Bollig, M., Tatschl, R., Wanker, R., Bachler, G., Ennemoser, A. Grantner, H., „Computerunterstützte Optimierung des Abgasnachbehandlungssystems für den neuen 1.8l Valvetronic Motor von BMW“, MTZ 11 (2001)



Pre-Processing



Post-Processing: 2D Results



Post-Processing: 3D Results