ABSTRACT

Future limits on emissions for both gasoline and Diesel engines require adequate and advanced systems for the aftertreatment of the exhaust gas. Computer models as a complementary tool to experimental investigations are indispensable to design reliable after-treatment devices such as catalytic converters and Diesel particulate filters. Therefore, the objective of this contribution is to present an integrated 1D to 3D simulation workflow of catalytic converters (TWC, DOC, SCR, …) and Diesel particulate filters. The parameters or sets of parameters are obtained by a fast and efficient 1D-approach of BOOST. They are readily transferable to the 3D simulation code FIRE to investigate detailed aspects such as spatial distribution of temperatures or heat losses. Thus, identical models predicting flow, energy and conversion of species of the exhaust gas were employed to both the 1D gas exchange/cycle and the 3D CFD simulation code.

This approach allows to carry out a basic analysis and to define first layouts for the exhaust system. Characteristic parameters of this first design stage are used for the multi-dimensional simulation to evaluate the overall performance including fine tuning of aftertreatment systems.

INTRODUCTION

The introduction of more stringent European and world-wide standards for engine emissions steadily increases the effort to develop new exhaust aftertreatment systems. In order to reduce costs and time, the application of reliable computer models became an indispensable part of any development in emission control and powertrain management. At early stages 1D simulation tools help perform basic system analysis and define first designs of aftertreatment devices. Multidimensional simulations are applied to evaluate the overall performance of fully integrated aftertreatment systems and to tune final designs.

This paper focuses on the modeling of the fluid flow and regeneration effects in a Diesel-Particulate-Filter “DPF” [4]. First the mathematical model is briefly described. Then the workflow approach for aftertreatment simulation is presented. Results are shown for the optimization of model parameters using AVL BOOST [1] including a comparison with experimental results. Finally, the present paper describes full 3D results using AVL FIRE [2] for the transient behavior of an exhaust gas line (Oxidation Catalyst and DPF) during a forced regeneration event.

MATHEMATICAL MODEL

Modeling of “Wall Flow Type” Particle Filters

The filter flow and regeneration model published by Bissett in 1984 [3] assumes that the thickness of the soot layer is so thin compared to the channel thickness that the change in the channel geometry can be neglected due to the presence of the particle layer. Furthermore, isothermal conditions throughout the filter are assumed. For very low soot loadings and rather large channel diameters this is surely a valid assumption. It simplifies the system of conservation equations significantly and therefore, it has been the basis for numerous models developed and presented during the last 20 years. Particularly the models published by Konstandopoulos and co-workers [5, 6] or Koltsakis and Stamatelos [7] rely on this assumption.

However, under urban and high-way driving conditions, particle filters are loaded with a soot mass of $m_{soot} = 8-12$ gr/ltr. This amounts to a thickness of the soot layer of approximately $h_{soot} = 0.2$mm, which reduces the cross section area of the channel (typically 1.44 mm x 1.44 mm) by 35%. Under extreme loading or engine operating conditions, these values may be exceeded, so that the change of channel geometry has to be accounted for under realistic operating conditions. Furthermore, experimental results suggest strongly (see Wanker et al. [8]), that a non-uniform distribution of the soot layer and non-uniform temperature distribution exists.
Therefore the FIRE/BOOST DPF model is designed to accurately account for the fluid dynamic behavior of a particle filter in the regime of cake filtration with channels of variable cross section areas and variable temperatures [9, 10, 11, 12, 13, 14 and 15].

Channel Fluid Dynamics and Pressure Drop

As ‘filter channel’ a pair of two channels is understood (see Figure 1). One, the inlet channel, is plugged at its end, and the other, the outlet channel, is plugged at its beginning. This pair of inlet/outlet channels is connected by a porous wall where the gas flows through and the soot particles are filtered. The following section describes the assumptions and governing equations for the flow inside a channel of a soot filter and an entire filter as applied under automotive conditions. First, the conservation equations for a single (inlet and outlet) channel under the influence of a soot layer are derived. This takes into account the feedback of the soot layer on the flow pattern of the gas inside the channel and thus, affects the deposition of soot on the channel walls.

For technical applications, the ratio of length to width of a channel is approximately L/aC~100. A dimensionless analysis reveals the length of the channel as the determining scale. Thus, the conceptual and computational complexities of a multi-dimensional and compressible flow are circumvented with a system of one-dimensional conservation equations, which simplifies the solution process significantly. Since loading and regeneration of a soot filter are transient processes, in the first approach the unsteady characteristics of the conservation equations have to be taken into account. However, a comparison of the time scales of the system, in particular the velocities of the flow and the growth of the soot layer, reveals that at least the gas phase processes can be assumed as quasi-steady. This assumption does not aggravate the accuracy of the system, however, it accelerates the solution process significantly. Under the above-mentioned assumptions, the flow in the inlet (“1”) and outlet (“2”) channel is assumed as a one-dimensional steady state flow as sketched in.

![Figure 1: Cross Section of a Filter Channel Consisting of an Inlet and Outlet Channel](image)

The differential conservation equations of mass for an inlet channel with variable cross section and an outlet channel are written as follows

\[
\begin{align*}
\frac{\partial \rho_1 v_1 (a_c - 2\delta_{\text{soot}})}{\partial x} &= -4 \rho_1 v_{\text{wall,1}} (a_c - 2\delta_{\text{soot}}), \\
\frac{\partial \rho_2 v_2}{\partial x} &= \frac{4}{a_c} \rho_2 v_{\text{wall,2}},
\end{align*}
\]

where \(a_c\), \(\delta_{\text{soot}}\), \(v_1\) and \(v_2\) are channel width, height of soot layer and velocities at a position in the inlet and outlet channel, respectively. The latter refer to quantities averaged over a cross section of the channel. Under the present conditions the gas is assumed to obey the equation of state in the form

\[
\rho_i = \frac{p_i}{RT_i} \quad \text{and} \quad \rho_j = \frac{p_j}{RT_j},
\]

where \(p_1\), \(p_2\), \(T_1\) and \(T_2\) stand for the gas pressures and temperatures of the inlet and outlet channels. The velocities \(v_{\text{wall,1}}\) and \(v_{\text{wall,2}}\) represent the lateral component of the velocity through the soot layer and the filter wall. Applying continuity to the wall flux entering the soot layer and leaving the wall into the outlet channel yields an expression for \(v_{\text{wall,2}}\)

\[
v_{\text{wall,2}} = v_{\text{wall,1}} \frac{\rho_1 (a_c - 2\delta_{\text{soot}})}{\rho_2 a_c}
\]

which is inserted into the conservation of mass of the outlet channel to give
The conservation equations of momentum are written as follows:

\[
\frac{\partial \rho_2 v_2}{\partial x} = \frac{4 \rho_1 v_{wall,1}}{a_C} (a_C - 2\delta_{soot})
\]

The conservation equations of momentum are written as follows:

\[
\frac{\partial \rho_1 v_1 (a_C - 2\delta_{soot})}{\partial x} = -(a_C - 2\delta_{soot})^2 \frac{\partial p_1}{\partial x} - F \mu v_1
\]

Due to low values of the velocity, transport of momentum perpendicular to the main direction of the flow is neglected. The shear stress exerted on the flow by friction along the channel walls is taken into account through a linear correlation between a loss coefficient F and the local channel velocity (see Shah, [16]). Thus, it represents the integral effect of shear transverse to the flow direction. The loss coefficient F depends on the shape of the channel. A constant value of F=28.454 (square channel) is assumed.

The filter wall and the soot layer are considered as a porous medium, through which the flow obeys the law of Darcy. For a non-negligible height of the soot layer, the velocity through the soot layer changes due to a varying cross section as shown in Figure 2.

**Figure 2: Cross Section of a Soot Layer**

Hence the wall velocities \(v_{wall,1}\) and \(v_{wall,2}\) and the pressure difference \(p_1 - p_2\) between the channels across the layer and the substrate are correlated as follows:

\[
p_1 - p_2 = \frac{\mu}{k_{soot}} \int_0^{\delta_{soot}} (y)dy + \mu \frac{\delta_{wall}}{k_{wall}} v_{wall,2}
\]

Here \(\delta_{wall}\), \(k_{wall}\), \(k_{soot}\) are the thickness and the permeability of the filter wall and the soot layer, respectively. The wall velocity \(v_w(y)\) as a function of the position \(y\) is derived from continuity through the soot layer in the following form:

\[
v_w(y) = v_{wall,1} \frac{(a_C - 2\delta_{soot})}{a_C - 2\delta_{soot} + 2y}
\]

Integration of Equation 7 and substitution of \(v_{wall,2}\) by Equation 3 yields the following expression for the pressure drop:

\[
p_1 - p_2 = \frac{\mu}{k_{soot}} (a_C - 2\delta_{soot})v_{wall,1} \ln \frac{a_C}{a_C - 2\delta_{soot}} + \mu \frac{\delta_{wall}}{k_{wall}} v_{wall,1} \frac{p_1 T_2}{p_2 T_1} \frac{(a_C - 2\delta_{soot})}{a_C}
\]

The following boundary conditions are applied:

\[
x = 0 : \quad v_1 = v_{in} \\
\quad v_2 = 0.0 \\
\quad p_1 = p_{in}
\]

\[
x = L : \quad p_2 = p_{out}
\]
The set of equations (1-10) represent the steady-state model for the flow through a particle filter. This boundary value problem is stepwise solved with an appropriate solver and its solutions are fed back to the flow-solvers of FIRE and BOOST.

**Soot Regeneration**

This section briefly discusses the FIRE/BOOST models for soot regeneration. As sketched in Figure 3 the soot layer within each inlet channel can be understood as fixed-bed (consisting of soot particles) that is flown through by gas and where chemical reactions take place. The important reactions for the soot regeneration are heterogeneous reactions between soot and gas species (e.g. O2, NO2) transported through the soot layer. Provided that transport effects are negligible in directions other than given by the wall velocity, a steady-state and 1D model over the soot height can be applied in each computational cell. Thus, in order to calculate the rate of regeneration FIRE/BOOST discretizes the soot layer over its height in each computational cell of the FIRE/BOOST mesh. This approach is called the Local-Layer-Discretization (LLD).

As explained in Figure 3 the soot layer is discretized in the direction of the wall velocity (normal to the particle filter wall) in the direction z. As shown in Figure 3 (A and B), the LLD model solves a continuity equation (Equation 11) and transport equations for the mass fractions of K species (Equation 12) in a coupled manner.

\[ \varepsilon_{L} U_{g} \frac{d \rho}{dz} = S_{\text{tot}} \quad S_{\text{tot}} = \sum_{k=1}^{K} S_{k} \]  

\[ \varepsilon_{L} U_{g} \rho \frac{d w_{k,g}}{dz} = S_{k} - w_{k,g} S_{\text{tot}} \quad k = 1 \ldots K \]

\( U_{g} \) is the gas velocity in the soot layer, \( \varepsilon_{L} \) is the layer porosity (constant), \( \rho_{g} \) is the gas density and \( w_{k,g} \) is the mass fraction of species k. The source term \( S_{\text{tot}} \) on the right hand side represents the mass added to the gas phase due to the heterogeneous combustion reactions. It equals the consumed soot at a certain point in the soot layer. In BOOST and FIRE the number of chemical species and/or reactions taken into account is arbitrary. However, in order to simplify the application, so called “pre-defined” kinetic models are available [15].

![Figure 3: Cross Section of a Soot Layer LLD-Concept; (A) Schematic of a Particle Filter Channel (wall flow type); (B) Discretized Soot Layer; (C) Sketched Mass Fraction and Gas Phase Mass Flow Profiles Across the Soot Layer](image)
WORKFLOW

Figure 4 displays the “Workflow-Concept” for aftertreatment simulations. The fast and robust 1D aftertreatment models (catalyst and DPF) of AVL BOOST are coupled with a code for the optimization of model parameters, currently iSIGHT is used. The choice of the objective functions and the optimization parameters is arbitrary. Typically we are optimizing kinetic parameters (regeneration behavior) and physical properties of the model (thermal behavior) using measurements (temperature, species conversions, pressure drop, …) as objective functions. As soon as the desired degree of accuracy is achieved the optimized parameters are available for the 3D CFD Code FIRE or the vehicle simulation code CRUISE (under development). The most important pre-requisites for these activities are that identical models and identical parameters are used in all simulation codes.

RESULTS 1D SIMULATION

Figure 5 shows the starting point and the final result of the parameter optimization process for the regeneration of a DPF using the BOOST 1D Aftertreatment model and iSIGHT. The transient behavior of the temperature at three different positions along the centre-line of the DPF is plotted. At the inlet of the DPF the temperature is increased (i.e. due to post-injection) in order to enforce and to control the regeneration process. According to this increase the DPF is heated up and the regeneration reactions are starting. With increasing temperature the amount of heat released from the oxidation of the soot particles is increasing. As a result a front of temperature is moving downstream through the DPF. The model is capturing these effects nicely and the agreement with the experiment is very good.
Figure 5: Regeneration of a DPF; Temperature at three different axial positions along the centre-line; Optimisation of Parameters using BOOST

RESULTS 3D SIMULATION

Figure 6: Simulation of the transient behaviour of an exhaust gas line (Diesel engine, DOC + DPF) during a forced regeneration event using FIRE.
Using the parameters determined with BOOST 1D Aftertreatment simulations a full 3D simulation for a complete exhaust gas line was set-up. Figure 6 shows contour plots of gas temperature, DPF and catalyst (DOC) temperature, soot mass and oxygen mass fraction at one distinct time during the transient regeneration process. The gas enters the DOC at a temperature of ~600K containing significant amounts of CO and C3H6 as they were produced by in-cylinder post-injections. At the time shown the light-off of the catalyst has already occurred and the heat-up of the gas in the catalyst can clearly be seen. The gas is leaving the catalyst at a temperature of ~900K, which is sufficient for initiating the regeneration downstream in the DPF. It is important to make sure that the oxygen content in the gas downstream of the DPF is still high enough to allow oxidation of the soot particles. Comparing the soot mass and the DPF temperature contour plots the heat-up of the DPF due to the heat released by the soot oxidation reactions can be seen. Non-uniformities in the local distribution of soot and temperature in the DPF are a result of flow distribution in front of and inside of the DPF as well as of losses to the ambient.

CONCLUSIONS

This paper presents new simulation models for flow and regeneration in a Diesel Particulate Filter. The models have been implemented into the 1D code BOOST and into the 3D code FIRE. A workflow is designed which makes it possible to automatically determine the necessary model parameters and to use them in both 1D and 3D simulations. The comparison with experimental results shows that the model accurately captures the relevant effects. Results of a 3D simulation of an exhaust gas line are presented. The same procedure can be carried out for each unit that is part of the exhaust gas line, i.e. SCR Catalyst, DENOX Catalyst or TWC.

REFERENCES