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ORIGINAL PAPER

Evaluation of Performance of Diesel Particulate Filters Through Integrated Multi-Scale Computer Calculations

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Abstract Wall-flow channel models and soot deposition models based on micro scale considerations are integrated into global 3D diesel particulate filter simulations. In addition, transient and steady-state simulations are combined to understand at the same time short- and long-time behaviour of the diesel particulate filter (DPF). The functionality of the simulation tool is achieved and correlations with measured data encourage the use of the model as a tool to predict DPF behaviour.

Keywords Particulate matter deposition · DPF · Flow modelling

1 Introduction

Diesel particulate filter systems are developed to increase the catalyst durability, filtering and catalytic emission reduction efficiency, as well as to decrease the system cost and packing size [1–4]. In the development process, computational fluid dynamics simulations have proved to be a valuable tool for testing different designs in addition to series of experimental “trial and error” operations [5, 6]. Still, this is by no means an easy task in diesel particulate reduction system design, since current computer simulations are unable to predict the long-time behaviour of DPF filters due to huge computational cost. In this work we demonstrate a combination of transient and novel steady simulations used to understand at the same time and in a systematic way the short-time behaviour of the filter and to obtain an understanding of its final state after long-time use. In addition, existing models for particulate matter deposition and heat transfer are extended to include effects resulting from processes at the micrometer scale [7]. This approach enables a reduction of peak temperatures during uncontrolled regeneration by advanced regeneration control based on a correct evaluation of the DPF filter state and the local catalytic chemical reaction distribution.

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2 Engine Test Bench Set-Up

The experimental boundary conditions are obtained for an exhaust manifold converter that consists of the NSR (NO_x Storage Reduction) and DPNR (Diesel Particulate-NO_x Reduction) catalyst. The details of the used engine and engine operation conditions are given in Table 1. Since one of the main objectives is to obtain detailed information about the chemistry-related heat transfer interaction inside the filters, the temperature distribution inside the filters is measured with thermocouples at 28 points, see Fig. 1. A common measurement procedure is established to minimize the systematic errors, while measuring two main regimes of catalyst—NO_x reduction and soot burning. For

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Table 1 Engine, after treatment, measurement equipment, and operation conditions data

Engine	2,231 cm^3 (4 cylinders), DI, T/C, EGR
Exaust after-treatment	Exhaust fuel injector, NSR (upstream), DPNR (downstream)
Measurement equipment	Two HORIBA gas analysers with sampling points at inlet, outlet, and between NSR&DPNR; 28 thermo couples; asynchronous dynamometer
Engine operation conditions	(a) 1,600 rpm, 45 Nm, inlet gas temp ~580 K, gas flow 18 g/s, 2.74 g soot/h
	(b) 1,600 rpm, 60 Nm, inlet gas temp ~600 K, gas flow 20 g/s, 2.46 g soot/h
	(c) 2,000 rpm, 120 Nm, inlet gas temp ~710 K, gas flow 44 g/s, 3.6 g soot/h
	(d) 2,000 rpm, 170 Nm, inlet gas temp ~750 K, gas flow 55 g/s, 2.83 g soot/h
	(e) Complete regeneration, inlet gas temp. ~1,000 K

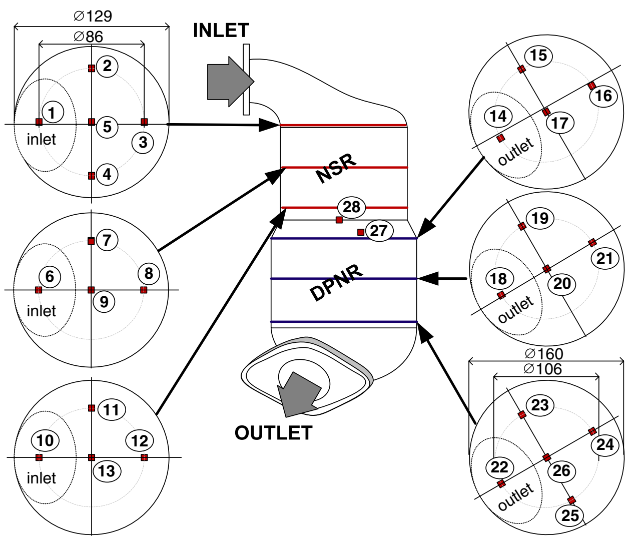

Fig. 1 Scheme of 28 thermocouples positioning in the cross-sections of the filter. The thermocouples in NSR and DPNR are oriented to match inlet and outlet pipe axis, respectively

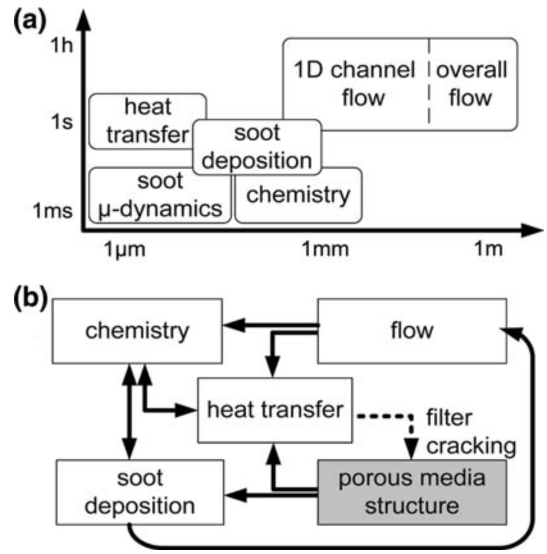

Fig. 2 Overall diagram of **a** length/time-scale positioning and **b** interaction of different processes included in the simulation scheme. Porous media micro-structure influences much of the heat transfer and soot deposition in the system

each engine operation condition: (1) DPF loading is measured until the pressure drop saturation at stationary conditions with the injection of fuel into the exhaust gas to consume oxygen and prevent particulate matter (soot) burning, (2) after loading, a normal operation point of the NSR/DPNR system is measured where fuel is periodically injected into the exhaust to alternatively reduce NO_x in the rich regime and burn soot in the lean regime, (3) lean regime is measured—in this condition the soot burning rate is high, while the NO_x removal rate is low. The filter was regenerated at the end of the experimental cycle, cf. operation point (e) in Table 1.

3 Models for Multi-Scale Simulations

Figure 2 gives an overview of different processes and their interactions, as seen in this study. The strategy used in this paper is to introduce fundamental micro-scale processes as sub-models in overall macroscopic fluid-dynamics simulations. In particular, additional equations are introduced to the standard DPF model, cf. Ref [2, 3], describing micro-scale aspects of soot deposition and heat transfer. DPF consist of a large number of sub-millimeter channels separated by micro-structured porous medium. Both heat transfer and particulate matter (soot) transport are strongly influenced by pore surface size, pores diameter distribution, and porous media wall thickness. Particulate matter (PM) is transported by diffusion and flow dynamics; if the flow velocity is small, particles will tend to accumulate at the entrance into the porous wall (see Fig. 3a, b, model parameters α_{diff}, β_1). As the particulate matter is accumulated inside the pores, these latter become narrower, and the pressure drop increases. The pores have a finite capacity—when pores are filled, PM will start to deposit in the channels creating soot cake and the pressure drop will reach a saturation point (since cake has small resistance to flow). At the same time, the accumulation rate, i.e., filtration efficiency will further increase since particles are caught by soot cake (parameter β_2). Particulate matter that

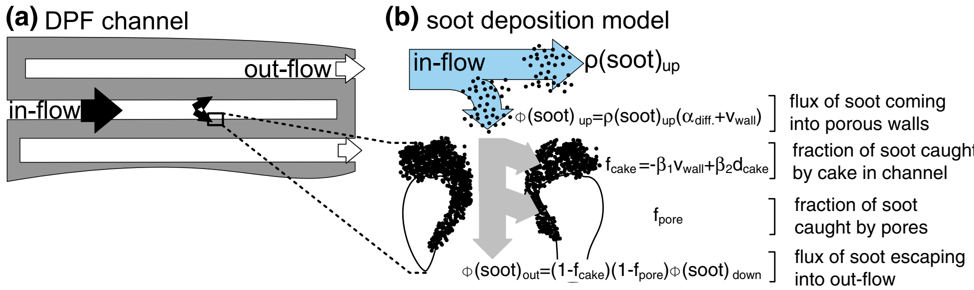

Fig. 3 Diagram of DPF wall flow filter channel is shown (**a**). The soot particles are collected at the surface of the pores and the inlet channel (**b**). The main equation for soot fluxes, using the fraction of soot caught at different points of the filter, is given. Coefficients β_1 and β_2 are model parameters

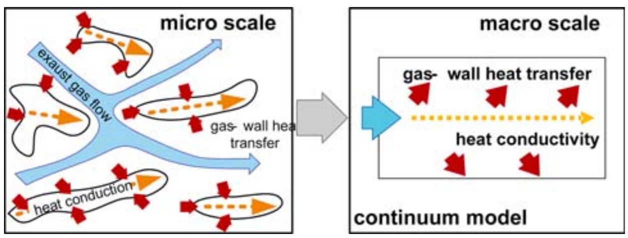

Fig. 4 Schematic diagram of micro-scale heat transfer simulations vs. macro-scale simulations. Heat transfer characteristics obtained at the micro scale is used to create macroscopic model

is not caught in soot cake or pores (f_{pore}) will leave the filter through downstream channels. Together with PM, heat is carried by the exhaust gas from the engine. Efficiency of heat absorption and conduction by the filter determines the temperature distribution inside filter. In the system used for this study, PM is burned by active oxygen generated in NO_x storage (NSR) and excessive oxygen coming from the engine under lean conditions. Since the burning reaction rate is strongly temperature dependent, a continuum model for heat transfer is developed which has heat transfer and conductivity rates equivalent to micro-scale flow model (see Fig. 4).

In order to bridge the time-scale gap between slow PM accumulation processes and fast chemistry, the stationary state solver is introduced. It uses the fact that after longer time in the filter all properties are constant in all points of the system. Therefore, time derivatives in model equations are equal to zero (though flow velocity is not zero). For the amount of deposited soot this approach has high convergence rate—stationary solution is achieved as soon as after a series of iterative calculations deposition by filtering and removal (burning) rates of the soot become equal. Since the stationary state is the state of the filter after a longer constant driving regime, the stationary solver is complementary to the standard transient solution, which gives the detailed evolution of the system with time (at much higher computational cost).

Figure 3 shows a schematic overview of the channel modelling. While the left side of the figure shows the channel overview, the right side shows a detailed view of the channel walls. Also the equations for modelling the soot flux at inlet and outlet of the pore structure within the channel walls are presented (Φ_{up} and Φ_{out}). The used parameters are α_{diff}, which is the soot diffusion, v_{wall}, the flow velocity through the channel wall pores and d_{cake}, the pore diameter. ρ(soot) represents the soot density. Furthermore, the soot fractions within cake deposition and pore deposition are used (f_{cake} and f_{pore}). Model parameters β_1, β_2 have to be fitted by the validation with experimental data.

4 Comparing Simulation and Test-Bench Results

The calibration of physical models is done by an adjustment of realistic inlet temperature and velocity profiles, gas composition, kinetic parameters such as Arrhenius pre-factors for catalytic chemical reactions, and heat transfer characteristics of the filter. Figure 5a–c show a comparison between the temperature distribution obtained in simulations and that in the experiment. The effect of intake flow on the heat distribution is well captured by the model.

Hydrocarbons carried by the exhaust gas from the engine are identified as the source of temperature differences in NSR in flow direction and along the filter profile, e.g., axis-1 and axis-2 in Fig. 5. As the exhaust gas from NSR is carried further downstream in DPNR, and the differences will exist also in DPNR. Also the time profiles of chemical species are well predicted by the model, an example for hydrocarbons is shown in Fig. 6.

The soot deposition model parameters (α_{diff}, β_1, β_2, and f_{pore}) are hard to be precisely measured. Therefore, they were roughly estimated to fit the few experimental data that

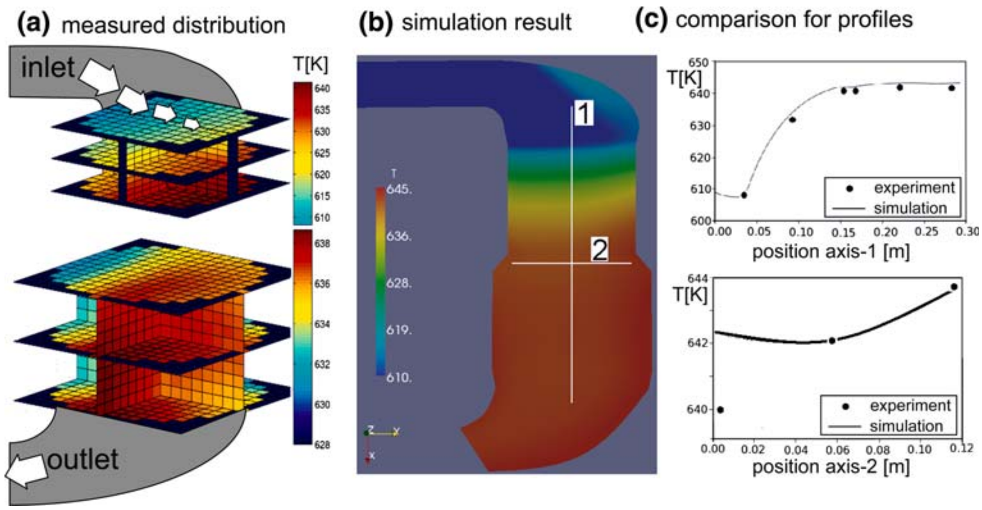

Fig. 5 Comparison of (**a**) measured and (**b**) simulated temperature distribution. An influence of flow profile on temperature distribution is visible. Diagrams (**c**) show more detail for temperature along axis-1 and axis-2, i.e., along and orthogonal, to flow direction, respectively

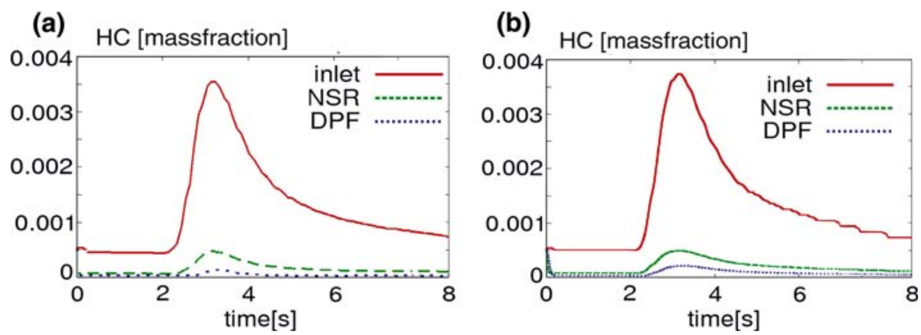

Fig. 6 Evolution of hydrocarbon mass fraction in time at inlet, after NSR and DPNR. **a** Experiment, **b** simulation

authors have made available. As such, the parameters and the soot deposition model represent the starting position for more research.

5 PM (Soot) Deposition–Burning Interaction

Starting from the stationary state, the regeneration of the DPNR filter is simulated. Figure 7a shows the thickness of the soot cake in filter channel. At the entrance into the filter where temperatures are lower, more soot is accumulated in the soot cake. Soot deposited in the cake has a positive feedback effect: more soot is already in the cake, more new soot will be deposited in the cake, cf. Fig. 7b. This is the reason why all soot is deposited in the soot cake at the beginning and no soot is deposited in the porous wall (see Fig. 7c). As the soot cake thickness is reduced, the deposition of soot in pores increases ($t = 10$ s). One should note that soot burning and soot deposition are independent processes. Therefore, if the soot cake is thick and cannot be removed during the lean regime, it will prevent new soot to deposit in wall pores. On the other hand, soot stored in the filter wall pores could be completely removed by burning. In such a scenario, the pressure drop would signal that there is little soot in the filter, while the soot is present in channels.

6 Simulations for Identification of Potential Filter Cracks

In this work, two compatible heat transfer models for porous media are developed in parallel: (1) a macro scale model suitable for macro scale simulations and (2) a micro scale model, which can give us information about the heat distribution on the level of the pores. Combining the two models we explored under realistic operational conditions the potential points of filter crack. As indicator maximal temperature gradient in the filter was used, since it is directly correlated to material stress, see Fig. 8. The observed relation of temperature gradient and ceramic material thickness is highly nonlinear, and ceramic bridges with diameter less then 50 μm are therefore highly sensitive to high temperature gradients.

7 Conclusions

In order to use DPF modelling as a predictive tool for real-world designs, it is important to develop reliable and time efficient 3D-models. In this work, a modelling approach is presented and validated against test bench measurements with special attention to exactly reproducing the temperature distribution and catalyst chemistry. The main results are:

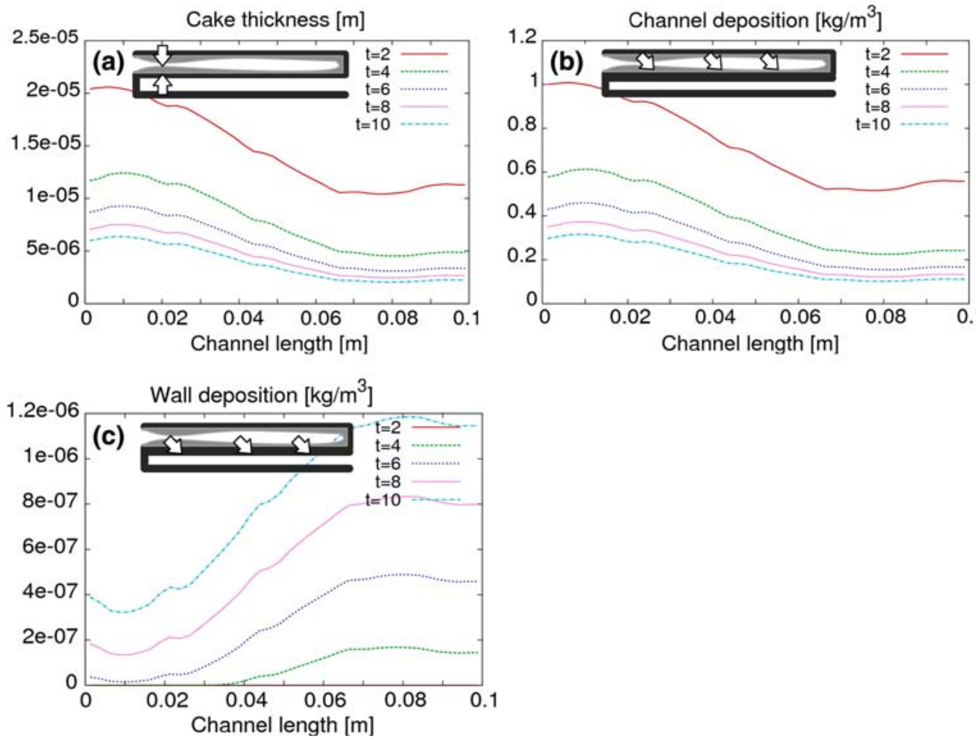

Fig. 7 Soot load distribution evolution in time during regeneration: soot cake thickness (**a**), deposition in channel (**b**) and deposition in wall (**c**). Different curves are separated by time interval 2 s

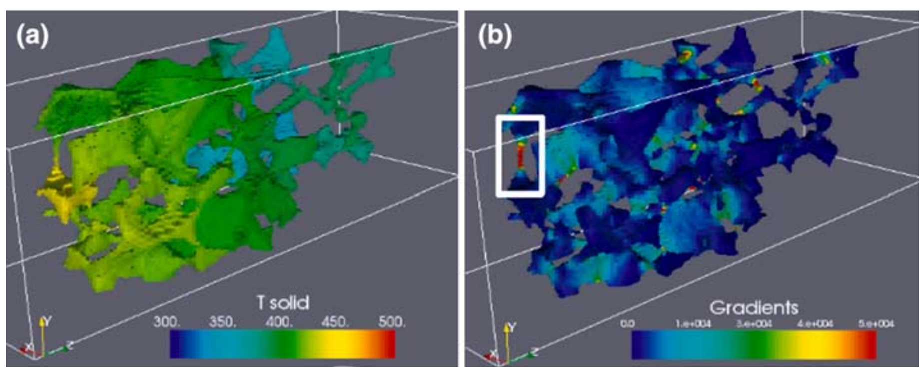

Fig. 8 Result of micro-scale simulation showing temperature (**a**) and temperature gradient (**b**) distribution. Initial filter temperature was 300 K and gas temperature 500 K, result after 2 s is shown. A typical area of high temperature gradient is denoted with a bold box

(1) A dynamic 3D calculation simulation tool is developed, which can predict the state of DPNR filter loading at both micro/macro length and at short/long time scales.
(2) The influence of temperature differences caused by flow profile on chemistry inside filters and soot deposition is understood.
(3) At the micro scale temperature gradients are understood which could result in filter cracking.
(4) Low time-cost of presented calculations makes them an efficient design tool.

The modelling approach hence builds on the multiscale link between the micro-structural evolution and the specific macroscopic exhaust system features with the objective to achieve major improvements in material design and catalyst lifecycle assessment.

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