Multi-scale modeling of catalytic filters for automotive exhaust gas aftertreatment

Petr Kočí[1]*, Martin Leskovjan[1], Marie Plachá[1], Marek Václavík[1], Martin Isoz[1], Emily Price[2], Vladimír Novák[2], David Thompsett[2]

1 University of Chemistry and Technology, Prague, Technická 5, Praha 166 28, Czech Republic;
2 Johnson Matthey Technology Centre, Sonning Common, RG4 9NH, United Kingdom

**Corresponding author: petr.koci@vscht.cz*

Highlights

- 3D XRT reconstruction of porous filter wall including distribution of catalytic material.
- Pore-scale simulation of flow, diffusion and reactions inside the reconstructed wall.
- Prediction of the permeability and conversion, linking with the full-scale model.
- Comparison with the measured pressure drop, analysis of inlet/channel/wall contributions.

1. Introduction

The newly introduced EURO 6c emission limits on particulate numbers are enforcing exhaust filters not only for Diesel engines (DPF = diesel particulate filter) but also for gasoline engines (GPF = gasoline particulate filter). Even if gasoline engines produce lower total soot mass, smaller particles are emitted so that their number can be relatively high. The exhaust aftertreatment system can be made more compact and less expensive by depositing the catalyst for conversion of gas pollutants directly on or into the porous wall of particulate filter (Figure 1). However, internal transport limitations may lead to an increased pressure drop and/or the hindered access of reactants to catalytic sites [1,2,3,4]. The loading and distribution catalytic material in the filter has to be controlled in order to achieve optimum performance of the device.

2. Methods

Series of particulate filters based on SiC and cordierite substrates were studied both bare (uncoated) and then coated with catalytic material – zeolite SCR for diesel applications or alumina-based TWC for gasoline applications. In-wall, on-wall and combined distributions of catalytic material were examined. The wall structure was characterized by MIP (porosity, pore-size distribution), 2D cross-section SEM and 3D XRT. The sample performance was tested in pressure drop, soot filtration and gas reaction experiments.

A newly developed multi-scale modeling methodology was applied to study the relations between the filter microstructure and performance of the entire device (Figure 1). 3D morphology of the filter wall including the actual distribution of catalytic material was reconstructed from X-ray tomography (XRT) images. The reconstructed medium was transformed into simulation mesh for OpenFOAM. Flow through free pores in the substrate as well as through the coated zones was simulated by porousSimpleFoam solver, while an in-house developed solver was used for component diffusion and reactions [4]. The obtained 3D pressure and concentration fields inside the wall were post-processed to evaluate the permeability and effectiveness factor. These results were employed as input parameters into the full-scale 1D+1D model of catalytic monolith channels [2], enabling to calculate the overall pressure drop of the device that consists of the inlet, channel, wall and outlet effects (Figure 1). The relative importance of the individual contributions to the overall pressure drop was validated by series of experiments with varying length of filter channels.

3. Results and discussion

The simulation results suggest that the gas predominantly flows through remaining free pores in the filter wall and/or cracks in the coated layer (Figure 1). The mass transport into the coated domains inside the filter wall is enabled mainly by diffusion. Large domains of compact catalytic coating covering complete channel wall result in a significant increase of pressure drop as the local permeability of the coating is an order-of-magnitude smaller than that of bare filter wall.

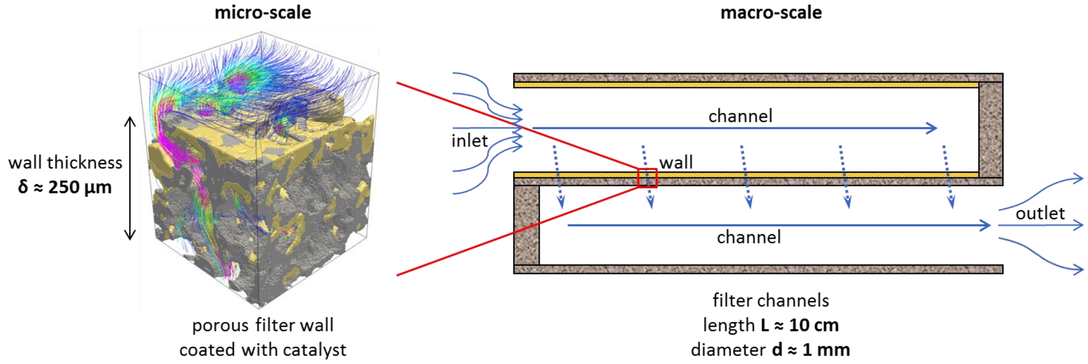

Figure 1. Multi-scale model of catalytic monolith filter. Left: 3D reconstructed wall (grey = substrate, yellow = coated catalytic material) with calculated flow field (streamlines) [4]. Right: Scheme of the filter channels simulated with full-scale 1D+1D model [2].

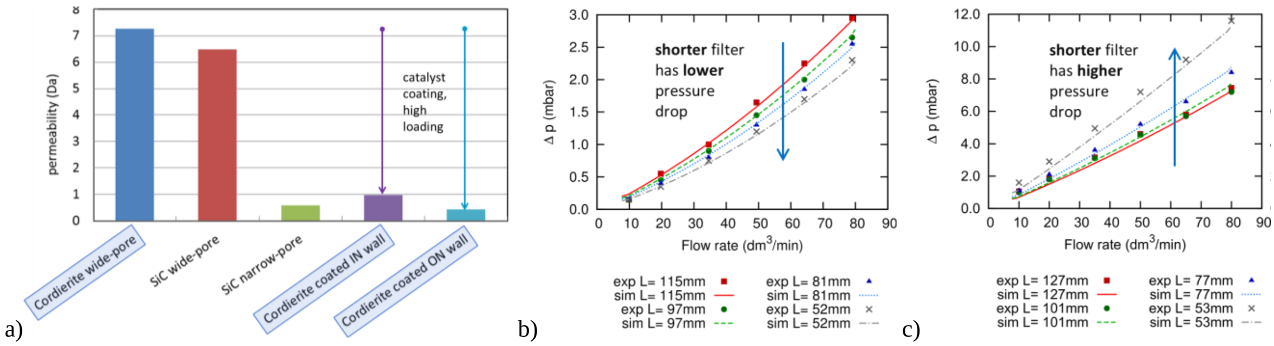

Figure 2. Prediction of filter pressure drop: a) permeability of the wall depending on its microstructure and catalyst distribution, b,c) full-scale model results vs. experiments with varying filter length L for wide-pore SiC (b) and narrow-pore SiC (c).

Examples of the predicted permeabilities depending on the filter wall microstructure and distribution of the catalytic material are given in Figure 2a. Figures 2b and 2c show the overall pressure drop measured in experiments and calculated by the full-scale model including the pressure losses at the inlet, outlet and along the monolith channels. The pressure drop in the wall dominates only in the case of narrow pores (Figure 2c).

4. Conclusions

The work introduces novel and systematic methodology for characterization, modeling and performance evaluation of catalytic particulate filters for automotive exhaust gas aftertreatment, enabling rational optimization of the material microstructure. The methods are applicable to a broad range of porous materials, including both diesel and gasoline particulate filters.

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Keywords

Multi-scale mathematical modeling; catalytic monolith filter; pressure drop; automotive exhaust gas aftertreatment.