From a 3D Reconstructed Porous Wall to the Effective 1D Model of Filtration in Catalytic Particulate Filters

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Highlights

- Particle deposition model was developed in a 3D digitally reconstructed filter wall.
- The model predictions were validated against time-resolved X-ray tomography scans.
- Effective 1D collector model was developed and compared to the detailed model.
- Spatially distributed collector sizes are necessary to obtain correct 1D deposition profiles.

1. Introduction

Catalytic particulate filters (CPFs) reduce exhaust gas emissions by simultaneously converting gaseous pollutants and capturing particulate matter. CPF is a monolith with a honeycomb structure with each channel plugged at one end. This forces the exhaust fumes to flow through the porous wall, filtering out the particulate matter. The wall is coated with a catalytic material to facilitate gas reactions. Careful design of CPFs is necessary to achieve high filtration efficiency and gas conversion while maintaining low pressure drop. To describe the impact of operating conditions and the CPF's geometry on its performance, an effective 1D+1D model is commonly used [1]. A more detailed 3D model has been developed to simulate the processes inside the realistic structure of the catalytic wall obtained from X-ray microtomography (XRT) [2,3]. This contribution aims at developing of computationally efficient collector models for 1D simulations of the particle filtration and accumulation in the catalytic filter wall. The goal is to obtain 1D particle deposition profiles over the wall comparable to those observed in detailed 3D simulations and XRT scans.

2. Methods

The generally accepted 1D approach to the filtration process was described by Konstandopoulos et al. [4] who adapted the correlations from Lee et al. [5]. The model is based on the unit collector model, where the porous wall is approximated by a packed-bed layer of solid spheres (collectors). When a particle collides with a collector, it is captured, and the diameter of the collector increases. It is assumed that only Brownian diffusion and interception are relevant mechanisms for CPF applications and other known mechanisms are neglected. The contributions depend mostly on the porosity of the wall and collectors' diameter, which both evolve during the filtration process. Alternative correlations were proposed, e.g. by Wurzenberger et al. [6]. The unit-collector model is implemented in our 1D+1D filter model [1] and validated against the 3D micro-scale model [2,3]. The 3D microstructure of a filter wall with the catalytic coating inside wall pores is analyzed from XRT images. The wall porosity and pore sizes are spatially averaged and represented either by a single value for the entire wall or a 1D profile over the wall.

3. Results and discussion

Filtration efficiency of the porous filter wall was calculated using different approaches for the single collector efficiency and compared with the pore-scale 3D model predictions, Figure 1a. The results suggest that the filtration efficiency predicted according to [5] is too high. Further analysis revealed that, in that case, the studied particles would be captured only thanks to the Brownian diffusion, Figure 1b.

However, 3D micro-scale simulations [2] suggest that the interception of 100 nm particles should be non-negligible. Ohara et al.'s measurements [7] showed that the minimum of filtration efficiency should be around 100 nm, which is not satisfied using the correlations according to Lee et al. [5]. This is better described by the collector efficiency correlations proposed recently by Wurzenberger et al. [6].

Another issue in the 1D modeling approach involves the porosity and pore size distribution over the wall. The pore mouths in the filter substrates designed for the in-wall coating of the catalyst are typically wider at the wall boundaries, see the profiles in Figure 2a evaluated from the XRT scan. The wider pores have lower local filtration efficiency resulting in most particles being captured somewhat deeper within the wall, where the narrower pore necks occur. Figure 2b confirms that using a realistic profile of pore sizes in the 1D model is essential for obtaining the correct particle deposition profiles. One sharp maximum is observed at the external wall surface, another local maximum is deeper inside the wall.

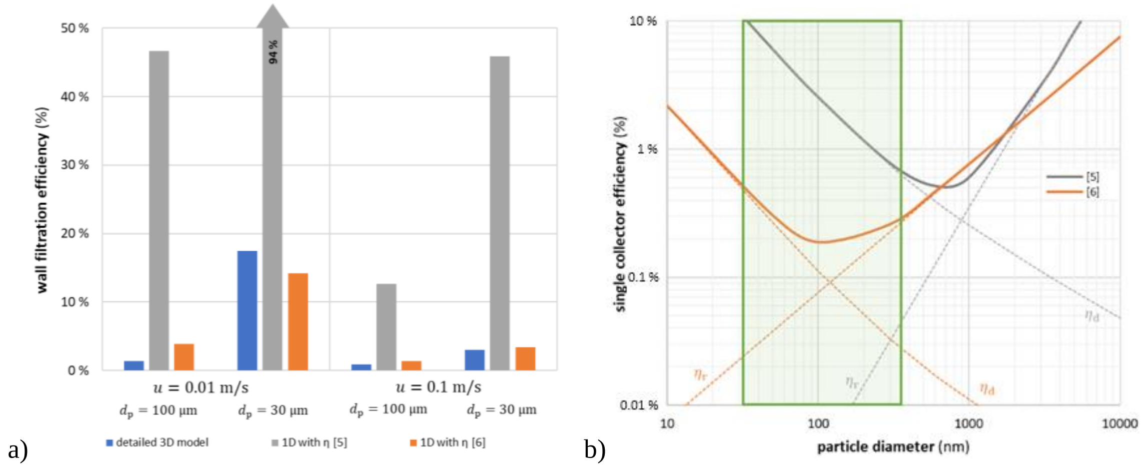

Figure 1. a) Filtration efficiency of clean filter wall, different approaches.
b) Contributions to overall single collector filtration efficiency. Green rectangle marks the area of interest.

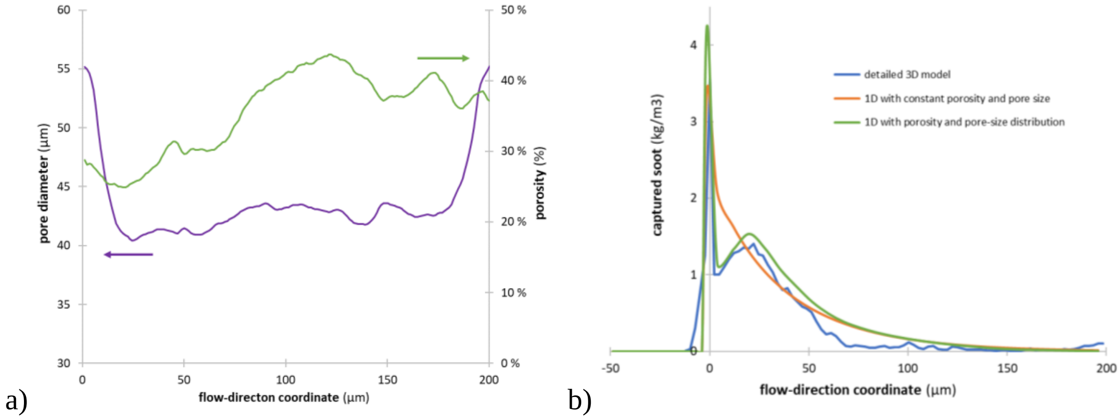

Figure 2. a) Profiles of pore size and porosity throughout filter wall.
b) Example of captured particles profiles inside filter wall.

4. Conclusions

The improved 1D model of particle filtration using unit collectors can provide reasonably accurate particle deposition profiles over the wall if the actual spatial distribution of pore sizes is considered instead of just a single mean value, Figure 2b. The developed model enables simulations for different filter wall configurations and operating conditions with little computational demands.

References

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Keywords
Exhaust gas aftertreatment; catalytic particulate filter; mathematical modeling.