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# Practically Relevant Ab Initio Filtration Simulation with Full-Detail Nanoparticle Aggregate Geometry

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As Diesel particulate filter (DPF) technology evolves towards multiply functionalised porous substrates, there is increased practical interest to predict in detail the soot deposition within or on the DPF wall. This work describes a framework for the ab initio yet practically applicable prediction of soot filtration behaviour which embodies the high fidelity reconstruction of the filter wall microstructure and a detailed representation of the soot aggregate particles across the relevant size spectrum of Diesel particulate. The basis of the framework is the calculation of Brownian particle trajectories and the determination of particle deposition based on particle geometry from a numerically generated soot aggregate library. The filter wall 3-D microstructure is obtained via so called process-mimetic digital reconstruction while the library of representative soot aggregates is generated via a cluster-cluster aggregation method using experimentally derived parameters for the mass-fractal scaling law describing soot aggregate morphology. The framework is validated against measurements of size-specific filtration efficiency of a commercial extruded honeycomb SiC DPF material.

High fidelity digital reconstruction of the filter wall microstructure begins with high resolution (<1 μm) SEM imaging of polished material sections. Comparison of the real filter wall material and the digital reconstruction is based on porosity and correlation information derived from sections such as in Fig.1(a,b) where the high fidelity of the digital reconstruction can also be gauged visually. The 3-D digital reconstruction (rendered in Figure 2(a)) is matched to the actual material porosity, wall thickness while the morphological resemblence is further validated on the basis of agreement between the two-point autocorrelation and the chord-length frequency distribution functions such as shown in Figure 2.(b,c). The sample of digital filter wall is placed in a computational domain that includes fluid space above/below the wall surfaces. The exhaust gas flow field is then computed within the clean porous wall by a finite volume method for incompressible steady flow implemented specifically for this application in which the porous microgeometry is represented by spatial occupancy enumeration in a uniform Cartesian grid.

Having obtained the solution for the exhaust gas flow field through th eporous wall, at the filtration conditions of interest, soot aggregates are then introduced sequentially at the inlet of the periodic domain and their trajectories are computed in a time-stepping manner according to the single particle Langevin equation [2,3]. The soot particle size distribution is sampled such that the porous wall sample is challenged by a statistically sufficient number of trial particles for each representative soot aggregate size class available in the soot library. Total filtration efficiency calculation takes into account the size distribution (Fig.3.b). The soot aggregate library used is generated with the the CCA algorithm described in [1] with morphology parameters (fractal dimension and prefactor) derived from a comparison of aerodynamic and mobility diameter measurements of soot from the 1.9 litre Fiat JTD test engine at APTL/Thessaloniki. For the results presented, eight discrete size classes are used to represent the soot size distribution. The location of particle insertion at the inlet of the computational domain is determined stochastically with uniform probability over the inlet boundary surface.

The initial (clean) size-specific filtration efficiency of a commercial DPF material (SiC wall flow honeycomb with nominal cell density 300 cells/in$^2$, 254 μm wall thickness, 11 μm pore size, 42% porosity) is measured in the diluted side stream exhaust of the APTL test engine at 60 °C and a filtration velocity of 1.5 cm/s. The experimental setup is based on a specially constructed holder-reactor for 35 × 35 × 50 mm DPF segment samples which is housed in a controlled temperature oven during the measurements. The SMPS 3936 system is used to measure the upstream/downstream soot concentrations while dilution ratio is determined by $NO_x$ analyser signals. The upstream/downstream particle size distributions and the filtration efficiency comparison are shown in Fig.4.

**Conclusions**

A framework for simulating the soot filtration process in a porous filter wall is presented, consisting of a combination of high fidelity and rigorously validated representation of the porous filter wall, calculation of the flow field within the porous wall microstructure and Brownian particle trajectory calculation and deposition of realistic representations of soot aggregates. On the basis of extensive use and favourable comparisons with experiment, such as the example shown, this framework has been found free of the need for empirical adjustment/correction parameters in predicting the initial/clean filtration efficiency of porous materials employed in Diesel particulate filters. Equally significant is that a novel numerical implementation of the deposition process has been developed that overcomes the scale disparity inherent in the problem and permits the coupling of the pore scale exhaust gas flow field and the deposition of fractal-like nanoparticles. The computational overhead is such that practical application of the framework is possible with calculation times, for a single simulation, on the order of 5 hours on a contemprary single core computer workstation.

## References


[1] Filipov A.V. et al.,Journal of Colloid and Interface Science 229, 261–273 (2000).

[2] Tien C., “Grannular Filtration of Aerosols and Hydrosols,” ISBN 0-409-90043-5, Butterworth Publishers, Stoneham, MA (USA) 1989.

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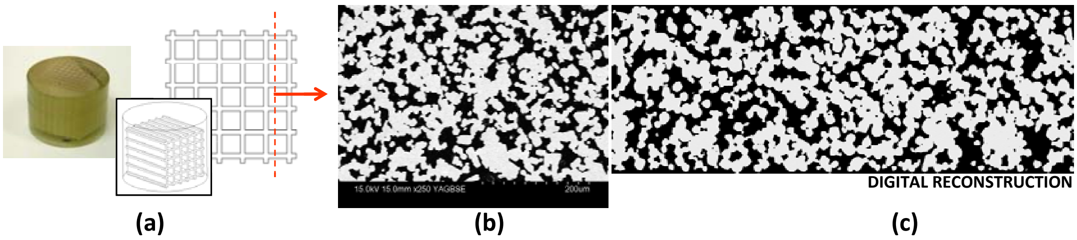



Figure 1. (a) Example of resin-impregnated sample and its sectionin for SEM imaging, performed by con-trolled grinding of the sample bottom face. (b) SEM section of the actual DPF material used in experimental measurements (multiple sticthed images). (c) Section of the reconstructed porous wall microgeometry.

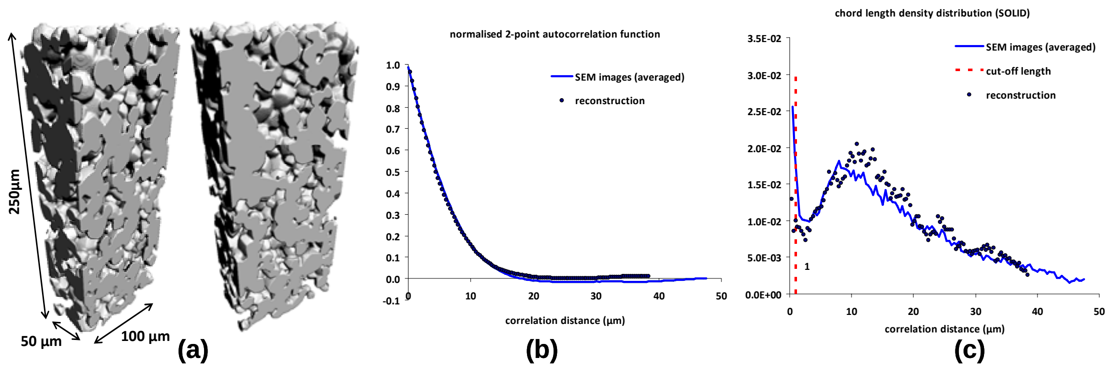
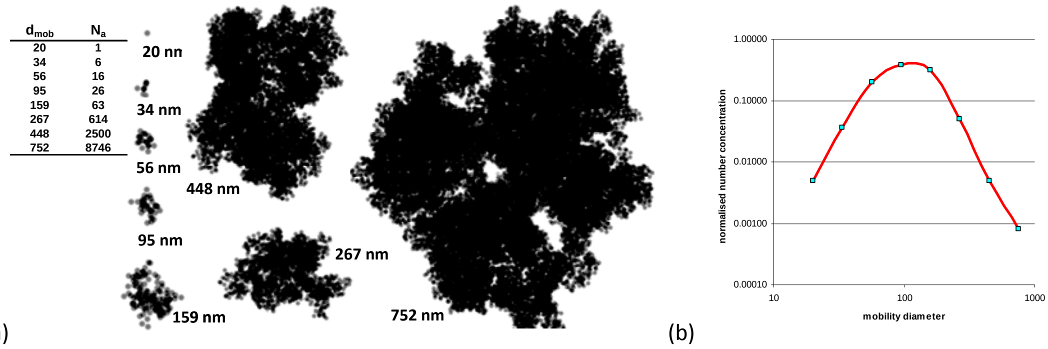
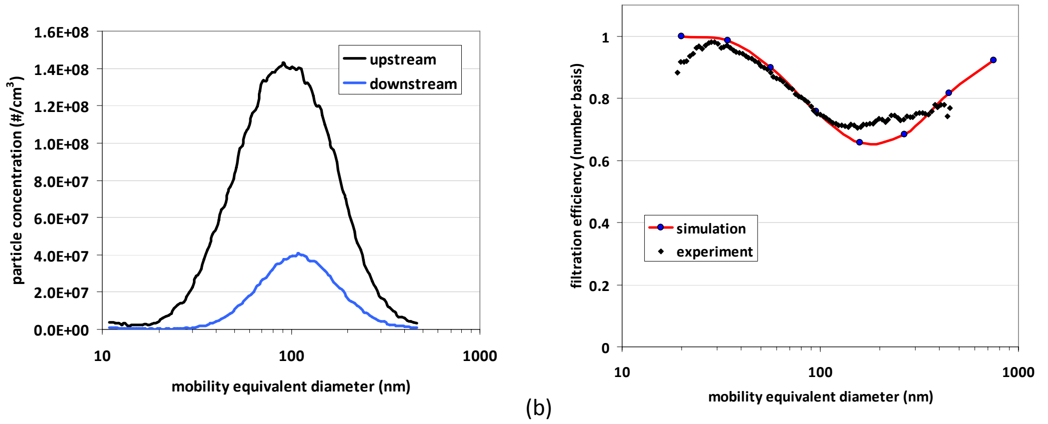



Figure 2. (a) Visualisation of the 3-D digital reconstruction of the DPF porous wall microgeometry modeled and depiction of the placement of the porous wall model within the computational domain. Domain size is for the commercial SiC material considered (left) is 22.5 million cells (including solid volume). Validation of the 3-D digital reconstruction of the DPF porous wall microgeometry on the basis of the normalised two-point autocorrelation functions (b), and the chord length frequency distribution (c).




(a) (b)

Figure 3. (a) Representative particles from the soot library of the APTL test engine (1900cc direct injection Fiat JTD engine / Euro3 homologation). (b) Distribution of relative particle concentration used in the filtration simulation for determining total mass and number basis capture efficiency.




(a) (b)

Figure 4. (a) Experimentally measured upstream and downstream particle size distributions. Filtration efficiency compa-rison of ab initio calculations against experimental measurements.

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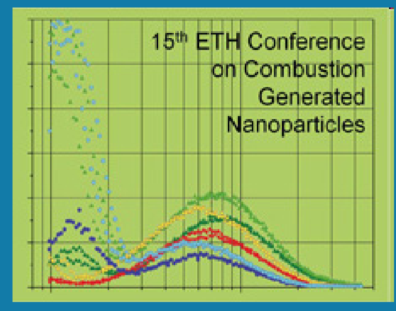



## ABSTRACT

A framework for the ab initio yet practically applicable prediction of soot filtration behaviour is shown which embodies the high fidelity reconstruction of the filter wall microstructure and a detailed representation of the soot aggregate particles across the relevant size spectrum of Diesel particulate. The basis of the framework is the calculation of Brownian particle trajectories and the determination of particle deposition based on particle geometry from a soot aggregate library. The filter wall 3-D microstructure is obtained via so called process-mimetic digital reconstruction while the library of representative soot aggregates is generated via a cluster-cluster aggregation method using experimentally derived parameters for the mass-fractal scaling law describing soot aggregate morphology.

## POROUS WALL DIGITAL RECONSTRUCTION

Reconstruction of the filter wall microstructure begins with high resolution (<1 μm) SEM imaging of polished material sections, as depicted in Fig.1(a). Comparison of the real filter wall material and the digital reconstruction is based on information derived from sections such as in Fig.1(b,c). The 3-D digital reconstruction (Figure 2(a)) is validated on the basis of porosity and two-point correlation functions such as shown in Figure 2.(b,c).

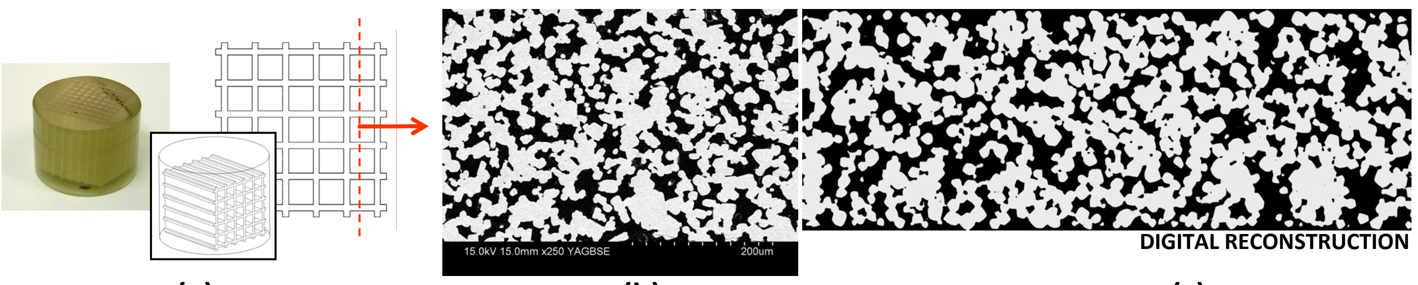



**Figure 1.** **(a)** Example of resin-impregnated sample and its sectionin for SEM imaging, performed by con-trolled grinding of the sample bottom face. **(b)** SEM section of the actual DPF material used in experimental measurements (multiple stitched images). **(c)** Section of the reconstructed porous wall microgeometry.

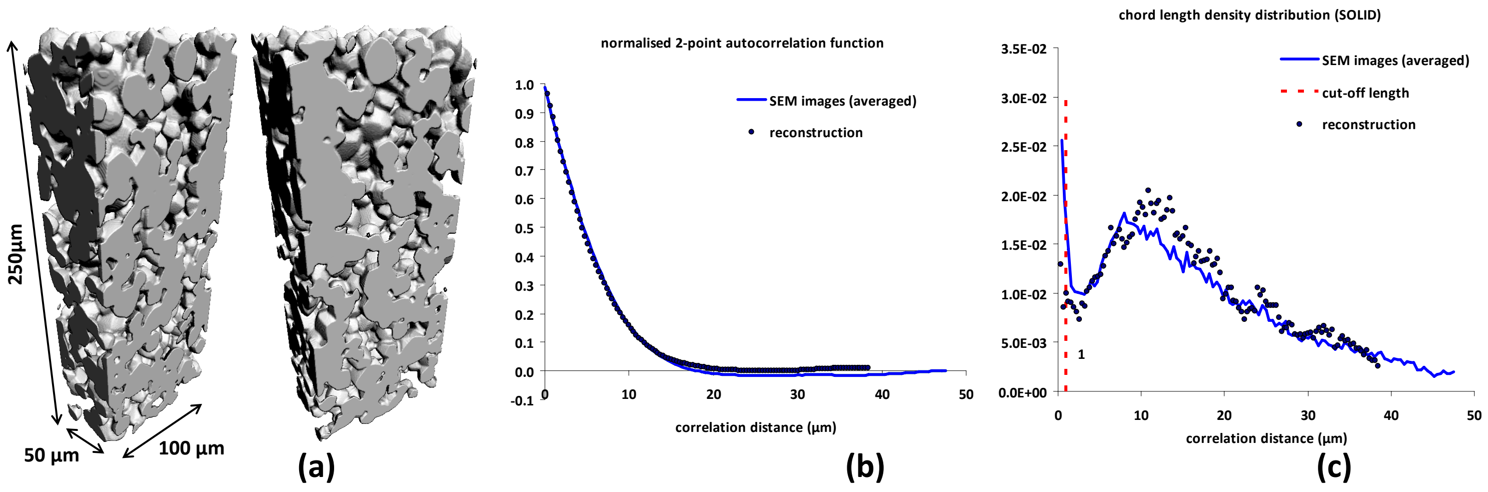



**Figure 2.** **(a)** Visualisation of the 3-D digital reconstruction of the DPF porous wall microgeometry modeled and depiction of the placement of the porous wall model within the computational domain. Domain size is for the commercial SiC material considered (left) is 22.5 million cells (including solid volume). Validation of the 3-D digital reconstruction of the DPF porous wall microgeometry on the basis of the normalised two-point autocorrelation functions **(b)**, and the chord length frequency distribution **(c)**.

## FILTRATION SIMULATION

The digital filter wall is placed in a computational domain that includes fluid space above/below the wall surfaces as depicted in Fig.3(a). The exhaust gas flow field is computed within clean porous wall by a finite volume method for incompressible or quasi-compressible steady flow. The soot aggregates are introduced at the inlet of the periodic domain and their trajectories are computed in a time-stepping manner according to the single particle Langevin equation [2,3]:

$$\underbrace{m_p \frac{d\mathbf{V}}{dt}}_{\text{total force on particle}} = \underbrace{-m_p \beta(\mathbf{V}-\mathbf{u})}_{\text{drag force}} + \underbrace{\mathbf{F}}_{\text{other forces}} + \underbrace{m_p \mathbf{A}(t)}_{\text{Brownian "force"}}$$

The soot particle size distribution is sampled such that the porous wall sample is challenged by a statistically sufficient number of trial particles for each representative soot aggregate size class. Total filtration efficiency calculation takes into account the size distribution (Fig.4).

The location of particle insertion at the inlet of the computational domain (Fig.3(c)) is determined stochastically with uniform probability over the inlet boundary surface.

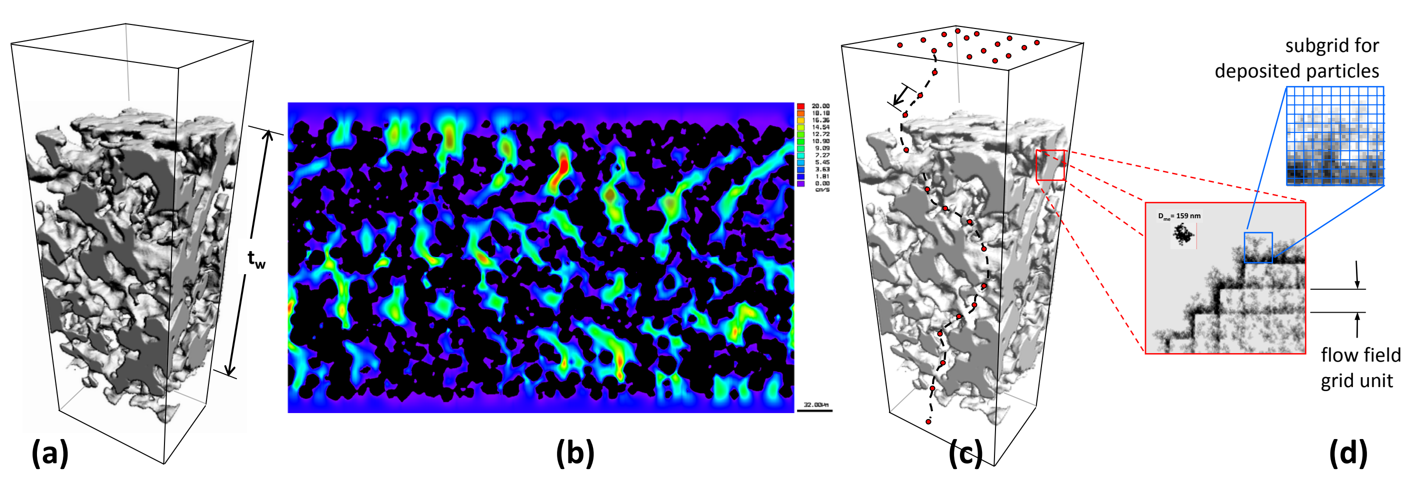



**Figure 3.** **(a)** Computational domain. **(b)** Flow field result for the commercial SiC material considered. Depiction of **(c)** soot particle introduction and trajectory calculation and **(d)** of the soot deposits sub-grid treatment.

## SOOT AGGREGATES LIBRARY

The soot aggregate library used is generated with the a CCA algorithm [1] with morphology parameters (fractal dimension and prefactor) derived from a comparison of aerodynamic and mobility diameter measurements of soot from the test engine at APTL/Thessaloniki. A discrete number of (eight) size classes is used to represent the soot size distribution.

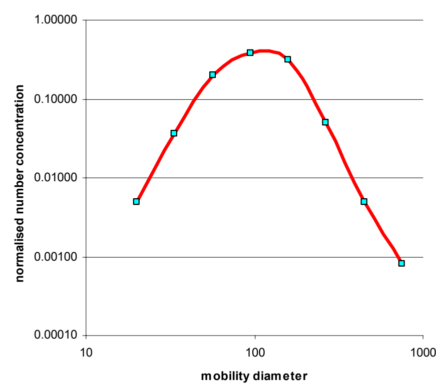
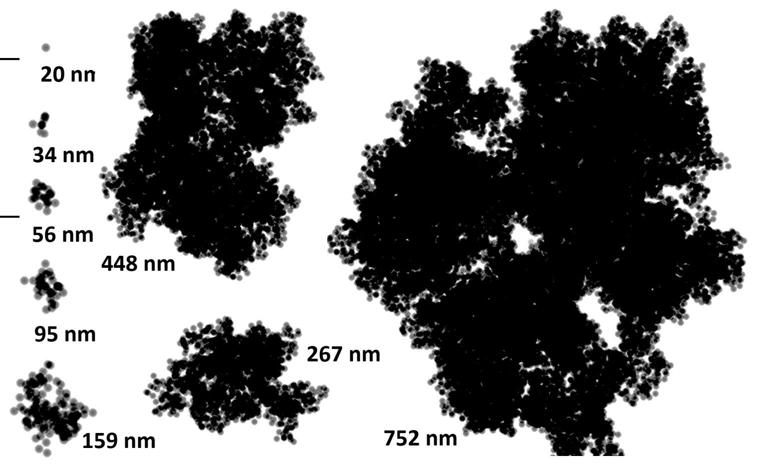



**Figure 4.** Distribution of relative particle concentration used in the filtration simulation for determining total mass and number basis capture efficiency.

**Figure 5.** Representative particles from the soot library of the APTL test engine (1900cc direct injection Fiat JTD engine / Euro3 homologation).

| $d_{mob}$ | $N_a$ |
|---|---|
| 20 | 1 |
| 34 | 6 |
| 56 | 16 |
| 95 | 26 |
| 159 | 63 |
| 267 | 614 |
| 448 | 2500 |
| 752 | 8746 |




## VALIDATION AGAINST EXPERIMENT

The initial size-specific filtration efficiency of a commercial DPF material (SiC wall flow honeycomb with 300 cells/in$^2$, 254 μm wall thickness, 11 μm pore size, 42% porosity) is measured in the diluted side stream exhaust of the APTL test engine at 60 °C and a filtration velocity of 1.5 cm/s. The experimental setup is based on a specially constructed holder-reactor for 35 × 35 × 50 mm DPF segment samples which is housed in a controlled temperature oven during the measurements. The SMPS 3936 system is used to measure the upstream/downstream soot concentrations while dilution ratio is determined by $NO_x$ analyser signals.

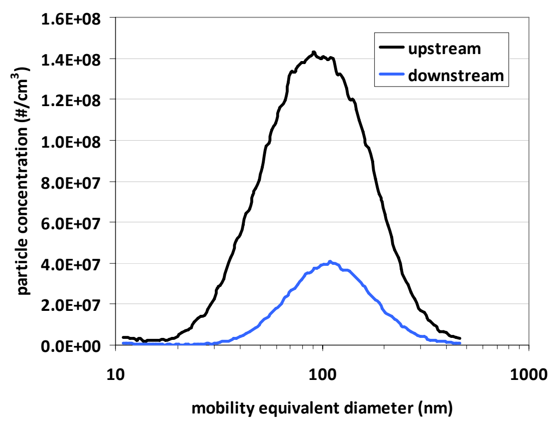



**Figure 7.** Experimentally measured upstream and downstream particle size distributions.

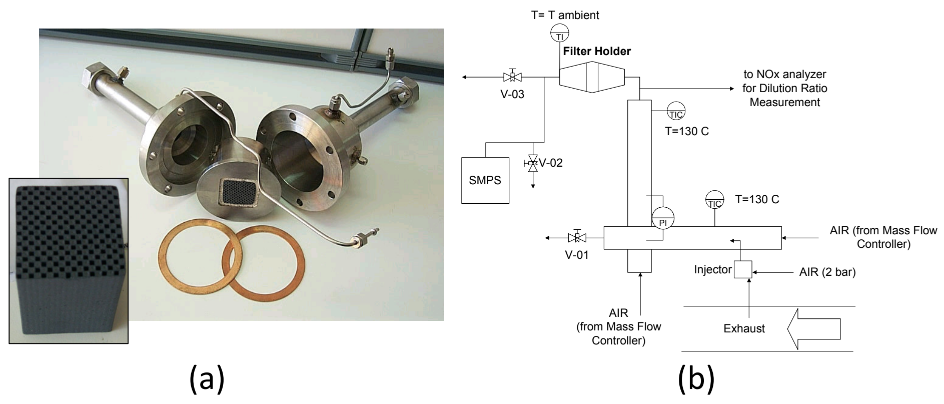



**Figure 6.** Experimental setup for the measurement of filtration efficiency with side-stream engine exhaust: (a) sample holder – reactor (inset: DPF material sample) and (b) setup flow diagram.

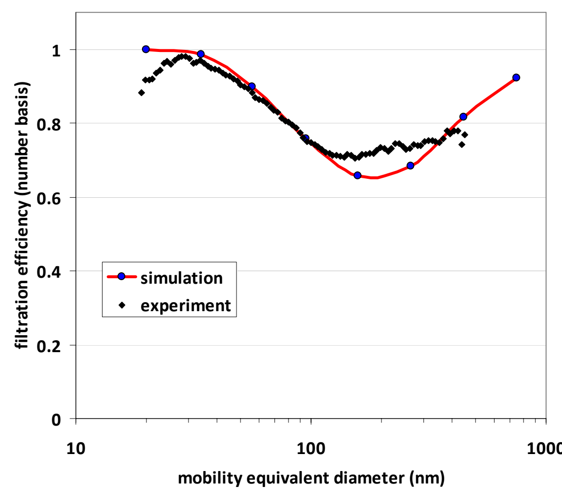



**Figure 8.** Filtration efficiency compa-rison of ab initio calculations against experimental measurements.

## CONCLUSIONS

The presented framework of simulating soot filtration process in a porous filter wall, consisting of a combination of:

- high fidelity and rigorously validated representation of the porous filter wall,
- calculation of the flow field within the porous wall microstructure and
- Brownian particle trajectory of realistic representations of soot aggregates,

has been found free of the need for empirical adjustment/correction parameters in predicting the initial/clean filtration efficiency of porous materials employed in Diesel particulate filters.

Equally significant is that a novel numerical implementation of the deposition process has been developed that overcomes the scale disparity inherent in the problem and permits the coupling of the pore scale exhaust gas flow field and the deposition of fractal-like nanoparticles. The computational overhead is such that practical application of the framework is possible with calculation times, for a single simulation, on the order of 5 hours on a typical single core computer workstation with 2 Gb of memory.

## REFERENCES

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