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Importance of filter's microstructure in dynamic filtration modeling of gasoline particulate filters (GPFs): Inhomogeneous porosity and pore size distribution

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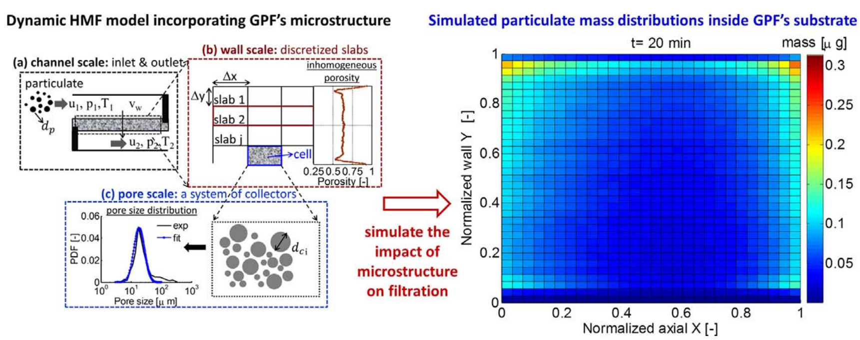
HIGHLIGHTS

- Microstructures of filters were characterized by X-ray CT and mercury porosimetry.
- A multiscale filtration model involving substrate's microstructure was developed.
- Micro- and macro-scopic filtration characteristics of GPF can be probed by the model.
- Filtration of realistic particulate from a SIDI gasoline engine was simulated.
- Microstructure of GPF substrate significantly influences filtration performance.

GRAPHICAL ABSTRACT



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ABSTRACT

The state-of-the-art multiscale modeling of gasoline particulate filter (GPF) including channel scale, wall scale, and pore scale is described. The microstructures of two GPFs were experimentally characterized. The pore size distributions of the GPFs were determined by mercury porosimetry. The porosity was measured by X-ray computed tomography (CT) and found to be inhomogeneous across the substrate wall. The significance of pore size distribution with respect to filtration performance was analyzed. The predictions of filtration efficiency were improved by including the pore size distribution in the filtration model. A dynamic heterogeneous multiscale filtration (HMF) model was utilized to simulate particulate filtration on a single channel particulate filter with realistic particulate emissions from a spark-ignition direct-injection (SIDI) gasoline engine. The dynamic evolution of filter's microstructure and macroscopic filtration characteristics including mass- and number-based filtration efficiencies and pressure drop were predicted and discussed. The microstructure of the GPF substrate including inhomogeneous porosity and pore size distribution is found to significantly influence local particulate deposition inside the substrate and macroscopic filtration performance and is recommended to be resolved in the filtration model to simulate and evaluate the filtration performance of GPFs.

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Nomenclature

PDF	probability density function
HMF	heterogeneous multi-scale filtration
GPF	gasoline particulate filter
SIDI	spark ignition direct injection
PFI	port fuel injection
PM	particulate mass
PN	particle number
DPF	diesel particulate filter
LBM	lattice Boltzmann method
PDF	probability density function
CT	computed tomography
PNNL	Pacific Northwest National Laboratory
SMPS	scanning mobility particle sizer
EOI	end of injection time
PSD	particle size distribution
m_p	particle mass
d_{pp}	primary particle diameter
D_{fm}	fractal dimension of the agglomerate
ρ_{pp}	primary particle density
$\rho_{eff,dm}$	effective density of particle
C	model constant
ρ_i	gas density
u_i	channel velocity
v_w	wall velocity
a	cell length
P_i	channel pressure
μ	gas viscosity
f	friction factor
w_s	soot cake thickness
w_w	wall thickness
k_s	permeability of soot
k_w	permeability of wall
ΔP	pressure drop across a filter
d_m	mobility particle diameter
N_{slab}	number of slabs
$PN(d_m)$	particle number at the diameter of d_m
$\eta(d_{ci},d_m)$	number filtration efficiency of a collector with a diameter of d_{ci} for a particle with a diameter of d_p
$\eta(d_m)$	number filtration efficiency
$E_{t,i}$	total single collector efficiency
L	wall thickness
d_{ci}	individual collector diameter in a collector cluster
$pdf_{d_{ci}}$	pdf of a collectors cluster
ε_j	porosity of the jth slab
l_{dc}	length scale of the filter collector

1. Introduction

Particulate matter (PM) emission from automotive combustion engines is one of the great concerns to our living environment and human health. When these particles are emitted to the atmosphere, they diminish visibility, absorb solar radiation and change the heat balance of the atmosphere, and settle on plants and inhibit photosynthesis [1]. Increased vehicular particle emissions can cause adverse health effects. Exposure to particles is associated with increased respiratory and cardiovascular diseases [2]. Driven by concerns on deteriorating ambient air quality and human health, measures are being taken across the world to adopt and enforce tighter PM emission regulations.

In North America, California LEV III light-duty emission regulations include a limit of 3 mg/mile PM starting in 2017 and a limit of 1 mg/mile PM in 2025 [3]. US environmental protection agency (EPA) Tier 3 requires a maximum tailpipe PM of 3 mg/mile over the FTP test cycle starting in 2017, which is closely harmonized with the California LEVIII PM regulations. Europe and China have particle number (PN) regulations to limit the fine particulates emitted from combustion engines. The Euro 6c regulation introduced a PN limit of 6E11#/km in addition to a particle mass limit of 7.2 mg/mile for SIDI engines [4]. In light of the particulate regulations discussed above, it appears that most modern SIDI vehicles and also some port fuel injection (PFI) vehicles will include a GPF to meet current and future mass- and number-based particulate emission regulations.

Diesel particulate filter (DPF) has been widely and successfully applied on diesel engines for decades [5]. However, there are several differences and challenges in operating GPFs compared to DPFs. First, the filtration regime is different between GPFs and DPFs. In diesel engine exhaust, there is a significant mass of large particles, which result in a rapid "soot cake" built up on the wall surface of a DPF. Once the "soot cake" is developed, filtration is dominated by the "soot cake" rather than the porous wall. On the other hand, SIDI engines generate less particulate emissions and have higher exhaust temperature compared to diesel engines [6–8]. As a result, it is not likely that a "soot cake" layer will be formed in GPFs [4]. Consequently, GPFs are operated in a "deep-bed" filtration regime for extended periods, during which the filtration efficiency may be low. Secondly, a higher exhaust temperature and a higher flow rate in boosted SIDI engines lead to a relatively high pressure drop across a GPF. Compared to diesel engines, SIDI engines are found to be more sensitive to the back pressure, which had a detrimental effect on engine performance and fuel economy [9]. Thirdly, the physical properties and chemical compositions of SIDI engine particulate differ significantly from diesel engines [10]. These physical properties and the chemical composition of the particulate are closely correlated to filtration and oxidation characteristics [11]. Moreover, the particulate emitted from SIDI engines is highly sensitive to operating conditions [11,12]. As a result of these differences, the microstructure of the filter substrate is expected to be critical for high filtration efficiency and low pressure drop GPFs.

Recent experimental studies have implied that the microstructure of the porous substrate significantly influence initial filtration performance. Kamimoto et al. found that surface pores open to the inflow channel made great contributions in trapping particulate through micro- and macroscopic visual diagnostics on cordierite and silicon carbide filters [13]. Moreover, distinct pore structures can greatly affect the "deep-bed" filtration and associated pressure drop. Low pressure drop can be achieved by reducing the pore size distribution range, which improves the homogenization of the microfiltration flow in porous substrate [14]. By using an ultraviolet (UV) microscope and a scanning electron microscope (SEM), Yapaulo et al. revealed the influence of a cordierite filter's microstructure on particulate deposition. They found that the majority of particulate deposited near the surface of the wall rather than penetrating into the wall [15]. Moreover, several studies demonstrated that high filtration efficiency and low back pressure can be achieved through optimized control of pore distribution and porosity of cordierite filters [16]. Merkel et al. showed that high filtration efficiency could be achieved in filters with narrow pore size distributions [17]. All these experimental studies show the importance of the substrate's microstructure in particulate filtration. A computational model that resolves the microstructure of the porous substrate is desirable to further this understanding.

Numerous approaches have been developed to simulate particulate filtration [18–20]. The Lattice Boltzmann method (LBM) is a widely accepted approach to simulate flow in porous media with complex geometry [18]. By solving the flow field within the pore space and conducting particle trajectory analysis [21], the filtration process can be simulated [22]. Although LBM is very helpful to understand the local