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Filtration and regeneration modeling for particulate filters with inhomogeneous wall structure

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ABSTRACT

A new advanced filtration model for diesel particulate filter (DPF) is presented. The model is able to account for the distribution of soot particle size and different material and filtration properties for non-homogeneous wall structures. The impact of a thin dense layer on top of the inlet channels of a DPF on filtration, pressure drop and passive regeneration is investigated using the model. In agreement with previous literature experimental studies, significant improvement in the filtration efficiency is shown. The increased pressure drop of the empty filter is quickly outbalanced during loading due to less soot accumulation inside the wall. The negative effect of the layer technology on passive regeneration of catalyzed filters is demonstrated by solving the reaction–diffusion equations in the wall.

1. Introduction

Filtration modeling for diesel particulate filters is traditionally based on the established filtration theory accounting for diffusion and interception mechanisms [1–3]. Due to the fact that engine emitted particulates are quite variable in size, a proper filtration model should be able to account for the actual particle size statistical distribution. Some issues related to the filtration modeling are linked to the description of the actual wall microstructure using simplified unit cell methods as well as the description of the soot particles geometry. Furthermore, the effect of the accumulated particles on the wall permeability and filtration performance poses a big challenge from the modeling point of view. In the present study, an advanced filtration model is presented addressing the above issues.

There have been several attempts to model the filtration efficiency of the wall-flow DPF in the recent literature [4–6]. In the present work, the presented new model is able to account for multiple layers inside or on top of the wall structure with variable geometrical/filtration properties. In parallel, a new approach to account for multi-disperse incoming soot particles is presented. The model is validated by experiments performed on the engine test bench using both homogeneous and non-homogeneous wall structures.

Special attention is given to the long-term effect on NO_2 regeneration in catalyzed filters. In this case, the lack of soot penetration in the catalyzed wall of DPF with non-homogeneous wall structures may have negative effects on the passive regeneration performance [7]. The prediction of this effect requires advanced modeling of the reaction–diffusion coupling in the catalyzed wall, which is briefly discussed in this paper.

2. Description of the advanced filtration model

The new filtration model is implemented in *axitrap*, the wall-through filters module of the software package *axisuite* [8]. The basic differential DPF model equations are summarized in Appendix, whereas more details can be found in previous publications [9–14]. The DPF model accounts for flow distribution, pressure drop, heat/mass transfer and soot oxidation in the filter. Intra-layer discretization in the catalyst and soot layer phase, coupled with the combined transport and reaction phenomena, allows for detailed simulation of the complex interactions of catalytic effects and soot oxidation.

The engine emitted particulates can be mathematically expressed by a particle number based log-normal distribution:

$$N = \frac{N_{tot}}{\sqrt{2\pi} \cdot \log\ \sigma} \cdot \exp\left[-\frac{(\log d_{part} - \log \mu_{part})^2}{2 \cdot \log^2 \sigma}\right] \tag{1}$$

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Nomenclature

Variables

b	geometric parameter
C	constant for the external Nusselt number expression
$c_{j,k}$	stoichiometric coefficient of species j in reaction k
c_m	molecular density
C_p	specific heat capacity
d_{grain}	grain diameter
d_{part}	mobility diameter
D_{part}	particle diffusion coefficient
d_{pore}	mean pore size
E_{wall}	layer filtration efficiency
f	geometrical parameter
h	convection coefficient
H	heat transfer per filter volume
k_b	constant for the external Nusselt number expression
k_p	soot layer permeability
k_s	substrate permeability
Ku	Kuwabara's hydrodynamic factor
m	constant for the external Nusselt number expression
N	particle number based log-normal distribution
N_{tot}	total particle number for unit volume
p	pressure
Pe	Péclet number
R	normalized radius
R_c	aggregate maximum radius
R_k	reaction rate
S	sum of heat sources
s_F	filter specific area
T	temperature
u, v	velocity
W_{cap}	wall saturation index
x, y, z	coordinates

Greek letters

α_1	constant in channel pressure drop correlation
Δw	layer depth
Δp	pressure drop
ε_{pore}	unit collectors porosity
η_D	diffusion grain efficiency
η_g	total grain efficiency
η_R	interception grain efficiency
λ	thermal conductivity
μ	dynamic viscosity
μ_{part}	geometric mean
ρ	density
σ	standard deviation

Subscripts

i	channel index
j	particle class
s	solid, ceramic substrate
w	wall-outlet channel interface
0	initial value

where N_{tot} is the total particle number for unit volume, μ and σ the geometric mean and standard deviation. The model simulates the soot emissions with several particle classes where each class has an equivalent mobility diameter d_{part} that follows the log-normal distribution. Furthermore each class is considered to be an aggregate cluster of primary carbon particles which has an equivalent maximum radius R_c shown in Fig. 1.

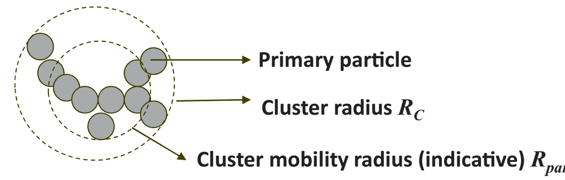

Fig. 1. Cluster radius vs. mobility radius.

The packing density is computed separately for each mobility diameter class. Then, the packing density of the deposit is computed as a weighted average, based on the accumulated mass of each particle class in the deposit.

The wall is discretized in several layers where each layer could have different microstructure properties in order to model non-homogeneous wall structures. The layer microstructure is described by a number of intralayer nodes of sphere unit collectors with porosity $\varepsilon_{pore,0}$ and mean pore size d_{pore}. The grain diameter of the sphere collector is calculated as:

$$d_{grain,0} = \frac{3}{2}\left(\frac{1-\varepsilon_{pore,0}}{\varepsilon_{pore,0}}\right) d_{pore} \tag{2}$$

The clean filtration efficiency is calculated taking into account the two main filtration mechanisms, diffusion and interception.

The single grain efficiency for particle class j is calculated for diffusion with the following equation:

$$\eta_{D,j} = 3.5\left(\frac{\varepsilon_{pore}}{Ku}\right)^{1/3} Pe_j^{-(2/3)} \tag{3}$$

where

$$Pe_j = \frac{u_w\, d_{grain,0}}{D_{part,j}} \tag{4}$$

$$D_{part,j} = \frac{C \cdot k_b \cdot T}{3 \cdot \pi \cdot \mu \cdot d_{part,j}} \tag{5}$$

The single grain efficiency for interception is calculated as:

$$\eta_{R,j} = 1.5\left(\frac{\varepsilon_{pore}}{Ku}\right)\frac{R_j^2}{(1+R_j)^m} \tag{6}$$

$$R_j = \frac{2 \cdot R_{c,j}}{d_{grain,0}} \tag{7}$$

$$m = \frac{3-2\varepsilon_{pore,0}}{3\varepsilon_{pore,0}} \tag{8}$$

The Kuwabara's hydrodynamic factor is calculated for sphere unit collectors as

$$Ku = 1 - \frac{9}{5}(1-\varepsilon_{pore})^{1/3} + (1-\varepsilon_{pore}) - 0.2(1-\varepsilon_{pore})^2 \tag{9}$$

The total single grain efficiency is calculated for each wall layer as:

$$\eta_{g,0,j} = \eta_{D,j} + \eta_{R,j} \tag{10}$$

This model assumes an empirical correlation to compute the effect of the wall soot loading on filtration efficiency. Firstly, a wall saturation index, ranging from 0 to 1, is calculated based on the following expression:

$$W_{cap} = \frac{\varepsilon_{pore,0} - \varepsilon_{pore}}{\varepsilon_{pore,0}} \tag{11}$$

which is then used to estimate loaded grain efficiency:

$$\eta_{g,j} = \eta_{g,0,j} + (1-\eta_{g,0j}) f(W_{cap}) \tag{12}$$