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Design of automotive flow-through catalysts with optimized soot trapping capability

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ABSTRACT

A hybrid model for accurate and computationally efficient simulations of the particle trapping characteristics of automotive flow-through catalysts is suggested in this paper. The new model is validated against the performance of a more elaborate, but computationally far more expensive model.

In this hybrid model, the trapping of the smallest particles is predicted using a computationally efficient submodel that can also be used for screening of new catalyst substrate designs. It is shown here that this screening model is very accurate for particles smaller than approximately 50 nm. A number of different catalyst designs are evaluated and compared using the screening model. In particular, the performance of a promising channel design with porous obstacles is evaluated. This design could potentially give over 70% reduction of small soot particles without a substantial increase in the pressure drop.

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1. Introduction

Particulate matter is formed during incomplete combustion in modern diesel and gasoline engines. When emitted to the ambient air, these submicron-sized particulates may end up in human lungs. It is estimated that one hundred thousand people die prematurely every year in Europe alone due to particulate matter from human activities [1]. In order to improve the air quality, forthcoming emission legislation for vehicles will focus not only on regulating the total mass of particulate matter emitted, but also the number of particles [2]. It is therefore likely that there will be a need to optimize the automotive emission control systems with respect both to the number and the mass of the particles emitted.

The so-called wall flow particulate filters in use today are very efficient, but still have unresolved issues regarding robustness and regeneration strategy. They also impose a fuel penalty by a marked increase in the total pressure drop over the exhaust gas aftertreatment system. It has been reported that particles smaller than 110 nm may be able to pass through the wall-flow filter uncollected [3]. A recent experimental study revealed a minimum in the particle trapping efficiency for particles of size around 100 nm in both cordierite and SiC wall-flow filters [4]. The possibility to introduce specific, application-tailored particle trapping capabilities to a preceding flow-through filter (e.g. the diesel oxidation catalyst or the three-way catalyst in gasoline applications) is therefore very attractive.

The different types of particulate matter have been shown to behave very differently in the exhaust catalyst [5]. Therefore, in order to optimize the overall trapping of particulate matter, a number of different measures will have to be undertaken. The purpose of the current work is twofold: (a) to identify these measures and (b) to find an optimal design tool for automotive oxidation catalysts depending on which type(s) of particulate matter one wishes to target specifically.

2. Background

In this paper, we will first motivate the introduction of particle trapping capabilities to the oxidation catalyst from the perspective of the overall performance of the aftertreatment system. We then use the previously published detailed model of Ström and Andersson [5] to evaluate the relative influence of the phenomena taken into account in that model. The results from this evaluation is used to suggest a new, simpler model. The performance of the simpler model is then compared to that of the full model, and a hybrid model is proposed that takes advantage of both the computational efficiency of the simpler model and the detailed information from the full model. A broad scanning of six geometrical designs of the

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Nomenclature

C_c	Cunningham correction factor
D	diffusivity ($m^2\ s^{-1}$)
D_p	pore diameter (m)
d_c	unit collector diameter (m)
d_h	hydraulic diameter (m)
d_p	particle diameter (m)
E	number trapping efficiency
g	gravitational acceleration ($m\ s^{-2}$)
$g(\varepsilon)$	geometric function
k_B	Boltzmann constant ($J\ K^{-1}$)
L	length (m)
m_p	particle mass (kg)
N_R	interception parameter
n	number of particles
P	pressure (Pa)
Pe	Peclet number
r	radial position (m)
Sh	Sherwood number
St	Stokes number
T	temperature (K)
t	time (s)
U	mean velocity ($m\ s^{-1}$)
u	velocity ($m\ s^{-1}$)
x	position (m)
x_i	mass fraction of species i
ε	porosity
η_{DR}	trapping efficiency due to Brownian motion and inertial effects
η_D	trapping efficiency due to Brownian motion
η_R	trapping efficiency due to inertial effects
μ	viscosity (Pa s)
ρ	density ($kg\ m^{-3}$)
ρ_p	particle density ($kg\ m^{-3}$)
τ_p	particle relaxation time (s)
τ_s	characteristic time scale (s)
Ω	rotational velocity (s^{-1})

oxidation catalyst is then carried out using the simpler model. These designs are motivated by a preceding theoretical analysis, and include both designs previously discussed in the literature as well as novel ones suggested here. The designs are compared in a results map, from which the most fuel efficient designs can be discerned. The possibility to further optimize these designs is finally discussed.

3. Advantages of particle trapping in the oxidation catalyst

We aim here to propose a strategy for the design of traditional automotive catalysts aiming to keep high the overall particle trapping efficiency of the complete exhaust gas aftertreatment system while keeping the fuel penalty to a minimum. In addition, the full system should be robust and reliable. It therefore becomes necessary to investigate what measures that can be undertaken in the oxidation catalyst to lower the pressure drop over a succeeding particulate filter and to increase its performance predictability.

When a conventional wall-flow particulate filter is clean (i.e. before the soot cake is formed), the most significant contribution to the pressure drop is caused by the gas flowing through the porous walls. The pressure drop over the wall can be estimated from Darcy's law with a Kozeny–Carman correlation for the permeability of the filter material, where D_p is the wall pore diameter and ε the effective porosity [6]:

$$\frac{\Delta P}{L} = 5.6\frac{\mu U}{\varepsilon^{5.5} D_p^2} \tag{3.1}$$

When the filter is loaded with soot, it is the soot content on and inside the channel walls that causes most of the pressure drop. The well-known Ergun equation gives the pressure drop for the flow through a porous bed (e.g. soot deposition layer) constituted of spherical particles of uniform size d_p:

$$\frac{\Delta P}{L} = 150\frac{(1-\varepsilon)^2 \mu U}{\varepsilon^3 d_p^2} + 1.75\frac{(1-\varepsilon)\rho U^2}{\varepsilon^3 d_p} \tag{3.2}$$

It should be stressed here that Eq. (3.2) is only an approximation of the pressure drop in the real application. In reality, a range of complex phenomena (e.g. degree of soot cake compaction, possible soot migration and blow-off effects) may influence the actual pressure drop. Eq. (3.2) is thus only used here as the basis for a qualitative discussion.

It is then evident from Eqs. (3.1) and (3.2) that a more densely packed soot bed and/or a more densely filled porous wall will cause significantly higher pressure drops. The effective porosities will be very much influenced by the smallest particles, as they will fill the voids in between the larger particles and inside the smallest pores. A reduction of the number of very small particles passed on from the oxidation catalyst to the particulate filter therefore has a large potential to decrease the pressure drop over the filter.

In addition, removal of the largest particles will significantly reduce the rate of soot accumulation in the filter, which will decrease the regeneration frequency. If the accumulation of soot is low enough, active regeneration of the filter may even be omitted.

Even in a situation where the new design of the oxidation catalyst channels causes an increase in pressure drop that outweighs the pressure drop gain in the wall-flow filter, the particle content of the filter will have a more narrow size distribution. For diesel and gasoline particulate matter, the particles of different size typically differ also chemically [7]. Since the oxidation behavior is largely dependent on the type of particles present, a more narrow compositional distribution will enhance the robustness and predictability of operation for the filter.

In addition, for gasoline applications it might be sufficient to remove a large fraction of the smallest particles to comply with emission regulations, as gasoline exhaust generally contains fewer and smaller particles than diesel exhaust [7]. A properly designed three-way catalyst may then spare the addition of a particulate filter altogether.

4. Solving for the gas flow

The work presented herein is based on modeling and simulation using computational fluid dynamics (CFD). Since the Reynolds numbers typically encountered in the flow of exhaust gases through monoliths are of the order of a couple of hundreds, it is possible to use a laminar flow model and solve the continuity equation with the incompressible Navier–Stokes equations:

$$\nabla \cdot u = 0 \tag{4.1}$$

$$\rho\left[\frac{\partial u}{\partial t} + \nabla\cdot(uu)\right] = -\nabla P + \nabla\cdot\left[\mu\left(\nabla u + \nabla u^T\right)\right] + \rho g \tag{4.2}$$

The boundary conditions used are that of a constant velocity over the inlet, a constant (atmospheric) pressure over the outlet, and no-slip at all walls. A constant velocity over the inlet is deemed a realistic inlet boundary condition since the dimensions of the channels are small in relation to the velocity gradients of the mean flow upstream the catalyst. In addition, the transition to a fully

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