

## A General 3D Model to Analyze Particle Transport Into a Partial-Flow-Particulate-Filter

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### ABSTRACT

Emission control efficiency and limited fuel consumption penalty and are the main design factors driving the development of engine-after-treatment exhaust systems according to both ACEA/DOE targets and continental regulations. The particulate-filter is certainly a critical technology to this aim as usually presents very high pm reduction efficiencies (even more than 90% on a mass basis depending on soot loading) leading however to a back pressure increase and eventually to an appreciable fuel consumption penalty. Nevertheless, it is in general discussion that health hazard related to particulate depends primarily on total number of emitted particles rather than on mass.

The partial-flow-filter has been recently developed presenting lower reduction efficiencies on a mass basis but also a reduced penalty on fuel consumption. As a selective capability of this filter in capturing the smaller particles has also been experimentally observed, technological and scientific interest in the development of design and analysis tools dedicated to this technology has developed. However, traditional 1D and 2D models cannot be directly applied to study this technology, as the coupling between fluid-dynamics and filtration must be properly taken into account by exactly modeling single channel geometry as it is.

Thus, in order to represent filtration effects by varying diameter class in partial-flow-filters, a 3D model has been coupled to a phenomenological filtration submodel taking into account Brownian diffusion and interception phenomena within an Eulerian transport framework for different particle classes depending on diameter. Results have been compared to experimental data and state that the model is able to represent the main occurring fluid-dynamic and filtration phenomena by varying mass flow rate and particle diameter.

### INTRODUCTION

Emission control and engine efficiency present a trade-off behaviour, so that, for example, the introduction of extremely high-efficient after-treatment systems increases fuel consumption and vice-versa. Moreover, the soon forthcoming NOx regulations [1] will force automotive companies to adopt complex after-treatment schemes using different technologies (DOC, LNT, LNC, SCR), partial-flow-filter) or integrated approaches (SCRi [2], DPNR [3]) to control PM and NOx simultaneously [1].

Engine fuel consumption is affected by these solutions due to the higher exhaust back pressures and to the complex control strategies required for optimized emission reduction. The after-treatment can then be seen as an integrated component that needs to be designed in close relationship with the engine.

Particulate filters are the most effective PM reduction devices. While this technology presents very high efficiency (even more than 90% on a mass basis, depending on soot loading), the resulting back-pressure may lead to an excessive cost in terms of engine efficiency. More recently, the different roles of PM characteristics such as particle mass, number and size have been addressed showing a strong impact of the particle number to human health and highlighting the role of nano-particles in urban pollution [4,5]. The scenario has also been enriched by the availability of more and more reliable experimental instruments (CPC for total number measurement, SMPS and ELPI for particle diameter distribution). The described factors drove in EU the PMP (Particle Measurement Program [6]) which finally fixed a limit of 6E11 particles/km for the forthcoming light-duty EURO 5-b/6 emission legislation. The particulate filter should therefore be designed to achieve not only a certain mass removal efficiency, but also a limited number of emitted particles. While engine out total number shows a high

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correlation between traditional gravimetric PM measurement and total number even by varying engine design technology [7], data downstream of the particulate filter are weakly correlated [8]. The two targets of limiting PM number and mass might be in fact separated since the maximum number typically occurs below 50 nm (nuclei mode, nano particles), while in terms of mass it occurs well above 300 nm (accumulation mode, ultrafine particles) (Figure 1). Moreover back pressure increase of the particulate filter (leading to fuel consumption increase) can be primarily related to the loaded PM mass. So, ideally, the particulate filter should be very efficient in the ultrafine range, to limit the emitted number of particles in the nuclei mode, while it might be less over the accumulation mode to not extremely penalize fuel consumption and related CO<sub>2</sub> emissions.

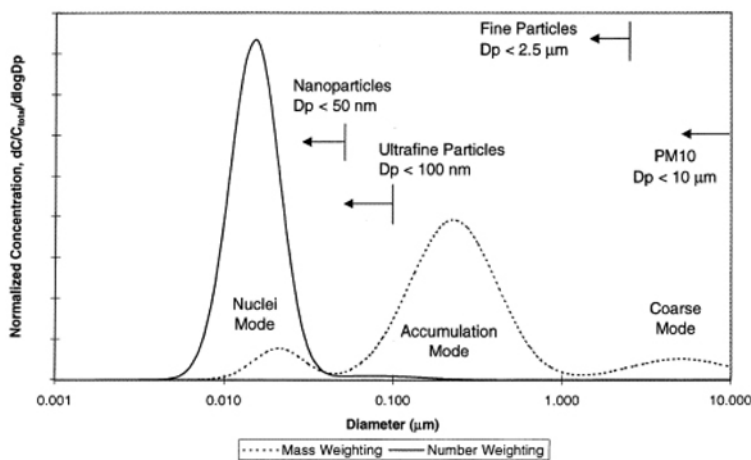


**Figure 1. Typical Diesel engine-out number and mass distribution [9].**

In this technological context, numerical modeling has played a key-role to better understand the influence of the design of after-treatment systems on filtration capabilities since several years, given the difficulties of measuring local flow and efficiency inside, for example, the particulate filter. In the first attempts, particulate filters were modelled via a 1D approach proposed first by Bissett [10], and then improved [11]. The cited approach led to good capabilities in terms of predictive reliability and computational efficiency, and allowed to analyze above all the filter back pressure increase as a function of time, engine and soot load and by adopting different regeneration techniques. The 1D approach has then been extended to 2D and 3D to get a more accurate description of the flow inside the single channel and the whole trap [12,13,14,15]. However, it has been demonstrated that traditional wall-flow filters [16] can be safely modeled via a 1D approach. It can be proven in fact that inside a single channel PM deposition rate actually depends only on channel axial abscissa [17].

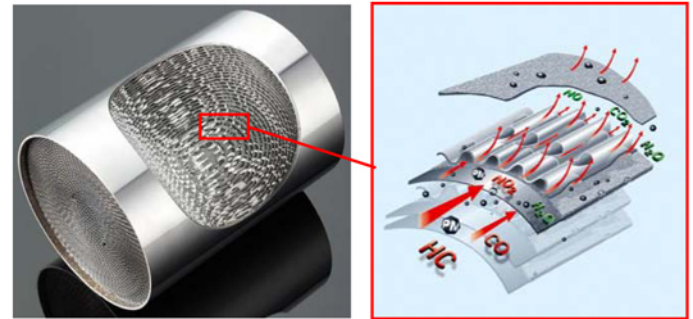


**Figure 2. partial-flow-filter (left); structure and principle of operation of a partial-flow-filter (right).**

The simulation analysis of the partial-flow-filter [18,19] (Figure 2), requires necessarily the use of advanced 3D techniques. In fact, the partial-flow-filter is constituted by corrugated foils supported by sintered metal PM-filtering flat foils (called in the rest of the paper fleeces or filtering material).

Each corrugated foil realizes a row of channels: all the rows are stacked and canned into the tailpipe (Figure 2, a). With this design the efficiency of the partial-flow-filter is determined by fluid-dynamic parameters such as the mass flow rate deviated on the filtering material, or the filtering material characteristics (porosity, permeability).

Partial-flow filter efficiency also depends on the number of blade-stages, which is a function of substrate length (i.e. 150 mm can correspond to up to 11 stages). The sketch plotted in Figure 2-b describes a twin-stage solution. As mentioned, the partial-flow-filter has been demonstrated to have a high potential in terms of total number efficiency in the range 10-300 nm [20].

The efficiency of filters with respect to particle number efficiency has not been addressed very often in the recent literature. Some fundamental works analyzed particle flow in a particulate filter single channel [21], and in the porous filtering material [22]. However, these papers have been focused primarily on PM accumulation into the filtering elements to represent the back-pressure increase rather than on efficiency as a function on different particle diameter classes.

Thus, moving from the given background, a 3D tool is presented in this paper to represent filtering efficiency in an automotive particulate filter depending on particle diameter. The 3D fluid-dynamic model is based on Eulerian transport of several particle diameter classes directly coupled to a filtration sub-model. The integrated model is able to calculate filtration efficiency depending on local flow into the filtering element and local filtration regime.

The model, which might be generally applied to any other kind of filter technology, is applied in this paper to the analysis of a partial-flow-filter to study the coupling between the flow and filtration capabilities of the material by varying operating conditions. In fact, the use of such accurate tools is mandatory for such device to represent the complex coupling between the 3D fluid-dynamic field and the local characteristics of filtration occurring into the filtering material and better understand the filtration potential in the 10-300 nm particle diameter range.

The model has been defined in the deep bed regime, and thus it is valid to represent the first hours of operation, or to represent the behavior of filters which are frequently regenerated.

## 3D FILTRATION INTEGRATED MODEL

### GENERAL DESCRIPTION

As stated above, a comprehensive and innovative 3D model is proposed in this paper, based on Eulerian transport of PM mass fractions, for 6 representative diameter classes: 10, 33, 66, 100, 150 and 300nm.

A single channel approach has been preferred, assuming the hypothesis that all the parallel channels of the filter behave in the same way from the fluid-dynamic point of view.

The flow is assumed to be laminar, since Re is in the order of 1000 in the highest flow operating conditions in real engine applications with respect to channel flow. The partial-flow-filter performance is analyzed in steady-state conditions. Governing equations are provided below, and have different forms depending on the described computational region which may be the porous filtering element (fleece) or the open channel, according to the sketch given in [Figure 3](#).

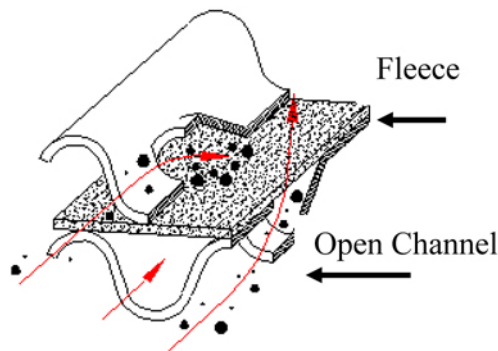


**Figure 3. Fleece and Open Channel Computational Regions.**

$$\nabla \cdot \rho \vec{u} = 0 \quad (1)$$

$$\nabla \cdot (\rho \vec{u} \vec{u} - \mu \vec{\nabla} \vec{u}) = -\vec{\nabla} \left( p + \frac{2}{3} \mu \nabla \cdot \vec{u} \right) \quad (2)$$

$$T = T_{\text{inlet}} \quad (3)$$

Eqs. (1), (2) and (3) are valid over the open channel region. Temperature has been retained homogeneous over all the domain, since the system may be reliably considered adiabatic committing a negligible error, if no regeneration processes occur. However, the effects of temperature on properties have been taken into account.

The fleece is treated as an isotropic porous medium. It is constituted by a wire mesh realizing a metal porous matrix. Its average properties are expressed in terms of porosity  $\epsilon$  that in turn is a function of wire diameter. Into the fleece, continuity and energy equation assumes the same form as [\(1\)](#) and [\(3\)](#), while momentum is reported below:

$$\nabla \cdot (\epsilon \rho \vec{u} \vec{u} - \epsilon \mu \vec{\nabla} \vec{u}) = -\epsilon \vec{\nabla} \left( p + \frac{2}{3} \mu \nabla \cdot \vec{u} \right) - \left( \frac{\mu}{\alpha} + \frac{C \rho}{2} |\vec{u}| \right) \vec{u} \quad (4)$$

Momentum losses due to porous material effects are taken into account via viscous and inertial effects respectively with coefficients  $\alpha$  and  $C$  (last term in [equation \(4\)](#)).

The carrier gas is supposed to be a single component with global properties equal to a typical composition of the exhaust gas of a Diesel engine.

PM mass fractions of the different diameter classes are transported according to the following equation:

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \vec{v} Y_i) = \nabla \cdot (\rho D_i \vec{\nabla} Y_i) + S_i \quad (5)$$

The particle transport equations do not concur to the overall mass balance, since their contribution may be retained negligible to that.  $D_i$  represents the Brownian diffusion coefficient, computed as a function of particle diameter and temperature as it follows:

$$D_i = \frac{Fk_b T}{3\pi\mu_g d_p} \quad (6)$$

The Cunningham factor  $F$  provides a correction for the transition from slip to continuum regime. It may be calculated as a function of the mean free path and particle diameter as it follows:

$$F = 1 + \frac{\lambda}{d_p} \left[ 2.34 + 1.05 \exp\left(-0.39 \frac{d_p}{\lambda}\right) \right] \quad (7)$$

The mean free path is calculated for air, a constituent similar to the carrier gas. At atmospheric pressure and 293 K (20°C), the mean free path is  $\lambda_{ref} = 66.4$  nm, while for other conditions the following formula can be used:

$$\lambda = \lambda_{ref} \left( \frac{P_{ref}}{P} \right) \left( \frac{T}{T_{ref}} \right) \left( \frac{1+110/293}{1+110/T} \right) \quad (8)$$

The different diameter classes are supposed to not have any interaction, i.e. agglomeration phenomena are not taken into account.

The term  $S_i$  in eq. (5) represents the source term to take into account particle deposition into the fleece. It is zero in the open channel region, while it is a function of particle diameter into the fleece according to eq. (9):

$$S_i = - \frac{4\rho|\vec{u}|Y_i\eta(1-\varepsilon)}{\pi d_f} \quad (9)$$

Eq. (9) comes directly from the definition of a single fiber total efficiency  $\eta$  (also called filtration submodel in the rest of the paper) which may be calculated by applying the “fan model” [23], which refers to a system of parallel and randomly oriented rows, each one consisting of a layer of parallel cylinder wires.

Among the different filtration mechanisms [24], only Diffusion (D), Interception (R) and combined Diffusion/Interception (DR) filtration mechanisms are taken into account, as inertial impaction mechanism can be neglected

since  $Stk \ll 1$  [25]. Stokes number  $Stk = \frac{\tau_V}{\tau_F}$  is defined as the ratio between the momentum particle response time  $\tau_V$  and a characteristic fluid-dynamic time  $\tau_F$ . In the case of

automotive particulate filter, if  $d_p < 300$  nm, the condition  $Stk \ll 1$  can be retained always valid.

A number of analytical models exist for the estimation of single fiber total efficiency  $\eta$  as a function of particle diameter and filtering material characteristics. The most common ones are single-fiber models of Kirsch and Stechkina [23], Liu and Rubow [26], Matteson and Orr 1987) [27], Davies [28], Brown [29], Rivers [30], Hinds [24] and Pontikakis et al. [31]. The filtration model presented in this paper is based on Hinds [24], and defined in eq. (10):

$$\eta = \eta_D + \eta_R + \eta_{DR} = APe^{-B} + C \left( \frac{\varepsilon}{k} \right) \left( \frac{R^2}{1+R} \right) + \frac{DR^{2/3}}{(kPe)^E} \quad (10)$$

where:

- A, B, C, D, E are empirical constants which depend on specific material properties, and must be tuned on an experimental basis, as it will be explained in a following section.

- $k$  = Kuwabara hydrodynamic factor defined as

$$k = -0.5 \ln(1-\varepsilon) - 0.52 + 0.64(1-\varepsilon) + 1.43\varepsilon \frac{\lambda}{d_p} \quad (11)$$

- $Pe$  = Peclet number

$$Pe = \frac{|\vec{u}|d_p}{D_i} \quad (12)$$

- $R$  = interception parameter

$$R = \frac{d_p}{d_f} \quad (13)$$

- $d_f$  = wire diameter.

Thus, in addition to the porosity  $\varepsilon$ , the diameter of the single fibres  $d_f$  creating the wire mesh is important to represent average filtration properties.

## COMPUTATIONAL DETAILS

The computational domain of the partial-flow-filter utilized for the calculations is plotted in Figures 4 and 5.

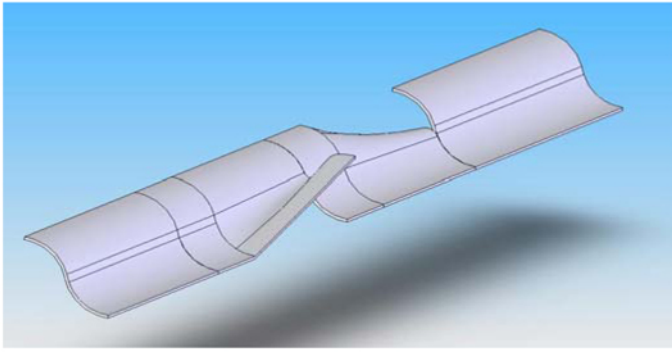


**Figure 4. Partial-flow-filter: 3D computational domain: corrugated foil layout.**

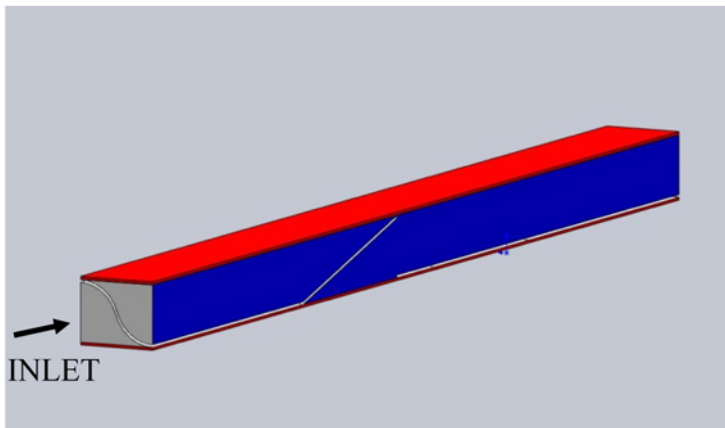


**Figure 5. Partial-flow-filter: 3D computational domain: single channel ensemble layout.**

The corrugated foil layout is highlighted in [Figure 4](#): it includes a single blade stage. The computational domain includes the gas channels obtained by the intersection of corrugated foils and fleeces, according to [Figure 5](#) sketch. To minimize the computational effort, symmetric boundary conditions have been applied to the axial sections (blue in [Figure 5](#)) of two neighbor half-channels. To the same aim, periodic boundary conditions have been applied to the fleece surfaces (red in [Figure 5](#)), that corresponds to the assumption that each row exchanges the same mass flow rate with the neighbor row. By this way, the computational domain is limited as much as possible realizing the so-called unit-cell approach, i.e. assuming that each channel behaves similarly to the neighbor. The validity of this hypothesis depends on flow distribution at the inlet of the whole filter, and usually this is safely verified in the central region of the whole device. Only a single blade stage has been represented in the domain since multi-blade filter efficiency  $EFF_{multi-stage}$  has been related to single-stage efficiency  $EFF_{stage}$  by the following assumption:

$$EFF_{multi-stage} = 1 - (1 - EFF_{stage})^{n_{stage}} \quad (14)$$

The assumption of purely serial multistage approach could not be safely done to take into account loading effects. In fact, first stages have higher soot deposition rate and then non-uniformity of stages over loading would bring to enhanced differences in terms of filtration efficiency. This is not the case of the present paper due to the fact that simulations and experiments refer only to the first minutes of operation or to frequently regenerated filters.

At the inlet section a homogeneous velocity profile is given to provide a certain engine mass-flow rate, while constant pressure has been imposed all over the outlet section. At the wall no-slip momentum conditions have been applied, since Re number falls in the laminar regime, i.e. all the flow length scales in the vicinity of the wall can be fully resolved.

The computational domain has been discretized into about 1M cells with 0.05 mm average grid-spacing, which allows to obtain independent-grid results safely.

PM mass fractions of the different diameter classes are provided at inlet and zero diffusive flux boundary condition is set on the walls and at the outlet. It is worth noting that the proper boundary condition on the walls should be zero PM mass fraction, due to the fact that particles hitting the wall gets trapped, but it could lead to an overestimation of filtration for higher diameter particles, due to the fact that numerical diffusion could be remarkable when diffusion coefficients are very low. To reduce as much as possible numerical diffusion contribution a quart-order accuracy discretization scheme has been used. The filtration model has been implemented into the Fluent commercial code via a ANSI-C UDF (User Defined Function) [32].

It is also worth underlining that [eq.\(5\)](#) can be written in non-dimensional form since  $Y_i$  is included in each of the terms of that equation. This in turn means that collection efficiency is not a function of actual soot mass fraction at the inlet. Actual soot mass fraction at the inlet only plays a role when loading effects cannot be considered negligible.

## ANALYSIS OF RESULTS

The standalone filtration sub-model has been first validated vs specific experimental data to characterize the performance of the filtering material, and prove the predictive capabilities of the phenomenological model defined by [eq. \(10\)](#). Then, the partial-flow-filter complete geometry has been analyzed in terms of different designs and inlet velocity operating conditions. The experimentally measured global efficiencies by varying diameter have been first compared to the 3D