

Modeling of the Soot Accumulation in DPF Under Typical Vehicle Operating Conditions

2010-01-2097

Published
10/25/2010

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ABSTRACT

The pressure losses across the different parts of a regenerative Diesel Particulate Filter (DPF) have been modelled and compared with the measured pressure loss and with the measured changes in the instantaneous weight of the DPF of a commercial automotive diesel engine. The comparisons were made in three operating conditions selected among those included in the transient cycle established in the European Emission Directive. The first one is a low-load mode, with high soot emissions and therefore with high contribution to the DPF charge. The second one is a medium-load mode, in which the balance of soot charge versus spontaneous soot regeneration leads to a slow DPF charging, the temperature at the exhaust manifold being high enough to permit active regeneration. The third one is a high-load mode, in which the spontaneous regeneration leads to a net DPF discharge, the active regeneration becoming useless. The model proposed uses computational fluid dynamics (Fluent ®) for validating the hypothesis of homogeneous pressure distribution in the conical inlet and along the filter channels. Once validated, a simplified model is used to estimate the effect of the morphology of soot agglomerates (porosity, specific surface, apparent density, fractal dimension, etc.) and of the soot oxidation reactivity on the DPF charging process. A precise estimation of the actual filter charge from the on-line measurement of the pressure difference up and downstream the DPF (considering the characteristics of the fuel used) would permit to optimize the engine regeneration strategies to be implemented in the Electronic Control Unit (ECU).

INTRODUCTION

Diesel particulate filter (DPF) is nowadays one of the most common technologies used in diesel vehicle engines to fulfill the current and future particulate matter emissions limits included in regulations EURO 5 and EURO 6. Wall-flow type traps are the most extended ones due to its high efficiency, generally above 90%. However, soot accumulation must be limited in the trap because otherwise the exhaust back pressure would increase up to unacceptable values, therefore moving the engine operating mode away from its optimized conditions. The trap must then be regenerated, this meaning that the soot is oxidized and converted to carbon dioxide mainly. There are active and passive regeneration procedures, the former ones increasing the exhaust temperature by late injection or specific post-burners or post-heaters located upstream the DPF, and the latter ones decreasing the soot oxidation temperature by means of additives or catalysts or taking advantage of the NO₂ formed in the oxidation catalyst. There are also combined methods called active-passive regeneration, such as the one used here [1].

An enhanced understanding of the particle accumulation and regeneration processes is essential for a proper calibration of the engine through the Electronic Control Unit (ECU) actuation, which, depending on the estimated mass of accumulated soot and on the current thermal conditions registered in the exhaust pipe, may decide either to set the engine into the regeneration mode, to advise the driver changing his driving condition to other more aggressive one favoring regeneration, or even to recommend the driver to stop in a garage for manual cleaning. The precise modeling of the mentioned processes under the most typical driving

conditions will help designers to optimize the engine performance and emissions as well as to extend the life of the DPF.

The main targets of the DPF modeling are, on the one hand, to relate the pressure drop across the filter to the accumulated mass of soot at any operating condition, and on the other hand, to predict the kinetics of soot accumulation, depending on the exhaust temperature. As the DPF temperature increases, soot oxidation becomes more significant. When the break even temperature (BET) is reached, oxidation compensates accumulation, this leading to no further increase in the pressure drop [2]. The BET depends on the operating mode, on the fuel used, on the eventual use of catalysts (in the filter) or fuel-borne additives and on the presence of an oxidation catalyst upstream the DPF, since the generated NO₂ favors downstream oxidation. Some of these parameters affect the morphology of soot agglomerates, and consequently their oxidation reactivity [2][3].

EXPERIMENTAL FACILITIES

Engine tests were carried out in a 4 cylinder, 4-stroke, turbocharged, intercooled, common-rail, 2.0 L Nissan diesel engine (model M1D) with rate power 110 kW, with intercooled EGR and equipped with oxidation catalyst (DOC) and regenerative wall-flow DPF. The engine was linked to an asynchronous electric brake Schenck Dynas III LI 250. The main specifications of the engine are given in Table 1, and those of the DPF (which is shown in Figure 2) are listed in Table 2. The brake control system permitted to measure and control the engine speed, throttle position and torque. The software INCA PC and the hardware ETAS ES 591.1 were used for the communication and management of the ECU. Since emissions are strongly dependent on the exhaust gas recirculation (EGR) ratio, it was important to keep this parameter fixed at a given mode. For this reason, the EGR valve was driven by means of the software INCA PC. Fuel consumption was measured with a gravimetric fuel balance AVL 733-S, and air consumption with a hot-wire sensor Siemens 5WK9628. The engine was also equipped with the necessary instrumentation for the measurement and monitoring of operating temperatures and pressure (intake air, fuel, lube oil, and specifically upstream and downstream the DPF).

Oxygen and carbon dioxide emissions were determined with a non-dispersive infrared analyser MIR, in order to obtain the oxygen partial pressure in the exhaust stream and the EGR rate. A dilution minitunnel Horiba MDLT 1304 was used to measure the particulate emissions. The soot content of the particulate matter was obtained after extracting the volatile fraction with a thermogravimetric analyser (TGA) TA Instruments Q500, following the method described in reference [4]. Finally, a scale (Kern DS 15K0.05) with 0.05 g

accuracy was used to measure the accumulated soot through eventual DPF weighing.

Table 1. Engine characteristics

Fuel injection system	Bosch CP1H high pressure pump electronically controlled (1600 bar)
Injection pressure	270 bar at idle (750 min ⁻¹) 1323 bar at full load (at 2000 min ⁻¹)
Max. rated power	111 kW (at 4000 min ⁻¹)
Max. rated torque	323.5 Nm (at 2000 min ⁻¹)
Cylinders arrangement	4, in line
Bore (mm)	84
Stroke (mm)	90
Swept volume (l)	2.0
Compression ratio	16:1

The exhaust configuration was modified to include a by-pass system, in order to enable the soot emissions measurements with and without DPF. These measurements provided the soot concentration upstream and downstream the DPF respectively, therefore enabling the estimation of its filtering efficiency (see Figure 1).

Table 2. DPF Characteristics

Material	Silicon Carbide (SiC)
Geometric configuration	Width (190 mm) Length (240 mm)
Structure	16/200
Catalyst	Coated with Pt 90 g/ft ³ (0.0032 g/cm ³)
Volume	4.1 L
Wall width (w_w)	0.4064 mm
Channel width (α)	1.3897 mm
Density of the monolith cells	31 cells/cm ²
Number of channels	4249
Crossed area	137.1 cm ²
Fraction of the crossed area opened in the monolith	0.29933
Filtering area	3.11153 m ²
Specific filtering surface (S_p)	758.91 m ² /m ³

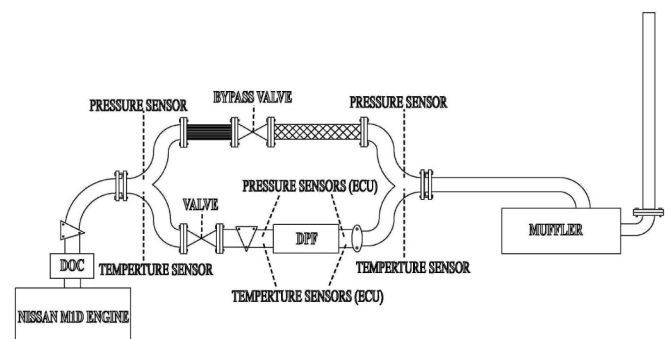


Figure 1. Configuration of the engine exhaust and bypass system



Figure 2. View of the DPF

Two samples of the soot emitted by the engine were taken for each of the three tested modes by means a vacuum pump at moderate temperature to avoid water condensation and a chemically resistant PTFE membrane Pall R2PL047. The first sample was used to measure the porosity of the soot accumulated in the filter cake with a porosimeter Micromeritics Gemini V 2380, following two methods: the BJH method developed by Barrett, Joyner, and Halenda [5] and the BET method developed by Brunauer, Emmett and Teller [6]. The measurements were made prior and after an external packing, for which a force equivalent to the pressure drop measured along the DPF (corresponding to each operating mode) was applied. The characteristics of the analysed soot cake corresponding to mode U9 are shown in Table 3 as an example.

Table 3. Measured characteristics of the unpacked and packed soot cake for mode U9

Soot cake	Unpacked	Packed
Packing pressure (hPa)	0	80
BET Surface area (m ² /g)	222.37	200.64
BET total volume of pores (cm ³ /g)	0.402	0.324
BJH absorption cumulative area of pores (m ² /g)	200.61	179.92
BJH Adsorption cumulative volume of pores (cm ³ /g)	0.388	0.309

From the results obtained with the BET method, and assuming an inherent soot density of 1850 kg/m³ [7], a porosity of $\varepsilon_{cake-up}=0.4267$ is obtained for the unpacked soot cake and a porosity of $\varepsilon_{cake-p}=0.3752$ is obtained for the packed soot. From the results obtained with the BJH method, porosities of $\varepsilon_{cake-up}=0.4179$ and $\varepsilon_{cake-p}=0.3636$ are obtained, they being around 2.5 % lower than those obtained with the BET method. The BET porosity results were finally selected for the pressure drop modeling.

The second soot sample (for each mode) was used to measure the activation energy and the pre-exponential factor of the Arrhenius-type equation simulating the oxidation process with air by means of the above mentioned thermogravimetric

analyser. The method for the determination of these parameters is described in reference [2].

SELECTED OPERATING MODES AND FUEL

Three engine operating modes were selected among the collection of steady operation modes that reproduce the New European Driving Cycle that the vehicles equipped with this engine must follow. After measuring all the engine emissions, pressures and temperatures in all modes reproducing the whole cycle, the mentioned three modes were selected by considering the following parameters: a) smoke opacity and particulate emissions, when the exhaust flow was conducted along the by-pass system, and b) pressure and temperature histories up and downstream the DPF, when the flow was conducted through it. The first mode (U9) is a low-load mode, belonging to the urban sub-cycle, with high soot emissions and therefore with high contribution to the DPF charge. The temperature at this mode remains always below the BET. The second mode (EU8) is a medium-load mode, belonging to the extra-urban sub-cycle, in which the balance of soot charge versus spontaneous soot regeneration leads to a slow DPF charging, the temperature at the exhaust manifold being high enough to permit active regeneration. The third one (EU16) is a high-load mode, also belonging to the extra-urban sub-cycle, in which the spontaneous regeneration leads to a net DPF discharge, the active regeneration becoming useless. These modes include all the processes which may take place in the DPF during the vehicle operation, and therefore, their modeling could be extrapolated to any other engine mode. Each of these modes was characterized by its engine speed, effective torque, brake mean effective pressure and EGR ratio. These values, together with the emissions and pressure and temperature losses along the DPF, are listed in Table 4. The engine was operated from cold (ambient) conditions until the DPF was charged up to its pressure drop limit (established by the ECU calibration) or until the pressure drop reached a stable value.

Table 4. Operating conditions and emissions of selected modes

Measured variables	Units	U9	EU8	EU16
PM (without DPF)	g/h	6.58	11.54	11.37
Maximum T upstream DPF	K	361	390	429
Maximum T downstream DPF	K	320.5	359	400
Pressure loss with clean DPF	hPa	4	6	13
Air flow	kg/h	77.71	103.61	186.95
Fuel flow	kg/h	3.90	5.34	9.25
Speed	rpm	1667	1972	2276
Torque	Nm	78	95	164
EGR (initial – final)	(%)	26.23 – 23.63	23.76 – 22.23	16.88 – 15.13
Oxygen molar fraction in the exhaust gas (initial-final)	(%)	6.99 – 6.24	7.32 – 5.90	5.56 – 5.56
Opacity (with DPF)	(%)	0.36	0.33	0.56
Opacity (without DPF)	(%)	14.64	17.40	3.10
Efficiency of DPF	(%)	98.18	98.66	82.38

Table 5. Fuel properties

ρ (kg/m ³) ^a	811
ν (cSt) ^b	1.99
LHV (MJ/kg) ^c	43.16
% C (in weight)	86.68
% H (in weight)	13.32
% O (in weight)	0
ppm S (in weight)	< 10 ^e
MW ^f	187.4 ^g
AFR _{st} ^h	14.59
Cetane Number	65.4 ^e

^aDensity, measured at 15°C;

^bKinematic viscosity, measured at 40°C;

^cLow heating value;

^eMeasured by fuel supplier;

^fMolecular weight;

^gCalculated using the Aspen-Advisor software;

^hStoichiometric air-fuel ratio.

In order to serve as a future reference fuel for studying the effect of fuel on the DPF charging process, the fuel used here is a net petroleum first-fill diesel fuel fulfilling EN-590 norm, with no FAME content, despite it is nowadays usual to find certain FAME content in the commercial fuels in Europe. It was supplied by Repsol. Its composition and main properties are presented in [Table 5](#).

CFD SIMULATION

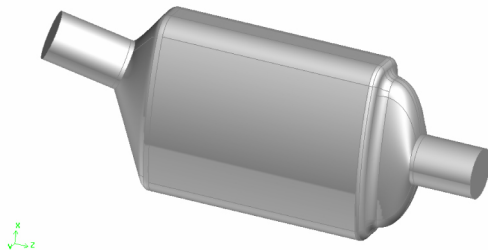


Figure 3. Geometry of the DPF

Previously to the simulation of the fluid-dynamic response of the DPF, the software GAMBIT was used to build up the mesh, this being adapted to the geometry shown in [Figure 3](#). The mesh was a hybrid one with hexahedrons in the filter and the channels and tetrahedrons with a prism layer at the wall in the cones. It was composed of 783581 cells. Fluent 12.1 was used for fluid-dynamic computation, for which steady regime was considered, as well as a simple second-order upwind interpolation for both pressure and velocity. A standard k- ϵ turbulence model and air (as fluid) were used, the viscosity of the latter being estimated with the Sutherland law. The diesel particulate trap was modeled as a porous medium based of the Darcy equation, with resistance coefficients adjusted to the experimental values. The temperature and pressure at the input and output sections were set as initial data, and the measured mass flow rate was used for confirmation of the

model accuracy. The walls were considered as adiabatic walls because skin temperature prediction was not the critical concern in this study. A residual convergence factor below 10^{-4} was always taken.

The results of the CFD simulation are presented in [Figures 4](#) and [5](#) for mode U9, in [Figure 6](#) for mode EU8 and in [Figure 7](#) for mode EU16. These results show, on the one hand, that pressure differences in the conical inlet are small with respect to the pressure losses along the DPF (see [Table 3](#)), and on the other hand, that the pressure field (and the velocity field although not shown here) becomes fairly uniform (therefore the radial mass transfer becoming negligible) at very small distances from the inlet section, this enabling the one-dimensional approach for the modelling of the pressure losses in a single channel.

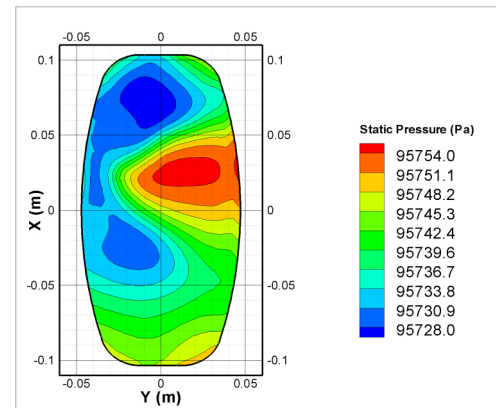


Figure 4. Pressure field in the DPF inlet section, mode U9

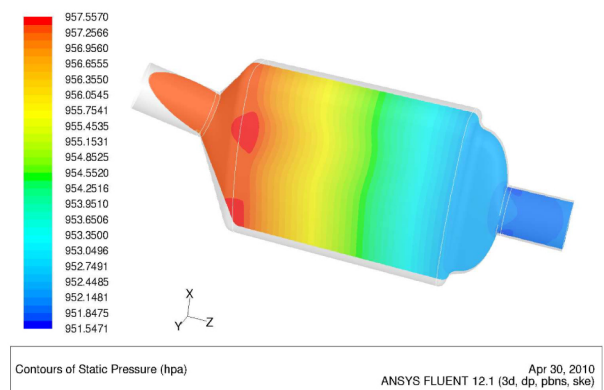


Figure 5. Pressure field along the DPF (hPa), mode U9