

Performance Assessment of a Multi-Functional Reactor Under Conventional and Advanced Combustion Diesel Engine Exhaust Conditions

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ABSTRACT

Current progress in the development of diesel engines substantially contributes to the reduction of NO_x and Particulate Matter (PM) emissions but will not succeed to eliminate the application of Diesel Particulate Filters (DPFs) in the future. In the past we have introduced a Multi-Functional Reactor (MFR) prototype, suitable for the abatement of the gaseous and PM emissions of the Low Temperature Combustion (LTC) engine operation. In this work the performance of MFR prototypes under both conventional and advanced combustion engine operating conditions is presented. The effect of the MFR on the fuel penalty associated to the filter regeneration is assessed via simulation. Special focus is placed on presenting the performance assessment in combination with the existing differences in the morphology and reactivity of the soot particles between the different modes of diesel engine

operation (conventional and advanced). The effect of aging on the MFR performance is also presented.

INTRODUCTION

Advanced Low-Temperature Combustion (LTC) technologies (such as the Homogeneous Charge Compression Ignition, HCCI) are successful in reducing simultaneously particulate and NO_x emissions. Still, the need for Diesel Particulate Filters will remain since advanced combustion is applicable to only a limited operating window (low to medium loads) and has to be combined with conventional combustion operation for higher engine loads [1, 2, 3]. The Low NO_x exhaust concentration during advanced combustion engine operation inhibits the NO₂-assisted (indirect) soot oxidation, causing difficulties in filter regeneration. In addition, the increased HC and CO concentration has to be taken into account when designing future emission control devices for the diesel engine.

This work concerns the evaluation of the Multi-Functional Reactor (MFR) for diesel exhaust treatment firstly presented in [4]. This paper presented the development efforts towards two novel aspects:

- A system design which exploits internal heat recovery.
- A multifunctional catalyst able to enhance the direct soot oxidation rate (i.e. through oxygen transfer), promote CO and HC oxidation and also promote the indirect (NO₂-assisted) soot oxidation.

Reference [4] described in detail the work towards the attainment of heat recovery and the advantages coming from it as well as the synthesis and application of the different catalytic functionalities on the filter substrate. A preliminary assessment demonstrated the improved performance of the full-scale MFR when compared to a Supplied for Assessment (SA) catalyzed wall-flow DPF (SiC, 6.66 in × 6 in, 300 cpsi, wall thickness 0.25 mm).

For the convenience of the reader, a summary of the data included in [4] is presented in the first section of the present paper. In the next section, the performance of the aged MFR is evaluated. Further on, simulation results with respect to the effect of the developed technology on the fuel consumption related to filter regeneration are presented. Then the MFR is assessed under advanced combustion engine operating conditions. Finally, the differences in the morphology and reactivity of soot particles from advanced and conventional combustion are examined.

PAST MFR DEVELOPMENTS

To enable heat recovery the target was to recover part of the energy released during the exothermic soot oxidation reaction. Due to the exothermic soot oxidation the downstream of the filter temperature is higher than the inlet temperature. The energy corresponding to the difference of the outlet and inlet temperatures was defined as the total recoverable energy (total heat released in the DPF as a result of the exothermic soot oxidation reaction). While several types of designs were considered, one specific design with the heat exchange function and the filtration function integrated with each other was chosen. This layout demonstrated significantly faster thermal response and more homogeneous in-filter temperature distributions during regeneration conditions compared to the standard wall-flow monolithic design. It also offered minimization of the heat losses to the environment during the filter operation compared to the conventional filter designs.

The catalyst incorporated a direct soot oxidation catalyst (base metal mixed oxide catalyst), a noble metal and Barium oxide (BaO). The doped mixed oxide catalyst was used for the enhancement of the direct soot oxidation rate. The noble metal (Pt) was used for the enhancement of the indirect soot

oxidation rate and the CO and HC conversion. BaO was included mainly to improve the local availability of NO₂ and “active” oxygen compounds for enhanced soot oxidation rate. The addition of the BaO was optimized towards this target and not the NO_x reduction due to the very low NO_x concentrations under LTC operating conditions. The Aerosol Based Synthesis (ABS) and the Aerosol Based Deposition (ABD) were used for the synthesis and application of the catalyst responsible for the direct oxidation of soot [5, 6, 7, 8]. Several formulations of Mixed Oxide Catalysts (MOC) have been investigated and the one with the optimal performance regarding soot oxidation and imposed filter pressure drop has been chosen. The BaO was added to the MOC precursor solution and synthesized and deposited simultaneously with the MOC. The Pt was incorporated into the catalyst layer upon the filter by the application of a washcoat and using a wet-chemistry technique, where the filter is impregnated into a solution of an appropriate Pt precursor.

Based on the above developments, a full-scale MFR was manufactured. The pressure drop of the full-scale MFR during soot loading was compared to the pressure drop of the full-scale wall-flow SA DPF that had the same filtration area under steady state engine operating conditions (1500 RPM, 3 bar BMEP). The evolution of the pressure drop as a function of the soot mass load for both systems is shown in the left graph of [Figure 1](#). The soot mass load is expressed in g of soot per m² of available filtration area. Such expression is constantly used by the authors as it allows the comparison of the pressure drop behavior during soot loading of different filter technologies. The filtration area is the relevant filter pressure drop parameter in contrast to the filter volume which is sometimes used in the literature. Before the start of the soot loading test the engine soot emission rate is gravimetrically measured. As the engine operates under constant conditions the engine soot emission rate is assumed to be constant throughout the test. The soot mass load is calculated from the engine soot emission rate assuming 100 % filtration efficiency. In the same graph the number-based MFR filtration efficiency is also presented. The number-based filtration efficiency was calculated from the measurements of the total number concentration upstream and downstream of the MFR via a Condensation Particle Counter (CPC) connected to a 3-stage mini dilution system.

For the evaluation of the regeneration ability of the MFR, the soot loaded filter was placed downstream of a standard (commercially available, cordierite, 1.8 L, 400 cpsi) Diesel Oxidation Catalyst (DOC) under steady state engine operating conditions (1500 rpm and 5 bar BMEP) corresponding to an inlet temperature of 340°C. HCs were injected upstream of the DOC to vary the filter inlet temperature in a step fashion. From the evolution of the pressure drop, during the regeneration, the soot oxidation rate

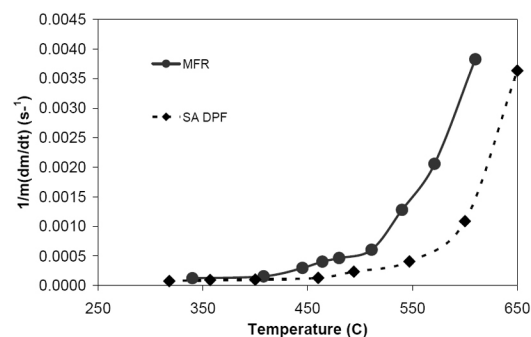
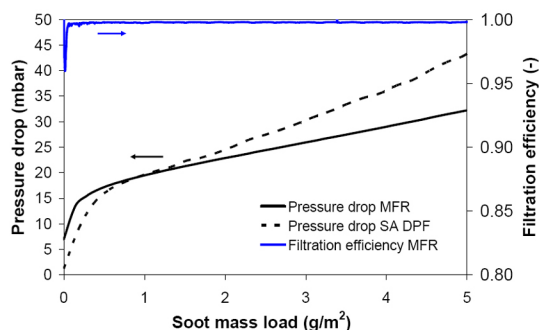


Figure 1. Study of the soot loading (left) and regeneration behavior (right) of the MFR and the SA DPF [4].

was calculated as a function of temperature by employing previously developed mathematical models [9,10]. In the right graph of Figure 1, the soot oxidation rate during such “step regeneration” test of the MFR and the wall-flow SA DPF with the same filtration area is illustrated as a function of the inlet filter temperature. Both filters exhibited similar soot oxidation rates up to 400 °C. However in the area of 450-550°C the MFR demonstrated highly improved soot oxidation activity, achieving a 3 times higher soot oxidation rate at 550°C compared to the SA DPF.

The performance of the full-scale MFR was also evaluated with respect to the exhaust gas conversion at steady state engine operating conditions. Good CO and HC oxidation performance was demonstrated while the NO₂-slip was negligible.

THE AGED MFR

AGING PROCEDURE

The aging procedure consisted of five consequent cycles. Each cycle included three steps. The first step referred to “soot loading” conditions (2000 RPM, 5 bar, exhaust temperature 310 C). The duration of the first step was 2 hrs. During the second step the MFR was operated at “regeneration” conditions (1500 RPM, 9 bar, exhaust temperature 500 C) for 1 hr. Finally, the “aging” step concerned engine operation at full load (3000 RPM, 10 bar, exhaust temperature 600 C) for 10 hrs. The same 3-step cycle was repeated five times. The entire procedure was equivalent to approximately 100,000 km of normal vehicle operation. The stated equivalency refers to the filter thermal exposure assuming filter regeneration every 500 km at 600 C with duration of 15 min. During this procedure the engine oil consumption was 470 g. A representative cycle is shown in Figure 2.

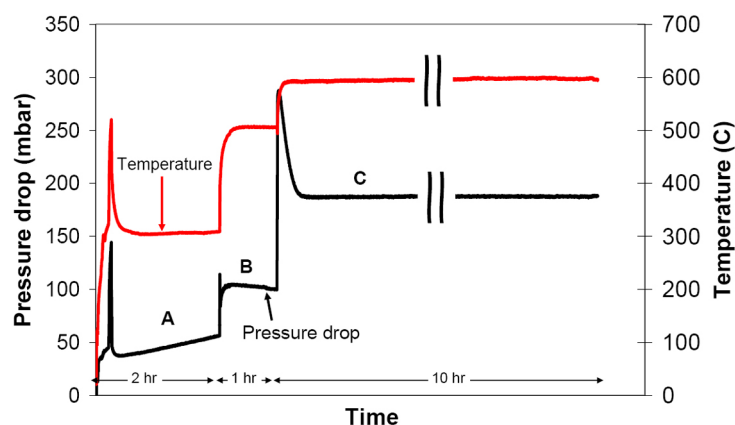


Figure 2. Pressure drop and temperature evolution during one cycle of the MFR aging procedure.

SOOT LOADING AND FILTRATION EFFICIENCY

The pressure drop of the fresh MFR sample was compared to the pressure drop of the aged prototype during soot loading. In both tests the filter was loaded with soot up to 5 g/m² at 1500 RPM, 3 bar BMEP and 250°C exhaust temperature. The aged MFR demonstrated somewhat increased pressure drop (approximately 20 %) compared to the fresh sample (Figure 3). This should be expected due to the ash particles accumulated during the aging procedure. The ash content of the engine oil was 0.95 % w/w. As the engine oil consumption was 470 g during the MFR aging, the amount of ash emitted from the engine should be approximately 4.5 g. The aging of the MFR did not cause any negative effect in the filtration efficiency of the MFR. On the contrary and even if this was very good from the fresh state, it became even better, probably due to the ash particles trapped by the filter.

The MFR was also tested under transient engine conditions. Twenty five New European Driving Cycles (NEDCs) were performed for the fresh and the aged MFR. The filtration efficiency was measured during the transient conditions by an opacity-meter and was found to be on average 98.5 % both for the fresh and the aged MFR. The results are shown in



Figure 3. Evolution of pressure drop during soot loading for the fresh and the aged MFR

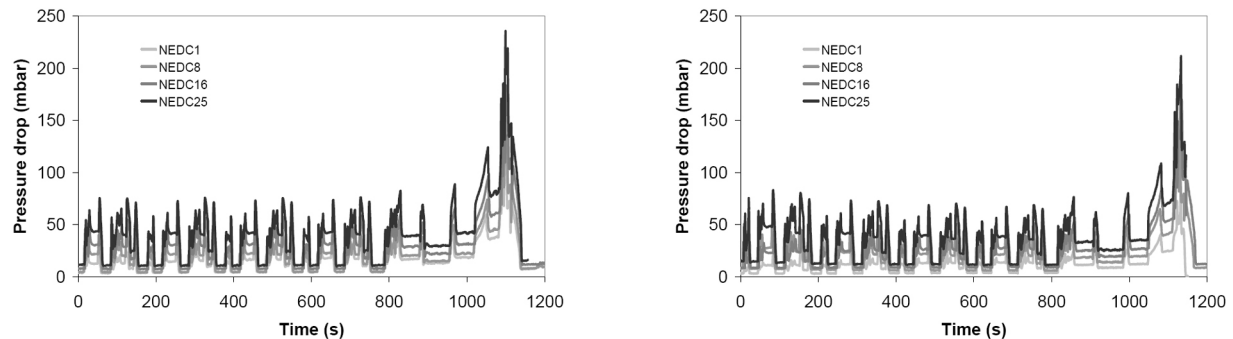


Figure 4. Evolution of the fresh (left) and aged (right) MFR pressure drop during the transient engine operation conditions

Figure 4. The pressure drop for the aged MFR is slightly decreased compared to the fresh MFR. This could be attributed to the lower engine soot emission rate during the testing of the aged MFR as the total soot mass collected by the fresh MFR was 18.2 g, while the total soot mass collected by the aged MFR was 16.3 g (measurements done by weighting the filter at clean and soot loaded state).

FILTER REGENERATION

In Figure 5 the variation of the soot oxidation rate with the inlet filter temperature is presented for the fresh and the aged MFR. The Figure includes data from “step regeneration” tests already described as well as data from “constant temperature regeneration” tests. In the second type of regeneration tests the filter is preloaded up to a certain amount of soot and then the inlet filter temperature is increased to a certain level (~ 500 °C) and kept constant until the filter is completely regenerated. Figure 5 reveals that the aging procedure did not have any significant negative effect on the soot oxidation rate and consequently the catalytic activity of the MFR. In fact, for temperatures higher than 500 °C, the soot oxidation rate is slightly increased for the aged MFR. This is inline with the results presented in [11] showing that ash particles can have an effect on the catalytic soot oxidation, which could be

positive or negative depending on the type of the catalytic coating involved. The regeneration of the aged filter was completed at 570 °C, therefore no soot oxidation rate measurement was done at 610 °C as was the case for the fresh MFR.

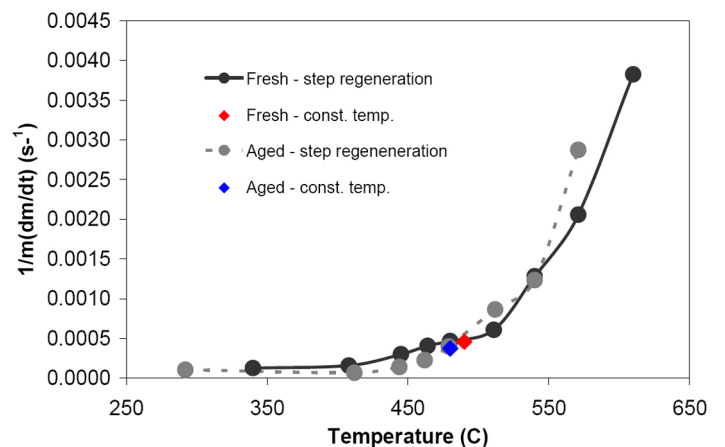


Figure 5. Soot oxidation rate as a function of inlet filter temperature for the fresh and the aged MFR

FUEL CONSUMPTION PREDICTION

For the prediction of the filter regeneration related fuel consumption all simulations were executed with the software GT-suite from Gamma Technology. GT-drive was one part of the software suite. The complete vehicle was set up including aerodynamic behaviour and mass inertia as well as transmission and engine characteristics. All transient data were taken from maps, which had been created with measured data. In this way also the engine characteristics regarding specific power, fuel consumption and emissions were integrated. To simulate the soot combustion and catalytic processes, the MFR and SA DPF were modelled in detail with GT-power with soot oxidation kinetic data obtained from small-scale tests described in [4]. The DOC (cordierite, 1.8 L, 400 cpsi, wall thickness 115 μm , Pt loading 90 g/ft^3) was modelled based on FEV's internally available experimental data. The sub-models were coupled with the GT-drive simulation, which provided the transient input in terms of exhaust gas temperature, mass flow rates and concentrations of gas components. The maps referred to an experimental car with FEV HECS engine (High Efficiency Combustion System) that is targeting NO_x -raw emission level below EU6 limits.

The engine data has been measured for standard operation and for a reference regeneration mode. In order to enable the simulation of different regeneration strategies and the related fuel penalties, the model required the possibility to change the amount of fuel that was injected in order to build up the required regeneration temperature. This was done by the model of an external fuel supply upstream of the DOC, which was not part of the real engine. Therefore in the model, fuel could be dosed directly into the exhaust system, where it was converted in the DOC to achieve the target exhaust gas temperature at the inlet of the MFR/SA DPF. In this way the external fuel supply either represents the late post injection in conventional regeneration strategies that is not converted inside the cylinder or an external fuel doser. Today systems with external fuel doser are in serial production with increasing market share. The conversion rate of the injected fuel within the DOC was implemented as a function of the DOC substrate temperature. The thermal inertia of the catalyst was taken into account in order to predict the correct heat up time of the system. Within the DOC module also the temperature raise of the exhaust gas in front of the MFR/SA DPF due to the exothermic HC conversion was calculated. The amount of fuel injection was setup in this way that ensured that all HCs were converted in the DOC. Thus, the dosing of fuel started only when the DOC temperature allowed the entire HCs amount to be oxidized. The combustion within the filter was simulated depending on the soot load, the oxygen concentration and the substrate temperature. To take into account the typically quite different temperature development in upstream and downstream areas of the MFR/SA DPF, the filter model consisted of 5 axial

slices. In each slice the Arrhenius equations of the local soot combustion and the equations for local heat exchange of the filter and the exhaust gas were solved. The soot load of the filter significantly influences the exhaust back pressure and consequently the engine operating point and the fuel consumption of the vehicle. The DPF pressure drop was implemented as a function of the soot load and was calibrated with test bench measurements [4].

Initial investigations in NEDC cycle with a real-time feasible, 0-D, Simulink model showed that the MFR offers a significant potential to lower the regeneration induced fuel penalty (Figure 6). The MFR fuel penalty advantage is increasing with decreasing regeneration temperature. This should be expected since catalytic soot oxidation is more important at lower temperatures. At higher regeneration temperatures, thermal soot oxidation is the key player, thus an advanced catalyst would contribute less at elevated temperatures.

Simulations with GT-Suite of MFR regenerations with typical regeneration temperature of more than 600 $^{\circ}\text{C}$ resulted in high substrate temperatures up to around 900 $^{\circ}\text{C}$ due to the high soot combustion rates unless the soot mass limit is properly adjusted (Figure 7). Due to the induced thermal stress the high substrate temperatures are not acceptable. Hence, the target temperature for the MFR was defined to 550 $^{\circ}\text{C}$, where the mean substrate temperature has its maximum below 700 $^{\circ}\text{C}$. For the SA DPF, the regeneration temperature was set at approximately 630 $^{\circ}\text{C}$ (common target regeneration temperature for catalyzed DPFs based on FEV's experience). Setting the regeneration temperature at lower than 630 $^{\circ}\text{C}$, would result in very low soot oxidation rate (as is evident in the experimental data in the right graph of Figure 1) and consequently very long regeneration duration and increased fuel penalty (as is evident in the simulation data in Figure 6) a fact that would be unjust for the comparison of the SA DPF with the MFR.

The results of the MFR fuel consumption simulations are compared with the ones of the SA DPF. The maximum soot load for the SA DPF was limited to 7 g/m^2 and for the MFR it was limited to 5 g/m^2 to avoid critical temperature peaks under thermo shock conditions. The implemented regeneration strategy switched back to standard engine operation, if a residual soot load of 0.5 g/m^2 had been achieved.

Table 1 gives an overview of the boundary conditions for the regeneration simulation. The NEDC was used as a base for the investigations of fuel consumption and exhaust emissions. The behavior of the tested filters under real driving conditions was also investigated. Therefore, beside the NEDC, three FEV standard off-cycle driving patterns, which are taken from measurements during test runs on roads