

Understanding of the Internal Crack Phenomenon inside Diesel Particulate Filter during Regeneration

Part 1: Modeling and Experiments

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ABSTRACT

This study deals with a coupled experimental and modeling approach of Diesel Particulate Filter cracking. A coupled model (heat transfer, mass transfer, chemical reactions) is used to predict the temperature field inside the filter during the regeneration steps. This model consists of assembled 1D models and is calibrated using a set of laboratory bench tests. In this set of experiments, laboratory scale filters are tested in different conditions (variation of the oxygen rate and gas flow) and axial/radial thermal gradient are recorded with the use of thermocouples. This model is used to build a second set of laboratory bench tests, which is dedicated to the understanding of the phenomena of Diesel Particulate Filter cracking.

INTRODUCTION

With the increasing stringency of European and global environmental standards regarding the emissions of particles eligible at the exhaust of diesel vehicles, the implementation of Diesel Particulate Filters (DPF) into the exhaust line is now mandatory on Diesel vehicles. To ensure the proper engine working, soot must be burned periodically. During this regeneration step under specific conditions (high amount of oxygen in the exhaust gas, low gas flow rate) the thermomechanical strength of the material might be exceeded, leading the filter to crack.

Mizutani *et al.* [1] studied the cracking phenomenon of SiC DPF. They carried out “back to idle” tests characterized by a sharp decrease of the exhaust gas flow rate and a high amount of oxygen in the gas. These “back-to-idle” tests showed that the appearance of cracks on the outer face of the filter was correlated with the radial thermal gradient measured close to the DPF outer face (measured between the center of a central

segment and the outside corner of the same segment). They also observed that when the maximum temperature gradient exceeds a threshold value, cracks systematically appear on the outer face. Briot *et al.* [2] showed the link between the intensity of maximum temperature gradient within the filter and the level of cracking of the filter. The level of cracking was characterized both by measuring the attenuation of the propagation velocity of an ultrasonic signal between a new filter and a damaged filter and by counting the number of internal cracks by visual analysis after cutting the monolith. This study also showed that a high density of cracks leads to a decrease of the system filtration efficiency (evaluated by measuring FSN index on filter before and after the severe regeneration).

This work takes place in the context of a study on understanding of DPF cracking phenomena. The two main objectives of this work are:

- refine the design criteria of DPF through a better understanding of the impact of crack on the filter substrate.
- reduction of costs associated with the evaluation of new substrates : development of laboratory bench test methods and simulation tools to reduce the engine bench tests.

Two simulation tools are developed. The first model described in detail in this paper allows us to simulate temperature field inside DPF during regeneration. These temperature fields will be used as input data in a finite element model that allows the prediction of the associated stress field.

Many authors have studied the phenomena of DPF cracks appearing during engine bench tests [3, 4, 5]. The aim of this

work is to develop a methodology to analyze the thermomechanical strength of DPF at a laboratory scale.

This paper presents a simulation tool able to predict the temperature field inside DPF during a regeneration step. This simulation tool is a multi-1D model composed of a set of 1D component interacting through thermal conduction and gas flow balance, as did some authors [6, 7] for axisymmetrical modeling. This approach is similar to that developed by Mizutani *et al.* [1] for multi-1D modeling. A set of laboratory bench tests is described and used to show the accuracy of the simulation tool. Finally, a second set of experiments aiming to understand the phenomena of DPF internal cracking at laboratory scale is introduced.

MODELING OF DPF REGENERATION

The DPF regeneration model was implemented in the Matlab environment as a C S-function. It takes into account the phenomena of heat transfer (conduction, convection and radiation), mass transfer (transport of oxygen and gases) and chemical reactions (combustion of soot).

MODEL DATA

The [figure 1](#) shows the basic input/output and state variables used in the model to describe the behavior of DPF and gives an example of simulation results (remaining soot mass and temperature field) for an engine bench test with a strong heterogeneity of the thermal field at the DPF inlet.

(See [Figure 1](#) after last section of paper)

SET OF REPRESENTATIVE CHANNELS

For symmetry reasons only a quarter of the inlet and outlet channel is described ([Figure 2a](#)). Each elementary model consists of a quarter inlet channel, the porous wall and a quarter of outlet channel. The 1D model is subdivided in the x direction into elements, whose length is approximately $\Delta x = 15$ mm ([Figure 2b](#)). Within each element, conductive heat transfer through the wall, convective heat transfer between the wall and the inlet/outlet channels, mass transfer and chemical reactions are taken into account.

(See [Figure 2](#) after last section of paper)

The set of channels was chosen considering the DPF macro geometry ([figure 3](#)).

(See [Figure 3](#) after last section of paper)

Due to the geometry of the laboratory bench test, the temperature field in front of the DPF is considered to be

axisymmetric. We also assumed that the soot loading is the same in the four quarters of the DPF. Following those assumptions, we considered that the behavior of the whole filter can be modeled with only one quarter of DPF.

On the filter outer skin, the heat flow Φ exchanged with the external environment takes into account the radiative and convective exchange:

$$\phi = h.S.(T_{out} - T_w^n(X, Y, Z, t)) + \varepsilon.\sigma.S. \dots (T_{out}^4 - (T_w^n(X, Y, Z, t))^4) \quad (1)$$

MODELING OF GAS FLOW

To simplify and accelerate the numerical calculation of mass transfer and pressure drop across the filter, we consider stationary flow conditions.

The description of the flow field is derived from the work of Mizutani *et al.* [1].

The main hypothesis of this work is the following:

- 1). No impact of the inlet cone shape on the DPF gas flow distribution
- 2). Pressure losses by friction of gas along the channel, contraction of the gas at the entry of inlet channels and expansion of gas at the exit of outlet channels are considered to be negligible to those induced by the passage of gas through the porous walls (simplification of the momentum conservation equation).
- 3). The pressure loss in the porous medium (soot and wall) is described by Darcy's law:

$$\Delta P(x, t) = \frac{-\mu.Q_{Gv}^w(x, t)}{k_{eq}.S_f}.\Delta w \quad (2)$$

These assumptions allow regarding the DPF as a set of parallel porous media, concerning the flow resistance. By equivalence with an electric circuit, the global flow resistance for the whole DPF can be computed from the local resistances, and the local flow within each element of the 1D model has the following analytical expression:

$$Q_{Gm}^f(X, Y, Z, t) = \frac{Q_{Gm}}{R(Y, Z, t) \sum \frac{1}{R(Y, Z, t)}} \quad (3)$$

CONTINUUM EQUATIONS

Mass conservation (1D)

The filtration gas flow field is determined from [equation 3](#) in the whole filter. The gas mass flow in the inlet (ic) and the outlet channels (oc) are derived from the filtration gas flow field using the mass conservation equation:

$$Q_{Gm}^{ic}(x + \Delta x, t) = Q_{Gm}^{ic}(x, t) - Q_{Gm}^{fic}(x, t) \quad (4)$$

$$Q_{Gm}^{oc}(x + \Delta x, t) = Q_{Gm}^{oc}(x, t) + Q_{Gm}^{foc}(x, t) \quad (5)$$

Energy conservation (gas phase)

The conservation equations in the inlet channel, outlet channel and within the porous medium (substrate and soot) respectively are presented below:

$$\begin{aligned} \rho_G^{ic} C_{PG} \Delta V_{ce} \frac{\partial T_G^{ic}(x, t)}{\partial t} = \\ Q_{Gm}^{ic}(x - \Delta x, t) C_{PG} T_G^{ic}(x - \Delta x, t) - \\ Q_{Gm}^{ic}(x, t) C_{PG} T_G^{ic}(x, t) - Q_{Gm}^{foc}(x, t) C_{PG} T_G^{ic}(x, t) + \\ h_{ic} S_{ic}(x, t) (T_S^{wic}(x, t) - T_G^{ic}(x, t)) \end{aligned} \quad (6)$$

$$\begin{aligned} \rho_G^w C_{PG} \Delta V_G^p \frac{\partial T_G^w(x, t)}{\partial t} = \\ Q_{Gm}^{fic}(x, t) C_{PG} T_G^{ic}(x, t) - Q_{Gm}^{foc}(x, t) C_{PG} T_G^w(x, t) + \\ h_p \Delta S_w (T_S^w(x, t) - T_G^w(x, t)) \end{aligned} \quad (7)$$

$$\begin{aligned} \rho_G^{oc} C_{PG} \Delta V_{cs} \frac{\partial T_G^{oc}(x, t)}{\partial t} = Q_{Gm}^{oc}(x, t) C_{PG} T_G^{oc}(x, t) - \\ Q_{Gm}^{oc}(x + \Delta x, t) C_{PG} T_G^{oc}(x + \Delta x, t) + \\ Q_{Gm}^{foc}(x, t) C_{PG} T_G^{oc}(x, t) + h_{oc} \Delta S_{oc} (T_S^{oc}(x, t) - T_G^{oc}(x, t)) \end{aligned} \quad (8)$$

Conservation of energy in the solid phase

The conservation of energy in the porous wall takes into account the heat transfer by convection with the gas flowing through the channels, the energy released by the combustion of soot, the conduction inside the 1D model and the conduction between the neighboring 1D models:

$$\begin{aligned} (\rho_s^w C_{PS} \Delta V_s^w) \frac{\partial T_s^w(x)}{\partial t} = \sum_{j=oc,ic} h_j \Delta S_j (T_G^j(x, t) - T_s^j(x, t)) + \\ h_w \Delta S_w (T_G^w(x, t) - T_s^w(x, t)) + \frac{\partial m}{\partial t} \cdot \Delta H_{soot \rightarrow CO_2} + \\ \frac{\lambda_s \cdot A_x}{\Delta x} \cdot (T_s^w(x - \Delta x) - 2 \cdot T_s^w(x) + T_s^w(x + \Delta x)) + \\ \sum_{N_{nc}} \frac{\lambda_{nc} \cdot A_{app}}{\Delta L_{nc}} \cdot \frac{1}{N_{neighbour. channels}} (T_s^{wnc}(x, Y_{nc}, Z_{nc}) - T_s^w(x, Y_w, Z_w)) \end{aligned} \quad (9)$$

In the equations presented above, simplifying assumptions are made to reduce the number of variables and allow the development of an efficient numerical algorithm. More details are presented in [reference \[8\]](#).

Soot combustion

Regarding soot loading, some assumptions are made to simplify the problem. The single soot layer model is retained (as compared to the two layers model proposed by Konstandopoulos *et al.* [9]). The assumption of a homogeneous loading in the filter at the beginning of the regeneration step is taken for the calculations.

In the studied application, the catalytic coating inside DPF allows the oxidation of CO to CO₂. We therefore consider that the enthalpy of combustion is the complete oxidation of carbon to CO₂. Soot is considered to be composed of two populations with different behaviors. The first part is mainly composed of carbon, while the second one corresponds to oxygenated species whose oxidation starts at 300°C to 400°C, with lower activation energy than the one of carbon [10]. Since the PGM loading of the filter is low and the soot-catalyst contact is poor in this type of DPF, we do not consider a catalyzed soot oxidation process.

The oxidation of total soot mass *m* at time *t* depends on the initial masses of soot A and B in the filter, temperature *T* and oxygen concentration in the exhaust gas:

$$\begin{aligned} \frac{dm}{dt} = \frac{dm_A}{dt} + \frac{dm_B}{dt} \quad \text{with} \\ \frac{dm_A}{dt} = -k_A \cdot e^{\frac{-E_{a_A}}{RT}} \cdot m_A(t) \cdot \chi_{O_2} \quad \text{and} \\ \frac{dm_B}{dt} = -k_B \cdot e^{\frac{-E_{a_B}}{RT}} \cdot m_B(t) \cdot \chi_{O_2} \end{aligned} \quad (10)$$

LABORATORY BENCH TESTS - KINETICS OF SOOT COMBUSTION

A set of experiments aiming at determining the kinetic parameters of soot combustion and heat transfer parameters in the DPF has been achieved.

The material used for these tests is R-SiC. These samples have been specially designed with dimensions (58*150mm) suitable for laboratory bench tests. They are made by assembling 4 segments connected by cement ([figure 4](#)).

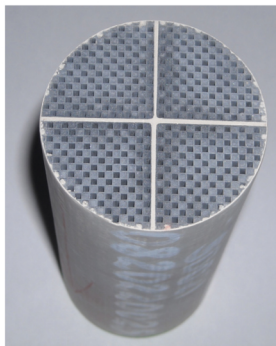


Figure 4. Laboratory scale R-SiC DPF filter

All samples are loaded with real Diesel soot, on a 2L Diesel engine bench test. The engine was performed on repeated extra-urban part of the New European Driving Cycle, until initial soot mass of 10g/L was loaded in the filters.

Samples were placed in an oven during a few minutes at 100°C and weighted, before and after the oxidation test.

[Table 1](#) summarizes the oxidizing conditions that have been tested.

(See [Table 1](#) after last section of paper)

During these experiments, the tested scenario was an increase of gas temperature at 15°C/min, followed by a temperature stabilization step (at 600 or 630° C). The impact of Gas Hour Space Velocity (GHSV) defined as the ratio of exhaust gas flow divided by the substrate volume has also been studied.

During each test, we recorded the temperature inside the monolith using 5 thermocouples (TCK-0.5 mm).

[Figures 5](#) and [6](#) present the thermocouple instrumentation used. In addition, we also recorded the temperatures 10 mm before (TCK6) and after (TCK7) the DPF and on the canning surface (TCK8).

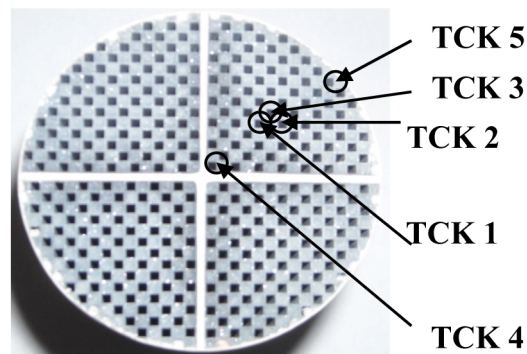


Figure 5. Thermocouples instrumentation (outlet face view)

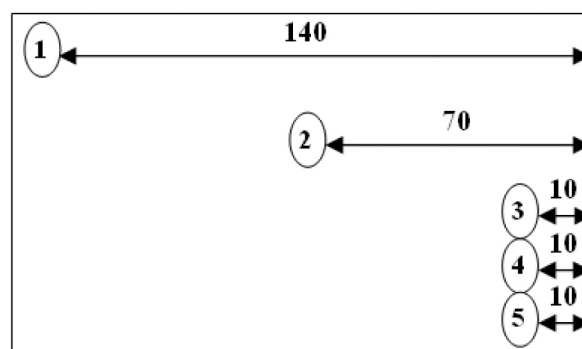


Figure 6. Thermocouples location (longitudinal view)

A gas analyzer was used to measure the amount of CO_2 (in ppm) after the DPF. [Figures 7](#) and [8](#) give an example of measurements for the test D ([table 1](#)).

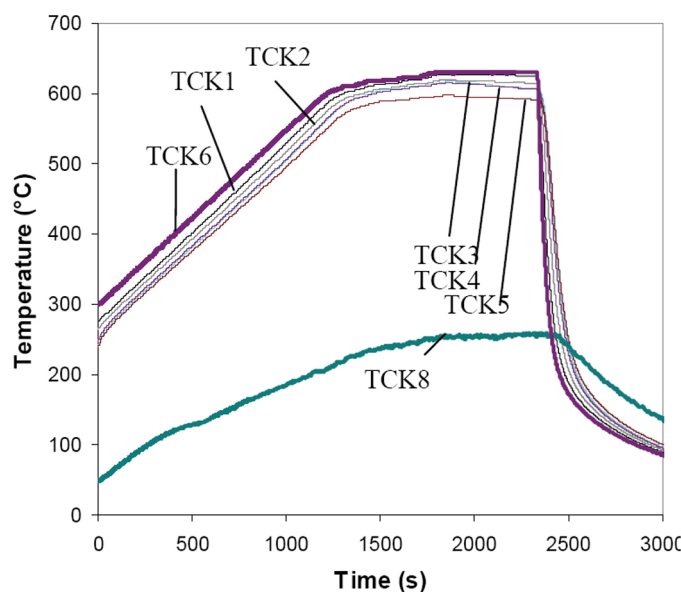


Figure 7. Measured temperatures during test D