Computer Aided Engineering of Diesel Filter Systems

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ABSTRACT

Increasingly stringent international diesel particulate emissions standards have re-established interest in Diesel filters. Modern Diesel engine technology, with computerized engine management systems and advanced, common rail injection systems, needs to be fully exploited in order to allow the application of efficient and durable Diesel filter systems, usually supported by catalytic aids, as standard equipment in passenger cars. Significant manpower, computational and testing resources are invested in this effort and mathematical models are indispensable in components', control and overall system optimization. In this paper, a model of Diesel filter operation adapted to work in Simulink environment is applied to regeneration control system optimization.

INTRODUCTION

Cellular ceramic diesel particulate filters with catalytic assistance have demonstrated the capacity to attain the extremely stringent particulate matter emissions of EPA Tier II and EURO 4 – EURO 5 standards, both for passenger cars and heavy duty vehicles. Diesel filter systems date back to the eighties [1]. Nevertheless, series application was not realized until recently, because of problems regarding filter reliability and durability, which were associated with the regeneration control of the filter [2]. During regeneration, the accumulated particulate matter is oxidized to CO_2 and CO. The soot oxidation reactions are followed by significant heat release, which may endanger the integrity of the filter under certain operating conditions: for example, during a sudden vehicle deceleration occurring shortly after the onset of regeneration in a heavily loaded filter, which results in high oxygen concentration and low mass flow rates in the filter inlet gas stream. To enable the onset of regeneration at low temperatures, Diesel filter systems currently installed on passenger cars are assisted by catalytic fuel additives or washcoated filters [3]. In addition, the capabilities of modern Diesel engine management and common rail injection systems (post injection) are employed to increase engine exhaust gas temperature when necessary. A Diesel oxidation catalyst and a NOx storage catalytic converter may also be present in the exhaust system. The design of an efficient system of this type is a demanding task. The need for engineering modeling tools has thus emerged [4, 5] in order to aid the Diesel filter and overall exhaust system design and optimization. Engineering models of Diesel filter regeneration should be developed having in mind the level of design optimization detail, data availability, computational cost and model consistency and reliability. For the concept analysis and preliminary design phase, simpler models are preferable. Difficulty in model development and validation grows rapidly with increase of model complexity, a fact that might create uncertainty about the reliability of highly complex models' results. Furthermore, sophisticated models with many degrees of freedom also require very detailed input data for their full exploitation, such as velocity profiles of the exhaust gas or complex reaction kinetics. Such data are not easy to get with the routine measurements that are usually employed in the framework of design engineering tasks. More sophisticated models also require higher expertise from the user, as well as higher computational and pre- and post-processing expenditure.

This paper addresses the control – oriented application of an engineering model of Diesel filter regeneration. The model is already applied in real world system design tasks, embodied in a complete methodology which comprises, apart from code development (including pre- and post-processing modules), code tuning and validation, experiment design and test data acquisition and quality assurance. It is a 1D model that has been extensively validated in the past [6, 7, 8]. The version employed in the current study runs in the MATLAB/ Simulink environment and mainly supports system and control design optimization. The support of detailed component design optimization tasks is also possible, based on the linking to commercial FEM software for the computation of the 3D temperature and stress field within the whole filter assembly [9].

CATALYTIC REGENERATION MODELING – SIMULINK IMPLEMENTATION

Chemical phenomena in Diesel filter regeneration include the combustion of the soot layer because of thermal and catalytic reactions and the adsorption, desorption and combustion of hydrocarbons contained in the soot particles (Volatile Organic Fraction – VOF content). The primary physical phenomena include heat conduction, convection and radiation in the filter and flow distribution in the channels, which interacts with axial and radial soot distribution within the filter. The first attempt to provide a mathematical description of the regeneration process of the soot layer was the pioneering work of Bissett [10] (zero-dimensional, averaged flow and soot distribution within the filter channels), which was extended to 1-D, also accounting for the axial heat conduction and the soot layer and flow distribution along the channel [11]. This work has been adopted and extended in [12], supported by experimental validation of high space velocity thermal regeneration events, with a systematic methodology of filter loading assessment by energy balances. It was further extended to cover catalytic regeneration, in zero-dimensions and also in 1-D [6]. During the last years, numerous models have been

presented in the literature along the same guidelines, with minor improvements and extension to higher dimensions, usually keeping the simplified reaction scheme of thermal Carbon oxidation. This limits their applicability because all Diesel filter systems in use today employ some catalytic aid. For this reason, the model presented here features an inclusive reaction scheme for the thermal and catalytic soot regeneration (Table 1).
The details of the mathematical treatment that refers to a unit computational cell, consisting of one inlet channel and four quarters of the four adjacent outlet channels, are given in [8]. The balance equations pertinent for regeneration modeling are applied to a fundamental volume of the cell of length Δz, where a soot layer of mass m and thickness w has accumulated. Exhaust gas species are consumed or produced as gas flows through the soot layer, which consists mainly of carbon and adsorbed hydrocarbons. Since the fuel additive takes part in the combustion process and the formation of particulate, the soot deposited in the filter contain bonded metal oxide particles, which are able to oxidize the Volatile Organic Fraction (VOF) and the Carbon at low temperatures.
The kinetic model employed herein accounts for catalytic soot oxidation by a Ce-based fuel additive, but does not include the effect for the VOF. The first step of the mechanism is oxidation of Ce_2O_3 by O_2 to produce CeO_2. The second step involves reduction of CeO_2 to Ce_2O_3 by carbon. The reactions along with their respective rate expressions and typical parameter values are given in Table 1. For the oxidation of Carbon and Ce_2O_3 by exhaust gas oxygen, the rate is proportional to the oxygen concentration in the exhaust gas. In the two reactions of catalyst assisted regeneration the quantity ψ, which represents the percentage of mol Ce being in its higher oxidation state CeO_2 , is employed. Also, the term ξ, defined as the concentration of catalyst in the soot layer is employed. This is a function of metal additive concentration in the fuel and the engine soot emissions accumulated on the filter wall. Both ψ and ξ are viewed as averaged quantities along the soot layer thickness.
As gas flows through the soot layer, its oxygen content is gradually depleted by reacting with carbon and Ceria. The resulting oxygen concentration profile through the soot layer is thus expressed by the oxygen mass balance:

$$\frac{\dot{m}_g}{A(x)}\frac{dy}{dx} = -M_g\left(k_1 + 0.5k_2 + 0.5k_5(1-\psi)\right)y \qquad (1)$$

Table 1 Reactions and rate expressions of the regeneration model, with typical kinetic parameter values

	Reaction	Rate expression	Pre-exponential factor (A) (mole/m^3,s)	Activation Energy (E) (kJ/mole)
1	$C + O_2 \longrightarrow CO_2$	$r_1 = k_1 y$	1E13	190
2	$C + 0.5O_2 \longrightarrow CO$	$r_2 = k_2 y$	5.5E10	150
3	$C + 4CeO_2 \longrightarrow 2Ce_2O_3 + CO_2$	$r_3 = k_3 \psi$	4.5E11	120
4	$C + 2CeO_2 \longrightarrow Ce_2O_3 + CO$	$r_4 = k_4 \psi$	4E8	80
5	$Ce_2O_3 + 0.5O_2 \longrightarrow 2CeO_2$	$r_5 = k_5(1-\psi)$	1E12	80
	where: $k_i = A_i e^{-E/R_g T}$, $i = 1 \ldots 5$			

The above mass balance may be solved to get the oxygen concentration profile, assuming of homogeneous soot layer temperature [10]. The solution yields the total consumption of oxygen through the soot layer, which is employed to calculate the rate of soot consumption because of both thermal and catalytic oxidation:

$$\rho_p \frac{dV}{dt} = \frac{M_C}{M_g}\frac{k_1 + 0.5k_2}{k_1 + 0.5k_2 + 0.5k_5(1-\psi)}\dot{m}_g \Delta y - M_C k_5 \psi V_p \qquad (2)$$

A mass balance is also formulated for ψ, which expresses the continuous transition of the catalytic additive between CeO_2 and Ce_2O_3 states. According to the CeO_2 mass balance, the rate of change depends on the additive oxidation and reduction reactions:

$$\xi\frac{d\psi}{dt} = -\frac{M_C}{\rho_p}(4k_3 + 2k_4)\psi + \frac{k_5(1-\psi)}{k_1 + 0.5k_2 + k_5(1-\psi)}\frac{\dot{m}_g}{\rho_p V_p}\frac{M_C}{M_g}\Delta y \qquad (3)$$

The two mass balance equations for soot and Ceria are solved with the respective initial conditions.
Finally, a heat balance equation, expressing the accumulation of heat in the soot layer and the ceramic wall because of reaction heat generation and heat conduction perpendicular to the soot layer and wall and (c) heat exchange between the gaseous and the solid phase, is integrated to yield the heat release rate dQ/dt

$$\frac{dQ}{dt} = \left(\rho_p c_{p,p} V_p + \rho_s c_{p,s} V_s\right) = \\ = -\frac{(\Delta H_1 k_1 + \Delta H_2 k_2)}{k_1 + 0.5k_2 + 0.5k_5(1-\psi)}\frac{\dot{m}_g}{M_g}\Delta y - (\Delta H_3 k_3 + \Delta H_4 k_4)\psi V_p + \dot{m}_g c_{p,g}\left(T - T_g^{in}\right) \qquad (4)$$

Now, the total pressure drop across the particulate layer and the ceramic wall can be expressed as the sum of the porous ceramic substrate pressure drop and the soot layer pressure drop. Following [13], pressure drop across the porous walls of the ceramic filters is approximated by Darcy's law, which may be written as follows by employing the concept of effective particulate layer thickness [14]:

$$\Delta p = p_{in} - p_{out} = \frac{\mu u_w w_s}{k_s} + \frac{\mu u_w m_p}{A_f \left(\rho k\right)_p} \qquad (5)$$

This formula allows, in principle, the backward approximate calculation of collected soot mass as function of measured filter backpressure at a certain engine and filter loading operation point, once an approximate value for the product $(\rho k)_p$, (soot layer density -times- permeability) is known for the specific engine – filter – operation point combination. Since the regeneration process is essentially three-dimensional, especially at low flowrates, and significant flow and soot maldistribution is reported [15,16], the problem of reliably correlating pressure drop with soot mass prohibits the use of pressure drop signal as a simple indicator of soot mass.

The above pressure drop and regeneration model equations are valid for each point *z* along the filter axis, but do not provide any information regarding axial profiles of temperature, pressure drop and mass distribution. This was first accomplished by Bisset [11] employing three balance equations: (i) the conservation of exhaust gas mass flow, (ii) the conservation of the axial component of momentum of exhaust gas and (iii) the conservation of the exhaust gas energy. The above balances, together with the Darcy correlation, are used to calculate the distribution of the gas velocities in the inlet and outlet channels and the velocities normal to the soot layer and wall. Once the velocities distribution has been calculated, the model computes the energy exchanged between the gaseous and solid phase. Finally, the axial temperature distribution along the wall is calculated. The heat balance implements 1D heat conduction and source terms for gas–solid heat convection and reaction enthalpy.

$$\left(\rho_1 c_{p,1} + \rho_2 c_{p,2}\right)\frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial z^2} + h_{in}\left(4/\ell\right)\left(T - T_{in}\right) + h_{out}\left(4/\ell\right)\left(T - T_{out}\right) + \frac{dQ}{dt} \qquad (6)$$

In the above equation, the heat source term *dQ/dt* expresses heat exchange due to perpendicular gas flow and reaction exothermy. The main I/O and control structure of the computational tool employed in this study is presented in Figure 1. The 1D model of filter operation is implemented as an S-Function in Simulink. Input data consist of time series of exhaust gas composition, soot emissions, temperature, mass flowrate and backpressure of the exhaust system downstream the filter, for the computational scenario (NEDC legislated cycle in the specific case study). Exhaust gas composition, soot emissions and exhaust gas temperature time series differ between normal engine operation and post-injection operation, thus, different sets of input time series are available, based on engine bench or chassis dyno measurements in the specific cycle. Also, the effect of engine exhaust backpressure on the engine operation, emissions and exhaust temperature time series is taken into account by specific approximations. The overall loop includes also the control algorithm that decides for the activation of post-injection, whenever specific conditions suggest the onset of regeneration (see next section).

EXPLOITATION OF THE COMPUTATIONAL TOOLS IN FILTER SYSTEMS DESIGN

The Diesel filter is usually placed downstream an oxidation catalyst. In order to avoid blocking of the filter by the accumulated particulate, the filter must be completely regenerated every 400 to 500 km, or partially regenerated in shorter intervals. Without the use of a catalyst, thermal regeneration takes place at exhaust gas temperatures exceeding 550 °C. Such temperatures are observed at near full load engine operation. In order to attain regeneration conditions during part load city driving of the vehicle (normal exhaust temperature levels after turbine and catalyst between 150 and 200 °C), additional equipment is required: When the engine management detects an overloaded filter, it can activate the post-injection capability of the common- rail injection. This leads to an increase in the cylinder temperature, which cannot be exploited to increase work on the piston due to the late timing of the post-injection. Thus, the reaction enthalpy of the post-injected fuel is mainly transferred to the exhaust. Usually, the post-injected fuel cannot burn completely, so we observe very high HC emissions, which are subsequently oxidized in the oxidation catalyst, finally resulting in a further increase of exhaust temperature downstream the converter, up to 450 °C. In order to effect regeneration at this lower temperature, it is necessary to employ catalytic aids, in our case study this is in the form of a fuel additive that is available in an additional storage tank and is automatically mixed in the fuel (by every refueling or by more precise dosing techniques). The design and control of the filter and regeneration system require demanding optimization, since they lead to an increase of fuel consumption of the order of 5% or more [17]. The fuel additive dosing strategy could also be subject to optimization.

An example of the use of the above-mentioned computational tools in the design optimization of a diesel filter system is briefly discussed in this section. First, an assessment of the model's kinetics parameters is carried out, based on the results of engine bench loading–regeneration experiments performed on one of the Laboratory engine benches. The experimental layout is presented in Figure 2 (143.8 mm diameter x 150 mm length, 200 cpsi/14 mils SiC filter fitted in the exhaust pipe of a 2-liter displacement HDI turbocharged passenger car engine with common rail injection system). Temperatures are measured at the inlet and the exit of the filter, and inside the filter, at characteristic points along a filter diameter. Exhaust emissions (CO, CO_2, NO_x and HC) are measured upstream filter. The O_2 concentration is measured by means of UEGO sensors installed upstream and downstream filter. The NEDC test sequence of operation points is programmed on the digital controlled dyno. The data acquisition and control computer is interfacing with the engine ECU and is capable of triggering the onset of regeneration by engaging the post-injection operation. The control algorithm for the activation of fuel injection is a subject of optimization in this case.

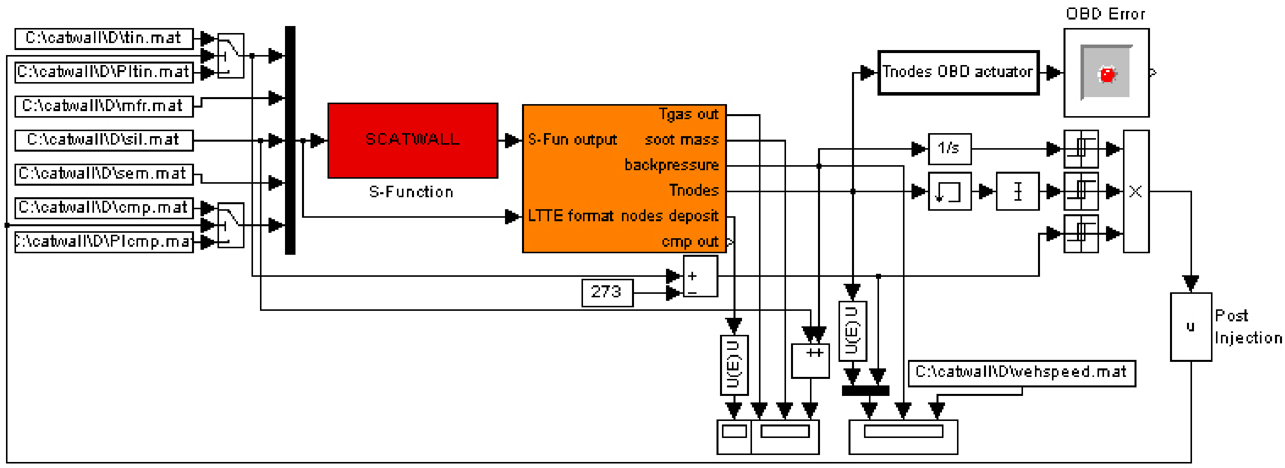

Figure 1 Simulink implementation of CATWALL 1D filter loading and regeneration model.

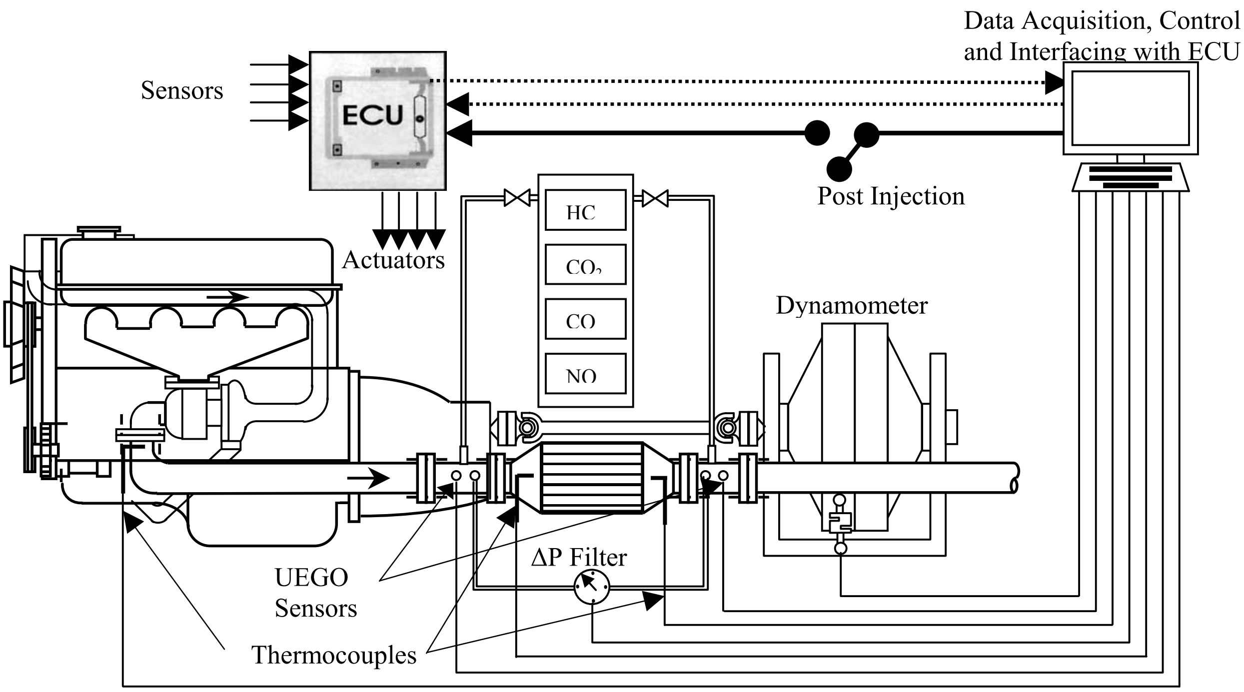

Figure 2 Experimental layout. Engine and digitally controlled dynamometer installation is shown along with exhaust gas analysers, main filter measurement lines, data acquisition and ECU interfacing system.

The kinetic parameter values employed are obtained by validation experiments, based on the experience from an extensive set of TGA analysis experiments of soot samples taken directly from the specific type of filter [18]. The values for the pre-exponential factor and the activation energy of each reaction are given in Table 1. In brief, the values of activation energies for catalytic oxidation correspond to dry soot oxidation for samples where the VOF content varies in the range between 2.5 and 8%. The pre-exponential factors were obtained by allowing a certain amount of tuning. Furthermore, the wall permeability, soot density and soot permeability times density were tuned to match the overall pressure drop behaviour of the specific system. Figure 3 shows an example output of the code in Simulink, which corresponds to the computed response of the filter wall temperatures along the filter axis and computed filter backpressure during operation of the reference vehicle in NEDC. A computation of this type (1180 sec of real operation) takes about 100 sec in a 2.4 GHz Pentium 4 PC.

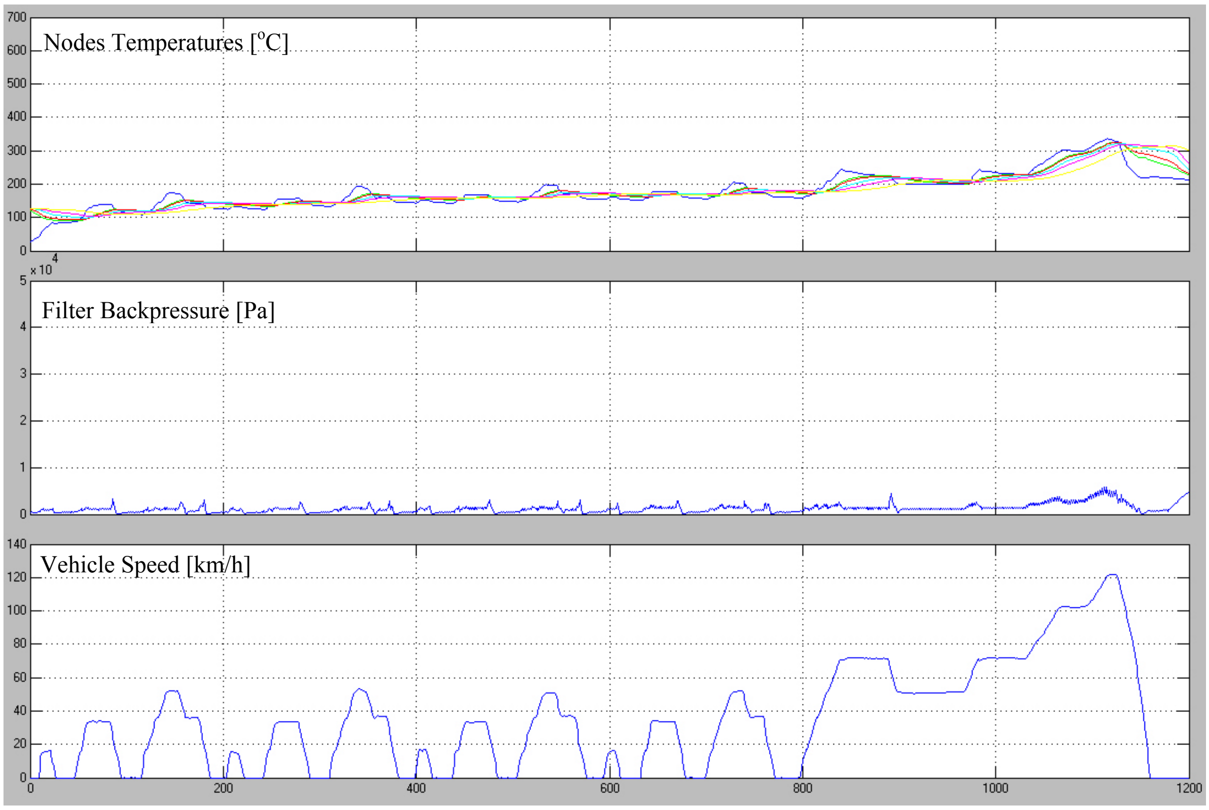

Figure 3 Computation of the clean filter wall temperatures and backpressure response to a repeated NEDC test scenario.Inlet temperatures are also shown, in blue color, to compare with node temperatures.

An important control aspect for this type of Diesel filter systems is associated with the activation of the post-injection operation, which enables regeneration of the loaded filter. The post-injection should be activated whenever the filter loading is found to exceed a critical value (Figure 4). Here, filter loading is no longer allowed to be expressed just by the instantaneous backpressure, as it happened with early Diesel filter systems. Actually, the mass of soot accumulated in the filter is what needs to be checked for exceeding a threshold value. But this can only indirectly be estimated, as function of filter backpressure, exhaust temperature, engine speed, a flow maldistribution factor, and an estimate of fuel additive ash accumulated in the filter [16]. The specific form of such a function and the threshold values is a subject of investigation by means of models and experiments.

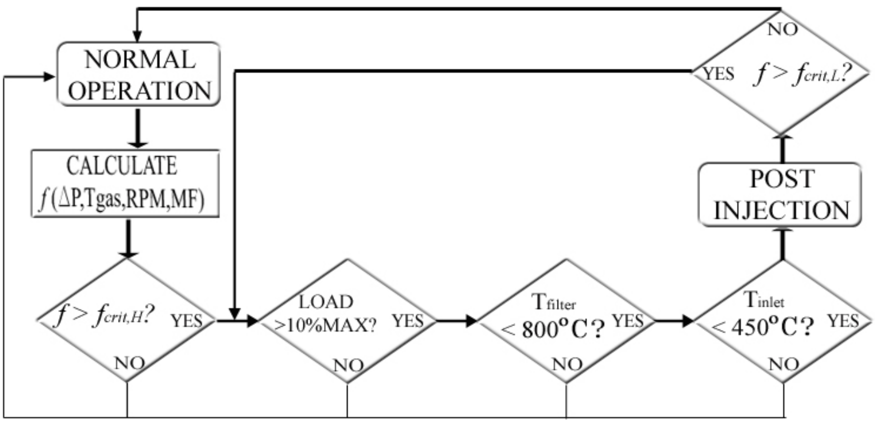

Figure 4 Indicative control strategy for post-injection activation in a fuel additive assisted Diesel filter system. After completion of the regeneration, the control returns the system to normal operation.

Once the critical filter loading threshold is exceeded, several additional checks should be carried out before activating post-injection (Figure 4). These checks should exclude the following incidences:

- if the exhaust temperature is sufficiently high (high load engine operation), it is neither necessary, not allowed to activate post-injection. Regeneration may proceed with normal engine operation.
- if the engine operation point is a very low load one, exhaust temperature levels cannot be raised sufficiently

for regeneration, even with the aid of post injection (it would just consume fuel).

- if the filter wall temperature is too high, post-injection must be avoided, to protect filter from overheating.

Once the above incidents are excluded, the control activates pots-injection. According to the control logic of Figure 4, post-injection operation can be switched off after the estimated filter soot loading is found to drop below a lower threshold value. The results of the run of Figure 5 should demonstrate how the Simulink model helps debugging the control system operation, in combination with limited engine bench or chassis dyno testing. In the specific run, which follows repeated operation of the vehicle according to the NEDC cycle for a number of hours, which corresponds to a few hundreds of kilometers covered, the soot mass accumulated in the filter had reached about 40 grams (see third diagram of Figure 5). This resulted in the increase of the backpressure levels, which can be seen by comparing the respective curves (second diagram, [Pa]) between Figure 3 and Figure 5. Based on the specific control programmed in the Simulink model, at about t=86 seconds of the current NEDC cycle, the calculated soot loading level exceeds the threshold value set and the post-injection is activated. The computed evolution of regeneration can be seen in the Figure 5. At about t=897 seconds, the estimated filter soot loading is found to drop below the lower threshold value and, again based on the specific control of the Simulink model, the post-injection operation is switched off. The degree of completeness of regeneration can be estimated by means of the calculated evolution of soot mass during regeneration (Figure 5).

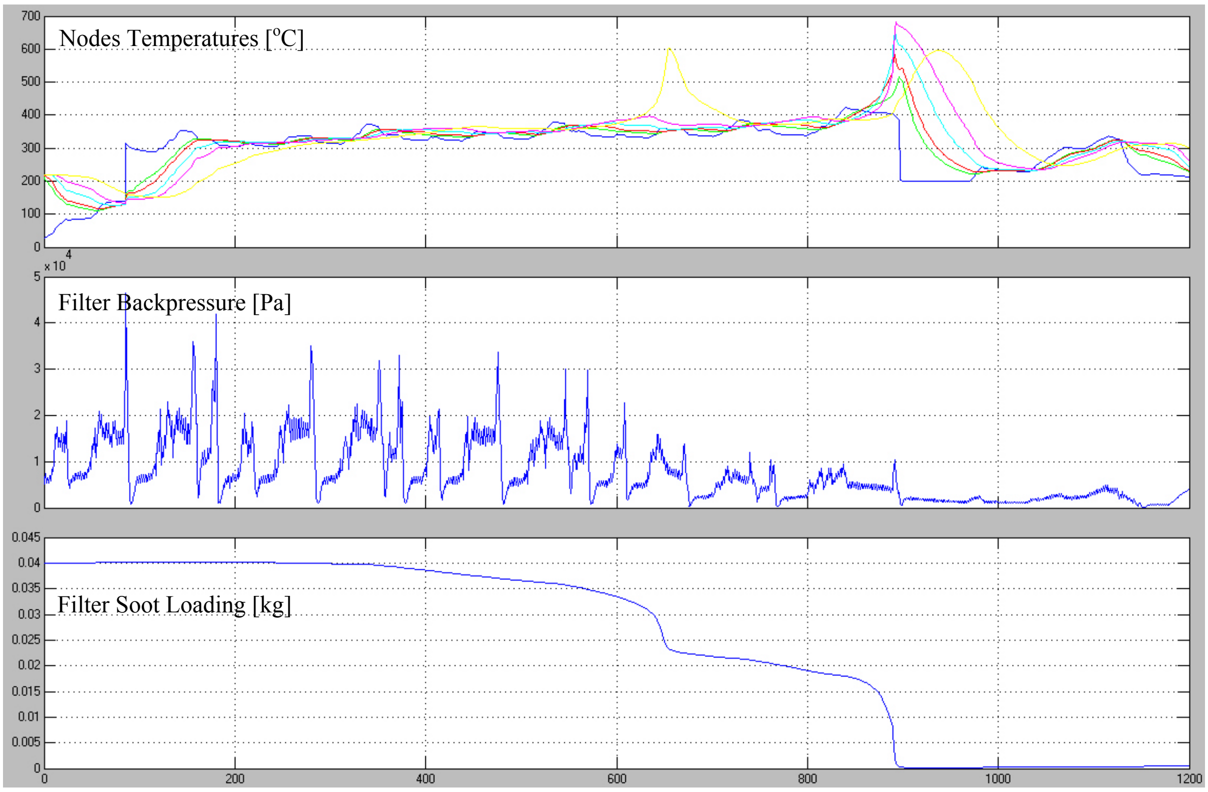

Figure 5. Computation of the heavily loaded filter wall temperatures (inlet temperatures are also shown, in blue color) and backpressure response, after repeated NEDC driving. Activation of post injection, calculation of the evolution of regeneration and return of the control to normal engine operation.

It should become clear by the above discussion that the development and validation of workable engineering models for Diesel filter regeneration behaviour is significantly more demanding than the development of their computational cores that are usually published in the literature with simplistic validation test cases. Nevertheless, engineering modeling has already shown great potential as an engineering design tool, also in this area, and its accuracy and application range is expected to develop more in the future, because of its increasing application in challenging design optimization tasks. Furthermore, as the on-board computers embodied in the ECU are becoming faster and better equipped with memory and networking capabilities, more detailed physical models of such complex systems are now demonstrating real time capability, and control system tools and theories are becoming more applicable to these complex systems.

CONCLUSIONS

A computational tool for the loading and regeneration of catalytically assisted diesel filters was customized to work in the MATLAB/Simulink environment, by adapting and further improving an existing filter channel model, featuring an inclusive reaction scheme for thermal and catalytic regeneration.

The Simulink implementation extends the potential of the model towards the prediction of the system's response to various control strategies. Thus, a useful computational tool for debugging control system operation for a Diesel filter- equipped vehicle has been developed. This tool is designed to work in synergy with routine engine bench or chassis dyno experiments A characteristic, real world case is presented in this paper, to demonstrate its capabilities and use in control system design optimization.

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