Diesel oxidation catalyst and particulate filter modeling in active – Flow configurations

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Abstract

A one-dimensional transient model is developed in order to carry out theoretical investigations on the active flow diesel aftertreatment configurations. Simulations are carried out to predict the thermal response of particulate filters during active flow regeneration operations. Results indicate that the active flow-control strategies can achieve higher energy efficiency in aftertreatment operations. The energy efficiency analysis is carried out using various active-flow configurations. The theoretical model is validated using the experimental results. Further empirical investigation is carried out in order to study energy efficiency of supplemental fuel in the active-flow configurations. Different engine operating modes are also investigated with the active-flow configurations. It is observed that diesel aftertreatment with active flow can significantly improve in the supplemental energy efficiency.

1. Introduction

In order to meet the stringent automotive emission regulations, increasing number of diesel vehicles around the world use catalytic converters. Diesel exhaust aftertreatment applications include Diesel Oxidation Catalyst (DOC), Diesel Particulate Filter (DPF) and NOx adsorber. In order to enable aftertreatment operations, diesel engines commonly require supplemental energy to raise the otherwise relatively low exhaust temperature [1]. The appropriate aftertreatment operation is largely dependent on the sufficient temperature level of the substrate. In order to improve the overall energy efficiency and keeping the most reactive conditions of the converters of the aftertreatment operation systems, measures are being adopted such as the supplemental fuel delivery, the heating of the exhaust gas and the active flow-control strategies that include the periodic alternating exhaust flow paths through the aftertreatment device [1–4]. Depending on the vehicle application an effective and efficient active flow control scheme can be developed with an objective to maintain conditions favorable to aftertreatment operations.

The supplemental energy input can be efficiently applied in the exhaust stream by combining various active flow-control strategies such as parallel alternating flow, flow stagnation and periodic flow reversal to reduce the overall energy penalty drastically. Different active flow schemes are shown in Fig. 1. It is important to develop a suitable theoretical model that can simulate aftertreatment operations under these active flow control configurations.

Several researchers have developed DOC and DPF models that can cater various flow control aftertreatment operation conditions [2,3]. The objective of the research presented in this paper is to develop a one-dimensional DOC–DPF model that can simulate aftertreatment operations and behaviors under extreme conditions of exhaust mass flow rates, oxygen concentrations and temperatures. In order to identify operating window for safe, effective and energy efficient regeneration, both numerical and experimental studies are carried out. Further experiments are carried out in order to perform an energy efficiency analysis of various active aftertreatment operations at low exhaust flow conditions.

The present study focuses on the evaluation of the energy efficiency on active-flow configurations of diesel aftertreatment systems. The active flow schemes include partial flow control of the exhaust gas through the parallel or reversal flow aftertreatment system with the addition of supplemental energy at the upstream of the aftertreatment system, operating at various flow rates and exhaust gas temperatures. The theoretical and empirical results of aftertreatment behaviors under these conditions are presented here.

A parallel flow system with DOC–DPF units operates in alternating cycles of filtration and regeneration with various space velocities. An active regeneration with external supplemental energy is relatively energy efficient with reduced space velocities, when the exhaust temperature is below the threshold limit for the aftertreatment operations. By sharing the operating cycle with other parallel devices, the partial flow restriction (PFR) operation can effectively reduce the supplemental energy consumption to successfully carry out active regeneration. For energy efficient operations, the PFR switches between different modes as shown in Table

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1.1. Different modes of flow control are made based on the requirements of the regeneration. Generally mode 1 operation is stayed over longer period of time as the rate of filtration is slower than the rate of regeneration. The flow control valve is placed in order to control the flow distribution during various modes of PFR operation as shown in Fig. 2. The PFR operates in sequence from modes 1 to 5.

Another active flow method is the periodic flow reversal operation, which is, in essence, a heat energy trap, performs an active heat recovery in addition to the heat retention capability of monolith solids. By cyclically alternating the direction of exhaust flow, a thermal wave is produced at the frequency of flow reversal, so that the central substrate temperature retained regardless of the variations in the exhaust gas temperature. The configuration of periodic flow reversal is shown in Fig. 3 [5].

2. Model formulations

This section presents the mathematical, chemical and physical phenomenon that describes energy, mass and momentum exchange characteristics in a single channel of the DOC and the DPF. The one-dimensional model equations are derived from the mass, momentum and energy conservation equations of a single channel inside the monolith DOC and DPF. References are taken from the works of Triana, Johnson and Konstandopoulos [6,7]. It is to be noted that over the past three decades, many researchers have developed one-dimensional transient models to simulate the chemical- and thermo-physical responses of the aftertreatment devices. One of the original models was proposed by Bisset Edward [8]. He proposed basic one-dimensional model accounting the various effects of flows inside the channels of DOC and DPF. Soon Kon-
standopolous and his co-researchers developed the model proposed by Bisset and included chemical effects on the thermal response in the aftertreatment devices [9]. Other researchers such as Johnson and Triana also contributed to the development of DOC and DPF model over next decades [7,10–13]. Till date the mathematical model developed to describe the thermo physical behavior in the DOC and DPF has been used to simulate aftertreatment operation under standard operating conditions. Comparatively less literature is available on the model’s capability to simulate active flow conditions such as flow stagnation that includes extreme conditions of flow rate. This model is calibrated with experimental data of thermal response of DOC and particulate regeneration of DPF.

2.1. DOC model

The Diesel Oxidation Catalysts are designed to chemically treat the raw exhaust gas by the oxidation of pollutant species such as carbon monoxide (CO), gas phase hydrocarbons (HC) and the volatile organic compounds such as soluble organic fraction (SOF) present in the diesel exhaust. Commonly used DOC is a honeycomb monolithic structure. The Nitrogen Oxide (NO) is also oxidized to nitrogen dioxide (NO2) at the temperatures from 270 °C to 430 °C [5]. The accumulated particulate matters (PM) are oxidized in the presence of NO2 inside DPF that is commonly located at the downstream of DOC in the aftertreatment systems. The effectiveness of the DOC in oxidizing CO and THC can be observed at temperatures above “light off” for the catalytic activity. At the temperatures below 250 °C, Palladium–Rhodium (Pd–Rh) catalysts that are commonly used in DOC, show relatively low reactivity. At the temperatures below “light off”, the surface reaction kinetics of the elemental chemical reactions governs the performance of DOC, while as at temperatures above “light off”, the diffusion of exhaust species from the gas to solid phase governs the performance characteristics of the DOC. The mass transfer process can be enhanced by incorporating design changes to the DOC cell structure, by increasing the surface area for the mass diffusion between the gas and solid phases. The present study is conducted to simulate the DOC performance in diesel exhaust condition with excess oxygen.

Three basic reactions are assumed to occur in DOC.

\[
\begin{align*}
\text{CO} + \frac{1}{2} \text{O}_2 & \rightarrow \text{CO}_2 \quad (1) \\
\text{C}_3\text{H}_6 + \frac{9}{2} \text{O}_2 & \rightarrow 3\text{CO}_2 + 3\text{H}_2\text{O} \quad (2) \\
\text{NO} + \frac{1}{2} \text{O}_2 & \rightarrow \text{NO}_2 \quad (3)
\end{align*}
\]

The hydrocarbon oxidation is represented by the Eq. (2) where the exhaust hydrocarbon is represented by C3H6. Different ranges of hydrocarbon present in the diesel exhaust. Depending on the diesel combustion mode the range of hydrocarbon in the exhaust gas may vary. In order to model Diesel after-treatment, the exhaust hydrocarbons may be assumed to mostly contain carbon chains ranging from C9 to C12 [14]. Therefore, considering the complications in modeling HC reactions at the ranges present in the typical diesel exhaust, a lower molecular weight of hydrocarbon family is used to simplify the model calculations.

A one-dimensional numerical model has been developed to simulate a single channel of the monolith substrate as shown in Fig. 4. The primary objective of the model is to carry out the transient thermal response simulation of the exhaust gas and the substrate wall. The model accounts for the convective heat transfer between the solid and the gas phase, and the conductive heat transfer. The effects of thermal radiation from the substrate wall to the surroundings are not considered in the model due to its intrinsic nature of simulation in one dimension along the direction of flow. In order to calculate the exothermic heat released from the chemical reactions, the chemical kinetics of the oxidation reactions in the catalyst surface are considered.
The exhaust species balance in the solid phase is dependent on the rate of mass diffusion, rate of catalyst surface adsorption and the rate of disappearance due to chemical reaction. Assuming quasi steady state of the energy balance in the solid phase, the rate of disappearance of reactant species is equal to the rate of adsorption of the species from the gaseous phase. The net rate of reaction is therefore controlled by the chemical kinetics when the rate of adsorption is higher than the rate of chemical reaction – the condition occurs mostly at the temperatures below light-off. However at temperatures above catalytic light-off, the rate of diffusion controls the rate of reaction since at these temperatures the rate of reaction is higher and thus the reaction is mostly controlled by the availability of the reactants.

The model treats the exhaust gas as an ideal gas. The compressibility of the exhaust gas is not considered due to the low operating pressures. The exhaust flow in the channel is assumed to be laminar due to low Reynolds number of the gas flow through the micro channels of the monolith substrate. In this paper, the effect of heat and mass transfer is simulated during heating of the substrate by the exhaust gas at different levels of exhaust flow rate and flow reversal switching frequencies through the monolith. The gas phase mass balance and the energy balance between the gas and the solid phase are derived from the mass and energy conservation laws. The convective heat transfer rate between the solid and the gas phase is the most dominant form of heat transfer that is responsible for the thermal behavior of substrate. In this particular study, the convective heat transfer coefficients is determined assuming fully developed laminar flow of exhaust gas with constant surface temperature.

The mass conservation of the exhaust gas is written in Eq. (4) in the partial differential form. The equation signifies that due to the rise or fall in the temperature of the exhaust gas through the channel, the exhaust gas density may vary. The variation in density will be compensated by the velocity variation through the channel.

$$\frac{d(p_c u_z)}{dz} = 0$$

(4)

The temperature variations of the exhaust gas through the monolith channel can be calculated from Eq. (5). The heat transfer between the solid and the gas phase is primarily due to forced convection at the solid to gas interface.

$$SVF \frac{\partial (p_c u_T g)}{\partial z} + (SSF)h(T_s - T_g) = 0$$

(5)

The convective heat transfer coefficient is a function of the exhaust gas conductivity, and the channel hydraulic diameter given by Eq. (6). The Nu number is determined assuming fully developed laminar flow of exhaust gas with constant surface temperature with the characteristic length of hydraulic diameter.

$$h = \frac{Nu \lambda_g}{d}$$

(6)

Assuming a homogeneous solid medium of the substrate, from the Fourier’s Law of heat conduction, the partial differential equation for the energy balance of the solid phase is derived and given by Eq. (7).

$$(1 - SVF)p_c \rho_c \frac{\partial T_s}{\partial t} = \lambda_s (1 - SVF) \frac{\partial^2 T_s}{\partial z^2} - hSSF(T_s - T_g) +SSF \sum_{i=1}^{3}(\Delta H_i)r_i$$

(7)

2.2. DPF model

The DPF design in various diesel applications is a ceramic porous wall flow honeycomb structure made of cordierite. The suspended particulate matters are filtered due to the deep bed filtration of the raw exhaust gas during its passage through the porous ceramic substrate wall. The unfiltered exhaust gas enters the inlet channel of the DPF whose outer end is plugged. The exhaust gas flows through the wall of the porous substrate resulting in the physical separation of the solid particulates of diameter exceeding 10 nm. The filtered exhaust gas is then allowed to pass through the outlet. The schematic single channel layout of DPF is shown in Fig. 5.

This section describes the loading and regeneration behavior of diesel particulate filters using filtration of solid particulates and chemical kinetics of soot oxidation. The DPF model describes the solid particulate matter deposition and subsequent oxidation of soot by O2 and NO2. The flow field calculation involves mass, momentum balance of the exhaust gas along the channel length. The initial boundary condition such as inlet pressure is calculated by iteration technique till the values converge to satisfy the principles of conservation for mass, momentum and energy.

The primary assumptions for the DPF model are similar to those for the DOC model except that the viscous friction is considered between the exhaust gas and the channel wall. The chemical reactions in the DPF regeneration model are represented as a one step global reaction given by Eqs. (8) and (9).

$$C + x_1O_2 \rightarrow 2 \left( x_1 - \frac{1}{2} \right) CO_2 + 2(1 - x_1) CO$$

(8)

$$C + x_2NO_2 \rightarrow x_2 NO + (2 - x_2) CO + (x_2 - 1) CO_2$$

(9)

The terms $x_1$ and $x_2$ are the coefficients of chemical selectivity for the reactions of PM with O2 and NO2, respectively. The chemical selectivity coefficients are dependent on the reaction rates of respective chemical reactions. In the Catalytic Diesel Particulate Filter (CDPF), the reaction rate for the particulate oxidation with oxygen is enhanced and therefore the chemical selectivity of the carbon oxidation with the available oxygen increases. The selectivity coefficients are given by Eqs. (10)-(13).

$$x_1 = 1 - \frac{f_{CO}}{2}$$

(10)

$$x_2 = 2 - \frac{g_{CO}}{1}$$

(11)

$$f_{CO} = \frac{1}{1 + p_{Y_1} \cdot Y_{O_2}^{\theta} \cdot e^{\theta Y_{O_2} / RT}}$$

(12)

$$g_{CO} = \frac{1}{1 + p_{Y_2} \cdot Y_{O_2}^{\theta} \cdot e^{\theta Y_{O_2} / RT}}$$

(13)

where $f_{CO}$ and $g_{CO}$ are the selectivity coefficient of CO formation from the soot oxidation by O2 and NO2, respectively.

The mass, the momentum and the energy balance equations are separately solved between the inlet and the outlet channels. The entire DPF channel is discretised into numerous small control volumes to solve the partial differential equations (PDE) individually for all the control volumes throughout the length of the DPF channel.

The mass transfer of exhaust gas for the inlet and outlet channels is given by Eqs. (14) and (15), respectively. The exhaust gas
density $\rho_{gw}$ in the filter wall is assumed to be same as of corresponding exhaust gas density in the inlet channel as denoted by $\rho_1$.

$$\frac{\partial}{\partial z}(\rho_1 u_1) = -\frac{4}{D_1^2} \rho_{gw} v_w$$  \hspace{1cm} (14)

$$\frac{\partial}{\partial z}(\rho_2 u_2) = \frac{4}{D_2^2} \rho_{gw} v_w$$  \hspace{1cm} (15)

The momentum balance of the exhaust gas in the inlet and outlet channels of the DPF is given by Eqs. (16) and (17), respectively. It is assumed that the axial momentum is affected by the change in velocity magnitude and the friction between the exhaust gas and the filter wall. The pressure drop across the filter wall between the inlet and the outlet channels is given by Darcy's Law given by Eq. (18). The law states that the pressure drop across the filter wall is dependent on the flow velocity, the thickness of the filter wall, the soot cake and their permeability. The dynamic viscosity of the exhaust gas is a temperature dependent variable that contributes to the pressure drop across the wall. It is assumed that the exhaust gas viscosity is a function of the wall temperature. The solid temperature is assumed to be uniform throughout the thickness of the particulate cake and the filter wall.

$$\frac{\partial p_1}{\partial z} + \frac{\partial}{\partial z}(\rho_1 u_1^2) = -F \mu u_1$$  \hspace{1cm} (16)

$$\frac{\partial p_2}{\partial z} + \frac{\partial}{\partial z}(\rho_2 u_2^2) = -F \mu u_2$$  \hspace{1cm} (17)

$$p_1 - p_2 = \frac{\mu}{K_p} \nu_w W_p + \frac{\mu}{K_i} \nu_w W_s$$  \hspace{1cm} (18)

The energy balance of the exhaust gas in the inlet and outlet channels is due to the net heat flux to the control volume, and the heat transfer to the substrate wall by convection. The gas phase heat transfers are given by Eqs. (19) and (20).

$$c_{pg} \rho_1 b_1 \frac{\partial T_1}{\partial z} = \frac{4}{D_1^2} h_1(T_s - T_1) - \frac{4}{D_1^2} \rho_{gw} \nu_w c_{gw} T_s$$  \hspace{1cm} (19)

$$c_{pg} \rho_2 b_2 \frac{\partial T_2}{\partial z} = \frac{4}{D_2^2} h_2(T_s - T_2) + \frac{4}{D_2^2} \rho_{gw} \nu_w c_{gw} T_s$$  \hspace{1cm} (20)

The energy balance of the substrate wall is considered by taking into account the convection heat transfer between the substrate and the exhaust gas at the inlet and the outlet channels, conduction heat transfer in the solid phase and the heat generation due to the exothermic soot oxidation. The solid phase in a loaded DPF channel is composed of the substrate and the soot cake. But the model assumes uniform solid temperature across the exhaust flow throughout the thickness of the soot cake layer and the solid substrate layer within a control volume remains same. The effect of conductive heat transfer across the soot layer is negligible to the effects of conduction along the length of the DPF channel due to the dimensional consideration.

$$\frac{\partial}{\partial z}[(\rho_{gw} c_{gw} W_s + \rho_p c_{wp} W_p) T_s] = h_1(T_1 - T_s) + h_2(T_2 - T_s)$$

$$-\lambda_s \frac{\partial}{\partial z} \left( \frac{\partial T_s}{\partial z} \right) - \lambda_w \frac{\partial^2 T_s}{\partial z^2} + \dot{q}_s$$  \hspace{1cm} (21)

With the mass, the axial momentum and the energy balance equations for the inlet and outlet channels of DPF, the flow field can be solved by numerical methods. The pressure drop is greatly influenced by the filtration and the oxidation of the accumulated soot cake in the DPF inlet channel. Therefore it is important to calculate the soot cake thickness in order to determine the pressure drop from the flow field calculation. The diffusion mass transfer dominates the species transport in the porous wall and the soot cake [8]. The chemical reactions in the gas phase are neglected due to its short residence time inside the DPF channel. The molar concentration of the reactant species like O$_2$ and NO$_2$ inside the DPF channel is assumed to be constant throughout the channel length for simplicity of calculation.

The conservation of the species can be expressed in terms of the molar concentrations of the reactant species and the rate of reaction in the embedded reaction sites. The total time derivative of the reactant species concentration is the sum of partial derivatives with respect to time and distance across the flow (i.e. distance along the particulate reaction site).

$$\frac{d(Y_k)}{dt} = \frac{\partial(Y_k)}{\partial t} + \frac{\partial(Y_k v_w)}{\partial y}$$

$$k = O_2, \text{ NO}_2$$  \hspace{1cm} (22)

From Eq. (22), it is seen that the time rate of change of molar concentration of reactants is governed by the balance between convective transport across the wall (y direction) and the chemical kinetics of the particulate oxidation. It is assumed that the chemical reactions are limited to its kinetics due to the extremely small reaction passage through the porous particulate filter layer. Experimental investigations by various researchers confirms that diffusion mass transfer rates are two orders of magnitude higher than the chemical reaction rates at the range of operating DPF regeneration temperatures (450–1400 °C) [7].

Assuming the order of oxidation reaction as $n_k$, the conservation equation of the reactant mole fractions are given by the steady state conditions for the overall rate of species accumulation. Equating the total time derivative of the reactant species concentration to zero the reactant species concentration equation can be as follows.

$$\frac{\partial (\rho_{gw} Y_k)}{\partial t} = -\frac{\partial (\rho_{gw} Y_k u_w)}{\partial y} - k_{kj} \rho_{gw} y_k k_{kj} = A_{kj} e^{(-e/kT)}$$  \hspace{1cm} (23)

The local reaction rate of particulate oxidation is represented by the modified Arrhenius form that is dependent on the temperature of the reaction site and the activation energy. The activation energy $E_j$ varies between different sites of reactions such as the thermal, the catalytic and the soot cake, (the subscript $j$ represents each reaction site). It is assumed that the thermal reaction site is embedded inside the porous particulate filter wall.

Assuming quasi steady state of reaction, the transient term of the Eq. (23) is neglected. Therefore the molar balance of the exhaust gas species across the DPF channel (y direction) is given by Eq. (24).

$$\frac{\partial}{\partial y}(\rho_{gw} u_w W_k) = -k_{kj} \rho_{gw} Y_k u_w$$  \hspace{1cm} (24)

The rate of O$_2$ or NO$_2$ depletion per unit wall surface area can be obtained by rearranging and integrating Eq. (24) across the wall thickness.

$$R_k = \int_{y=0}^{\infty} s_k k_{kj} \rho_{gw} Y_k dy$$  \hspace{1cm} (25)

where $s_k$ is the specific surface area of soot particulate [13]. Therefore smaller the size of soot, greater will be the surface area of soot oxidation for a given mass of soot loading in a DPF channel. This will lead to a higher rate of oxidation with higher specific surface area of oxidation.

The soot layer depletion rate during the regeneration process is a mathematical product of the rate of oxidation reaction and the order of reaction. The overall rate of change of soot cake thickness is given by:

$$\rho_{soot} \frac{\partial \delta_w}{\partial t} = -\sum_k \left( \frac{M_k}{M_s} \right) R_k + \omega_{acum}$$  \hspace{1cm} (26)

In the two layer model developed (Konstandopolous et al., 2000) the particulate layer thickness is divided into the thermal layer and catalytic layer [8]. A similar model treatment of the soot...
oxidation phenomenon is adopted to estimate soot oxidation embedded inside the porous filter walls. The filtration and the accumulation mechanism of the exhaust particulate are modeled and integrated with the regeneration model in order to simulate simultaneous regeneration and accumulation. The particulates are initially deposited on the porous filter wall by Brownian diffusion through the direct interception that is considered the deep bed filtration. But as soon as the porous filter wall is saturated with the accumulated soot, the particulate matter starts accumulating over the filter wall to form soot cake inside the wall of the inlet channel. In the following simulations the accumulation mechanism is modeled based on the assumption that the soot deposition is dependent on the flow field of the exhaust gas at the inlet channel and the filter wall. The rate of soot accumulation in a control volume is dependent on the influx of soot and the wall flow velocity, and is inversely proportional to the inlet flow velocity. Higher the inlet flow velocity, greater the chance of bulk soot been carried over to the next control volume of the inlet channel.

\[
\frac{\partial \left[ (\rho u) \right]}{\partial z} = -k_{\text{acc}} \left[ (\rho u) \right] v_w 
\]  

\[
\dot{\omega}_{\text{accum}} = k_{\text{acc}} \left[ (\rho u) \right] v_w \frac{\dot{m}_i}{\dot{m}_i \left( \frac{1}{2} N_c \right)} 
\]

The soot accumulation rate is estimated from the above equation. The inlet exhaust mass is only passed through the inlet channels of DPF which is only half of the total number of channels in the DPF \((N_c)\). The mass flow rate of the exhaust gas at the intake of DPF gives an estimate of how much soot is carried over to DPF for the filtration or the accumulation. In general high soot accumulation coefficient \((k_{\text{acc}})\), represents the less flow ability of particulates along the inlet channel. The mass flow rate of the exhaust gas at the inlet of DPF channel is given by:

\[
\dot{m}_i = \rho v_i \left( \frac{N_c}{2} \right) 
\]

In the DPF model, the effect of porosity may change the pressure drop across DPF. However the combined porosity of the filter wall varies across the soot and porous filter layer. Variations in exhaust soot property, however large, cannot affect the overall combined porosity, because the soot layer porosity is generally contributes only 10–15% of overall porosity. Variations across the soot layer and the filter wall are often neglected for thermal response calculation due to the complexity of such model and also due to the fact that less than 1% of thermal variation may occur across the soot layer and substrate wall. Therefore directional variations are carefully considered for the model development as shown in Fig. 6.

The equations are solved numerically by applying computational fluid dynamics (CFD) techniques using finite volume approach. The PDE are discretised into simple arithmetic forms and the discretised equations are solved simultaneously within a time loop of the simulation. The scalar variables such as temperature, pressure species concentration, etc., are solved along with vector flow field parameters such as velocity and mass flux by semi-implicit pressure linked equation. However the energy equation for gas phase in DOC is solved using explicit method. The discretised momentum and energy equations are solved using tri-diagonal matrix algorithm (TDMA) using forward elimination and backward substitution for fast and efficient solution. The initial boundary condition for pressure at the inlet of DPF is solved iteratively till the flow continuity convergence criterion is reached. The solution at every iteration step is checked for convergences, boundedness and transportability to avoid solution divergence. In order to apply the pressure velocity equation in the DPF the channel is divided into a staggered mesh formation of small control volumes. The scalar variables are solved at every node whereas the vector variables are solved at every faces using central differencing scheme. The simulation code setup in brief is given in Fig. 7.

3. Results

A single cylinder engine is set up with a DOC and a DPF to perform tests on active and passive flow-control strategies to enable aftertreatment operation. Simulation results are compared with experimental results in a DPF regeneration experiments performed in a dedicated DPF system as shown in Fig. 8. The experimental setup is placed with thermocouples placed at various positions in order to record temperature along the length of DPF channel. Further experiments and simulations reported in this work are carried out using a DOC–DPF setup with the specification tabulated in Table 3.1.

In order to validate the regeneration model, a simulation case with initial soot loading of 5 g/L and initial substrate temperature of 250 °C is compared with an experimental result. The initial soot load is assumed on the basis of the initial pressure drop for the DPF. Thermocouples are located at four different locations inside
the substrate channel as given in Table 3.2. The model is validated by tuning number of chemical kinetics, thermal and flow field parameters in order to match the pressure drops and the temperatures of the substrate within the acceptable limits of tolerance. Regeneration model is validated by comparing the simulated thermal response and pressure drop of the DPF with the experimental data. Figs. 9 and 10 show that the simulation predicts the pressure drop across DPF within ±5%.

From Figs. 11 and 12 it is seen that the simulation and the experimental data are in reasonable agreement with one another. The simulated pressure drop is within ±0.25 kPa and the temperatures are comparable within ±70°C with the experimental results. It is noticed that the timing of the regeneration is governed by the reaction kinetics. The simulation model is therefore able to predict the timing of the regeneration response based on the chemical kinetics calculations. Based on the validation some important calibration parameters describing the thermo physical process during DPF regeneration are tabulated in Table 3.3. Simulations are also carried with the same set of calibration parameters with lower initial soot loading (3 g/L) and higher exhaust flow rate (~100 g/s). The initial pressure drop across DPF is measured 3.2 kPa as shown in Fig. 13. Simulation results with the following transient test are fairly accurate with the prediction of the pressure drop and regeneration response in the DPF. The pressure drop across DPF initially rises because of the rise of exhaust temperature inside DPF channel. The subsequent drop in pressure is due to the lower resistance offered to the wall flow due to depletion of soot cake thickness. The DPF thermal response is shown in Fig. 14.

3.1. Simulation results

Simulations are carried out with the various active flow conditions for the DOC–DPF systems. The objectives of the theoretical investigations are to carry out the thermal response and the energy efficiency analysis with different active flow strategies in the diesel aftertreatment system. The main focus of the simulation is to study DPF regeneration and to get a better understanding of the various pathways to initiate safe and efficient regenerations in the DPF. The energy required initiating such conditions in the DOC and the DPF are quantified.

3.1.1. Gas temperature variation

The cases with different initial temperatures and the inlet gas temperatures (Table 3.4) are simulated to analyze the energy required to initiate and sustain regenerations inside DPF. The inlet

![Fig. 8. Dedicated DPF setup.](image)

<table>
<thead>
<tr>
<th>Table 3.1</th>
<th>DOC–DPF specification.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>Unit</td>
</tr>
<tr>
<td>DOC diameter</td>
<td>5.66 in.</td>
</tr>
<tr>
<td>DOC length</td>
<td>6 in.</td>
</tr>
<tr>
<td>DOC wall thickness</td>
<td>8 mil</td>
</tr>
<tr>
<td>DOC cell density</td>
<td>400 cpsi</td>
</tr>
<tr>
<td>DPF diameter</td>
<td>5.66 in.</td>
</tr>
<tr>
<td>DPF length</td>
<td>6 in.</td>
</tr>
<tr>
<td>DPF wall thickness</td>
<td>19 mil</td>
</tr>
<tr>
<td>DPF cell density</td>
<td>200 cpsi</td>
</tr>
<tr>
<td>Substrate material</td>
<td>Cordierite</td>
</tr>
<tr>
<td>Catalyst alloy</td>
<td>Pt–Pd</td>
</tr>
</tbody>
</table>

![Fig. 9. Pressure drop vs. flow rate (0 g/L).](image)

<table>
<thead>
<tr>
<th>Table 3.2</th>
<th>Thermocouple positions in DPF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid temperature (°C)</td>
<td>Location (z/L) in the monolith</td>
</tr>
<tr>
<td>T1</td>
<td>0.1</td>
</tr>
<tr>
<td>T2</td>
<td>0.4</td>
</tr>
<tr>
<td>T3</td>
<td>0.6</td>
</tr>
<tr>
<td>T4</td>
<td>0.9</td>
</tr>
</tbody>
</table>

![Fig. 10. Pressure drop vs. flow rate (5 g/L).](image)

![Fig. 11. Regeneration response comparison.](image)
The temperature of the exhaust gas can be varied by installing an exhaust gas heater similar to the one used in the experiment at the flow rates ranging from 2 to 15 g/s. The rise in the exhaust temperature depends on the exhaust gas flow rate and the energy supplemented by the exhaust heater. The supplemental heat energy can be effectively delivered at the low exhaust space velocities corresponding to the low flow rate loop of the PFR system. The experimental results indicate that if the DOC is placed before the DPF, the setup will facilitate to accomplish the regeneration provided that the DOC attains catalytic "light off". Once the "light off" condition is reached, the DOC catalytic activity can be sustained by controlled addition of the supplemental fuel. The exothermic reactions of fuel oxidation inside the DOC channels counterbalance the convective heat loss to the cooler exhaust gas. The exhaust gas picks up the convective heat from the DOC channel and helps to sustain the regeneration in the DPF in the downstream.

In the following simulations the DOC is positioned before the DPF so that the catalytic activity in the DOC helps to achieve regeneration conditions in DPF. A sufficient amount of external fuel is injected in the upstream of DOC with the initial temperature of DOC just above the temperature to sustain catalytic activity. The simulation results of the transient thermal response along with the fraction of soot regeneration (i.e., regeneration efficiency) are presented for different cases. The soot profiles at different time as the regeneration progresses are also shown from Figs. 15–21. An energy efficiency comparison (Fig. 22) is made by analyzing the fraction of soot regenerated with the total quantity of the supplemental energy delivered for the purpose. It is assumed that the supplemental fuel injected in the exhaust stream

![Fig. 12. Regeneration thermal response.](image1)

![Fig. 13. Regeneration Response comparison.](image2)

![Fig. 14. Regeneration thermal response.](image3)

![Fig. 15. Transient results (Case S1A).](image4)
is fully vaporized before entering to the DOC. The supplemental fuel delivery rate of 50 mg/s in an exhaust stream of approximately 10 g/s corresponds to 5000 ppm by mass of THC by mass fraction as indicated in Table 3.4. It is assumed that the supplemental fuel is represented by the THC in the exhaust stream of the active flow control embedment.

The simulations are repeated with other inlet temperatures of the exhaust gas and the initial temperatures of the substrate. The progress of regeneration in DPF with the 5 g/L initial soot loading is compared between the different cases of the initial substrate temperatures and the inlet exhaust gas temperatures and shown in Fig. 22. It is observed that if the temperature is kept below the DOC “light off”, then the regeneration in DPF is not initiated. The simulation results demonstrate that the DOC–DPF system is capable of the regeneration once the temperature is maintained above 290 °C. The supplemental energy required to carry out the regeneration towards the completion is given by Fig. 23. It is evident that in order to initiate and complete the regeneration by energy efficient methods, an additional supplemental heater may be needed in the diesel exhaust system. The offset of additional heater cost, the PFR setup and the additional heat energy can be recovered by the energy saved during the regeneration process in DPF.
3.1.2. DPF soot accumulation

The operating condition of the exhaust and DPF is kept constant while the exhaust gas flow rate and the soot concentration in the exhaust are varied as shown in Table 3.5. Between the cases S2B and S2C a comparison is made for wall flow rate and soot accumulation profile because between these conditions, the net soot filtration are comparable. The conditions are summarized in Table 3.6.

Simulations are performed in order to generate soot accumulation profile under different conditions. The simulation model assumes that the soot accumulates over the existing soot cake (5 g/L initial soot load). The local wall flow velocity of the exhaust gas through the accumulated soot layer and the porous substrate bed is shown in Fig. 24 for Case S2A. The accumulated soot profile variation with time for Case S2A is presented in Fig. 25. The soot accumulation rates at different local positions (z/L = 0.01, 0.25, 0.5, 0.75, 1) are compared for Case S2A and are presented in Fig. 26. It is been observed from the simulation results that the wall flow velocity doesn’t vary with the progressive soot accumulation in the inlet channel. This is consistent with the overall mass balance of the exhaust gas. Because the overall mass flow rate of the exhaust gas is kept constant throughout the soot accumulation process, the pressure drop across the channel rise without the

Table 3.5
Simulation matrix (Case S2).

<table>
<thead>
<tr>
<th>Cases</th>
<th>Soot</th>
<th>Flow rates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>60 mg/m³</td>
<td>90 mg/m³</td>
</tr>
<tr>
<td>S2B</td>
<td>80 g/s</td>
<td></td>
</tr>
<tr>
<td>S2A</td>
<td>53 g/s</td>
<td>S2B</td>
</tr>
<tr>
<td>S2C</td>
<td></td>
<td>S2A</td>
</tr>
</tbody>
</table>

Table 3.6
Fixed exhaust condition (Case S2).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exhaust temperature</td>
<td>200</td>
<td>°C</td>
</tr>
<tr>
<td>DPF initial temperature</td>
<td>200</td>
<td>°C</td>
</tr>
<tr>
<td>Exhaust O₂</td>
<td>10</td>
<td>%</td>
</tr>
<tr>
<td>Exhaust NO₂</td>
<td>100</td>
<td>ppm</td>
</tr>
<tr>
<td>Initial soot load</td>
<td>5</td>
<td>g/L</td>
</tr>
</tbody>
</table>
change in the wall flow velocity. The local pressure drop across the channel is dependent on the accumulated soot layer permeability and thickness. Therefore the pressure drop is increased with the accumulation of soot in the inlet channel as shown in Fig. 27 for Case S2A. A comparison of the accumulated soot profile over a time period of 1200 s is done and presented in Fig. 28.

3.1.3. Active flow DPF regeneration

DPF soot regeneration is simulated using the same model in order to calculate transient soot profiles and the related flow and temperature field along the DPF channel under various active-flow configurations. In active-flow configurations, the exhaust gas is controlled to attain the suitable quantity and quality for an efficient and safe DPF regeneration. In order to initiate the regeneration, the external energy is supplemented to the exhaust stream in the form of fuel, electrical heating or microwave heating. In the following section, simulations are carried out by varying the exhaust flow rate and supplemental energy delivery rate may be varied by changing parallel flow paths through the aftertreatment system. The simulation matrix is shown in Table 3.7. A uniform soot-layer thickness at the initiation of the regeneration is assumed as the initial boundary condition to the simulations presented in this section.

The progress of the DPF regeneration of the local soot layer and the exhaust flow profile through the filter wall along the DPF channel length are presented in this section. The local wall flow rates and soot thickness profiles are presented in Fig. 29–31. The simulation cases are expanded to other exhaust mass flow rates keeping the total supplemental fuelling rate constant. The simulation results indicates that at higher flow rates (>50 g/s) the convective heat transfer from the cooler exhaust gas subside any surface catalyst activity in the DOC and subsequently resulting in lower regeneration rate in the DPF placed downstream of the DOC. The regeneration progress as a percentage of soot oxidized of the initial soot load is presented for the various cases of exhaust flow rate in Fig. 32. A subsequent energy analysis is carried out based on the regeneration progress and supplemental fuel delivered (assuming

![Fig. 27. Soot accumulation rate (Case S2A).](image)

![Fig. 28. Accumulated soot profile (1200 s).](image)

![Fig. 29. Local wall flow (Case S3B).](image)

![Fig. 30. Local soot thickness (Case S3B).](image)

![Table 3.7 Simulation conditions (Cases S3).](image)
LHV 42.9 kJ/g) and is shown in Fig. 33. The analysis is also performed to quantify the energy required for the regeneration with the variations in exhaust flow rates in Fig. 34.

From the wall flow and the soot profile transient simulation results it can be observed that thicker soot layer offers more resistance to the passage of exhaust gas through the local wall region. This result is consistent with the observations made by various other researchers [8,7]. It is also observed that with the increase in exhaust flow rate, soot regeneration is more uniformly distributed along the channel length and conversely at lower flow rate the regeneration occurs with local soot burning as shown in Figs. 30 and 31. This can be explained that at lower exhaust flow rate, the oxygen supply to the regions of unburned soot is limited by the local exhaust flow through the soot layer and the filter wall. Other numerical investigations with the model reveal that at lower flow rate, the soot regeneration is associated with local overheating and significant loss of heat energy. On the other hand, at higher flow rates, the exothermic reactions in DOC are superseded by the convective heat transfer affecting in loss of catalytic activity and subsequently loss of regeneration conditions in DPF. From Fig. 34 it is seen that there are specific conditions favorable to regeneration with the variations of exhaust flow rate. At high flow rates, due to low diesel exhaust temperature, the DOC catalyst does not achieve “light off” and at very low flow rates, the limited supply of exhaust oxygen in the soot layer cannot provide favorable conditions to sustain regeneration.

Further simulations are carried out in order to investigate the influence of variations of the exhaust oxygen concentration (that is subjected to the diesel engine load variation) on the regeneration efficiency during partial flow operation mode of active flow schemes. In this investigation, attempts are made to identify the critical operating modes of partial flow system during transient engine operations. Due to minimal oxygen present in the exhaust stream at high load engine conditions, aftertreatment reactions in DOC and DPF may suffocate, thereby deactivating aftertreatment operation resulting in increased total energy consumption. On the other hand recovery of exhaust oxygen during transient high to low load operation may also increase the chance of unsafe and uncontrolled regeneration in the DPF.

Simulation with different exhaust flow velocities and exhaust oxygen concentrations are carried within the conditions of partial flow operation. Supplemental energy to initiate regeneration (20% of regeneration) and subsequent completion of the regeneration (with 80% of initial soot been regenerated) are calculated and shown in Fig. 35. It is observed that exhaust oxygen concentration
plays a vital role in the supplemental energy efficiency in the con-
ditions of partial flow operation due to limited availability of ex-
haustr oxygen for the regeneration reaction. Simulation also
indicates substrate overheating (temperature above 1400 °C) with
4 g/s and exhaust oxygen concentration of 20%. This indicates there
is a critical operating boundary for the DPF operation of during
load transients in partial flow restricting conditions.

In order to isolate the factors influenced by the exothermic
reactions in DOC on the mechanism of DPF regeneration, the rise
in the exhaust gas temperature through the DOC channels with
the variations in the supplemental fuelling are calculated. It is ob-
served if the DOC is operated above the catalytic “light off” condi-
tions (i.e. ~290 °C) the supplemental fuel is completely burnt
inside the DOC channels at the partial flow operating conditions.
This is supported by the fact that at low flow rates, the exhaust
gas has more time to burn completely in the DOC flow channels
than normal passive flow conditions of high flow rates. Due to this
increase in residence time of supplemental fuel in DOC, the rise in
exhaust temperature is almost linearly proportional to the supple-
mental fuelling rate, as shown in Fig. 36.

3.2. Experimental results

Empirical analysis is carried out in this study in order to further
validate on the supplemental fuel energy delivery strategies and its
effect in active-flow configurations. The thermal response of the
DOC–DPF system is recorded at different supplemental energy fuel
supply rates at different engine speed and load conditions. Diff-
ferent modes of external fuel injection rate are applied to raise the
temperature of the DOC–DPF system to enable aftertreatment
operation. A small gasoline injector, operated at 200 kPa pressure,
is used for external supplemental energy delivery. An electric hea-
ter (0.8 kW) heats up the exhaust stream to aid in diesel vaporiza-
and mixing with the exhaust stream.

The space velocities of the exhaust gas across the DOC–DPF sys-
tem at different engine operating conditions are given in Table 3.8.
In a six-cylinder diesel engine these low space velocities will cor-
respond to the conditions of partial flow restriction (PFR) across
the aftertreatment device. Therefore the experiments reported in
this paper are an appropriate representation of PFR.

Tests have been carried out to investigate the heating process of
the DOC–DPF with three different external fuel injection rates at
two engine speeds. The engine operating conditions were kept
similar at both the speeds to prevent any bias in the results. The
different modes of external fuel injection at 1400 RPM are shown in
Fig. 37. A relative fuel injection rate (RFIR) has been defined as
the ratio of the external fuel injection rate to the exhaust flow rate.
These external fuel injection tests are carried out to attain a fixed
temperature rise (ΔT ~ 280 °C) in the DOC and to maintain the fi-
nal temperature of the substrate at approximately 550 °C. During
modes 2 & 3, the fuel injection is initially higher to obtain faster
heating of the substrate. The fuelling rate is then reduced to that
of mode 1 to maintain the same final temperature for all the
modes.

The overall thermal response of the substrate for the test is
shown in Fig. 38. The system is allowed to cool down to the initial
temperature before starting the fuelling for the next testing mode.
The results indicate that a higher fuel injection rate results in a fas-
ter heating up of the substrate. On an energy efficiency basis, how-
ever, the same may not hold true as shown later in the energy
efficiency analysis.

The same tests were then repeated at 1800 RPM to investigate
the influence of the higher exhaust flow rate on the thermal re-
sponse of the aftertreatment. The RFIR for the three modes of
external fuel injection is shown in Fig. 39 and the test results are
given in Fig. 40. The temperature rise (ΔT ~ 340 °C) in the DOC
was kept constant in each testing mode.

The results show that the substrate heats up faster at a higher
exhaust flow rate for similar fuelling modes. This can be explained

Table 3.8

<table>
<thead>
<tr>
<th>Engine speed (RPM)</th>
<th>Engine torque (Nm)</th>
<th>Space velocity (1/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1400</td>
<td>37</td>
<td>21280</td>
</tr>
<tr>
<td>1800</td>
<td>38</td>
<td>28373</td>
</tr>
</tbody>
</table>

Fig. 36. Exhaust temperature in DOC.

Fig. 37. Modes of external fuel injection (1400 RPM).

Fig. 38. Overall thermal response of aftertreatment (1400 RPM).
by the fact that convection heat transfer rate and oxygen supply rate increases at higher exhaust flow rates.

3.2.1. Energy efficiency analysis

An energy efficiency analysis has been carried out for the empirical results presented above. Due to the difference in the temperature rise ($\Delta T$) for the two exhaust flow rates under consideration, the specific energy consumption is defined by the authors for comparing different cases [15]. Fig. 41 shows the energy efficiency comparison between various modes of operation and the absolute energy consumed to raise and maintain the temperature rise of ($\Delta T$) in the aftertreatment given in Table 3.9. It is observed that with the results presented in this analysis the specific energy consumed is less at the high flow rate than at the low flow rate. At 1800 RPM, due to the increase exhaust flow rate the rate of heat transfer increases, which may be attributed to faster reaction rates. However, it can be seen that the substrate cools down quickly at 1800 RPM compared to 1400 RPM. At higher flow rates, the convection heat transfer rate increases between the exhaust gas and the substrate. Thus, the thermal retention ability is reduced at higher flow rates.

At 1400 RPM, mode 2 gives the highest efficiency, whereas at 1800 RPM, mode 3 results in the highest efficiency. Observations reported in previous publications by authors also show a similar trend of energy consumption [16]. At a high fuelling rate, the exhaust gas becomes rich in combustibles and therefore has less chance to get oxidized completely. The time and temperature required to complete the oxidation of the rest of combustibles inside the DOC can be optimized by a combination of two or more fuel injection rates during the heating process.

4. Concluding remarks

A one-dimensional DOC and DPF model has been developed in order to perform simulations of active flow diesel aftertreatment configurations. Simulations are carried out in order to investigate various active flow conditions for DPF regeneration. The simulation results are compared with a set of experimental data for DPF regeneration. Based on the theoretical investigations, energy efficiency analysis is carried out between various active flow control aftertreatment operations. A preliminary energy efficiency analysis has also been carried out with the empirical data of various active flow aftertreatment control schemes.

Theoretical investigation indicated that soot oxidation inside DPF requires considerable less supplemental energy at the exhaust temperatures exceeding “light off” for DOC operation with external fuel injection as compared to lower exhaust temperature. A supplemental exhaust gas heater can effectively reduce overall energy penalty to efficiently regenerate DPF. This may be attributed to the higher thermal availability in the process of electrical heating when compared with the exothermic heat release due to fuel oxidation.

Simulation results indicate that at low-exhaust flow-rate operation regimes, the DPF regeneration requires less supplemental energy, providing that there is enough oxygen left in the exhaust for completing the soot oxidation reaction inside DPF channels. At the conditions of exhaust gas stagnation (e.g., no exhaust flow), the soot oxidation may seize to occur due to the unavailability of oxygen inside the DPF.

Depending on the engine operating modes, the exhaust oxygen concentration may vary in the exhaust stream. At low exhaust flow rates, variations in exhaust oxygen concentration may significantly affect the oxidation reaction efficiency of a DOC–DPF system.

Particulate regeneration is dependent on the factors such as the availability of oxygen in the soot layer due to the exhaust wall flow and the exhaust temperature. It is observed from the simulation results that soot profile gives an indication of the local soot oxidation rate. It is also observed that the higher the local soot oxidation rate, the higher is the tendency of substrate overheating and local thermal stress.

Variations across the channel length are neglected in model consideration. It is observed that with the results presented in this paper, large portion of exhaust pressure drop across DPF is attributed due to the soot layer distribution profile across DPF channel.
In active aftertreatment control strategies, critical supplemental energy may be used to maintain the exhaust temperature above the “light-off” temperature, at those locations where the catalyst may exhibit best performance. Thus, the catalyst coating can be strategically placed at most reactive regions thereby reducing overall cost in precious metal coating.

From the empirical investigation it is observed that if engine exhaust contains substantial amount of combustible substances, overheating can be predicted and prevented by increasing the flow rate with unidirectional flow control. The energy utilization efficiency of the external fuel injection can be optimized with both the engine operating condition and substrate-operating conditions including external fuelling strategies.

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