Development of a Catalyzed Diesel Particulate Filter Multi-zone Model for Simulation of Axial and Radial Substrate Temperature and Particulate Matter Distribution

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Abstract The catalyzed particulate filter (CPF) is an important exhaust aftertreatment subsystem that is managed by the electronic control unit (ECU) of an engine. CPFs need periodic regeneration to avoid temperature exotherms and excess engine back pressure. To this end, a multi-zone particulate filter (MPF) model was developed in this research to serve as a simulation tool to provide on-board diagnostics (OBD) data for managing CPF active regeneration (AR). The MPF model runs in real time within the ECU to provide feedback on temperature and particulate matter (PM) loading distribution within each axial and radial zone of the filter substrate. The MPF model accounts for the internal and external heat transfer mechanisms, inlet temperature distribution using the fully developed boundary layer concept, and PM oxidation by thermal (O₂)- and NO₂-assisted oxidation mechanisms. A calibration procedure was developed to calibrate the PM kinetics and heat transfer coefficients of the MPF model. The model shows the good capability to predict temperature and PM loading distribution within the filter.

Keywords Diesel particulate filter model · ECU based particulate filter model · Temperature distribution · Particulate loading distribution · Diesel exhaust emission control

Abbreviations

AR Active regeneration
 B10 Diesel blend (ULSD) with 10% Biodiesel

B20 Diesel blend (ULSD) with 20% Biodiesel
 CFD Computational fluid dynamics
 CPF Catalyzed particulate filter
 CO₂ Carbon dioxide
 DOC Diesel oxidation catalyst
 DPF Diesel particulate filter
 ECU Electronic control unit
 MPF Multi-zone particulate filter
 MTU Michigan Technological University
 NO₂ Nitrogen dioxide
 NO Nitrogen monoxide
 OBD On-board diagnostics
 O₂ Oxygen
 PO Passive oxidation
 PM Particulate matter
 SCR Selective catalytic reduction
 ULSD Ultra-low-sulfur diesel
 1-D One dimensional
 2-D Two dimensional
 3-D Three dimensional

Nomenclature

A_{amb} Surface area of outer surface [m²]
 $\bar{A}$ Average cross-sectional area [m²]
 A_{O_2} Pre-exponential for thermal (O₂) PM oxidation [m K⁻¹ s⁻¹]
 A_{NO_2} Pre-exponential for NO₂-assisted PM oxidation [m K⁻¹ s⁻¹]
 $A_{f,i,j}$ Cross-sectional area perpendicular to direction of heat transfer [m²]
 $A_{r,i,j}$ Area normal to direction of heat transfer in the radial direction [m²]
 $A_{s,i,j}$ Combined surface area of both inlet and outlet channels [m²]
 C Constant [–]

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c_f	Specific heat of filter material [$\text{J kg}^{-1} \text{K}^{-1}$]	$\dot{Q}_{\text{conv}}$	Convection between channel gases and filter wall [W]
C_{NO_2}	CPF inlet NO_2 concentration [ppm]	$\dot{Q}_{\text{rad}}$	Radiation between channel surfaces [W]
C_{O_2}	CPF inlet O_2 concentration [ppm]	$\dot{Q}_{\text{reac}}$	Total energy released during PM cake exothermic reactions [W]
c_p	Constant pressure specific heat [$\text{J kg}^{-1} \text{K}^{-1}$]	$\dot{Q}_{\text{reac,NO}_2}$	Energy released during NO_2 -assisted PM cake exothermic reactions [W]
C_{PM}	CPF Inlet PM concentration [mg m^{-3}]	$\dot{Q}_{\text{reac,O}_2}$	Energy released during thermal (O_2) PM cake exothermic reactions [W]
c_s	Specific heat of PM cake [$\text{J kg}^{-1} \text{K}^{-1}$]	rc_i	Radial distance of a zone from centerline [m]
d	Side length of square channels [m]	Δr	Effective zone radius [m]
D	Overall diameter of the CPF [m]	R_u	Universal gas constant [$\text{J gmol}^{-1} \text{K}^{-1}$]
E_{O_2}	Activation energy for thermal (O_2) PM oxidation [J gmol^{-1}]	$\dot{S}_{c(th)}$	Thermal (O_2)-assisted PM cake oxidation rate [$\text{kg C}_{(s)} \text{m}^{-3} \text{s}^{-1}$]
E_{NO_2}	Activation energy for NO_2 -assisted PM oxidation [J gmol^{-1}]	$\dot{S}_{c(\text{NO}_2)}$	NO_2 -assisted PM cake oxidation rate [$\text{kg C}_{(s)} \text{m}^{-3} \text{s}^{-1}$]
$F1$	Temperature factor [–]	S_p	Specific surface area of PM [m^{-1}]
$F2$	Mean to surface temperature ratio [–]	t	Time [s]
F_{3-1}	Radiation view factor between inlet of the channel to filter wall [–]	T	Average gas temperature of channels [K]
F_{3-2}	Radiation view factor between outlet of the channel to filter wall [–]	T_{amb}	Ambient temperature [K]
h_{amb}	Ambient convective heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]	T_{exit}	Filter exit gas temperature [K]
h_g	Convective heat transfer coefficient [$\text{W m}^{-2} \text{K}^{-1}$]	Tf	Temperature of combined filter and PM cake [K]
ΔH_{reac}	Heat of reaction for carbon oxidation via O_2 [J kg^{-1}]	T_{in}	CPF inlet temperature [$^{\circ}\text{C}$]
$J1$	Radiosity of channel inlet surface [W m^{-2}]	T_m	Mean exhaust gas temperature [K]
$J2$	Radiosity of filter wall surface [W m^{-2}]	T_s	Wall inner surface temperature [K]
$J3$	Radiosity of channel outlet surface [W m^{-2}]	T_r	Temperature at a given radial location [K]
k_{O_2}	Rate constant for thermal (O_2) PM oxidation [m s^{-1}]	$\bar{t}_{s,i,j}$	Average PM cake thickness in each zone [m]
k_{NO_2}	Rate constant for NO_2 assisted	$\bar{t}_s$	Average PM cake thickness across entire CPF [m]
k_g	Thermal conductivity of channel gas [$\text{W m}^{-1} \text{K}^{-1}$]	$\bar{t}_{s_i}$	Average PM cake thickness in each radial zone [m]
L	Axial length [m]	u	Representative velocity in each zone [m s^{-1}]
L_t	Total length of CPF [m]	u_I	Average inlet channel velocity [m s^{-1}]
ΔL	Effective zone length [m]	u_{II}	Average outlet channel velocity [m s^{-1}]
Δt	Solver Time step [s]	u_s	Average velocity through PM layer [m s^{-1}]
$\dot{m}$	Instantaneous exhaust mass flow rate [kg s^{-1}]	u_{si}	Average velocity through PM layer in each radial zone [m s^{-1}]
$\dot{m}_{i,j}$	Mass flow rate entering each zone [kg s^{-1}]	u_w	Average velocity through wall layer [m s^{-1}]
$ms_{i,j}$	Mass of PM in each zone [kg]	u_{wi}	Average velocity through wall layer in each radial zone [m s^{-1}]
ms_t	Total mass of PM retained [kg]	V	Total volume of a zone [m^3]
$\dot{m}_{\text{total}}$	Total mass flow rate into CPF [kg s^{-1}]	V_e	Empty volume in each zone [m^3]
Nc_i	Number of cells in each radial zone [–]	V_{es}	Empty volume accounting for PM cake [m^3]
Nc_t	Total number of cells [–]	V_f	Volume of filter in each zone [m^3]
Nu_{avg}	Average Nusselt number of the inlet and outlet channel	V_s	PM cake volume in each zone [m^3]
Nu_{inlet}	Nusselt number of the inlet channel	V_t	Total volume of the filter [m^3]
Nu_{outlet}	Nusselt number of the outlet channel	W	Exhaust gas molecular weight [kg kmol^{-1}]
Pe_w	Peclet number of wall [–]	$W^{c(s)}$	Molecular weight of carbon [kg kmol^{-1}]
P_{in}	CPF inlet gas pressure [kPa]	W_{O_2}	Molecular weight of oxygen [kg kmol^{-1}]
$\dot{Q}_{\text{cond,axial}}$	Axial conduction [W]	W_{NO_2}	Molecular weight of nitrogen dioxide [kg kmol^{-1}]
$\dot{Q}_{\text{cond,radial}}$	Radial conduction [W]	x	Diameter ratio of CPF or DOC [–]

Y	Mass fractions [–]
y	Axial location [–]

Greek Variables

a	Thermal diffusivity [$\text{m}^2 \text{s}^{-1}$]
a_{O_2}	O_2 oxidation partial factor [–]
a_{NO_2}	NO_2 oxidation partial factor [–]
ε_r	External radiation coefficient [–]
λ	Effective thermal conductivity of PM cake and filter [$\text{W m}^{-1} \text{K}^{-1}$]
λ_f	Thermal conductivity of filter [$\text{W m}^{-1} \text{K}^{-1}$]
λ_s	Thermal conductivity of PM cake [$\text{W m}^{-1} \text{K}^{-1}$]
ρ	Exhaust gas density [kg m^{-3}]
ρ_i	Exhaust gas density in each radial zone [kg m^{-3}]
ρ_f	Filter density [kg m^{-3}]
ρ_s	PM cake density [kg m^{-3}]
σ	Stefan-Boltzmann constant [$\text{W m}^{-2} \text{K}^{-4}$]

Subscripts and Superscripts

i	Radial direction
j	Axial direction

1 Introduction

Diesel particulate filters play a key role in meeting current and future particulate emission standards for diesel engines. One of the disadvantages of the diesel particulate filter is the need for periodic active regeneration. Regeneration is necessary to avoid an increase in engine exhaust back pressure as the particulate matter (PM) accumulates in the filter substrate. The active regeneration oxidizes PM which reduces engine back pressure and fuel consumption caused by increased back pressure/pumping work. However, active regeneration also consumes fuel. An experimental study by Rose et al. showed that there are overall fuel consumption penalties due to the increase in back pressure and the extra fuel required for active regeneration. The results showed a 3.3 % fuel penalty for a Euro 5 compliant 1.4-L turbocharged diesel engine with B10 fuel during the New European Driving Cycle [1].

The knowledge of PM mass retained as a function of time is the vital input for an effective and efficient active regeneration strategy. This is mainly because the PM loading beyond an acceptable level can lead to a damaged catalyzed particulate filter (CPF) and underloading leads to frequent regeneration events and hence excess fuel consumption and CO_2 emissions. The current engine electronic control unit (ECU) controls the PM loading using an internal PM estimator model. The PM estimator relies on the calibrated engine PM maps; pressure drop across the CPF and temperature measurements

to determine PM mass retained and regeneration frequencies [2].

Advanced regeneration strategies involve simplified CPF models that run real time within the ECU to provide more accurate feedback on current PM loading of the filter substrate. By applying simplified models that are similar to the ones used during design, development, and application of CPFs, the regeneration frequency and duration can be optimized based on vehicle operating conditions which determine engine operating conditions. This would lead to fuel consumption savings and resulting CO_2 emission reductions and also a potential increase in the durability of the CPF.

The optimum regeneration frequency and duration rely on the accurate prediction of temperature distribution within the filter. Due to the heat transfer and cake PM oxidation, CPF filter temperature varies spatially (both axial and radial directions) and affects the regeneration efficiency of the filter as the PM oxidation reactions are highly temperature dependent. Hence, the accurate prediction of temperature distribution within the filter substrate will aid in the optimum regeneration frequency and duration. The prediction of temperature distribution within the filter also provides robust diagnostics capability by monitoring the CPF temperature (as a virtual sensor) at several locations within the filter. The other use of the temperature distribution prediction could be as an alternative to a conventional CFD model to calculate axial and radial temperature distribution of the substrate. This could reduce significant simulation time and resources during the design and development phase of diesel particulate filters.

Hence, the model-based approach presented in this paper would enable the use of simplified MPF models that run fast enough in the ECU to predict temperature distribution within the filter and the PM cake oxidation. This paper describes a new MPF model for modeling temperature distribution in a CPF and the local cake PM oxidation.

The overall objective of this study is to develop a computationally efficient MPF model for predicting CPF temperature distribution and PM oxidation. The model should require limited calibration effort and needs to be validated with experimental data.

To present the approach to fulfill the above objective, the paper is organized into four components of research:

1. Review the literature related to modeling of heat transfer in the CPF substrate and the PM density distribution including experimental data.
2. Develop a MPF model that is capable of simulating filter substrate temperature and PM oxidation during passive oxidation and active regeneration within the axial and radial zones of the CPF.

3. Develop a calibration procedure for the heat transfer within the substrate and to the ambient including PM kinetics (NO_2 - and O_2 -assisted PM oxidation) locally.
4. Calibrate the MPF model using the experimental data [3–6] to arrive at a common set of MPF model calibration parameters for all experiments.

2 Background and Literature Review

The literature review is organized in two parts. First, the use of simplified models (0-D and 1-D) for ECU-based controls from previous studies is explored including the heat transfer models and their assumptions. Second, the simplified multi-dimensional modeling efforts (2-D and 3-D) in CPF modeling were studied along with their benefits and limitations related to modeling accuracy and computational efficiency.

2.1 CPF Models for ECU-Based Controls

CPF models can be incorporated in the ECU to monitor and optimize CPF performance along with the engine performance. Such a CPF model for CPF regeneration was described by Kladopoulou et al. [7] using a lumped parameter model. This was a 0-D model and the simulation relied on time dependence of input parameters. The spatial dependence (axial and radial directions) was assumed to be negligible. This lumped model included an external heat transfer mechanism by considering external ambient heat transfer through convection. Subsequently, further advanced model-based control techniques were explored by many researchers to simplify conventional 1-D models for real-time ECU application with reasonable accuracy and computational speed compared to conventional map-based control approaches as presented by Rose et al. [2].

The real-time implementation of a 0-D CPF model along with 1-D DOC model was presented by Nagar et al. [8] and showed that the 0-D CPF model was able to predict the average filter substrate temperature within 25 °C. They also highlighted the difficulty of initiating regeneration based on ΔP (difference between inlet and outlet pressure of CPF) measurement and concluded that PM loading provides a more reliable criterion to trigger CPF filter regeneration than using ΔP values. The CPF model by Nagar et al. assumed internal convective heat transfer from filter substrate to exhaust gas as a mechanism to dissipate the energy release during PM oxidation. However, the model ignores any conductive heat transfer within substrate.

Mulone et al. presented the 1-D CPF model for ECU application for steady-state [9] and transient operating conditions [10]. The model is based on the single channel representation of the CPF. The model was able to predict axial variation in the PM loading. However, the model ignored radial temperature gradients and the radial PM loading distribution in the CPF.

The resistance node methodology presented by Depcik et al. [11] provides a simplified and computationally efficient modeling approach to predict axial and radial temperatures of the filter. However, this model assumes uniform inlet temperature and ignores the inlet temperature variation along the radial direction of the CPF.

2.2 Simplified Multi-dimensional CPF Modeling

Konstandopoulos et al. [12] developed a multichannel model using a multiphase continuum approach to simulate spatial non-uniformities in the filter (axial and radial directions). The multiphase continuum model was derived from the discrete multichannel description of the CPF. The model worked in a CFD code framework to include the partial differential equations in the CPF model. The conduction, convection, and radiation heat transfer within the filter were considered in the model. With inlet radial non-uniformities in velocity and temperature, the model showed partial regeneration of the filter. The partial regeneration mainly occurred at the periphery of the filter as the PM at the periphery of the CPF was not oxidized due to lower temperatures in this region. This continuum model is computationally expensive as it involved a system of several ordinary and partial differential equations and the equations have to be solved in a 3-D domain.

Yi [13] developed a 3-D macroscopic model for predicting PM loading within the filter. The model was based on grouping the channels with reasonably uniform inlet conditions and solving each group using 1-D model equations. This established a link between 1-D and 3-D models and reduced the complexity of detailed 3-D simulations. The model did not consider PM oxidation (passive oxidation and active regeneration) within the filter and also neglected heat losses from the substrate can of the filter. The model showed PM distribution within the filter over a period of time and also indicated that PM distribution evolves to uniform when simulated without inlet and outlet connections (uniform inlet velocity). The model showed significant non-uniform radial and axial distribution of PM when simulated with inlet and outlet connections attached to the substrate and highlighting the need for multi-dimensional analysis to determine the actual PM distribution within the filter.

2.3 Proposed MPF Model

The non-uniform flow and temperature at the inlet of the filter affect both axial and radial PM distribution within the filter. This would cause localized heating and excess thermal stress due to heterogeneous oxidation of PM under high temperature and a high PM loading condition. This affects the durability of CPF systems. Previous 0-D and 1-D studies ignore these effects; thus, this study focuses on developing a multi-zone modeling approach (axial and radial zones) of the CPF for ECU applications.

The new MPF model proposed in this work is capable of predicting both temperature and PM loading distribution within the CPF in the axial and radial directions. The model considers varying CPF inlet temperature conditions to account for the thermal boundary layer development at the inlet of the CPF, heat transfer within the filter, and also heat dissipation to the ambient including conduction, convection, and radiation heat transfer. PM cake oxidation by O_2 and NO_2 is also considered.

As will be shown later in the paper, the proposed model can predict non-uniform distribution of the filter loading and temperature within the filter substrate and it requires significantly less simulation time compared to the multi-dimensional CPF models in the literature.

3 Experimental Data

A 2007 inline 6-cylinder turbo charged direct-injection common rail Cummins ISL 8.9-L diesel engine rated at 272 kW with DOC and CPF aftertreatment devices was used for this study. The detailed specifications of the engine and aftertreatment system are shown in references [3, 4]. The brief specifications of the CPF used in this study are shown in Table 1.

Experimental data collected by Shiel et al. [3, 5] and Pidgeon et al. [4, 6] at 18 different operating conditions are used to calibrate and validate the model developed in this study. The test summary of 18 experiments (6 passive oxidation and 12 active regeneration experiments) used in this study is shown in reference [14]. The experiments were performed with three fuels—ULSD, B10, and B20 blends. The properties of test fuels used for the experiments are documented in references [3, 4]. The detailed test setup, test matrix, and instrumentation are explained in reference [3] for the passive oxidation experiments and reference [4] for the active regeneration experiments.

The passive oxidation and active regeneration experiments start with 600 °C cleanup phase followed by stage 1 loading of

filter with a DOC inlet temperature of 265 ± 10 °C for 30 min. Then the stage 2 loading starts and continues to achieve a target filter loading of 2.2 ± 0.2 g/L. Upon completion of stage 2 loading, the test was continued further with the ramp up phase (RU) for 15 min. Following the RU phase, for the passive oxidation experiments, the engine was operated at the passive oxidation test conditions (for PO-B10-16 experiment, the CPF inlet conditions are temperature 408 °C, 61 ppm NO_2 , 209 ppm NO_x , and 7.1 % O_2) for a specified duration (43 min for PO-B10-16 experiment). For active regeneration experiments, following the RU phase, the engine was operated at an active regeneration ramp phase for 10 min (or until DOC inlet temperature has stabilized at 325 ± 10 °C) and then the active regeneration phase for a predetermined duration (26 min for AR-B10-1 experiment) at the specified CPF inlet conditions (temperature 530 °C, 4 ppm NO_2 , 119 ppm NO_x , and 7.8 % O_2 for AR-B10-1 experiment). Upon completion of passive oxidation phase for passive oxidation experiments and active regeneration phase for active regeneration experiments, the filter was loaded at stage 3 loading condition for 30 min and then the test was continued further with stage 4 loading for 60 min. The filter was weighted at the end of each stage. The engine operating conditions for all four stages of the loading are the same.

The experimental data from these tests (temperature distribution and PM loading) are used in this study for the calibration of the internal and external heat transfer of the MPF model and also the PM kinetic parameters.

3.1 CPF Temperature Distribution

Having temperature distribution data is critical for this study to validate the MPF model since predicting temperature distribution within the CPF is one major contribution from this study. The experimental temperature distribution data were collected from references [5, 6]. For each of the 18 experiments in this study, temperature distribution within the CPF was measured using 16 ungrounded K-type thermocouples to determine temperature distribution within the filter during each test. These data were used for the heat transfer model calibration and validation of the MPF model simulation data. The CPF thermocouple layout and specifications of the thermocouples are shown in references [5, 6].

The CPF thermocouples were placed at four axial locations (at a distance of 32, 98, 152, and 273 mm, respectively, from the end of the filter) and four radial locations (at diameters of 0, 110, 190, and 244 mm). The temperature distribution measured by thermocouples (C1–C16) for AR-B10-1 experiment at 5.63 h (15 min after fuel dosing) is shown in Fig. 1. Figure 2 shows the radial temperature distribution measured by thermocouples C1–C4 during the entire test duration.

From Figs. 1 and 2, the following trends are observed. The temperatures are varying in both the axial and radial directions.

Table 1 Specifications of the CPF used in the experiments

	CPF	Units
Substrate material	Cordierite	–
Cell geometry	Square	–
Diameter	267	mm
Length	305	mm
Cell density	31 (200)	cells cm^{-2} (cells in^{-2})
Cell width	1.49	mm
Wall density	0.45	$g\ cm^{-3}$
Specific heat	891	$J\ kg^{-1}\ K^{-1}$
Thermal conductivity	0.84	$W\ m^{-1}\ K^{-1}$

Fig. 1 Measured CPF temperature distribution during AR-B10-1 experiment at 5.63 h (15 min after fuel dosing)

The radial variation of temperature is comparatively higher (up to 40 °C) than the axial variation in temperature (up to 12 °C). The radially decreasing temperature is attributed to external ambient heat transfer of the filter and inlet flow/temperature maldistribution, and the axially increasing temperature is attributed to the oxidation of PM within the filter during active regeneration along with the heat transfer. Without the PM oxidation, the temperature would drop axially due to heat transfer.

4 Model Development

4.1 Overview

The MPF model presented in this paper is an extension of the 0-D lumped models developed by Kladopoulou et al. [7] and Johnson et al. [15]. The model development presented in this

Fig. 2 Measured CPF temperature distribution during AR-B10-1 experiment for thermocouples C1–C4

paper is based on the resistance node methodology presented by Depcik et al. [11]. In the MPF model, the CPF is modeled as a user configurable number of axial and radial zones as shown in Fig. 3.

The filter and gas energy equation is employed at each zone. The energy equation considers the heat transfer within the filter and external to the filter through convection, conduction, and radiation heat transfer modes. The PM oxidation model is also applied in each zone and the model considers PM oxidation by thermal (O_2)- and NO_2 -assisted mechanisms using inlet O_2 and NO_2 concentrations. The model also takes into account the inlet temperature distribution assuming the fully developed boundary layer at the inlet of the CPF. The coefficients used for generating the temperature profile at the inlet of the filter are explained later in the paper. The model outputs are temperature distribution within the filter substrate, total PM mass retained, and PM loading distribution within the filter. The inlet channel, outlet channel, PM cake layer, and substrate wall velocity equations are also included in the model to allow future work for predicting species concentration within the filter substrate. The model assumptions are outlined as follows:

1. The inlet PM deposits uniformly over the entire volume of the filter substrate and all the PM deposits as a cake.
2. The PM inlet rate into the each zone is assumed to be the ratio of volume of each zone to the total volume of the filter. In other words, no maldistribution of inlet PM is considered.

R = Radius of the filter
 L = Length of the filter
 r_1, r_2, r_3 and r_4 = Radial distance of each zone from centerline
 $\Delta r_1, \Delta r_2, \Delta r_3$ and Δr_4 = Effective zone radius
 $\Delta L_1, \Delta L_2, \Delta L_3$ and ΔL_4 = Effective zone length

Fig. 3 4×4 Multi-zone CPF model schematic. R radius of the filter; L length of the filter; r_1, r_2, r_3 , and r_4 radial distance of each zone from centerline; $\Delta r_1, \Delta r_2, \Delta r_3$, and Δr_4 effective zone radius; and $\Delta L_1, \Delta L_2, \Delta L_3$, and ΔL_4 effective zone length

- Species concentrations (O_2 and NO_2) are assumed to be uniform in each zone of the filter and are equal to inlet concentrations.
- Back diffusion of NO_2 due to the catalyst wash coat is not considered.
- Gaseous hydrocarbon oxidation within CPF is not considered.
- PM cake layer and substrate wall are at the same temperature. In other words, no temperature gradient across the PM cake layer and substrate wall is considered.
- A fully developed boundary layer exists at the inlet of the CPF.
- The exhaust gas mixture is assumed to be an ideal gas.
- The exhaust gas has the same properties as air at 1 atm pressure. Properties are considered as a function of temperature. CPF inlet species concentrations (CO_2 , O_2 , N_2 , and H_2O) are used for the calculation of molecular weight of the exhaust gas.

4.2 Discretization

Discretization of the filter volume is done in both the axial (ΔL) and radial directions (Δr) as shown in Fig. 4. Figure 4 shows the physical representation of the CPF channels with uniform deposition of PM in the cake layer along the walls of inlet channel. In the MPF model, the full volume of the filter is discretized into a user-configurable number of axial and radial zones. Each zone is comprised of multiple inlet and outlet channels. The schematic representation of the channel geometry for each zone is shown in Fig. 5. Each zone consists of the filter substrate, PM cake, and empty volume for inlet and outlet channels. The multi-zone model discretization equations are presented in Appendix A.

4.3 Filter Temperature Equations

The energy stored in the filter is due to the (a) heat conduction along the length of the filter ($\dot{Q}_{\text{cond,radial}}$), (b) heat conduction

ts = Thickness of the cake layer, d = Channel width

Fig. 4 Schematic of the CPF channel geometry with the PM cake layer ts =thickness of the cake layer, d =channel width

Fig. 5 Schematic for a zone of the MPF model

along the radial direction of the filter ($\dot{Q}_{\text{cond,radial}}$), (c) convection between the filter and the channel gas ($\dot{Q}_{\text{conv}}$), (d) energy released during oxidation of the PM cake ($\dot{Q}_{\text{reac}}$), and (e) heat transfer due to radiation exchange between channel surfaces ($\dot{Q}_{\text{rad}}$). The energy flow through the wall is neglected as there will be no distinction between inlet and outlet channels in the MPF model in this work. Hence, the energy equation for the filter is as follows:

$$\left(\rho_s c_s V s_{i,j} + \rho_f c_f V f_{i,j} \right) \frac{dTf_{i,j}}{dt} = \dot{Q}_{\text{cond,axial}} + \dot{Q}_{\text{cond,radial}} + \dot{Q}_{\text{conv}} + \dot{Q}_{\text{reac}} + \dot{Q}_{\text{rad}} \quad (1)$$

where Tf is the filter substrate temperature.

The detailed formulation for the terms used in Eq. (1) is explained in Appendix A.

The convection heat transfer between the filter substrate and the channel gas is calculated using the following equations [11, 19]:

$$\dot{Q}_{\text{conv}} = h_g A s_{i,j} (T_{i,j} - Tf_{i,j}) \quad (2)$$

The convective heat transfer coefficient (h_g) is calculated using the fully developed Nusselt number correlation based on the flow Peclet and Reynolds number through the wall for a square channel configuration. Depcik et al. [16] determined Nusselt number correlations from the historical references for Prandtl number of 0.72 (approximately air). Recently, Bissett et al. [17] and Kostoglou et al. [18] derived Nusselt number correlations for wall-flow monoliths for the parameter range applicable for the diesel particulate application. From reference [17], the polynomial approximations of Nusselt numbers for $Re_w < 3$ are given as

$$Nu_{\text{inlet}} = 2.98 + 0.60Pe_w - 0.143Re_w \quad (3a)$$

$$Nu_{\text{outlet}} = 2.98 - 0.40Pe_w \quad (3b)$$

In the MPF model, as there is no distinction between inlet and outlet channel, the average Nusselt number is used for

computing the heat transfer coefficient for the combined inlet and outlet channel and it is given as

$$Nu_{avg} = Nu_{inlet} + Nu_{outlet} = \frac{h_g d}{k_g} \quad (3c)$$

where

Nu_{avg}	Average Nusselt number of the inlet and outlet channel
Nu_{inlet}	Nusselt number of the inlet channel
Nu_{outlet}	Nusselt number of the outlet channel
k_g	Thermal conductivity of channel gas
Pe_w	Peclet number of wall
Re_w	Reynolds number of wall
As_{ij}	Combined surface area of inlet and outlet channels.

4.4 PM Oxidation

The PM oxidation equations include PM oxidation by thermal (O_2)- and NO_2 -assisted reactions. The total rate of PM mass oxidation in the cake due to thermal- and NO_2 -assisted oxidation is equal to [16],

Total rate of PM oxidation

$$= \text{PM oxidation by thermal } (O_2) \\ + \text{PM oxidation by } NO_2 \text{ assisted} \quad (4)$$

$$\frac{d(ms_{i,j})}{dt} = \frac{S_p \rho_{i,j} Y_{i,j} O_2 k_{O_2} W_c}{\alpha_{O_2} W_{O_2} \rho_s} ms_{i,j} - \frac{S_p \rho_{i,j} Y_{i,j} NO_2 k_{NO_2} W_c}{\alpha_{NO_2} W_{NO_2} \rho_s} ms_{i,j} \quad (5)$$

where

$$\frac{d(ms_{i,j})}{dt} = \text{Rate of PM mass oxidized in each zone}$$

In Eq. (5), the pressure term for computing the exhaust gas density ($\rho_{i,j}$) is assumed to be constant.

The details of formulation for the terms used in Eq. (5) is explained in [Appendix A](#).

4.5 Velocity Equations

Using average gas velocity equations for the entire filter substrate from reference [11], the average velocity through the PM cake (u_{si}) and wall layers (u_{wi}) for each radial zone is

$$u_{si} = \frac{\dot{m}_{i,j}}{4\rho_{i,j} \frac{Nc_i}{2}(d-2.\overline{ts_i}) L_t} \quad (6)$$

$$u_{wi} = \frac{u_{si}(d-2.\overline{ts_i})}{d} \quad (7)$$

The average velocity through the inlet channel (u_I) and outlet channel (u_{II}) for each radial zone can be determined as

$$u_I|_{i,j} = u_I|_{j-1} - \frac{4u_{si}}{d-2.\overline{ts_i}} \Delta L_{j-1} \quad (8)$$

$$u_{II}|_{i,j} = u_{II}|_{j-1} + \frac{4u_{wi}}{d} \Delta L_{j-1} \quad (9)$$

The detailed formulation of Eqs. (6) to (9) are explained in [Appendix A](#).

4.6 Temperature Distribution at Filter Inlet

The radial temperature distribution at the inlet of the filter is due to the thermal boundary layer development as explained in references [12, 19–21]. In order to account for the thermal boundary layer development, the empirical temperature factor profile is determined by analyzing experimental data from the 18 runs.

The temperature profile at the inlet of the CPF is not constant across the radial direction for the data in Figs. 1 and 2. This is mainly because of the thermal boundary layer development in the upstream of exhaust pipes and the DOC. The thermal boundary layer develops when the exterior surface of the pipe is exposed to a different temperature than the fluid flowing through the pipe. If the air temperature of outer surface is lower than the exhaust gas temperature, then the temperature of the exhaust gas in contact with the inner surface decreases and causes a subsequent drop in temperature of the exhaust gas in other regions of the pipe. This leads to the development of thermal boundary layer (similar to velocity boundary layer).

For a fully developed flow, the temperature factor shown below is constant across the length (temperature profile is constant). Hence, from reference [19],

$$\frac{\partial}{\partial x} \left[\frac{T_s(y) - T(r, y)}{T_s(y) - T_m(y)} \right] = 0 \quad (10)$$

$$\text{Temperature Factor} = \frac{T_s - T_r}{T_s - T_m} = C \quad (11)$$

where

T_m	Mean exhaust gas temperature
T_s	Wall inner surface temperature
T_r	Temperature at a given radial location
y	Axial location.

For this modeling work, the temperature factor at the inlet of CPF was determined by analyzing the C1, C2, C3, and C4 thermocouple measurements. Figure 6 shows the temperature

Fig. 6 Temperature factor profile at filter inlet

factor calculated using Eq. (11) for all 18 runs at 0.42 h. The horizontal axis is the CPF diameter ratio, 0 means center of the filter and 1.0 means outer diameter of the filter. The 3rd-order polynomial equation was used as the curve fit to represent the temperature factor for a given diameter ratio of the CPF and is given by

$$\begin{aligned} \text{Temperature Factor } (x) = & -2.493x^3 \\ & + 1.0585x^2 - 0.3285x \\ & + 1.7631 \end{aligned} \quad (12)$$

where x is the diameter ratio at a given location.

The diameter ratio is the ratio of CPF diameter at a given measurement location to the maximum CPF diameter. From Fig. 6, the temperature factor is almost constant up to CPF diameter ratio of 0.4 (indicating uniform temperature) and drops to 0 value (minimum temperature) at the CPF diameter ratio of 1.0 (outer radius of the filter). The maximum gradient in the temperature factor is observed at the CPF diameter ratio of 0.8 to 1.0, showing that 50 % of the radial temperature reduction is in the 20 % of the filter section closest to the outer radius of the filter. From Appendix B, the minimum substrate temperature at the outer surface ($R=133$ mm) is 4.3 % lower than mean substrate temperature at the inlet ($\frac{T_m}{T_s} = 1.043$).

The detailed procedure for developing the thermal boundary layer temperature factor and other coefficients used in the MPF model are explained in Appendix B. Using Eqs. (11, 12) and knowing the temperature at one radial location/zone of the CPF inlet, the temperatures at the other radial locations can be determined. The MPF model uses one CPF inlet temperature sensor data (T_{in}) to develop thermal boundary layer profile for the remaining zones at the CPF inlet.

4.7 Numerical Solver

The model formulation involves simulation of the time-varying temperature within the CPF from node to node. Hence, an explicit solver scheme was used to determine the temperature at each time step. The explicit solver estimates the filter substrate temperature for a time step (t) using temperature values from the previous time step ($t-1$). This approach is relatively simple to setup and program. However, Δt must be less than the limit imposed by stability constraints [19, 22]. The temperature for the new time step with the explicit solver method can be expressed mathematically as (for $i=2$ to i_{max} and $j=1$ to j_{max})

$$\begin{aligned} \text{Temp\_filter\_new}_{i,j} = & \text{Temp\_filter\_old}_{i,j} + \dots \\ & + \frac{\dot{Q}_{\text{cond.axial}} + \dot{Q}_{\text{cond.radial}} + \dot{Q}_{\text{conv}} + \dot{Q}_{\text{reac}} + \dot{Q}_{\text{rad}}}{(\rho_s c_s V_{s,i,j} + \rho_f c_f V_{f,i,j})} \Delta t \end{aligned} \quad (13)$$

where

Δt is the time step for the solver.

The explicit method is easy to use, but it is not unconditionally stable and the largest permissible value of Δt is limited by the stability criterion. For larger time steps, the explicit method oscillates widely and diverges from the actual solution. In general, the stability criterion is satisfied when the primary coefficients of all temperature terms in the Eq. (13) are greater than or equal to zero for all nodes [19]. Since the time step for each term is different, the practical approach to this problem is to use the most restrictive time step. From reference [19], the 1D convection problem for a plane wall, the time step is expressed as

$$\Delta t \leq \frac{\Delta x^2}{2\alpha \left(1 + \frac{h\Delta x}{k}\right)} \quad (14)$$

where, Δx is the discretization length (minimum of ΔL or Δr), α is the thermal diffusivity of the filter substrate. However, considering the heat transfer between filter and channel gas, α is minimum at the gas side and hence

$$\alpha = \frac{k_g}{\rho c_p} \quad (15)$$

where

k_g	Thermal conductivity of exhaust gas
ρ	Density of exhaust gas
c_p	Specific heat capacity of exhaust gas
$h=h_g$	Convective heat transfer between filter substrate and channel gas.

Using the Eqs. (14) and (15), the initial values of time step can be determined. The MPF model includes conduction, convection, and radiation terms together. By iteration from the above initial guess, the stable time step of 0.01 s was determined to work for up to a 20×20 multi-zone formulation in this work.

5 Model Calibration

5.1 Inputs and Outputs

The MPF model has 4 sets of input variables, 15 constants, and 7 calibration parameters. The model needs to be parameterized in order to simulate the temperature and PM mass loading distribution within the filter substrate. The input variables include

- 1) Instantaneous exhaust mass flow rate ($\dot{m}$)
- 2) CPF inlet concentrations (C_{PM} , C_{NO_2} , and C_{O_2})
- 3) CPF inlet temperature (T_{in})
- 4) CPF inlet gas pressure (P_{in}).

The constants of the MPF model are listed in Table 2. The model constants C1 to C6 were determined from the thermal boundary layer formulation as explained in Appendix B. There are two groups of unknown calibration parameters in the MPF model. These two groups include (i) PM oxidation parameters and (ii) heat transfer coefficients. These two groups of parameters are determined by using optimization techniques and the experimental data.

5.2 Calibration Process

For the model calibration and results presented in this work, the 10×10 MPF model was used which runs about 12 times faster than real time on a laptop with 12-GB RAM, 64-bit and inter core i7 processor. However, the optimum number of zones for an ECU application can be determined by running

Fig. 7 Model calibration flow chart

the model at different levels of discretization (axial and radial zones). This discretization study along with the detailed model validation is ongoing work and will be covered in the next research paper.

The overall objective of the calibration process was to simulate the axial and radial PM loading distribution to agree with the total experimental PM mass retained within 3 g. This was achieved by the two-step calibration process shown in Fig. 7.

- 1) Calibration of PM oxidation: PM kinetic parameters (A_{NO_2} , E_{NO_2} , A_{O_2} , and E_{O_2}) are determined in this step. The calibration of PM kinetic parameters from the engine experiments are preferred over synthetic gas-based lab reactor experiments because the engine experiments provide representative PM composition, residence time, and operating temperatures of the filter for calibration. Hence, the PM kinetic parameters determined from the engine experiments can be directly used in the MPF model.

Table 2 MPF model constants

Symbol	Description	Units	Values
F	Radiation view factor	[–]	0.011
C1	DOC radial temperature distribution factor 1	[–]	–2.493
C2	DOC radial temperature distribution factor 2	[–]	1.0585
C3	DOC radial temperature distribution factor 3	[–]	–0.3285
C4	DOC radial temperature distribution factor 4	[–]	1.7631
C5	DOC mean to surface temperature ratio	[–]	1.0425
C6	DOC temperature sensor offset	[–]	$0.0273 \cdot T_{in} - 2.4996$
ρ_{pm}	PM density	kg m^{-3}	104
S_p	Specific surface area of PM	m^{-1}	5.5×10^7
$C_{p_{air}}$	Specific heat of air	$\text{J kg}^{-1} \text{K}^{-1}$	Using Eq. (66)
μ	Dynamic viscosity of air	N s m^{-2}	Using Eq. (67)
λ_f	Thermal conductivity of substrate wall	$\text{W m}^{-1} \text{K}^{-1}$	1
λ_p	Thermal conductivity of PM cake layer	$\text{W m}^{-1} \text{K}^{-1}$	2.1
α_{O_2}	O_2 combustion partial factor	[–]	0.8
α_{NO_2}	NO_2 combustion partial factor	[–]	1.75

The objective of the first step is to minimize the error between the simulation and the total experimental PM mass retained.

- 2) Calibration of heat transfer coefficients: convective and radiation heat transfer coefficients (h_{amb} and ε_r) are determined from this step. In addition, the filter substrate density (ρ_f) is found. The substrate density along with other thermophysical properties (thermal conductivity, substrate density, and PM density) of the filter changes during the filter loading. Hence, in order to simulate the change in thermophysical properties of the filter, the filter substrate density is also considered as the one of the calibration variables in the MPF model. Depcik et al. [11] showed in his model calibration efforts that the model accuracy could be improved during temperature rise portion of the experiment by optimizing the filter substrate density. The objective of this step is to minimize the RMS temperature error between the simulation and the experimental data measured by the 16 CPF thermocouples during the stage 1 and 2 loading phases of the experiments.

The calibration process starts with the initial assumption of calibration parameters. The initial values of the calibration parameters were determined from the references [11, 14, 23, 24]. All 18 runs are simulated and the results are compared with the experimental data. To improve the model accuracy, the calibration process is repeated if the PM mass loading error exceeds 3 g and the RMS temperature distribution error exceeds 15 °C. Details about the calibration process for the two steps are explained next.

5.2.1 Step 1: PM Kinetics Calibration Procedure

The objective of the PM kinetics calibration procedure is to simulate the experimental total PM mass retained within the filter at each of the four stages of loading. This was achieved by determining NO₂-assisted PM oxidation kinetic parameters (A_{NO_2} and E_{NO_2}) and thermal (O₂)-assisted PM oxidation kinetic parameters (A_{O_2} and E_{O_2}) from the experimental runs (passive oxidation and active regeneration). The error term e_m in Fig. 7 represents the error between simulated and experimental PM mass retained at each of the four stages of loading.

The tasks involved in the PM kinetics calibration are the following:

1. Determine the NO₂-assisted PM kinetics (A_{NO_2} and E_{NO_2}) from the passive oxidation experiments keeping other parameters constant. Optimization is done in Matlab® using Nelder-Mead Simplex method [25]. Matlab function *fminsearch* is used to minimize the error between MPF model simulation and the experimental PM mass retained. The error value of 1 g is used as the target for the Simulink design optimization at the end of each of the stages of loading.
2. Use the NO₂-assisted PM kinetics (from task 1) to determine the thermal (O₂)-assisted PM kinetics from the active regeneration experiments keeping other parameters constant in the model.
3. From the PM kinetics determined from tasks 1 and 2, use the Arrhenius plots to determine the optimum PM kinetic parameters for each type of fuel.
4. From tasks 1, 2, and 3, determine one set of PM kinetic calibration parameters (A_{NO_2} , E_{NO_2} , A_{O_2} , and E_{O_2}) for each type of fuel (ULSD, B10, and B20)

5.2.2 Step 2: Heat Transfer Coefficients Calibration

Similar to step 1, Nelder-Mead Simplex optimization method [24] is used to calibrate the heat transfer coefficients in the MPF model. The heat transfer coefficients and filter density values are varied keeping all other parameters constant in the model. The objective of the optimization routine is to minimize the RMS temperature error between the simulation and the experimental temperature data measured by the 16 thermocouples during stages 1 and 2 of the loading phase of the experiment. The RMS error of 2 °C is used as the target for optimization.

The resulting model parameters from the 2-step calibration procedure are shown in Tables 3 and 4. Simulation results and experimental validation of the MPF model with calibrated parameters are provided in the next section.

Table 5 shows the standard deviation (1 sigma) of the activation energy and pre-exponential between the experiments

Table 3 Calibrated parameters of the MPF model for PM kinetics for three different fuels

PM oxidation	Symbol	Description	Units	ULSD	B10	B20
NO ₂ -assisted	A_{NO_2}	Pre-exponential for NO ₂ -assisted PM oxidation	$\text{m K}^{-1} \text{s}^{-1}$	0.0088	0.0083	0.0085
	E_{NO_2}	Activation energy for NO ₂ -assisted PM oxidation	kJ g mol^{-1}	60.8	64.1	63.1
Thermal (O ₂)	A_{O_2}	Pre-exponential for thermal (O ₂) PM oxidation	$\text{m K}^{-1} \text{s}^{-1}$	0.982	1.004	1.029
	E_{O_2}	Activation energy for thermal (O ₂) PM oxidation	kJ g mol^{-1}	158.1	151.8	148.9

Table 4 Calibrated heat transfer coefficients and filter density for the MPF model

Symbol	Description	Units	Values
h_{amb}	Convection heat transfer coefficient	$\text{W m}^{-2} \text{K}^{-1}$	8.1
ε_r	External radiation coefficient	[-]	0.16
ρ_{filter}	Filter density	kg m^{-3}	449

for all three types of fuel used based on an analysis of the Arrhenius plots of the data.

6 Results and Discussion

Using the single set of calibration parameters (Tables 3 and 4) determined from the calibration process, the MPF model simulations of one passive oxidation (PO-B10-16) and one active regeneration (AR-B10-1) experiment were studied. The results are presented in the following section.

6.1 Temperature Distribution

Figure 8 shows the radial temperature distribution of the PO-B10-16 experiment measured by C13–C16 thermocouples (shown as continuous line) and the temperatures simulated by the MPF model (shown as dotted line) at the outlet of the filter (273 mm from the filter inlet). As shown in Fig. 8, the MPF model simulation closely follows the experimental data (within 5 °C excluding the temperature spikes related to experimental procedure and transition phases of moving in and out of PO phase of the experiment) during the entire experiment.

Figure 9 shows the axial temperature distribution of the thermocouple measurements at the center of the filter ($R=0$ mm). As shown in Fig. 9, the simulation and experimental data shows that the temperature of the substrate is nearly constant during the experiment along the length of the filter (axially 32, 153, 207 and 273 mm from the front of the filter).

Figure 10 shows the temperature distribution measured by all 16 thermocouples and temperatures simulated by the MPF model at 4.73 h (15 min after switching to passive oxidation engine operating condition). The engine operating condition at 4.73 h is chosen to compare the model predictability at high temperature regions of the experiment. From Fig. 10, it is

Fig. 8 Radial temperature distribution at filter outlet (PO-B10-16 experiment)

evident that the MPF model follows the experimental data. The maximum absolute temperature difference between the experimental and simulation data is 5 °C. From Fig. 10, the filter substrate temperatures for radius less than 80 mm are almost same. A slight temperature increase (1–2 °C) in axial direction is due to the local PM oxidation. The substrate temperature close to the wall shows a slight decrease in temperature due to the dominant convection and radiative heat loss to the ambient compared to the local PM oxidation.

Figure 11 shows the radial temperature distribution for the AR-B10-1 experiment as measured by the C13–C16 thermocouples and the temperatures simulated by the MPF model at the outlet of the filter (273 mm from the filter inlet). The MPF model is within $-24/+6$ °C to the experimental data (excluding the temperature spikes related to the experimental procedure and the transition phase of moving in and out of AR phase of the experiment). The temperatures close to the outer surface of the filter substrate ($R=122$ mm) showed the maximum temperature deviation during the active regeneration phase of the experiment compared to the other locations of the filter substrate. The temperature simulated by the MPF model during loading (0 to 5.0 h) and post loading (6.3 to 7.3 h) phase of the experiment is within (7 °C) to the experimental data.

Figure 12 shows the axial temperature distribution of the thermocouple measurements at the center of the filter ($R=0$ mm). As seen from Fig. 12, the temperature stays constant

Table 5 PM kinetics parameters standard deviation summary between runs

PM oxidation	Symbol	Description	Units	ULSD (%)	B10 (%)	B20
NO ₂ assisted	A_{NO_2}	Pre-exponential for NO ₂ -assisted PM oxidation	$\text{m K}^{-1} \text{s}^{-1}$	3.8	0.6	NA
	E_{NO_2}	Activation energy for NO ₂ -assisted PM oxidation	kJ mol^{-1}	1.1	1.2	NA
Thermal (O ₂)	A_{O_2}	Pre-exponential for thermal (O ₂) PM oxidation	$\text{m K}^{-1} \text{s}^{-1}$	1.4	2.5	4.5 %
	E_{O_2}	Activation energy for thermal (O ₂) PM oxidation	kJ mol^{-1}	0.8	0.2	0.9 %

Fig. 9 Axial temperature distribution (PO-B10-16 experiment)

during the experiment along the length of the filter (axially 32, 153, 207, and 273 mm from the front of the filter) which is similar to the trends observed during the passive oxidation experiment PO-B10-16. The MPF simulation model follows the experimental data within (+18/−15 °C).

Figure 13 shows the temperature distribution measured by all 16 thermocouples and temperatures simulated by the MPF model at 5.63 h which is 15 min after the start of fuel dosing in order to compare the model predictability at the high-temperature region of the experiment. From Fig. 13, the MPF model follows the experimental data and the maximum temperature difference between the experimental and the simulation data is (−20 °C) at the upper right corner of the plot (filter substrate length >250 mm and radius >120 mm).

From Fig. 13, the experimental filter substrate temperature shows an increase in temperature (10–12 °C at filter radiuses below 40 mm) axially due to the local PM oxidation, and the substrate temperature close to the wall shows a lower increase

Fig. 10 Temperature distribution for PO-B10-16 experiment at 4.73 h (15 min after switching to PO engine operating condition)

Fig. 11 Radial temperature distribution at filter outlet for AR-B10-1 experiment

in temperature axially (5 °C approximately) due to the dominant convection and radiative heat loss to the ambient compared to the local PM oxidation. From Fig. 13, the MPF simulation model also shows an increase in temperature (4.4 °C) in the axial direction due to PM oxidation; however, the magnitude of the increase is low compared to the experimental data.

6.2 PM Mass Retained

Figure 14 shows the comparison of PM mass retained for the experimental data and simulation model along with the model cumulative for inlet PM and oxidation masses for PO-B10-16 experiment.

The measured PM masses at the end of each stage of the experiment (stage 1 to 4) are marked with plus markers in Fig. 14. NO₂-assisted PM oxidation is the dominant mode of PM oxidation shown by a dashed line because of the NO₂

Fig. 12 Axial temperature distribution for AR-B10-1 experiment

Solid lines: Experimental Data
Dashed lines: MPF Model Simulation

Fig. 13 Temperature distribution for AR-B10-1 experiment at 5.63 h (15 min after start of fuel dosing)

concentration (61 ppm). The thermal (O_2)-assisted PM oxidation is low (<1.3 g) compared to NO_2 -assisted PM oxidation due to the lower exhaust gas temperature during the PM oxidation (408 °C at 4.49 to 5.22 h).

Table 6 shows the comparison of measured and simulated PM mass retained in the CPF at the end of each stage. From Table 6, the MPF model simulated the PM mass retained within the filter substrate with the maximum absolute error of 1.3 g between experimental and the simulated PM mass retained at the end of the stage 2 loading phase of the experiment.

Figure 15 shows the comparison of PM mass retained for the experimental data and simulation model along with the model cumulative for inlet PM and oxidation masses for AR-B10-1 experiment. From Fig. 15, thermal (O_2)-assisted PM oxidation is the dominant mode of PM oxidation during

Fig. 14 Comparison of PM mass retained in the experimental data and simulation model along with the model cumulative for inlet PM and oxidation masses for PO-B10-16 experiment

Table 6 Comparison of experimental PM retained measured to MPF model output PM retained at the end of each stage for PO-B10-16 experiment

Stage	Time [hrs]	Expt. [g]	Model [g]	Diff. [g]
1	0.47	4.3	4.3	0
2	4.23	36.5	37.8	1.3
3	5.70	26.0	26.6	0.6
4	6.70	35.1	35.9	0.8

active regeneration as shown by the dotted line because of the increased reaction rate due to the higher exhaust gas temperature (530 °C at 5.38 to 5.82 h) and O_2 concentration (7.8 %). The overall PM oxidized by thermal (O_2)-assisted PM oxidation is 82 % whereas the NO_2 -assisted PM oxidation is 18 % due to the lower NO_2 concentration in the exhaust gas.

Table 7 shows the comparison of experimental PM mass retained to the MPF model simulated PM mass retained. From Table 7, the maximum absolute error between the experiment and the simulation is 2.8 g at the end of stage 2 loading condition.

Figure 16 shows the PM mass loading distribution at the end of PM oxidation by passive oxidation during the PO-B10-16 experiment. The minimum PM mass loading is 1.1 g/L up to the filter radius of 80 mm and increases to a maximum value of 1.8 g/L at the outer radius of the filter substrate. This is mainly due to the lower exhaust gas temperature at the outer radius of the filter due to the ambient convective and radiative heat transfer compared to the center of the filter substrate.

Figure 17 shows the PM mass loading distribution at the end of the PM oxidation during the AR phase of the experiment. From Fig. 17, the PM loading at the end of active regeneration varies significantly. The minimum PM mass loading is 0.2 to 0.4 g/L up to a filter radius of 80 mm and increases to a maximum value of 2.4 g/L at the outer radius of the filter substrate. This is mainly due to the lower exhaust gas

Fig. 15 Comparison of PM mass retained in the experimental data and simulation model along with the model cumulative for inlet PM and oxidation masses for AR-B10-1 experiment

Table 7 Comparison of experimental PM retained measured to MPF model output PM retained at the end of each stage for AR-B10-1 experiment

Stage	Time	Expt.	Model	Diff.
	[hrs]	[g]	[g]	[g]
1	0.49	4.0	4.8	0.8
2	4.97	43.2	46.0	2.8
3	6.34	18.3	17.0	-1.3
4	7.34	27.9	27.6	-0.3

temperature at the outer radius of the filter due to the ambient convective and radiative heat loss compared to the center of the filter substrate.

From the above simulation and experimental results analysis, the MPF model shows good capability in predicting temperature distribution, PM mass retained, and filter loading distribution within the filter substrate. For an ECU application, computational time is the key requirement for successful implementation of model-based control approach such as one presented in this paper. In general, the model with fine discretization is good for accuracy but takes long computational time. Hence, it is necessary to carry out a parametric study to determine the optimum required number of zones in the MPF model for aftertreatment control applications. This discretization study along with the detailed model validation is an ongoing work and will be covered in the next research paper.

Fig. 16 Simulated PM mass loading distribution along axial and radial directions at 5.19 h—end of PM oxidation by passive oxidation for PO-B10-16 experiment **Fig. 17** Simulated PM mass loading distribution along axial and radial directions at 5.82 h—end of PM oxidation by active regeneration for AR-B10-1 experiment

7 Summary and Conclusions

A new MPF model was developed for simulating filter substrate temperature and PM loading distribution within the filter. The model was parameterized through a two-step calibration procedure using 18 sets of data from the passive oxidation and active regeneration experimental data from references [3–6]. The model was calibrated with sample passive oxidation and active regeneration experimental data, and the model shows good capability in predicting the temperature distribution and filter loading within the filter substrate.

The specific conclusions from this work include

1. The MPF model to predict axial and radial temperature and filter loading distribution within the filter substrate was developed. The model accounts for heat transfer within and external to the filter and PM cake oxidation by O_2 and NO_2 .
2. The radial temperature distribution initiates well before the inlet of the CPF and affects the distribution for the entire length of the CPF. This radial temperature distribution can be characterized using thermal boundary layer equations. For the CPF presented in this study, 50 % of overall radial temperature reduction is in the 20 % of filter section close to the outer radius of the filter.
3. The detailed two-step MPF model calibration procedure was developed. A single set of PM kinetic parameters for each fuel type (Table 3) was found, and a single set of heat transfer coefficients (Table 4) was found for the all 18 runs.
4. The new MPF model simulation results show good capability in predicting temperature distribution (within $-24/+$

6 °C), PM mass retained (within $-1.3/+2.8$ g), and filter loading distribution within the CPF.

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Appendix A—MPF Model Development Equations

The total volume of each zone (V), empty volume (V_e), and filter volume (V_f) are [11]

$$V_{i,j} = \pi(r_i^2 - r_{i-1}^2) \Delta L_j \quad (16)$$

$$V_{e,i,j} = N_{c_i} d^2 \Delta L_j \quad (17)$$

$$V_{f,i,j} = V_{i,j} - V_{e,i,j} \quad (18)$$

The inlet PM is assumed to be deposited uniformly over the entire volume of filter; hence, mass of PM deposited in each zone is calculated as

$$ms_{i,j} = \frac{ms_t V_{i,j}}{V_t} \quad (19)$$

The average thickness of PM cake in each zone is calculated using total PM mass, PM density, and channel geometry as follows [21]:

$$ts_{i,j} = \frac{1}{2} \left[d - \sqrt{d^2 - \frac{ms_{i,j}}{N_{c_i} \Delta L_{i,j} \rho_s}} \right] \quad (20)$$

The empty volume while accounting for PM is calculated as follows (V_{es}):

$$V_{es,i,j} = \frac{N_{c_i}}{2} \left[(d - 2ts_{i,j})^2 + d^2 \right] \Delta L_j \quad (21)$$

Finally, the PM cake volume is calculated as

$$V_{s,i,j} = V_{i,j} - V_{f,i,j} - V_{es,i,j} \quad (22)$$

The detailed calculations and assumptions in discretization are explained in reference [11].

Filter Temperature Equations

The energy balance in the filter is affected by (a) heat conduction along the length of the filter (axial conduction), (b) heat conduction along radial direction of the filter (radial conduction), (c) convection between filter and channel gas, (d) energy released during oxidation of PM cake, and (e) heat transfer due to radiation exchange between channel surfaces. The energy flow through wall is neglected as there will be no distinction between inlet

and outlet channels [11]. Hence, the energy balance equation for the filter is

$$\left(\rho_s c_s V_{s,i,j} + \rho_f c_f V_{f,i,j} \right) \frac{dT_{f,i,j}}{dt} = \dot{Q}_{\text{cond.axial}} + \dot{Q}_{\text{cond.radial}} + \dot{Q}_{\text{conv}} + \dot{Q}_{\text{reac}} + \dot{Q}_{\text{rad}} \quad (23)$$

where T_f is the filter substrate temperature.

The axial and radial conduction along the length of the filter is calculated using resistance node methodology [11, 18]:

$$\dot{Q}_{\text{cond.axial}} = \lambda_{i,j} A_{f,i,j} \left[\frac{T_{f,i,j+1} - T_{f,i,j}}{\frac{1}{2}(\Delta L_{j+1} + \Delta L_j)} + \frac{T_{f,i,j-1} - T_{f,i,j}}{\frac{1}{2}(\Delta L_{j-1} + \Delta L_j)} \right] \quad (24)$$

$$\dot{Q}_{\text{cond.radial}} = \lambda_{i,j} A_{r,i,j} \left[\frac{T_{f,i+1,j} - T_{f,i,j}}{\ln(rc_{i+1}/rc_i)} + \frac{T_{f,i,j-1} - T_{f,i,j}}{\ln(rc_i/rc_{i-1})} \right] \quad (25)$$

$$A_{f,i,j} = \frac{V_{f,i,j} + V_{s,i,j}}{\Delta L_j} \quad (26)$$

$$A_{r,i,j} = 2\pi \Delta L_j \quad (27)$$

$$\lambda_{i,j} = \frac{\lambda_f V_{f,i,j} + \lambda_s V_{s,i,j}}{V_{f,i,j} + V_{s,i,j}} \quad (28)$$

The convection heat transfer between filter and channel gas is calculated using the following equations [11, 16]:

$$\dot{Q}_{\text{conv}} = h_g A_{s,i,j} (T_{i,j} - T_{f,i,j}) \quad (29)$$

The convective heat transfer coefficient (h_g) is calculated using the following fully developed Nusselt number correlation based on flow Peclet number through the wall for $Re_w < 3$ is given as [18]

$$Nu_{\text{inlet}} = 2.98 + 0.60 Pe_w - 0.143 Re_w \quad (30a)$$

$$Nu_{\text{outlet}} = 2.98 - 0.40 Pe_w \quad (30b)$$

In the MPF model, as there is no distinction between inlet and outlet channel, the average Nusselt number is used for computing the heat transfer coefficients and it is given as

$$Nu_{\text{avg}} = Nu_{\text{inlet}} + Nu_{\text{outlet}} = \frac{h_g d}{k_g} \quad (30c)$$

The combined surface area A_s is calculated as follows [11]:

$$A_{s,i,j} = \frac{N_{c_i}}{2} [4(d - 2ts_{i,j}) + 4d] \Delta L_j \quad (31)$$

The energy released during exothermic reactions is given by [11]

$$\dot{Q}_{\text{reac,th}} = -\frac{ms_{i,j}}{\rho_s} \dot{S}_{c(th)} \Delta H_{\text{reac,th}} \quad (32)$$

$$\dot{Q}_{\text{reac,NO}_2} = -\frac{ms_{i,j}}{\rho_s} \dot{S}_{c(NO_2)} \Delta H_{\text{reac,NO}_2} \quad (33)$$

$$\dot{Q}_{\text{reac}} = \dot{Q}_{\text{reac,th}} + \dot{Q}_{\text{reac,NO}_2} \quad (34)$$

where $\dot{S}_{c(th)}$ is the PM mass lost due to thermal (O_2) oxidation of PM and $\dot{S}_{c(NO_2)}$ is the PM mass oxidized due to NO_2 -assisted combustion.

The gas energy balance equation for the channel gas entering and leaving the zone is given by

$$\rho c_p A s_{i,j} \Delta L_j \frac{dT_{i,j}}{dt} = \dot{m}_{i,j} c_p (T_{i,j-1} - T_{i,j}) - \dot{Q}_{\text{conv}} \quad (35)$$

$$\dot{m}_{i,j} = \dot{m}_{\text{total}} \frac{Ves_{i,j}}{\sum_i Ves_{i,j}} \quad (36)$$

where T is the average channel gas temperature. The average channel gas temperature that lumps inlet and outlet channel is used in the gas energy balance equations.

Radiation between the channel surfaces

In the MPF model, each zone is treated as an enclosure as shown in Fig. A1. The surface 3 is the substrate wall with PM cake (black body radiation), and surfaces 1 and 2 are the inlet and outlet of this enclosure (the gas interface between the zones) which are assumed to be black for simplicity of the analysis and moreover radiation escaping surfaces 1 and 2 will be absorbed in to the adjacent black surface.

Assuming channel gas is completely transparent to thermal radiation and the surfaces are black, the net radiation heat transfer between filter wall (surface 3) can be determined as follows [19]:

$$\dot{Q}_{\text{rad}} = -As_{i,j} (F_{3-1}(J_3 - J_1) + F_{3-2}(J_3 - J_2)) \quad (37)$$

$$J_1 = \sigma T_{i,j-1}^4 \quad (38)$$

$$J_2 = \sigma T_{i,j}^4 \quad (39)$$

$$J_3 = \sigma T_{f,i,j}^4 \quad (40)$$

The effect of internal radiation is very small at lower temperatures and could be more important over 600 °C and could

improve the model accuracy during uncontrolled regeneration events [23].

PM Oxidation Equations

The PM oxidation equations include PM oxidation by thermal (O_2)- and NO_2 -assisted reactions. The chemical reaction expression for thermal (O_2) oxidation is [11]

Similarly, the reaction equation for NO_2 -assisted oxidation is given by [16, 23]

The oxidation of PM mass on the surface due to thermal and NO_2 -assisted oxidation is equal to

$$\dot{S}_{c(th)} = -\left(S_p \rho_{i,j} Y_{i,j,O_2} k_{O_2}\right) \frac{W_{c(s)}}{a_{O_2} W_{O_2}} \quad (43)$$

$$\dot{S}_{c(NO_2)} = -\left(S_p \rho_{i,j} Y_{i,j,NO_2} k_{NO_2}\right) \frac{W_{c(s)}}{a_{NO_2} W_{NO_2}} \quad (44)$$

The Arrhenius reaction rate for thermal- and NO_2 -assisted reaction is equal to

$$k_{O_2} = A_{O_2} T f_{i,j} \exp\left[-E_{O_2} / (R_u T f_{i,j})\right] \quad (45)$$

$$k_{NO_2} = A_{NO_2} T f_{i,j} \exp\left[-E_{NO_2} / (R_u T f_{i,j})\right] \quad (46)$$

Velocity Equations

From Depcik et al. [11], the average inlet channel velocity can be determined as

$$u_l|_{z=0} = \frac{\dot{m}_{\text{total}}}{\rho \frac{Nc_t}{2} (d - 2\bar{ts})^2} \quad (47)$$

Using the Eq. (47), the radial zone velocity (mass flow is axially same for each zone) is calculated as

$$u_l|_{z=0} = \frac{\dot{m}_{i,j}}{\rho_{i,j} \frac{Nc_i}{2} (d - 2\bar{ts}_i)^2} \quad (48)$$

where $\bar{ts}_i$ is the average PM cake thickness in each radial zone

Fig. A1 Schematic of an enclosure (zone) for the radiation heat transfer model

Table B1 CPF inlet temperatures measured by C1–C4 thermocouples and temperature factor

Radial distance in mm	Temperature ID	Temperature at 0.30 h in C	Temperature at 5.8 h in C	Diameter ratio	Temperature factor at stage 1—loading 0.3 h	Temperature factor at active regeneration—5.8 h
0	C1 (measured)	268.6	542.7	0.00	1.70	1.76
55	C2 (measured)	268.9	539.8	0.41	1.72	1.63
95	C3 (measured)	263.2	529.3	0.71	1.17	1.16
122	C4 (measured)	255.6	513.1	0.91	0.42	0.44
133	Ts (extrapolated)	251.3	503.2	1.00	0.00	0.00
	T_m (calculated)	261.5	525.6			
	T_m/T_s	1.041	1.045			
	Avg T_m/T_s	1.043				

Surface temperature (T_s) in Table B1 was extrapolated from C1–C4 thermocouple measurements as shown in Figs. B1 and B2

and $\frac{N_{ci}}{2}$ is the number of inlet channels in each radial zone.

From Depcik et al. [11], average velocity through the PM cake (u_s) and wall layers (u_w) is

$$u_s = \frac{\dot{m}_{total}}{4\rho \frac{N_{ci}}{2}(d-2.\overline{ts}) L_t} \quad (49)$$

$$u_w = \frac{u_s(d-2.\overline{ts})}{d} \quad (50)$$

Writing Eqs. (49) and (50) for each radial zone is

$$u_{s_i} = \frac{\dot{m}_{i,j}}{4\rho_{i,j} \frac{N_{ci}}{2}(d-2.\overline{ts}_i) L_t} \quad (51)$$

$$u_{w_i} = \frac{u_{s_i}(d-2.\overline{ts}_i)}{d} \quad (52)$$

From Depcik et al. [11], average velocity through the inlet channel (u_I) and outlet channel (u_{II}) is

$$u_I|_j = u_I|_{j-1} - \frac{4u_s}{d-2.\overline{ts}} \Delta L_{j-1} \quad (53)$$

$$u_{II}|_j = u_{II}|_{j-1} + \frac{4u_w}{d} \Delta L_{j-1} \quad (54)$$

Writing Eqs. (53) and (54) for each radial zone,

$$u_I|_{i,j} = u_I|_{i,j-1} - \frac{4u_{s_i}}{d-2.\overline{ts}_i} \Delta L_{j-1} \quad (55)$$

$$u_{II}|_{i,j} = u_{II}|_{i,j-1} + \frac{4u_{w_i}}{d} \Delta L_{j-1} \quad (56)$$

The detailed formulations of Eqs. (48, 49, 52, 53, and 54) are found in reference [11].

Filter Temperature Boundary Conditions

At the inlet of MPF model (for nodes $i=1$ to i_{max} and $j=1$), the temperature profile is calculated using the thermal boundary layer Eq. (12) and the CPF inlet temperature at a given location. At the center of the filter (for $i=1$, $j=1$ to j_{max}) due to the symmetry, the boundary condition equals to [11]

$$\left. \frac{dT}{dr} \right|_{r=0} = 0 \quad (57)$$

Fig. B1 CPF temperature profile at 5.8 h **Fig. B2** CPF temperature profile at stage 1 loading 0.3 h

Fig. B3 Temperature factor

At the exterior of the CPF ($i=i_{\max}, j=2$ to $j_{\max}$), the following equation is used to calculate the radial conduction heat transfer

$$\begin{aligned} \dot{Q}_{\text{cond.radial}} = & \lambda_{i,j} A_{r,i,j} \frac{T_{f,i-1,j} - T_{f,i,j}}{\ln(rc_i/rc_{i-1})} \\ & + h_{\text{amb}} A_{\text{amb}} (T_{\text{amb}} - T_{f,i,j}) \\ & + \varepsilon_r \sigma A_{\text{amb}} (T_{\text{amb}}^4 - T_{f,i,j}^4) \end{aligned} \quad (58)$$

The surface area of the CPF is calculated as follows

$$A_{\text{amb}} = \pi D \Delta L_j \quad (59)$$

Appendix B—Thermal Boundary Layer Curve Fits and Coefficients

As shown in Fig. 6, the temperature factor for all 18 runs is identical. Hence, AR-B10-1 experiment was used as the reference experiment for calculation of thermal boundary layer coefficients. The temperatures measured by thermocouples C1–C4 were used for calculation of temperature factor.

The temperature factors [19] were calculated using Eq. 60. The sample calculation at $R1=0$ mm is shown as follows:

Fig. C1 Air properties' plot at 1 atm pressure [26]

$$\text{Temperature factor} = \frac{T_s - T_r}{T_s - T_m} \quad (60)$$

where T_m = Mean exhaust gas temperature

T_s = Wall inner surface temperature

T_r = Temperature at a given radial location

$$\begin{aligned} \text{Temperature factor @ R1, 0 mm @ 5.8 hrs} &= \frac{503.2 - 542.7}{503.2 - 525.6} \\ &= 1.76 \end{aligned}$$

Figure B3 shows the plots of temperature factors for stage 1 loading at 0.3 h (a sample point at low-temperature region of the test) and active regeneration at 5.8 h (a sample point at high-temperature region) test conditions. From Fig. B3, it is evident that the temperature varies significantly between 0.3 (262 °C) and 5.8 h (523 °C), the temperature factor profile looks similar for both conditions, confirming that the one factor can be applied for the entire duration of the test. The following equation represents temperature factors of both test conditions with R^2 value of 1.00 (Fig. C1).

$$\begin{aligned} \text{Temperature Factor @ } x &= -2.493x^3 \\ &+ 1.0585x^2 - 0.3285x \\ &+ 1.7631 \end{aligned} \quad (61)$$

Where x is the CPF diameter ratio.

Using Eq. 60 and knowing the temperature at any radial location at the CPF inlet, the temperatures at the other radial locations can be determined as shown below

$$\frac{T_s - T}{T_s - T_m} = F1 = \text{Temperature Factor} \quad (62)$$

$$\frac{T_m}{T_s} = F2 = \text{mean to surface temperature ratio} \quad (63)$$

Combining Eqs. (62) and (63) yields

$$\frac{T_s - T}{T_s - F2 \cdot T_s} = F1 \quad (64)$$

$$F1(T_s - F2 \cdot T_s) + T - T_s = 0 \quad (65)$$

Example calculation: To find temperature T_s , assume we have a temperature measurement $T=539.8$ °C at $x=0.41$. From Eq. (61), $F1=1.63$ for $x=0.41$. Then substituting $F2=1.043$ (from Table B1), $F1=1.63$, and $T=539.8$ °C in Eq. (65), the T_s can be calculated as follows:

$$1.63(T_s - 1.043 \cdot T_s) + 539.8 - T_s = 0$$

and $T_s = 504.4$ °C. Similarly, temperatures at other locations can be determined using Eq. (62).

Appendix C—Model Calibration Inputs

The multi-zone model uses the following air properties relationship based on data in reference [26].

The Eqs. (66) and (67) were developed using the table values in reference [26] for specific heat and dynamic Figure C1 shows the plot of table values from reference [26] as a function of air temperature for specific heat and dynamic viscosity along with their model curve fits.....

$$\begin{aligned} \text{Specific heat} = & 3.7835E-05T^2 - 2.0196E-01T \\ & + 9.8135E + 02 \end{aligned} \quad (66)$$

$$\begin{aligned} \text{Dynamic viscosity} = & 1.3126E-11T^2 + 4.2194E-08T \\ & + 1.7843E-05 \end{aligned} \quad (67)$$

Where T is the temperature of the channel gas at each zone for the multi-zone model.

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