

Combining the Classical and Lumped Diesel Particulate Filter Models

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ABSTRACT

The growing presence of Spark Ignition Direct Injection (SIDI) engines along with the prevalence of direct injected Compression Ignition (CI) engines results in the requirement of Particulate Matter (PM) exhaust abatement. This occurs through the implementation of Gasoline Particulate Filters (GPFs) and Diesel Particulate Filters (DPFs). Modeling of GPFs and DPFs are analogous because of the similar flow patterns and wall flow PM capture methodology. Conventional modeling techniques include a two-channel (inlet/outlet) formulation that is applicable up to three-dimensions. However, the numerical stiffness that results from the need to couple the solution of these channels in compressible flow can result in relatively long run times. Previously, the author presented a lumped DPF model using dynamically incompressible flow intended for an Engine Control Unit (ECU) in order to generate a model that runs faster than real time using a high-level programming language. Building on the favorable outcomes of temperature evolution from this prior effort, this work enhances the model to predict compressible flow gas dynamics in order to match the evolution of pressure drop. Another enhancement is the inclusion of deep bed filtration within the wall, and the transition to the cake layer. Results show comparable temperature profiles with the dynamically incompressible model with a pressure drop that follows appropriately by linking through the ideal gas model. However, solving chemical species as an independent equation separate from compressible flow still deviates significantly from the classical two-channel approach.

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INTRODUCTION

The control of PM that emanates from SIDI and CI engines is of significant concern for the automotive industry. This is because PM can infiltrate the alveoli in humans and transport toxic chemicals absorbed on the surface of the particle, subsequently leading to lung related illnesses [1]. As a result, the automotive industry now widely implements PM filtration in the exhaust. In particular, DPFs are used for CI engine exhaust with GPFs currently being considered for SIDI engines.

The operation of a DPF (or analogous GPF) includes the storage of PM in and on top of a porous wall with its eventual regeneration in an oxidative environment. This can be accomplished actively utilizing O_2 or passively by employing NO_2 ; often through synchronization with an upstream Oxidation Catalyst. This need to modulate device operation has led to the development of simulation tools in order to reduce the number of experiments needed by predicting the pressure drop through the device and its temperature evolution. Broadly speaking, the models typically fall into one of two categories; those designated to operate within an Engine Control Unit (ECU) [2] and the classical two-channel approach [3].

The ECU approach is designed for computational speed and is still often based on the two-channel model originally posed by Bissett [4]. In a previous effort by the author, the research in this area was reviewed and a derived model was generated that used dynamically incompressible flow to simulate the flow through the device while

creating lumped zones in order to predict the temperature evolution. Utilizing a high-level coding language that runs significantly slower than traditional programming languages [5], the filter temperature evolution could be predicted relatively accurately in a faster than real time manner. This was because only one term in the governing energy equations was influenced by compressible flow. However, decoupling temperature and pressure by using dynamically incompressible flow (effectively negating the ideal gas law), the model was unable to simulate the pressure drop during warm-up and PM regeneration experiments.

As a result, this effort seeks to merge the two models by simulating temperature using the ECU approach while estimating the pressure drop using the two-channel methodology. In specific, the temperature profile through the device is generated by the ECU version that is then utilized as a constant within the two-channel model removing the need to solve for the channel temperatures. Moreover, deep bed filtration is included in the model formulation in order to simulate the pressure drop evolution in the device more accurately. Finally, model run times are given in order to document the computational expense of the combined model.

DPF MODEL DERIVATION

In a previous effort, instead of simulating both the inlet and outlet channels along with a porous wall model derivation followed a lumped approach through the creation of a variable number of zones

[2]. The prior efforts found that temperature could be computed in this manner effectively when compared to the classical two-channel approach because only one variable was affected. As a result, this work will employ the lumped approach for temperature while bringing in the classical approach for the pressure drop through the filter. For brevity, a succinct summary of the previous model formulation is presented and only the new variables are defined since the rest of the parameters are available in the previous paper.

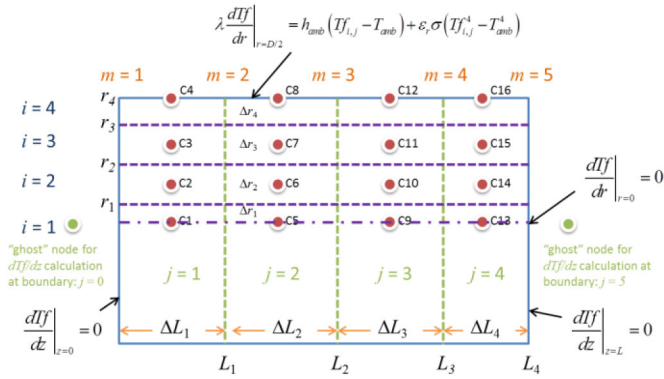


Figure 1. Graphical schematic of the lumped DPF model illustrating pertinent lengths, boundary conditions, and subscript nomenclature.

Filter and Gas Energy Equations

The energy equation for the filter includes an energy storage term on the left hand side:

$$\left(\rho_s c_s V_{s,i,j} + \rho_f c_f V_{f,i,j} \right) \frac{dT_{f,i,j}}{dt} = \dot{Q}_{cond,axial} + \dot{Q}_{cond,radial} + \dot{Q}_{conv} + \dot{Q}_{wall} + \dot{Q}_{reac} \quad (1)$$

with the right hand side adding the influences of axial conduction along the filter ($\dot{Q}_{cond,axial}$), radial conduction in the normal direction ($\dot{Q}_{cond,radial}$), convection between the channel gases and the filter wall ($\dot{Q}_{conv}$), an enthalpy flow through the wall ($\dot{Q}_{wall}$), and the influence of the PM exothermic reactions ($\dot{Q}_{reac}$). Of note, the subscript nomenclature indicates i for the radial direction and j for the axial direction as indicated in Figure 1.

Writing a lumped energy equation for the gas employing an average gas temperature that includes both the inlet and outlet channels equals:

$$\bar{\rho}_j c_p V_{es,i,j} \frac{dT_{i,j}}{dt} = \dot{Q}_{in} + \dot{Q}_{out} - \dot{Q}_{conv} \quad (2)$$

The left hand side describes the energy stored by the gas that is often considered negligible. However, keeping this term allows this equation to be solved with other equations as an array of Ordinary Differential Equations (ODEs).

The prior modeling effort employed dynamically incompressible flow; hence, only one value for gas density was utilized throughout the entire DPF in Eqn. (2). In this effort, a single representative inlet

and outlet channel will be employed in order to calculate the pressure drop of the DPF using compressible flow. Therefore, in Eqn. (2), the gas density is evaluated as an average of inlet and outlet channels:

$$\bar{\rho}_j = \frac{1}{2} \left[\frac{1}{2} (\rho_{I,m} + \rho_{I,m+1}) + \frac{1}{2} (\rho_{II,m} + \rho_{II,m+1}) \right] \quad (3)$$

with the subscript nomenclature of m employed in order to differentiate between values at the boundaries of Figure 1 and those computed in the middle of the zones (i.e., i & j). This is required in order to synchronize with the common boundary conditions for the classical two-channel model. Moreover, the subscripts I and II refer to the inlet and outlet channels, respectively, of the classical model.

Since only one representative set of channels will be simulated, the value of temperature will be a weighted average in the radial direction:

$$\bar{T}_j = \sum_i \frac{\dot{m}_{i,j} T_{i,j}}{\dot{m}_{total}} \quad (4)$$

However, as just indicated, these values are defined in the middle of the zone. Therefore, they must be translated to the boundary temperatures of each zone:

$$T_{III,m} = T_{inlet} \quad @ z = 0 \quad (5)$$

$$T_{III,m} = \frac{1}{2} (\bar{T}_{j-1} + \bar{T}_j) \quad @ 0 < z < L_i \quad (6)$$

$$T_{III,m} = \bar{T}_j \quad @ z = L_i \quad (7)$$

with the last assumption indicating that the exit temperature change over the half-cell is negligible. Of note, for the temperature exiting the DPF, this is the same boundary condition utilized in the previous effort.

Now, from this information, the temperature derivative between the boundaries can be specified as:

$$\left. \frac{dT_{III}}{dz} \right|_m = \frac{T_{III}|_{m+1} - T_{III}|_m}{\Delta L_j} \quad (8)$$

This will act as a constant within the ODE solver for the channel equations, effectively removing the need to employ the conservation of energy in the solver. In other words, the lumped model will provide the temperature profile through the DPF and the channel equations will simply employ this result.

PM Mass Equations

The previous effort only employed a PM mass balance for the cake layer and neglected deep bed filtration. This has been expanded here based on the unit collector model pioneered by Konstandopoulos and Johnson [6] and later updated by Konstandopoulos et al. [7, 8, 9, 10]. This effort slightly modifies this model for inclusion in the lumped zone approach.

In the model, there are now equations for both the PM stored in the wall (mw) and cake layer (ms), respectively:

$$\frac{d(mw_{i,j})}{dt} = \Phi_{i,j} \dot{m}s_{i,j} - \chi_{i,j} mw_{i,j} \quad (9)$$

$$\frac{d(ms_{i,j})}{dt} = (1 - \Phi_{i,j}) \dot{m}s_{i,j} - \chi_{i,j} ms_{i,j} \quad (10)$$

where Φ is a partition coefficient that determines the fraction of mass collected in the first slab that contributes to cake formation. It is calculated using the characteristic dimension of a unit spherical collector (dc and dc_0 for the initial value of an unloaded wall):

$$\Phi_{i,j} = \frac{dc_{i,j}^2 - dc_0^2}{(\psi b)^2 - dc_0^2} \quad (11)$$

with ψ a calibration constant and b equal to the unit cell diameter:

$$b^3 = (1 - \varepsilon_0) dc_0^3 \quad (12)$$

and ε_0 is the porosity of a clean filter. The initial value of the collector diameter of an unloaded wall is calculated as:

$$dc_0 = \frac{3}{2} \left(\frac{1 - \varepsilon_0}{\varepsilon_0} \right) d_{pore} \quad (13)$$

where d_{pore} is the pore diameter of the filter. Of note, this is a characteristic dimension of a solid “spherical” collector. The numerator $(1 - \varepsilon_0)$ indicates the amount of the pore that is the solid fraction; whereas, the denominator (ε_0) is the open fraction of the pore.

The current value of the unit spherical collector is based on the amount of deposited particulate in the wall:

$$\frac{4\pi}{3} \left(\frac{dc_{i,j}}{2} \right)^3 = \frac{mw p_{i,j}}{\rho_{sw}} + \frac{4\pi}{3} \left(\frac{dc_0}{2} \right)^3 \quad (14)$$

Effectively, this equation determines the diameter of a unit spherical collector (hence, volume as indicated through third power) as a function of the volume of PM per pore and the initial unit spherical collector value. Investigating Eqn. (14), one can see that this equation effectively grows the solid fraction of the pore that is used to capture the PM through the mechanisms of Brownian diffusion and interception.

The volume of PM per pore involves the entire PM that is stored in the wall zone that is currently being analyzed, divided by the total number of pores (Np) in the wall at the current location:

$$mw p_{i,j} = \frac{mw_{i,j}}{Np_{i,j}} \quad (15)$$

$$Np_{i,j} = \frac{Veo_{i,j}}{\frac{4\pi}{3} (d_{pore}/2)^3} \quad (16)$$

where the denominator is an equivalent pore volume and Veo is the empty volume of the wall at the location under analysis:

$$Veo_{i,j} = \varepsilon_0 V_{f,i,j} \quad (17)$$

It is anticipated that Np is grossly overestimated as it assumes that all pores will be available for PM capture, which is untrue. This is remedied through ρ_{sw} , the packing density of the PM particles in the filter structure. This is taken as a calibration constant in this effort similar to Konstandopoulos et al. [11] that found values for this parameter between 8.26 and 14.10 kg m⁻³. Of note, the methodology presented in this paper deviates from the conventional unit collector approach that divides the filter wall into slabs and tracks the amount of particulate accumulated in each slab. This version is no longer dependent on a discretization in the wall direction, and instead lumps all PM capture into a single slab. Hence, the value of the packing density will be different from the previous studies indicated.

The mass flow rate to the wall comes from previous efforts of the author [12, 13]:

$$\dot{m}s_{i,j} = \bar{\rho}_j \bar{u}_s Y_d S_{i,j} \quad (18)$$

utilizing the average gas density, the mass fraction of PM in the inlet channel gas (Y_d), and the average wall flow velocity to the surface since it does not change significantly in the axial direction:

$$\bar{u}_s = \sum_m u_{s,m} / Nz \quad (19)$$

where Nz is the number of boundaries and the calculation for $u_{s,m}$ is provided later in this paper. The inlet channel surface area for the particular zone under analysis: