

Development of a Particulate Filter Model for the Prediction of Backpressure: Improved Momentum Balance and Entrance and Exit Effect Equations

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ABSTRACT

The development of a one-dimensional model for the prediction of backpressure across a gasoline or diesel particulate filter (PF) is presented. The model makes two innovations: Firstly, the term for momentum convection in the gas momentum balance equations includes the loss (or gain) of axial momentum in the direction perpendicular to the channels; neglecting this results in the momentum convection term being too large. Secondly, equations for the pressure change due to the abrupt contraction at the PF entrance and for abrupt expansion at the exit are derived which take into account the fact that the velocity profile across the channels is not flat; often workers have used equations appropriate for high Reynolds numbers which assume flat velocity profiles.

The model has been calibrated/tested against cold flow data for more than one length of PF. The use of more than one length allows along-filter pressure losses to be separated from entrance and exit effects.

A simulation study has been carried out to investigate the relative magnitude of the different contributions to backpressure, *viz.* across-wall losses (Darcy and Forchheimer), along-channel losses (viscous and inertial) and entrance and exit effects.

Finally, other workers have recently published a PF model in which the effect of the wall Reynolds number on the friction factors, Nusselt numbers and momentum transport has been included. The influence of these modifications on the backpressure and outlet temperature prediction has been investigated and found not to be significant over the range of conditions tested.

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1. INTRODUCTION

Particulate Matter (PM) [1,2,3,4] emitted in the exhaust of internal combustion engines is detrimental to the human health and the environment. Studies have shown that exposure to PM may cause health problems such as premature death, asthma, lung cancer and other pulmonary and cardiovascular problems [3,4,5]. Diesel PM is also a major source of carbon black, which has a high global warming potential (albeit a short lived one) [6]. PM influences atmospheric visibility and can lead to the soiling of buildings [7]. Diesel Particulate Filters (DPF) [4,8] have been extensively and successfully used to remove PM from the exhaust of diesel engines for around 20 years [8,9,10]. More recently, with the introduction of legislated limits for particulate number, Gasoline Particulate Filters (GPF) are being introduced to control ultrafine particulate emissions from gasoline direct injection engines [4,11,12].

As this work applies equally to DPFs and GPFs, the term Particulate Filter (PF) will be used to refer to both.

Computer simulation has become an important tool for designing aftertreatment systems [13,14], enabling a wide range of parameters and scenarios to be investigated more quickly and cost effectively than a purely experimental, "trial and error" approach. Simulation can also be used gain insights into the emissions control system which are not readily obtained by measurement.

This paper concerns the development of a PF model for backpressure prediction. Most one-dimensional PF models are based on the pioneering work of Bissett [15]. Since that work numerous models for PFs with various improvements have been published, *e.g.* [16,17, 18,19,20,21,22,23,24,25]. An extensive review of the development of PF models has been written by Koltsakis et al. [26].

Probably the most significant advance in PF modelling in recent years has been made by Bissett, Kostoglou and Konstandopoulos [27,28]. Previously, PF models have assumed that the gas flow in the channels is not significantly influenced by the flow through the porous walls. These workers have investigated this, publishing correlations which enable the effect of the gas flow out of or into channels through the porous walls to be incorporated into the usual one-dimensional PF model framework.

This work describes the development and application of a one-dimensional model for a PF. The model makes two innovations. Firstly, the term for momentum convection in the gas momentum balance equations includes the loss or gain of axial momentum in the direction perpendicular to the channels; neglecting this results in the momentum convection term being too large. Secondly, equations for the pressure change due to the abrupt contraction at the PF entrance and for abrupt expansion at the exit are derived which take into account the fact that the velocity profile across the channels is not flat.

The rest of the paper is structured as follows: The experimental section (section 2) describes the collection of data for model calibration and for model input for drive cycle simulations. The development of the model is described in section 3 and model calibration in section 4. The following section (section 5) describes application of the model to investigate the relative magnitude of the different contributions to backpressure, *viz.* across-wall losses (Darcy and Forchheimer), along-channel losses (viscous and inertial) and entrance and exit effects, and how these vary with flow rate, PF length, temperature, etc. Finally, (section 6) the effect of the model modifications proposed by Bissett, Kostoglou and Konstandopoulos [27,28] to account for the impact of wall flow is investigated.

2. EXPERIMENTAL

2.1 Cold Flow Experiments

Cold flow measurements were made on uncoated, 4.5 and 6.0 inch (114.3 and 152.4 mm) long, 4.66 in (118.4 mm) diameter cordierite PFs supplied by the same manufacturer. The cell density was 300 cpsi (465 000 cells per m²) and the wall thickness 8 thou (0.20 mm). The parts were of the same type/material, *i.e.* with the same porosity, mean pore diameter, etc.

Backpressure measurements were made with a SuperFlow® SF1020 ProBench flow bench [29]. The key design points of this equipment for this work are shown in the schematic in Fig. 1 (top). During testing, air is drawn into the top of the part from the room. On leaving the part, this air expands into a large plenum, which has a cross-sectional area approximately 60 times that of the PFs tested in this work. Since, the inlet of the PF is at atmospheric pressure, it is clear that the pressure within the PF is sub-atmospheric. This contrasts with a PF on a vehicle (Fig. 1, bottom) where the exit is at (or close to) atmospheric pressure and the pressure within the PF is above atmospheric pressure.

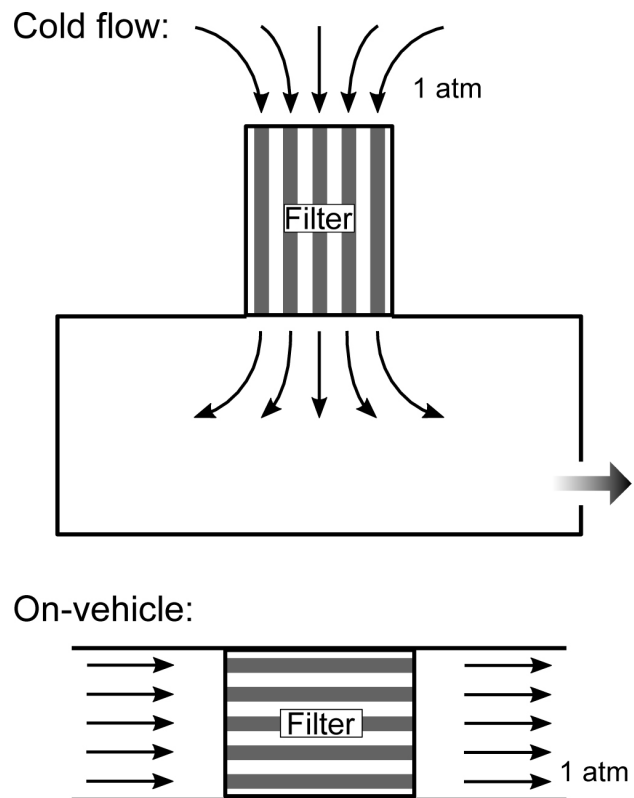


Figure 1. Schematics of the two PF configurations considered in this work, *viz.* cold flow (top) and on-vehicle (bottom). Note that atmospheric pressure is at the PF inlet with the cold flow configuration and at the outlet with the on-vehicle configuration.

2.2 Hot Flow Data

As input for transient simulations data for a 1.6 L gasoline passenger car measured on a chassis dynamometer over a class 3 Worldwide harmonised Light vehicles Test Cycle (WLTC) [30,31] was used. The test was run according to standard procedures. This data file was used purely for input to the model (gas temperature and mass flow); no measurements of PF backpressure or outlet temperature were available for comparison with simulation results. A temperature measured 25 mm in front of the catalyst position was used as input to the PF model.

3. DEVELOPMENT OF MODEL

This section describes the derivation of a one-dimensional model for a PF. The model is based on the one by Bissett [15], but with various improvements, such as allowing for the constriction of the inlet channel by the soot cake and compressible flow. The model makes two innovations: Firstly, the term for momentum convection in the gas momentum balance equations includes the loss (inlet channel) or gain (outlet channel) of axial momentum in the direction perpendicular to the channels; neglecting this results in the momentum convection term being too large. Secondly, equations for the pressure change due to the abrupt contraction at the PF entrance and for abrupt expansion at the exit are derived which take into account that fact that the velocity profile across the channels is not flat.

While this paper only covers simulations of symmetric filters, where the inlet and outlet channels have the same dimensions, for completeness the model will be derived (with the exception of the across-wall pressure drop) for the case where the inlet and outlet channels have different dimensions. Similarly, while this paper does not include soot-loaded PFs, the model derivation will include the presence of soot in the channels.

The model makes the following assumptions:

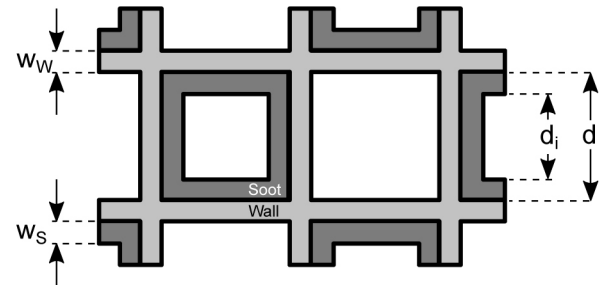
- Uniform flow distribution at the entrance to the PF.
- Negligible radial temperature gradient across the catalyst.
- Reactant gases are dilute so that changes in the amount of substance (and hence gas volume) with reaction can be ignored, *i.e.* this is a trace system.
- The channels are square in cross section.
- The flow profile in the channels is unaffected by the flow to/from the porous walls of the channels.
- The flow profile is unaffected by the presence of PM due to the low concentration of PM in the exhaust gas.
- The gas velocity, pressure and temperature profiles along the channels are at steady-state as the gas residence time is short compared to the transient behaviour of the PF.
- Negligible pressure gradients across the width of the channels.
- The pressure drop across the soot cake and PF wall can be described by Darcy's law with the Forchheimer extension; any effect of slip flow is neglected.
- Adiabatic behaviour, *i.e.* no heat losses to the surroundings.
- Axial transport of heat in the solid phase by conduction.
- Heat is transported along the channels by convection; axial conduction through the gas in the channels is negligible in comparison.
- Conduction of heat through the gas in the channels to the channel walls in the direction perpendicular to the channels is significant and can be described by heat transfer terms.
- Negligible heat transport by radiation since those portions of the long thin channels that have significant view factors with each other are expected to have similar temperatures.
- Uniform temperature across the PF wall and soot cake in the direction perpendicular to the channels at each axial location, *i.e.* the PF wall and soot cake temperature varies axially, but *not* in the through-wall direction.
- The gas passing through the soot cake and PF wall has the same temperature as the soot cake and PF wall due to efficient heat transfer.
- Soot is only located only as a cake; soot in the wall is not considered.
- Ideal gas behaviour within the PF, *i.e.* the gas within the PF is compressible.
- The gas is incompressible during contraction as the gas enters the PF and during expansion as the gas leaves the PF.
- Heat capacities and viscosity are temperature dependant.

The focus of this paper is on backpressure prediction; simulation of reactions occurring over a catalytic coating on the PF and soot accumulation and removal by oxidation will not be discussed in this work.

3.1 Dimensions / Geometry

The model is one-dimensional, describing a single inlet channel-outlet channel pair. Figures 2 and 3 show cross-sectional and longitudinal schematics of the PF with the dimensions marked.

Symmetric:



Asymmetric:

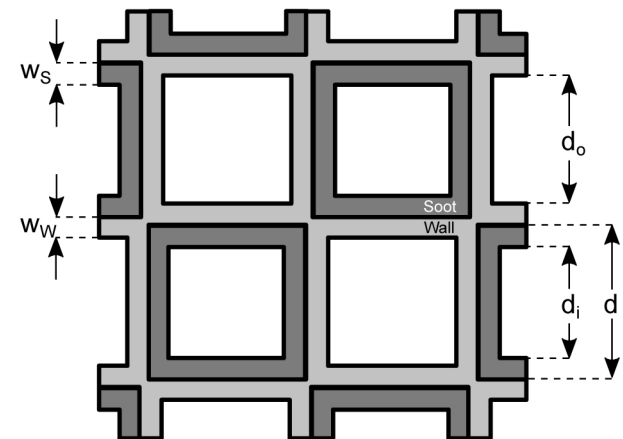


Figure 2. Schematic diagrams of the cross section of symmetric (top) and asymmetric (bottom) PFs showing the dimensions. The darker shading represents the soot cake in the inlet channels.

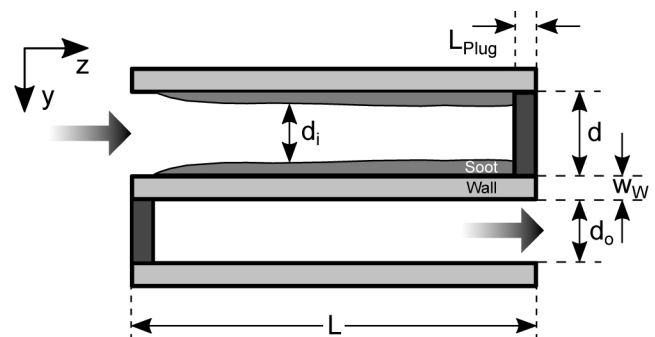


Figure 3. Longitudinal schematic of a PF showing the dimensions.

The channel width of the soot-loaded inlet channel, d_i , is related to the soot-free width of the inlet channel, d , and the soot loading, S (mass of soot per unit volume of PF), by

$$d_i = \sqrt{d^2 - \frac{2S}{\rho_{Cell} \rho_S}} \quad (1)$$

where ρ_S is the packing density of the soot cake and ρ_{Cell} is the cell density, *i.e.* the number of channels per unit cross-sectional area of the PF. For segmented PFs, ρ_{Cell} should be for the whole filter (including the cement between the segments), not just a segment.

The open cross-sectional area of the soot-free PF in the region away from the plugs (*i.e.* the cross-sectional area of the empty channels) divided by the cross-sectional area of PF, ϵ , is given by:

$$\epsilon = \frac{(d^2 + d_o^2) \rho_{Cell}}{2} \quad (2)$$

The open area fraction of the front and rear faces of the PF, ϵ_i and ϵ_o , are given by:

$$\epsilon_i = \frac{d_i^2|_{z=0} \rho_{Cell}}{2} \quad (3)$$

$$\epsilon_o = \frac{d_o^2 \rho_{Cell}}{2} \quad (4)$$

where $d_i^2|_{z=0}$ indicates the value of d_i^2 at $z=0$, *i.e.* the front of the PF.

Since ideal gas behaviour is assumed, gas density is given by,

$$\rho = \frac{PM}{RT} \quad (5)$$

where M is the molecular mass of the gas and R is the molar gas constant.

3.2 Gas Phase Balance Equations

When deriving the gas balance equations, it is important to remember that the axial velocity of the gas in the channels is not uniform across the width of the channels, but rather varies across the channels, being fastest along the centre of the channels and slowest at the channel walls. Thus, the variables V_i and V_o represent the *average* gas velocity in the inlet and outlet channels (respectively) at a given axial location. The average velocity is given by the volumetric flow divided by the cross-sectional area of the channel. The mass flux of the gas in the channels, ϕ_i and ϕ_o , will also be referred to; again these quantities refer to averages across the channel (mean mass flux = mass flow in channel divided by the cross-sectional area of the channel). In the derivation, it is necessary to refer to the variation in gas velocity across the channel. In this case the variable u will be used. Note that $V_i = \langle u_i \rangle$ and $V_o = \langle u_o \rangle$, where the angle brackets indicate the average over the cross section of the channels.

As with gas velocity, the temperature of the gas in the channels will also vary across the width of the channels, *e.g.* because of heat transfer with the walls of the PF and the velocity distribution across the channels. Thus, the variables T_i and T_o refer to the mixing cup or bulk temperature of the gas in the inlet and outlet channels.

Variations in pressure across the width of the channels will be ignored. Thus, P_i and P_o refer to the pressure of the gas in the inlet and outlet channels at a given axial location; the same value applies across the whole width of the channels.

3.2.1 Gas Mass Balance

The mass balance for the inlet channels is given by:

$$\frac{\partial d_i^2 \rho_i V_i}{\partial z} = -4d \rho_{g,w} V_w \quad (6)$$

where V_w is the superficial through-wall velocity and $\rho_{g,w}$ the density of the gas as it passes through the soot cake and the PF wall. The term on the left represents the net rate of mass loss per unit length of PF due to gas convection along the inlet channel and the term on the right the rate of mass loss per unit length due to flow through the wall. The “4” arises from the fact that the channels have four sides. Note that since d_i varies along the length of the PF, d_i must be included in the derivative.

The inlet channel mass balance can also be expressed in terms of the inlet channel and through-wall mass fluxes, ϕ_i and ϕ_w , where $\phi_i = \rho_i V_i$ and $\phi_w = \rho_{g,w} V_w$. Thus,

$$\frac{\partial d_i^2 \phi_i}{\partial z} = -4d \phi_w \quad (7)$$

Similarly, the outlet channel mass balance is given by,

$$\frac{\partial \rho_o V_o}{\partial z} = \frac{4d \rho_{g,w} V_w}{d_o^2} \quad (8)$$

Or in terms of the mass fluxes,

$$\frac{\partial \phi_o}{\partial z} = \frac{4d \phi_w}{d_o^2} \quad (9)$$

The outlet mass balance equations (Eq. (8) and (9)), are similar to those for the inlet channel balance (Eq. (6) and (7)), except for the change in sign of the wall flow term (gas is entering the channel through the walls rather than leaving) and that since d_o is a constant it can be taken out of the derivative. Note that both V_w and ϕ_w are referenced to the dimension d , so that they still appear with d in the outlet channel mass balance.

3.2.2 Gas Momentum Balance

Typically, PF models have used axial momentum balance equations resembling the following:

$$\frac{\partial P_i}{\partial z} = -\frac{1}{d_i^2} \frac{\partial d_i^2}{\partial z} \rho_i V_i^2 - \frac{F \mu_i V_i}{d_i^2} \quad (10)$$

$$\frac{\partial P_o}{\partial z} = -\frac{\partial \rho_o V_o^2}{\partial z} - \frac{F \mu_o V_o}{d_o^2} \quad (11)$$

where μ_i and μ_o are the viscosity of the gas in the inlet and outlet channels.

Each term in these equations can be interpreted as the net rate of gain in axial momentum per unit volume by different causes. Alternatively, they can be interpreted as the resultant force in the z-direction applied to the gas per unit volume by different sources. From left to right, the terms correspond to i) the force applied to the gas in a volume element by pressure; ii) the rate of momentum gain by convection (or alternatively the force required to accelerate the gas); and iii) the force due gas viscosity, which retards flow. The form of the viscosity term is explained in [Appendix A](#).

The momentum convection terms in [Eq. \(10\)](#) and [\(11\)](#) describe the net rate of gain of z-momentum (*i.e.* momentum in the axial direction) per unit volume across a volume element due to gas entering and leaving in the z-direction. However, for the case of the inlet channel, this term neglects the loss in z-momentum due to the net flow of gas out of the element in directions perpendicular to the channel axis towards the wall. As a result, the net rate of change in momentum due to convection is overstated and this term is larger than it should be. The same applies for the outlet channel, but with the “signs reversed”, *i.e.* the outlet channel term neglects the gain in z-momentum due to the net flow of gas into the element in directions perpendicular to the channel axis away from the walls and towards the centre of the outlet channel. Again, this results in the net rate of change in momentum due to convection being overstated and a term which is larger than it should be. Therefore, we propose a new momentum convection term, which is much closer to including the loss or gain of axial momentum in the direction perpendicular to the channels. The reason why this has been previously neglected, is that PF models are generally derived assuming that the flow field in the channels is not changed by the gas flow to/from the walls so that gas velocities in the direction perpendicular to the axis are taken to be zero.

In this development, only the momentum convection term will be considered. The momentum convection term from the most general form of the momentum balance equation for fluids is $-\nabla \cdot \rho \mathbf{u} \mathbf{u}$ [32]. The z-component of this is:

$$-\frac{\partial \rho u_x u_z}{\partial x} - \frac{\partial \rho u_y u_z}{\partial y} - \frac{\partial \rho u_z u_z}{\partial z} \quad (12)$$

Applying the product rule to each derivative gives:

$$-\rho u_x \frac{\partial u_z}{\partial x} - \rho u_y \frac{\partial u_z}{\partial y} - \rho u_z \frac{\partial u_z}{\partial z} - \dots - u_z \left(\frac{\partial \rho u_x}{\partial x} + \frac{\partial \rho u_y}{\partial y} + \frac{\partial \rho u_z}{\partial z} \right) \quad (13)$$

The mass balance under steady-state conditions is $\nabla \cdot \rho \mathbf{u} = 0$ [32]. Therefore, the bracketed term in the above equation is zero, which leaves:

$$-\rho u_x \frac{\partial u_z}{\partial x} - \rho u_y \frac{\partial u_z}{\partial y} - \rho u_z \frac{\partial u_z}{\partial z} \quad (14)$$

Along the centre line of the channel, $u_x \partial u_z / \partial x$ and $u_y \partial u_z / \partial y$ are zero on symmetry grounds; away from the centre line these terms will be non-zero. The exact values of these terms will depend on the flow field (*i.e.* the value of $\mathbf{u}$ as a function of position). However, for the inlet channels it seems likely that $u_x \partial u_z / \partial x$ and $u_y \partial u_z / \partial y$ will increase in magnitude with proximity to the channel walls; u_x and u_y will likely increase towards the walls with the gathering flow to the walls, while the typical parabolic-like velocity profile associated with laminar flow (which still broadly occurs for square channels with wall flow, albeit with more some more complicated behaviour close to the walls of the inlet channels [27,28]) will result in $\partial u_z / \partial x$ and $\partial u_z / \partial y$ (mostly) increasing in magnitude from the centre line to the walls.

Nevertheless, we chose to neglect $u_x \partial u_z / \partial x$ and $u_y \partial u_z / \partial y$, making the usual assumption in PF modelling that the flow field in the channel is unaffected by the (relatively slow) flow to/from the walls, which would result in these terms being zero. Neglecting these terms at this stage is conceptually no different from neglecting $\partial \rho u_x u_z / \partial x$ and $\partial \rho u_y u_z / \partial y$ in [Eq. \(12\)](#) as is done to give the momentum convection terms in [Eq. \(10\)](#) and [\(11\)](#). This leaves just one term:

$$-\rho u_z \frac{\partial u_z}{\partial z} \quad (15)$$

Strictly speaking, this term only refers to the convection of z-momentum at a single set of coordinates. For including in the z-momentum balance equation of a one-dimensional model, this equation needs to be averaged over the channel cross section by integrating over the cross section and dividing by the cross-sectional area of the channel. To do this, it is assumed that the z-component of the velocity (u_z) can be expressed as $u_z = \langle u_z \rangle f(x,y)$ [27,28].

Substitution of this into [Eq. \(15\)](#) gives:

$$-f^2 \rho \langle u_z \rangle \frac{\partial \langle u_z \rangle}{\partial z} \quad (16)$$

Note that in this equation only f is a function of x and y , so it is only this term that needs averaging over the cross section. Averaging [Eq. \(16\)](#) over the cross section of the channel gives:

$$-\alpha \rho \langle u_z \rangle \frac{\partial \langle u_z \rangle}{\partial z} \quad (17)$$

$$\text{where } \alpha = \frac{\iint_{\text{channel}} f^2 dx dy}{\iint_{\text{channel}} dx dy} = \frac{\langle u_z^2 \rangle}{\langle u_z \rangle^2}$$

The right hand term in this expression is obtained by substituting $u_z = \langle u_z \rangle f(x,y)$ for f in the integral. Equation (17) is the final form of the improved momentum convection term. Thus the new momentum balance equations are:

$$\frac{\partial P_i}{\partial z} = -\frac{\alpha \rho_i V_i}{d_i^2} \frac{\partial d_i^2 V_i}{\partial z} - \frac{F \mu_i V_i}{d_i^2} \quad (18)$$

$$\frac{\partial P_o}{\partial z} = -\alpha \rho_o V_o \frac{\partial V_o}{\partial z} - \frac{F \mu_o V_o}{d_o^2} \quad (19)$$

The α term in these equations is the momentum flux correction factor which serves to correct for the non-flat velocity profile across the channel (remember $\langle u^2 \rangle \neq \langle u \rangle^2$). As Bissett, Kostoglou and Konstandopoulos [27,28] have pointed out, such a term should also appear in the momentum convection terms of the “old” equations (Eq. (10) and (11)), but this is rarely seen in the literature. For developed laminar flow in a square channel with non-porous walls, $\alpha=1.377$ [28].

Another way of looking at the “old” and “new” momentum balance equations is that if one starts with the momentum convection term from most general form of the momentum balance equation for fluids, $-\nabla \cdot \rho \mathbf{u} \mathbf{u}$ [32], and takes the term for convection of z -momentum in the z -direction, one gets $\partial \rho u_z^2 / \partial z$, the term in the old momentum balance (Eq. (10) and (11)). If, on the other hand, one starts with the momentum convection term from the Navier-Stokes equation, $\rho \mathbf{u} \cdot \nabla \mathbf{u}$ [32], and takes the term for convection of z -momentum in the z -direction, one gets $\rho u_z \partial u_z / \partial z$, the term in the new momentum balance (Eq. (18) and (19)). Note that the use of this Navier-Stokes term does not require the assumption of incompressible flow since only steady-state conditions are being considered.¹

The only other model we have found to consider the convection of z -momentum in the transverse direction was by Wurzenberger and Kutsch [20]. This model includes the effect in the inlet channel momentum balance, but not in the outlet channel balance. Their momentum balance equations like most neglect the velocity profile across the channels. However, although differently expressed, their inlet channel momentum balance is mathematically equivalent to Eq. (18) with $\alpha=1$, except that they have d_i^2 appearing outside of the derivative in the momentum convection term instead of inside.

¹ From a standard identity [33], which is easily proved by multiplying out the terms:

$$\nabla \cdot \rho \mathbf{u} \mathbf{u} = \rho \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{u} \nabla \cdot \rho \mathbf{u}$$

Under steady-state conditions the mass balance is $\nabla \cdot \rho \mathbf{u} = 0$ [32] and hence $\nabla \cdot \rho \mathbf{u} \mathbf{u} = \rho \mathbf{u} \cdot \nabla \mathbf{u}$.

It is useful to compare the magnitude of the “new” and “old” momentum convection terms. Under isothermal conditions and when the pressure change across a volume element is not large enough to cause a significant change in gas density, ρ can be considered a constant. Under these conditions, $\partial \rho V^2 / \partial z$ (the “old term”) is equal to $2\rho V \partial V / \partial z$, which is twice the new momentum convection term.

A comparison of predicted backpressure as a function of flow rate for the new (Eq. (18) and (19)) and old (Eq. (10) and (11)) momentum balance equations for both $\alpha=1$ (flat velocity profile) and $\alpha=1.377$ (realistic velocity profile) is shown in Fig. 4. At low flow rates, the lines coalesce indicating that the momentum convection term is insignificant under these conditions. At higher flows, it is clear that the new momentum convection term results in a lower backpressure prediction than the old one and that allowing for a velocity profile across the channel ($\alpha=1.377$) results in a higher prediction than if a flat velocity profile is assumed ($\alpha=1$).

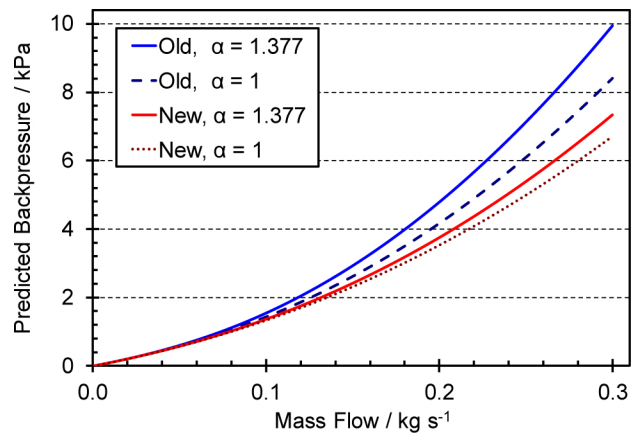


Figure 4. Comparison of predicted backpressure for different versions of the momentum convection term in the gas momentum balance equations. (300/8, 4.66×6 in PF; 20°C; on-vehicle configuration (Fig. 1, bottom); $L_{\text{plug}} = 0$ mm)

Since the gas velocity decreases along the inlet channel, the momentum convection term in both old and new the momentum balance equations (Eq. (10) and (18)) is positive. As a result, at sufficiently high flow rates, these equations will predict (perhaps surprisingly) that pressure will increase along the inlet channel. As the new momentum convection term is smaller than the old one the tendency for this to happen is reduced, but the effect is not prevented.

Since d_i varies along the length of the PF, d_i must be included in the derivative of the momentum convection term ($\partial d_i^2 V_i / \partial z$ or $\partial d_i^2 \rho_i V_i / \partial z$) in the inlet channel momentum balance (both new and old forms, Eq. (10) and (18)), although not everybody does this [17,18,19,23,25]. In contrast, d_i should not appear in the $\partial P / \partial z$ term. Most workers have written their $\partial P / \partial z$ term without d_i in the derivative [17,18,19,20,21,23,25] (although there are exceptions [22]), but, in general, the reason for this has not been made clear. The only explanation we have been able to find is that this is required “to balance the forces” [21,26]. We have found that including d_i in the pressure derivative results in the prediction unphysical pressure and velocity profiles during soot loading, so this is an important point.

Therefore, it seems worth explaining why d_i does *not* appear in the $\partial P_i / \partial z$ term. Consider Fig. 5, which represents two elements of the inlet channel of length δz across which the width of the channel changes due to variation in the soot loading. The forces acting on the gas in the left hand element in the axial (z) direction are indicated. The net (or resultant) force acting on the gas in the axial direction is given by:

$$\text{Net force} = A_z P_z - A_{z+\delta z} P_{z+\delta z} - (A_z - A_{z+\delta z}) P_{z+\delta z} \quad (20)$$

where A_z & $A_{z+\delta z}$ and P_z & $P_{z+\delta z}$ are the cross-sectional area and the pressure at positions z & $z+\delta z$. The first two terms after the equals sign are the forces acting on the gas in the element from the left by the upstream gas and from the right by the downstream gas. The third term is the force on the gas exerted by its “container”, in this case the (soot-lined) channel walls. Since $\delta z \rightarrow 0$, in calculus terms the channel width changes in a stepwise fashion across the element (Fig. 5), rather than there being a continuous change in cross section.

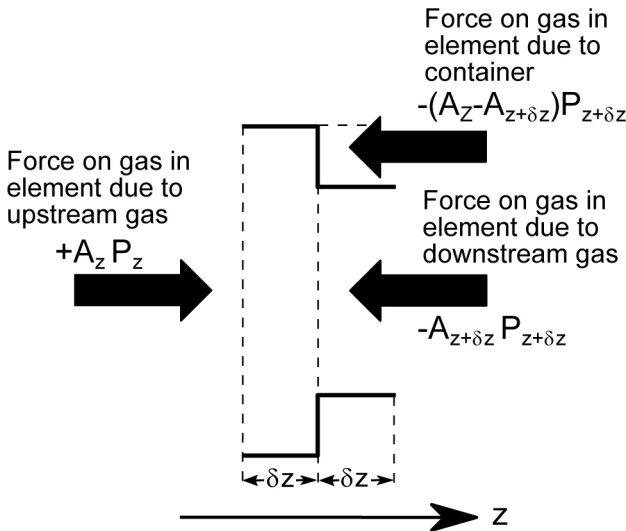


Figure 5. Diagram of two elements of soot-loaded inlet channel showing the forces acting on the gas in the left hand element in the z -direction. P_z and A_z are the pressure and cross-sectional area at axial coordinate z . In calculus terms, since $\delta z \rightarrow 0$, the channel width changes in a stepwise fashion rather than continuously.

Simplifying the equation:

$$\text{Net force} = A_z (P_z - P_{z+\delta z}) \quad (21)$$

Dividing this by δz and as $\delta z \rightarrow 0$, gives the derivative $-A \partial P / \partial z$, i.e. the pressure derivative with the cross-sectional area appearing outside of the derivative. Note that the same conclusion would be reached if the channel width changed in the opposite direction to that depicted in Fig. 5. Incidentally, this consideration did not arise in Bissett's original model [15] as he assumed that the inlet channel width did not change with soot loading.

The momentum balance equations (Eq. (18) and (19)) have so far been presented in a form that is not practical for solving with a Boundary Value Problem (BVP) solver as the derivatives $\partial d_i^2 V_i / \partial z$

and $\partial V_i / \partial z$ are not readily available. For the inlet channel balance, this can be remedied by writing $\partial d_i^2 V_i / \partial z$ as $\partial (d_i^2 \phi_i / \rho_i) / \partial z$, substituting in Eq. (5) for the density and applying the product rule to the resulting derivative. Substitution of this result into Eq. (18) gives:

$$\left(1 - \frac{\alpha \phi_i V_i}{P_i}\right) \frac{\partial P_i}{\partial z} = -V_i \left[\alpha \left(\frac{1}{d_i^2} \frac{\partial d_i^2 \phi_i}{\partial z} + \frac{\phi_i}{T_i} \frac{\partial T_i}{\partial z} \right) + \frac{F \mu_i}{d_i^2} \right] \quad (22)$$

This equation contains only derivatives that are known; it defines $\partial P_i / \partial z$, while the other derivatives are given by Eq. (7) and (26). A similar expression applies for the outlet channel:

$$\left(1 - \frac{\alpha \phi_o V_o}{P_o}\right) \frac{\partial P_o}{\partial z} = -V_o \left[\alpha \left(\frac{\partial \phi_o}{\partial z} + \frac{\phi_o}{T_o} \frac{\partial T_o}{\partial z} \right) + \frac{F \mu_o}{d_o^2} \right] \quad (23)$$

3.2.3 Gas Energy Balance

In terms of the specific enthalpy, H_i , the gas energy balance for the inlet channel is:

$$\frac{\partial d_i^2 \phi_i H_i}{\partial z} = 4d_i h_i (T_w - T_i) - 4d \phi_w C_{pg,w} T_w \quad (24)$$

where h_i is the heat transfer coefficient for heat transfer between the gas in the inlet channel and the PF wall, T_w is the temperature of the soot cake and the PF wall and $C_{pg,w}$ is the specific heat capacity at constant pressure of the gas passing through the soot cake and the PF wall.

From left to right, the terms in Eq. (24) correspond to the rate of enthalpy loss per unit length of PF by convection along the inlet channel; the rate of energy gain per unit length due to heat transfer between the gas in the channel and the PF wall (or soot cake for a soot-loaded PF); and the rate of enthalpy loss per unit length due to flow through the wall.

Substituting in $dH_i = C_{pg,i} dT_i$,² where $C_{pg,i}$ is the specific heat capacity of the gas in the inlet channel, gives,

$$C_{pg,i} \frac{\partial d_i^2 \phi_i T_i}{\partial z} = 4d_i h_i (T_w - T_i) - 4d \phi_w C_{pg,w} T_w \quad (25)$$

Note that $C_{pg,i}$ appears outside the derivative. Applying the product rule to the derivative and substituting in Eq. (7), gives the final equation for the inlet channel gas energy balance,

$$C_{pg,i} d_i^2 \phi_i \frac{\partial T_i}{\partial z} = 4d_i h_i (T_w - T_i) + \dots + 4d \phi_w (C_{pg,i} T_i - C_{pg,w} T_w) \quad (26)$$

² The full version of this equation is as below [34], but the second term is zero for an ideal gas:

$$dH = \left(\frac{\partial H}{\partial T} \right)_p dT + \left(\frac{\partial H}{\partial p} \right)_T dp + \left[\frac{1}{\rho} - T \left(\frac{\partial \phi}{\partial T} \right) \right] d\rho$$

Analogously, the outlet channel energy balance is:

$$C_{pg,o} d_o^2 \phi_o \frac{\partial T_o}{\partial z} = 4d_o h_o (T_w - T_o) + \dots + 4d \phi_w (C_{pg,w} T_w - C_{pg,o} T_o) \quad (27)$$

This differs from the inlet channel balance predominantly in the effective change in the sign of the ϕ_w term as gas is entering the channel through the wall rather than leaving it.

The heat transfer coefficients, h_i and h_o , are calculated from the Nusselt number, Nu , and the thermal conductivity of the gas in the inlet and outlet channels (λ_i, λ_o), thus from the definition of Nu :

$$d_i h_i = Nu \lambda_i \quad (28)$$

$$d_o h_o = Nu \lambda_o \quad (29)$$

In this model, Nu is assumed to be a constant. The effect of Nu being a function of the wall Reynolds number, Re_w , will be considered in [section 6](#).

In deriving the inlet channel energy balance, it has been assumed that the gas leaving the inlet channels through the walls has the same temperature as the PF wall (Eq. 24)). This recognises that the gas temperature varies across the width of the channel with the gas close to the PF wall (or soot cake, if there is one) having the same temperature as the wall (or soot cake) due to efficient heat transfer with the wall and the low velocity of the gas close to the wall (due to the no slip boundary condition (*i.e.* gas in the channel adjacent to the wall having zero axial velocity) and the low through-wall velocity resulting from the large filtration area). This approach was used in Bissett's original model [15] and has been used by other workers [24,35]. However, this assumption also results in an apparent paradox in that if ϕ_w is sufficiently large, Eq. (26) predicts that T_i will increase along the inlet channel when $T_i > T_w$, which clearly contradicts thermodynamics. To avoid this apparent paradox, many workers have developed models in which it is assumed that the gas leaving the inlet channel through the walls has a temperature of T_i instead of T_w [18,21,22,23,25,26]. More recently, Bissett, Kostoglou and Konstandopoulos [27,28] have resolved this apparent paradox by showing that h_i in fact increases with ϕ_w (more specifically with Re_w) at a rate which ensures that $\partial T / \partial z$ can never have "the wrong sign". Therefore, there is no reason not to use the original approach where the gas leaving the channel through the PF wall has a temperature of T_w and indeed Bissett et al. [27,28] argue that this approach is preferable for a number of reasons. (However, others remain unconvinced [26], stating that the Bissett, Kostoglou and Konstandopoulos' work relies on a fixed gas temperature at the channel wall boundary, the value of which is not known *a priori*).

As Bissett et al. [27] have pointed out, the terms in the final form of the inlet channel energy balance (Eq. (26)) correspond (from left to right) to i) the enthalpy change in the portion of the gas entering a

volume element that continues along the channel, ii) the total heat flux at the walls (due to conduction through the gas [15,28]), and iii) the change in enthalpy of the remaining portion of the gas entering the volume element which leaves through the PF wall. For the latter term, the enthalpy change is associated with the fact the gas enters the element with a mixing cup temperature of T_i , but leaves at a temperature of T_w . With the first term, the enthalpy change is associated with the change in mean gas temperature (T_i) across the element. This physical interpretation is possible because of the splitting the derivative in Eq. (25) into terms corresponding to gas passing along the channel and gas exiting through the wall.

3.2.4 Boundary Conditions for Gas Balance Equations

Since there are six differential equations (Eq. (7), (9), (22), (23), (26), (27)), six boundary conditions are required. For the on-vehicle configuration (Fig. 1, bottom), these are:

$$d_i^2 \phi_i|_{z=0} = 2\dot{m} / \rho_{cell} A \quad (30)$$

$$\phi_i|_{z=L} = 0 \quad (31)$$

$$\phi_o|_{z=0} = 0 \quad (32)$$

$$P_o|_{z=L} = (P_5 - P_6) + P_{atm} \quad (33)$$

$$T_i|_{z=0} = T_{in} \quad (34)$$

$$T_o|_{z=0} = T_w|_{z=0} \quad (35)$$

where A is the cross-sectional area of the PF, $\dot{m}$ is the total mass flow into the PF and $(P_5 - P_6)$ is the pressure change due to expansion of gas as it leaves the PF; P_5 and P_6 refer to pressures at specific locations defined in Fig. 6. The evaluation of $(P_5 - P_6)$ is described in [section 3.5.1](#).

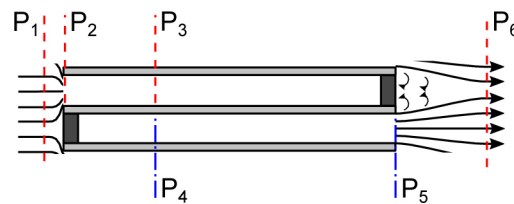


Figure 6. Schematic of a PF defining locations 1-6 at which it is useful to refer to the pressure. Note that while P_1 , P_2 , P_5 and P_6 are at fixed locations, P_3 and P_4 can be at any point along the PF provided that they are both at the same axial coordinate. P_1 and P_6 are in regions of developed flow, before the contraction into the PF front face and after the expansion out of the rear face. Based on a figure by Konstandopoulos [36].

In words, the boundary conditions are that the inlet mass flux and temperature are known (Eq. (30) and (34)); that the gas mass flux at the end of the of the inlet channel and the state of the outlet channel is zero (Eq. (31) and (32)); that the pressure at the end of the outlet

channel is equal to the external pressure plus the change in pressure due to expansion as the gas leaves the PF (Eq. (33)); and that since the gas at the start of the outlet channel (if there were any) is stagnant (Eq. (32)) it must have the same temperature as the PF wall at the same axial location (Eq. (35)).

For the cold flow configuration (Fig. 1, top), where atmospheric pressure is at the PF inlet rather than the outlet, Eq. (33), is replaced by:

$$P_i|_{z=0} + (P_1 - P_2) = P_{atm} \quad (36)$$

where $(P_1 - P_2)$ is the pressure loss due to contraction of the gas as it enters the PF (Fig. 6). The evaluation of this is described in section 3.5.2. In words, this boundary condition is that the pressure at the start of the inlet channel plus the pressure change due to gas contraction at the PF entrance is equal to the external pressure.

3.3 Across-Wall Pressure Drop

The pressure drop across the soot cake and PF wall can be described by Darcy's law with the Forchheimer extension. Since gas density and hence through-wall gas velocity (at constant mass flow) vary with pressure, this equation is written in differential form:

$$-\frac{\partial P}{\partial y} = \frac{\mu V_w}{k} + \beta \rho_{g,w} V_w^2 \quad (37)$$

where y is the distance through the soot cake and PF wall, k is the permeability and β is the Forchheimer constant. Both k and β are properties of the porous media through which the gas flows. The first term on the right hand side of the equals sign is Darcy's law and the second term the Forchheimer term.

Darcy's law³ [37] and the Forchheimer extension⁴ [38] are both empirical laws originally developed for the flow of water across beds of sand. However, they have been extensively used for the prediction of pressure drop across all sorts of porous media. Both Darcy's law [39,40] and Darcy's law with the Forchheimer extension [41,42] have subsequently been derived from first principles. Darcy's law describes pressure drop across the porous media due to viscous losses and the Forchheimer extension the pressure drop due to inertial effects.

Equation (37) needs to be solved for the soot cake and PF wall. The soot cake in the inlet channel can be divided into four trapezoidal sections (Fig. 2), each of which sits on a slab shaped section of wall. This geometry, together with the dimensions, is depicted in Fig. 7. In this work we only consider flow through the wall of symmetric PFs, where the wall cross section is rectangular; asymmetric PFs represent an additional level of complexity as the flow path through the PF wall is non-trivial [35]. Since this model allows for the variation in gas

density (and hence through-wall velocity) with pressure, it is necessary to rewrite Eq. (37) in terms of the through-wall mass flux. Thus, for the PF wall Eq. (37) becomes:

$$-\frac{\partial P}{\partial y} = \frac{\mu_w \phi_w}{k_w \rho_{g,w}} + \frac{\beta_w \phi_w^2}{\rho_{g,w}} = \frac{RT_w}{PM} \left[\frac{\mu_w \phi_w}{k_w} + \beta_w \phi_w^2 \right] \quad (38)$$

In the right hand expression, Eq. (5) has been substituted for $\rho_{g,w}$. k_w and β_w refer to the permeability and Forchheimer constant of the wall.

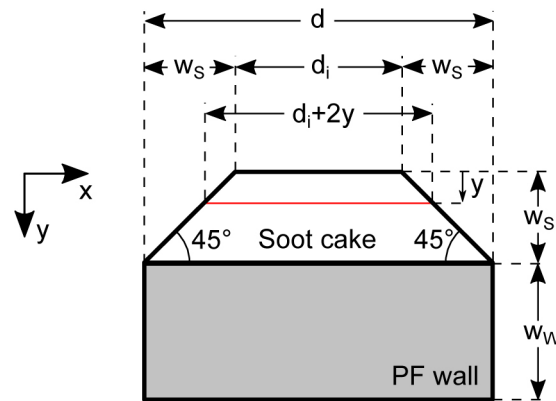


Figure 7. Diagram of the trapezoidal soot cake and wall slab geometry showing dimensions.

Similarly, for the soot cake Eq. (37) becomes:

$$-\frac{\partial P}{\partial y} = \frac{RT_w}{PM} \left[\frac{\mu_w \phi_w}{k_s} \frac{d}{d_i + 2y} + \beta_s \phi_w^2 \frac{d^2}{(d_i + 2y)^2} \right] \quad (39)$$

where k_s and β_s refer to the permeability and Forchheimer constant for the soot cake. Note that $d_i + 2y$ is the width of the soot cake at a distance y from the "top" (or channel side) of the soot cake as depicted in Fig. 7. Here it has been assumed that the flow through the soot cake can be modelled by assuming that the gas flow simply spreads out to fill the expanding cross-sectional area of the soot cake. Thus the gas velocity through the soot cake varies with $d/(d_i + 2y)$. Note also that since the temperature is assumed to be constant through the soot cake and PF wall, μ_w and T_w apply to both Eq. (38) and (39).

Equations (38) and (39) are first order differential equations with separable variables, which can be solved to give:

$$P_i^2 - P_o^2 = \frac{RT_w}{M} \left[\left(\frac{2w_w}{k_w} + \frac{d}{k_s} \ln \left(\frac{d}{d_i} \right) \right) \mu_w \phi_w + \dots + \left(2\beta_w w_w + \beta_s d^2 \left(\frac{1}{d_i} - \frac{1}{d} \right) \right) \phi_w^2 \right] \quad (40)$$

Thus the pressure drop across the soot cake and PF wall, is a quadratic in ϕ_w . This can be solved using the usual equation for the solution of a quadratic to give ϕ_w as a function of P_i and P_o , which is what is actually required for numerically solving the gas balance equations.

³ Compared to the modern form of Darcy's law, Darcy's original equation [37] lacks the viscosity term.

⁴ In Forchheimer's original paper [38], pressure drop per unit length of column for water flowing through a column of sand was modelled by two equations, viz. $aV + bV^2$ and mV^n , where a , b , m and n are constants. The former equation would appear to be the origin of the modern Forchheimer extension to Darcy's law.