

Methodology for Modelling a Combined DPF and SCR Catalyst with the Porous Medium Approach in CFD

S. F. Benjamin and C. A. Roberts
Coventry Univ.

ABSTRACT

In an attempt to reduce particulate and NO_x emissions from Diesel exhaust, the combined DPF and SCR filter is now frequently chosen as the preferred catalyst. When this device functions effectively it saves valuable packaging space in a passenger vehicle. As part of its development, modelling of its emissions performance is essential. Single channel modelling would seem to be the obvious choice for an SCR filter because of its complex internal geometry. This, however, can be computationally demanding if modelling the full monolith. For a normal flow-through catalyst monolith the porous medium approach is an attractive alternative as it accounts for non-uniform inlet conditions without the need to model every channel. This paper attempts to model an SCR filter by applying the porous medium approach. The model is essentially 1D but as with all porous medium models, can very easily be applied to 3D cases once developed and validated. The model is described in full in this paper and values for all the key parameters are presented. The filter is assumed to collect soot in the inlet channels, but only the outlet channels are coated with SCR washcoat, as in the most recent devices. This aims to avoid back diffusion of NO₂ that promotes soot and NO_x reactions. But it is necessary to modify the pressure loss expression term to account for the smaller size of the washcoated outlet channel. The SCR model integrated into the CFD coding is simple and based on a scheme available in the literature. This includes the standard and fast SCR reactions and ammonia adsorption and desorption. NO and ammonia oxidation are also included and are important during the high temperature regeneration phase. The detail of the flow at the channel scale is not modelled but the species can be modelled at the channel scale for the monolith by application of source terms in the species transport equation. The source terms are evaluated in user subroutines in commercial CFD software. The species levels of NO, NO₂ and NH₃ in the flow coming through the filter wall, in the pores in the wall and in the flow in the downstream channel are all modelled as a function of distance along the brick. The simplifying assumptions on which this model is based are stated in this paper. The model produces plausible output when run as a demonstration case for a 1050 s soot storage period at 550 K, followed by a 150 s regeneration period at 900 K, and then for a further soot storage period at 550 K. The simulations are in qualitative agreement with the expected performance of a combined DPF and SCR in a real Diesel exhaust. An attempt has been made to apply the model to a real case based on data available in the literature so that its output can be validated.

CITATION: Benjamin, S. and Roberts, C., "Methodology for Modelling a Combined DPF and SCR Catalyst with the Porous Medium Approach in CFD," *SAE Int. J. Engines* 7(4):2014, doi:10.4271/2014-01-2819.

INTRODUCTION

Passenger cars with Diesel engines are now in common usage because of good fuel efficiency and relatively low emissions of CO and hydrocarbons. Particulate emissions and NO_x, however, remain challenging as the emissions regulations become ever more restrictive. The DPF is established as the method of choice for the removal of particulates and SCR catalysts have been shown to be effective in removing NO_x. Recently, the DPF and the SCR have been combined into a single unit, sometimes called an SCR filter (SCR filter) or WFSR (wall flow SCR). This combined device occupies less space in the exhaust system than a separate filter and SCR catalyst for aftertreatment. As with all aftertreatment devices, it is desirable that the emissions performance of the device can be modelled.

The geometry of the DPF, the catalysed DPF and the combined SCR/DPF is by its nature more complex to model than the flow-through multi-channel catalyst substrate.

There are at least three separate research teams working on the issue of SCR filter modelling who have published widely. Haralampous et al. [1, 2] began some years ago by modelling catalysed DPFs; they have published extensively on catalysed DPFs where the catalyst was intended to promote the regeneration, which occurred by oxidation of soot with either oxygen or NO₂. Their modelling approach was mathematically rigorous with the full model description presented as a set of equations in their papers. They later moved on to modelling

combined DPF-SCR devices [3, 4]. In these later papers they have utilised the specialised software package Axisuite to solve the equations.

York et al. also investigated catalysed DPFs initially [5, 6]. But by 2012 [7] this team had also turned their attention to the SCRF. They attempted to model the performance of an SCRF and also to validate their model. Unfortunately, their model is not readily applicable by other users because some details, including kinetic constants, are not presented. Park et al. [8] have also published a paper, which is specifically a modelling study of SCR-DPF devices. They mention the mass transfer in the inlet and outlet channels of the DPF being influenced by suction at the wall in the inlet channels and blowing at the wall in the outlet channels, which is a detail that is not commented upon by most authors. They have published again on this topic [9] and have investigated mass transfer differences between flow-through and wall-flow devices. In this later paper they suggest that wall-flow devices are less efficient in converting NO_x than flow-through devices, but their paper is not focused on developments to the model itself.

In an SCRF, the flow passing through the porous walls of the filter into adjacent channels is orthogonal to the main flow direction through the substrate as a whole. This implies that modelling the individual channels may be necessary to describe the detail of the processes within the catalysed filter when developing a CFD model. A single channel modelling approach will provide a complete description of a situation where the main flow direction is aligned with the channels as in a normal multi-channel catalyst, or if several channels are modelled, it can follow the flow through the wall from channel to channel in a DPF. For a normal flow-through catalyst substrate there is a computational option, which is modelling using the porous medium approach. This considers the whole substrate as an analogous porous medium and has the advantage of computational efficiency. The mesh size is often coarser than the cross sectional dimensions of the channels and so a smaller number of computational cells is required for a large 3D model. In 2007, an attempt was made by the authors to model a DPF using the porous medium approach. This was an evaluation exercise and was computationally successful, although the model was not fully validated [10]. For the DPF or the newer combined DPF/SCR it may initially appear counter-intuitive to model the device using the porous medium approach. The advantages of the porous medium approach, however, make the attempt to model the combined DPF and SCR in this way worthwhile. The detail of the flow at the channel scale is not modelled by this approach but the species can be modelled at the channel scale for the monolith by application of source terms in the species transport equations. The attempt reported in this paper demonstrates that modelling in this way is indeed feasible for assessing conversion efficiency. The SCR kinetic model integrated into this model is based on a scheme published by Olsson et al. [11]. Soot oxidation is included as in an earlier paper by the authors [10] and a reaction rate for the reaction between soot and NO₂ can also be included; Ahmadinejad et al. [12] and

Zouaoui et al. [13] have both investigated the kinetics of the reaction between soot and NO₂. The model as presented in this paper is essentially a demonstration model but it has been applied to real cases and compared with data presented in the literature [14]. The model as developed and described here is essentially 1D but the advantage of the porous medium approach is that, once validated, it can very easily be adapted and extended to 3D cases.

Park et al. [8] present a useful comparison between the time scales for convection and diffusion in a combined DPF-SCR device. They suggest that convection along the channel and diffusion to the filter wall have the same time scale in the inlet channel but that diffusion along the inlet channel is 4 orders of magnitude slower and hence negligible. This is presumably also true in the outlet channel. When the flow passes through the filter wall, diffusion in the flow direction and diffusion to the catalyst surface are an order of magnitude faster than convection through the wall. Other authors have made different assumptions, and most do not comment on any diffusion occurring in the direction of the net convective flow through the wall. Ahmadinejad et al. [12] assume that reactants reach the soot by convection only and so did not consider diffusion. Watling et al. [7] state that diffusion to the surfaces from convective flow both through the wall and along the channels should be considered in an SCRF model. They apply mass transfer terms to account for this. This diffusion issue does present a challenge to the application of the porous medium approach to an SCRF as any gradient in concentration through the wall must be assumed to be linear. Nevertheless a transfer coefficient can be applied to the bulk flow through the wall to allow for lateral diffusion to the sites within the wall. This is discussed later in this paper.

The aim of this work is to demonstrate that the combined DPF/SCR or SCRF can be modelled as a homogeneous entity using the porous medium approach. The aim is to develop a model that will circumvent the need to use representative single channels when modelling cases with a complex 3D flow field. The time advantage achieved when using smaller numbers of computational cells with the porous medium approach is considerable. This report gives full details of the model, which is developed in Star-CD Version 4.14. The source terms, which are discussed in detail in this paper, have been coded into user subroutines of the CFD code. This is a novel approach to modelling this device which has flow passing through the filter walls in directions orthogonal to the main flow direction. The model developed in this paper is 1D but is readily transferable to 3D geometries.

ASSUMPTIONS MADE IN FORMULATING THE POROUS MEDIUM DPF-SCR MODEL

When modelling any multichannel catalyst substrate as an analogous porous medium in Star-CD, the gas phase and solid pore phase species concentrations are both properties of the porous fluid cells. The DPF-SCR or SCRF that is modelled in this

paper has a washcoated SCR layer only in the outlet channel. A schematic diagram is shown in Figure 1. When modelling an SCRf, the inlet species concentration ($\rho_{in} C_{in}$) and mass fraction C_{in} are known. There are four other locations where the species mass fractions are solved for and are of particular interest. Those four locations are: in the porous wall after the soot layer, in the gas filled pore within the SCR washcoat layer, in the gas as it flows from the SCR washcoat layer into the outlet channel, and in the gas flow along the outlet channel.

The general conservation equation for chemical species is the transport equation. Equation (1) is the full 3D version of this equation.

$$\frac{\partial(\rho C)}{\partial t} + \nabla \cdot (\rho U C) - \nabla \cdot \left[\left[\frac{\mu_t}{\sigma_s} + \rho D \right] \nabla C \right] = \dots$$

$$= Source \text{ kg m}^{-3} \text{ s}^{-1}$$

(1)

The three terms of this equation on the left are the transient term, the convective term and the diffusion flux term. The source term on the right hand side is only applicable within the porous medium computational cells when the porous medium approach is implemented, for example in a multichannel catalyst substrate. In that case the source term describes the net effect of diffusion of species between the gas stream and the washcoat pores at the channel wall as a mass transfer process. So, in effect, the source term replaces the diffusion flux term in the direction normal to the flow direction. This is achieved by using a mass transfer coefficient. The diffusion flux in the flow direction in a porous medium is usually assumed to be negligibly small compared with the convective flux. To model an SCRf, for the purposes of this paper, it is possible to consider a hypothetical channel pair and solve eq. (1) in the y and z directions only. Equation (1) is written in its 1D form as eq. (2), for axial flow along the analogous porous medium, with the diffusion flux term suppressed, which is achieved within Star-CD by the choice of values for σ_s and D.

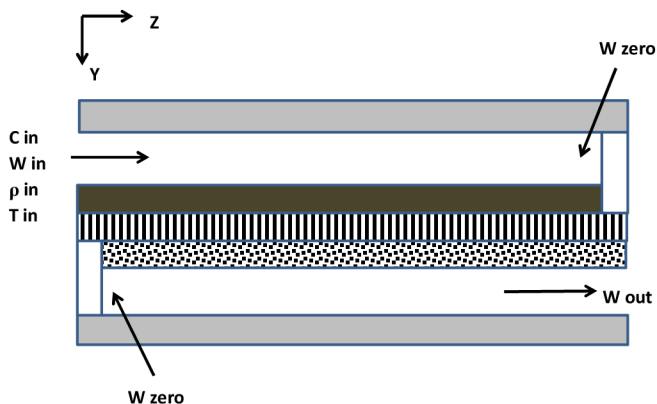


Figure 1. Schematic diagram of a combined SCR/DPF or SCRf or WFSR showing the detail of one wall between a hypothetical channel pair. Soot layer is black; porous wall is shown striped; SCR washcoat layer is dotted black. Blocked channel ends are shown in white. W is velocity in z direction.

$$\frac{\partial(\varepsilon \rho C)}{\partial t} + \frac{\partial(\varepsilon \rho W C)}{\partial z} = Source \text{ kg m}^{-3} \text{ s}^{-1}$$

(2)

In an SCRf the pores where the reactions will take place are accessed by the flow as it passes through the tortuous passages in the SCR washcoated layer. In that layer, where the net flow direction is normal to the SCRf channels, the magnitudes of mass transfer by convection and by diffusion are closer in magnitude, because the net flow velocity through the wall is low. The second order diffusion term in the y direction may therefore not be negligible in some cases but it has been neglected in this model as a first approximation for the purposes of demonstration of the model methodology. For flow through the porous layer in the net y direction, the general equation, eq. (1), is rewritten as eq. (3). Transfer to the pores in the washcoat, which is a lateral diffusion process within the porous wall, is dealt with by the source term, using a mass transfer coefficient that is referenced in Appendix A.

$$\frac{\partial(\varepsilon \rho C)}{\partial t} + \frac{\partial(\varepsilon \rho V C)}{\partial y} = Source \text{ kg m}^{-3} \text{ s}^{-1}$$

(3)

The model described here aims to simulate the combined DPF/SCR as a homogeneous entity using the porous medium approach. In order to achieve this and to model the detail of the processes in these dual-channel devices, numerous assumptions are necessary, which are listed here. These assumptions in turn require adaptations to be made to the equations solved within the CFD code Star-CD.

- [1]. It is assumed that there is no mass transfer occurring between adjacent channel pairs.
- [2]. Table B1 in Appendix B lists the species defined in the model. The gas concentrations (ρC_g) are those in the inlet channel. The concentrations (ρC_{ps}) are post the soot layer, which means the concentrations in the wall after the soot reactions have occurred. The pore concentrations (ρC_{pore}) are the local concentrations inside the SCR washcoat layer. The concentrations (ρC_w) as the gas leaves the wall are the gas phase concentrations in the flow that passes through and out from the wall in the y direction at each specified z location. The ammonia storage in the wall, characterised by parameter θ , is similarly a function of z. The outlet channel concentrations (ρC_{out}) are the gas phase concentrations in the flow, which in the real SCRf convects in the z direction along the outlet channel towards the exit.
- [3]. The simulation assigns a convective velocity in the z direction to each computational cell when the combined DPF/SCR is considered as a whole and modelled as an equivalent porous medium. This is not the true convective velocity in either the upstream or the downstream channel. It is an effective velocity for a hypothetical channel pair. Detailed modelling of the upstream channel is circumvented since the function of this channel is only soot filtration as modelled previously for a simple non-catalysed DPF [10].

- [4]. In the outlet channel downstream of the porous wall the convective velocity varies from zero at $z = 0$ up to the convective velocity corresponding to the full mass flow rate at the exit from the channel of the SCR. The assumption is made that the mass flow distributes itself uniformly when it enters the wall from the inlet channel. This necessitates coding strategies in the user subroutine for the species source terms to force the CFD solver to calculate values that represent the true mass fractions, and hence concentrations, in the downstream channel.
- [5]. The nominal wetted area A_v (m^2/m^3 substrate) is based on all the channels of an SCR. The filtration area is approximately half of this because soot accumulates only in the inlet channels. When only the outlet channels are coated with washcoat and SCR catalyst, then the wetted area in the outlet channels is smaller than the filtration area offered by the inlet channels. This is because the washcoat layer thickness is accounted for in the evaluation of the wetted SCR surface area in the outlet channels.
- [6]. The parameter V_w is a measure of the pore volume in the SCR washcoat layer per m^3 of bulk substrate and is dependent upon SCR geometry, the SCR washcoat properties and its loading. An estimated value for an SCR is about 0.05 m^3 pore volume / m^3 substrate, assuming the washcoat porosity is in the range 50 - 60 %.
- [7]. The soot layer thickness in the inlet channel is negligible initially but the wall is assumed already permeated with soot so that soot accumulates on the surface as a cake. The filter is 100 % efficient in removing soot from the flow.
- [8]. There is no significant diffusion or reaction of species in the inlet channel so that the concentrations of the incoming species are uniform along the inlet channel. Change in the concentration of NO , O_2 and NO_2 by reaction with soot occurs as the flow passes through the soot layer. The reaction rates for the soot reactions are calculated using the gas phase NO_2 and O_2 concentrations.
- [9]. The SCR reactions take place in the pores in the SCR washcoat layer. There is mass transfer between the flow through the washcoat layer and the pores in the layer; the pore phase concentrations are used to calculate the reaction rates for the SCR reactions. The mass transfer coefficient for transfer between the flow through the SCR washcoat layer and the pores is discussed in [Appendix A](#) of this paper.
- [10]. The concentration of the species NO , NO_2 and NH_3 in the flow that passes into the downstream channel is controlled by reactions that have already occurred as the flow has passed through the soot layer, and through the catalytically active washcoat layer on the wall in the outlet channel.
- [11]. In the outlet channel there is convection in the z direction, but negligible diffusion in the z direction. There can be exchange by diffusion, however, in the y direction between the outlet channel flow and the relatively slow flow through the SCR washcoat layer. This is accounted

for in the model by a mass transfer source term. The mass transfer coefficient is calculated in the normal way in the demonstration model reported here. The wall flow velocity is very low and so the transfer coefficients will be a fair approximation to the real situation. But Hwang et al. [15] consider the effect of suction (which occurs in the inlet channel) and blowing (which occurs in the outlet channel) on wall heat transfer; and there will be a similar effect on mass transfer. The model may need to be modified to account for this at a later stage of its development.

- [12]. If both the inlet channels and outlet channels are coated in SCR washcoat, the soot layer forms directly adjacent to an SCR washcoat layer. There can be back-diffusion of species from the SCR washcoat layer to the soot layer. This back diffusion is particularly significant when NO_2 is present [1]. This is because NO_2 interferes with the soot oxidation during the regeneration. This back diffusion is not currently accounted for in the model described in this paper. The geometry on which this model is based is different because the filter wall separates the SCR layer from the soot cake layer, which is where most of the soot resides.

FORMULATION OF SOURCE TERMS FOR COMBINED DPF-SCR MODEL

The general forms of the transport equation were given in [eqs. \(1\), \(2\), \(3\)](#). Applying the porous medium approach in CFD requires that diffusion is suppressed in the porous medium; but where there is diffusion in the porous medium, which must be accounted for in the model, this is achieved with source terms. In order to account for all of the assumptions discussed in the previous section, the equations and their source terms will take various forms, which are discussed in detail in this section.

The modelling of the two soot species in [Table B1](#) of Appendix B is based on the non-catalysed DPF model previously developed [10]. The contents of the soot cake layer increases from approximately zero to a value that is very large when expressed as a mass fraction of the fluid (gas). In order to solve the transport equation in the CFD model, a multiplier (10^4) is introduced so that $[\text{true mass fraction} \times 10^{-4}]$ is solved for in the case of this scalar. For the rest of the defined species the mass fraction is solved for, and the species are dealt with as now described.

NO , NO_2 , O_2 and NH_3 Concentrations in the Inlet Channel and the Bulk Gas Phase

[Equation \(4\)](#) describes the conservation of gas species for a hypothetical channel pair assuming that there is no mass transfer or gas phase reaction occurring as the species travel from the inlet to the outlet of the monolith. Hence the source term is zero in [eq. \(4\)](#), as indicated in [Table B1](#) in Appendix B. The concentration ($\rho_{\text{air}} C_g$) can be described as the bulk species concentration in the whole substrate and will remain constant at the inlet concentration if density is unchanged. The density ρ_{air} approximates the exhaust stream density.

$$\frac{\partial(\rho_{air}W_s C_g)}{\partial z} + \frac{\partial(\varepsilon \rho_{air} C_g)}{\partial t} = 0 \quad (4)$$

Note that W_s is the superficial velocity in the z direction for the bulk porous medium, not the inlet or outlet channel velocity. The porosity of the SCR is the void fraction ε , so that

$$\rho_{air} W_s = \varepsilon \rho_{air} W$$

In eq. (4) the diffusion flux term has been suppressed in the porous medium, but normal values for the diffusion coefficients do apply, however, in the fluid. Values for diffusion coefficients are shown in Table B1. A small mesh has been used for model development, see Figure 2, and the inlet and outlet fluid ducts are shown in blue. In the fluid ducts, the normal RANS equations are solved. The demonstration model presented here is a simple 1D case. In more complex and 3D models there will be a temporal and spatial distribution of inlet velocity and species concentration at the front face of the SCR. The bulk concentration will therefore change as a consequence of both varying inlet conditions and heat transfer in the monolith.

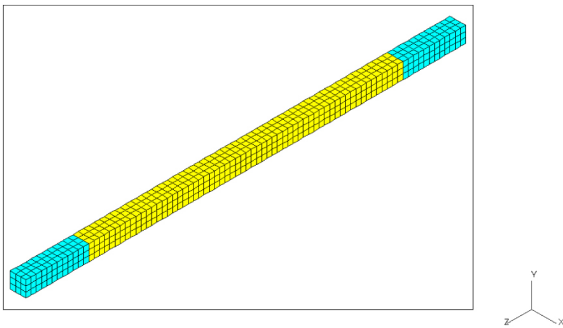


Figure 2. The computational mesh for the combined DPF/SCR or SCR model with 756 cells each 2.5 mm × 2.5 mm × 2.5 mm; Inlet duct from $z = 0$ to $z = 30$ mm (12 cells); Porous medium between $z = 30$ mm and $z = 180$ mm (60 cells); Outlet duct from $z = 180$ mm to $z = 210$ mm (12 cells).

NO, NO₂, and O₂ Concentrations in the Wall After Reactions with Soot

The flow passes through the soot cake layer in the y direction. The convective term is not included on the left hand side of eq. (5) but is accounted for in the source term. The flow enters the soot layer with concentration ($\rho_{air} C_g$) and leaves with concentration ($\rho_{air} C_{ps}$). The significance of this term is discussed further in relation to eqs. (6), (7), (8). Equation (5) also has diffusion suppressed so that it cannot occur in the z direction in the porous medium.

$$\frac{\partial(\varepsilon \rho_{air} C_{ps})}{\partial t} = \frac{M'(C_g - C_{ps})}{V_{sub}} + \sum SRR \quad kg \ s^{-1} m^{-3} \ reactor \quad (5)$$

The rates for the soot reactions are calculated with gas phase concentrations of NO, NO₂ and O₂.

The quantity M' is the total mass flow rate in kg/s that passes through the DPF/SCR. The quantity V_{sub} is the volume of whole substrate that filters and converts the species in the mass flow. Hence, a value for the mass flow rate in kg/s/m³ substrate is derived in eq. (6). This value applies to the bulk flow through the substrate in the z direction but also to bulk flow through the wall in the y direction, as demonstrated by eqs. (6), (7), (8). Note that $[V_{sub}/L]$ m² is the superficial cross-sectional area of the equivalent continuum through which all the mass flows in the z direction, and A_{filt} (m²/m³) is the wall filtration area per unit volume through which all the flow passes in the y direction.

For the net flow through the porous medium in the z direction with velocity W_s

$$\frac{M'}{V_{sub}} = \frac{W_s \rho_{air}}{L} \quad kg \ s^{-1} m^{-3} \ substrate \quad (6)$$

Also, for flow through the wall in the y direction with superficial velocity V_{wall}

$$M' = V_{wall} \rho_{air} [V_{sub} A_{filt}] \quad kg \ s^{-1}$$

From eq. (7)

(7)

From eq. (7)

$$\frac{M'}{V_{sub}} = V_{wall} \rho_{air} A_{filt} \quad kg \ s^{-1} m^{-3} \ substrate \quad (8)$$

Thus the local value for mass flow rate per unit volume can be found by using the local values of W_s and ρ_{air} in the CFD model, which are temperature dependent, but dividing by the full length of the substrate in the z direction as in eq. (6). Equations (6), (7), (8) show that the net bulk flow into a computational cell (kg/s/m³) is the same for both channel-pair and through-the-wall modelling. This is also applied in the next section.

NO, NO₂, NH₃ and O₂ Concentrations in the Flow Leaving the SCR Wall Layer

For the concentrations in the flow that has passed through the wall, the convective term in the z direction is not included. Equation (9) also has diffusion suppressed so that it cannot occur in the z direction in the porous medium. Three separate terms make up the source term in eq. (9).

$$V_w \frac{\partial(\rho_{air} C_w)}{\partial t} \quad kg \ s^{-1} m^{-3} \ reactor = \left\{ M' \frac{(C_{ps} - C_w)}{V_{sub}} + \dots \right. \\ \left. + K_{mi} \rho_{air} (A_v/2)(C_{out} - C_w) + K_{pore} S_A \rho_{air} (C_{pore} - C_w) \right\} \quad (9)$$