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Modelling of secondary particulate emissions during the regeneration of Diesel Particulate Filters

Chung Ting Lao[a], Jethro Akroyd[a], Nick Eaves[a], Markus Kraft[a,b] *

[a]*Department of Chemical Engineering and Biotechnology, University of Cambridge, UK*
[b]*School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore*

Abstract

Significant nanoparticle emission during the regeneration of Diesel Particulate Filters (DPFs) has been observed in experiments. A numerical reactive-flow model is coupled with a sectional particle method and phenomenological filtration model to describe the behavior of the DPF, and in particular the evolution of soot particle size distribution. The ability of the model to predict the pressure drop and flow profile in the DPF is critically assessed against experimental and simulated results from the literature. The capability to describe the impact of oxidative fragmentation on the size distribution of trapped particles is demonstrated. The model is shown to be able to qualitatively describe the decrease in average soot particle size during regeneration which will allow better prediction of particle number emissions.

Keywords: Exhaust after-treatment, Diesel Particulate Filter (DPF), Regeneration, Particle Number (PN)

1. Introduction

Diesel Particulate Filters (DPFs) are essential to meet particulate emission standards for diesel engines worldwide. A Particle Number (PN) limit was introduced by the European Union (EU) in 2011 which was later adopted by China, India and South Korea. Secondary particulate emission has been observed in experiments during the "regeneration" – combustion of trapped soot in order to avoid excessive pressure drop – of loaded DPFs [1]. This phenomenon may lead to potential violation of the PN limit. It is speculated that oxidative fragmentation is responsible for secondary

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* Corresponding author. Tel.: +44-1223-748-999
E-mail address: mk306@cam.ac.uk

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particulate emission because the average diameter of the particles observed during secondary emissions is approximately 30 nm, significantly lower than that of the inlet particle population (100 nm). A general reactive-flow model coupled with a sectional model to describe the evolution of the trapped soot particles is developed to predict secondary emissions from DPFs. The proposed model is validated against existing data and the capability of the model to predict the evolution of particle size distribution in the DPF is demonstrated.

Nomenclature

A	Heat transfer area (m^2)
C	Heat capacity (J/K)
E	Filtration efficiency
F	Friction factor
H	Enthalpy of formation per unit mass (J/kg)
h	Heat transfer coefficient (W/m^{2}K)
k	Permeability (m^2)
L	Length (m)
M	Molar mass (kg/mol)
m	Gas mass (kg)
$\dot{m}$	Gas mass flow rate (kg/s)
N	Particle number density (1/m^3)
n	Number of mole of gas molecules (mol)
P	Pressure (Pa)
R	Universal gas constant (J/molK)
r	reaction rate (mol/m^{3}s)
S	Particle process source term (1/m^{3}s)
T	Temperature (K)
U	Specific internal energy (J/kg)
V	Gas volume (m^3)
v	Gas velocity (m/s)
Y	Gas mass fraction (kg/kg)
ρ	Gas density (kg/m^3)
μ	Dynamic viscosity (Pa.s)
υ	Stoichiometry coefficient

Subscript

g	gas
i,j	Reactor index
l	Reaction index
s	solid
η	Section index
χ	Species index

2. Method

2.1. Reactor Network

The proposed model may be classified as "single-channel model". It assumes that the inlet conditions are identical for all channels in the monolithic DPF. A pair of representative DPF channels is modelled as a network of ideal constant-volume continuous stirred tank reactors (CSTRs). Each CSTR represents a volume element of the DPF channels as shown in Figure 1.

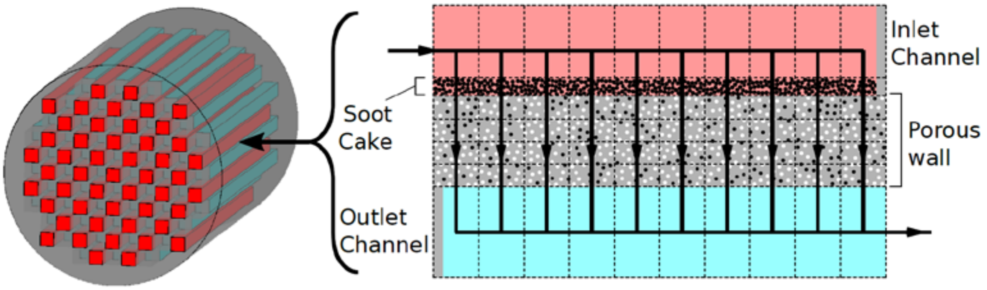

Fig. 1. Single channel model representation of a monolithic diesel particulate filter (DPF).

The gas phase is described by the ideal gas law:

$$P_i V_i = n_i R T_{g,i} \tag{1}$$

Please refer to the nomenclature section for the meanings of parameters in the equations. The flow in the DPF is modelled in terms of “connections” between the reactors. The flow-rate of each connection depends on the pressures of reactors at either end of the connection. The gas flow into and out of each reactor in the inlet and outlet channels is calculated using the Bernoulli equation:

$$P_{in} + \frac{1}{2}\rho_{in} v_{in}^2 + F v_{in}^2 = P_{out} + \frac{1}{2}\rho_{out} v_{out}^2 \tag{2}$$

The gas flow across the reactors corresponding to the soot cake and the porous wall between the channels is calculated using Darcy’s Law:

$$P_{in} - P_{out} = \frac{\mu v L}{k} \tag{3}$$

The gas in each reactor is considered to be perfectly mixed. The number of mole of gas-phase species in each reactor depends on the inflow/outflow and reactions:

$$\frac{dn_{\chi,i}}{dt} = \sum_{\forall j} \frac{\dot{m}_{ji} Y_{\chi,j}}{M_\chi} - \sum_{\forall j} \frac{\dot{m}_{ij} Y_{\chi,i}}{M_\chi} + V_i \sum_{\forall l} \nu_{\chi,l} r_{l,i} \tag{4}$$

In addition to the gas phase, a solid phase may be present in each CSTR which represents the heat capacity of the ceramic substrate. The gas phase temperature and solid phase temperature are given as:

$$C_{g,i} \frac{dT_{g,i}}{dt} = h_i A_i (T_{s,i} - T_{g,i}) + \sum_{\forall j} \dot{m}_{ji} \sum_{\forall \chi} [Y_{\chi,j}(H_{\chi,j} - H_{\chi,i}) + \frac{RT_{g,i}}{M_\chi}(Y_{\chi,j} - Y_{\chi,i})] +$$

$$V_i \sum_{\forall \chi} U_{\chi,i} M_\chi \sum_{\forall l} \nu_{\chi,l} r_{l,i} \tag{5}$$

$$C_{s,i}\frac{dT_{s,i}}{dt}=h_iA_i(T_{g,i}-T_{s,i}) \tag{6}$$

The DPF is considered to be adiabatic in this paper. The heat transfer between the gas and wall is assumed to be rapid such that the gas phase temperature is approximately equal to the solid phase temperature.

2.2. Particle model

A sectional method is implemented to describe the population of soot particles. The soot particles are assumed to be purely carbonaceous. The mass ranges of particles are logarithmically divided into discrete sections. The number density of particles in each section in the channel reactors are calculated analogously to equation 4. In the soot cake and porous wall region, where particles are being filtered, the particle number densities are given as:

$$\frac{dN_{\eta,i}}{dt}=E_{\eta,i}\dot{N}_{\eta,ji}+S_{\eta,i} \tag{7}$$

where the flow is from reactor j to reactor i. The particle source term S in equation 7 includes the effect of regeneration and oxidative fragmentation. In this paper, regeneration is described by the following equation:

$$C_n+O_2\rightarrow C_{n-1}+CO_2 \tag{8}$$

The fragmentation kernel is implemented as described in Ref. [2]. It assumes that the rate of fragmentation is proportional to the rate of oxidation and the mass of the original particle is split evenly into two daughter particles. The filtration efficiency E in equation 7 accounts for the soot loading behavior in the DPF. It is calculated using the unit collector model [3], which considers filtration by both Brownian diffusion and interception.

To the best of the authors' knowledge, this work is the first attempt to consider oxidative fragmentation in a numerical DPF model. Previous works in the literature have not considered the change of soot particle size distribution during the regeneration process.

3. Results and discussion

3.1. Flow profile

The ability of the proposed model to describe the velocity profile in a clean DPF is validated against experimental obtained data from Ref. [4]. Figure 2 shows good agreement between the experimental data and the simulation. Significant non-uniformity in wall flow profile is commonly observed for clean DPFs.

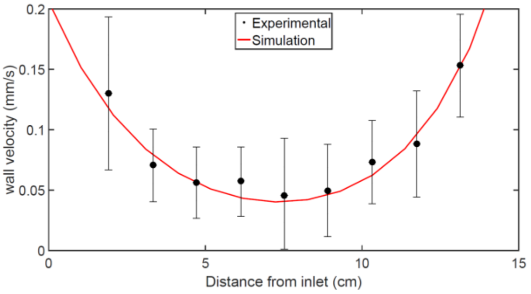

Fig. 2. Comparison of predicted and measured [4] through-wall velocity profile.

3.2. Filtration behaviour

During the loading stage, soot particles are trapped inside the DPF. Particles start to deposit in pores of the substrate, leading to a rapid increase in the overall pressure drop. As loading continues, the pores will eventually become blocked, preventing further loading of the wall. A layer of soot deposit is formed on the interface between the inlet channel and the wall. This is commonly referred as the “soot cake”. The overall pressure drop continues to increase with soot loading, but at a lower rate. The overall pressure drop during soot loading calculated by the proposed model is compared against simulation data [3] in Figure 3. It is shown that the model is in good agreement with the literature model and the typical two-stage behavior of soot filtration is captured.

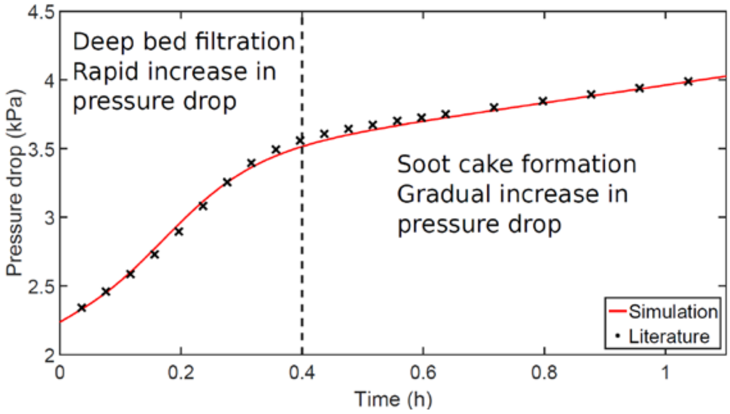

Fig. 3. Comparison of predicted overall pressure drop of DPF during soot loading by literature model [3] and proposed model.

3.3. Regeneration validation and demonstration

Excessive pressure drop across the DPF is detrimental to the engine performance. The DPF must be periodically regenerated to reduce the pressure drop by oxidizing the trapped soot particles. A regeneration event simulated using the proposed model is shown in Figure 4. In this case, the wall and the trapped soot are heated by increasing the temperature of the gas feed. Once the wall temperature reaches 700 K, the regeneration reaction (equation 8) starts to proceed rapidly, leading to rapid regeneration and a spike in the wall temperature. It is shown in Figure 4 that the proposed model is in good agreement with literature data [5] for both the wall temperature profile and the soot mass profile.

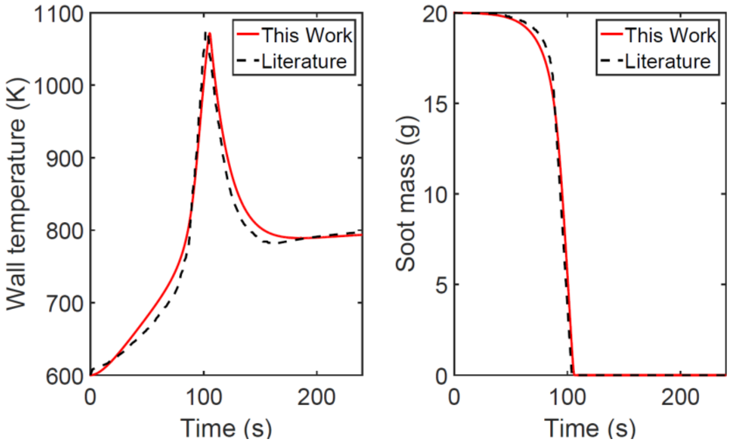

Fig. 4. Comparison of predicted wall temperature and soot mass during regeneration by literature model [5] and proposed model.

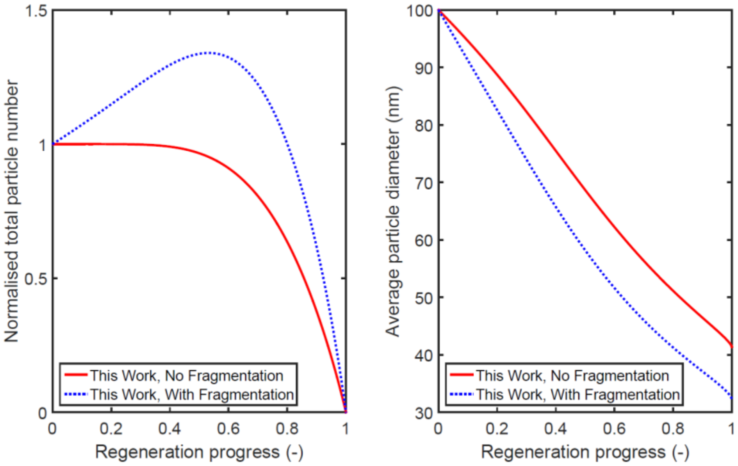

Fig. 5. Impact of fragmentation on total particle number and average particle diameter during regeneration.

In addition to predicting the temperature of the filter and the mass of trapped soot, the proposed model can capture the evolution of soot particle size distribution during regeneration. The calculated total particle number during regeneration is shown in Figure 5. Oxidation on the surface of the trapped particles leads to a decrease in particle size. In addition, any fragmentation of the particles during this oxidation leads to an increase in the total particle number and a further decrease in the average particle size. Both these types of behavior are able to be captured by the proposed model. In this particular case, fragmentation causes the maximum total particle number to increase to 33% above its initial value, with a corresponding decrease in the average particle size. The ability of the model to simulate the decrease in size of soot particles and the increase of particle number will allow better prediction of particle number emissions.

4. Conclusion

A reactive-flow model coupled with a sectional particle method and phenomenological filtration model is proposed to simulate the loading and regeneration of diesel particulate filters. Predictions of the flow profile, filtration and regeneration behavior are in good agreement with literature data. The proposed model is able to capture the evolution of the particle size distribution of the trapped soot. A particle breakthrough mechanism will be implemented in the model to describe the secondary particulate emission during DPF regeneration.

Acknowledgements

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