Growth Dynamics & Microstructure of Soot Deposits in Diesel Particulate Filters

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Motivation

Transient filtration model validation for cordierite, SiC, woven, non-woven & gradient porosity filters

Deposit microstructure vs. Peclet number

Application to On-Board trap soot load estimation

Conclusions

Future outlook
Motivation

- Soot deposit is major contributor to filter $\Delta P$. Need to study its microstructure vs. growth mechanism

- Need reliable soot deposit (and filter) microstructural properties as input for DPF Simulators

- Develop on-board soot sensing methods in conjunction with filter management and control
Dynamics of Particle Deposition in Filters

Collected Mass (gr)

Pressure Drop (kPa)

Flow

Soot in porous medium

Cake filtration

Soot cake

Deep bed filtration
Clean Filter Flow Resistance Descriptors

Standardized Measurement Methodology (Konstandopoulos et al. 2002)

\[ \Delta P = \frac{\mu Q}{2V_{trap}} (\alpha + w_s)^2 \left[ \frac{w_s}{k \alpha} + \frac{8FL^2}{3\alpha^4} \right] + \frac{\rho Q^2 (\alpha + w_s)^4}{V_{trap}^2 \alpha^2} \left[ \frac{\beta w_s}{4} + 2\zeta \left( \frac{L}{\alpha} \right)^2 \right] \]

\[ k = ? \quad \zeta = ? \]

\[ \Delta P \]

adequate pipe length to ensure flow uniformity

\[ \sim 10_u \quad \sim 100_u \]

95% Confidence Interval

[Graph showing pressure drop vs flow rate with 95% confidence interval]
Application to characterize catalyzed DPFs
Filtration mechanisms in extruded DPFs

**Brownian diffusion**

- Peclet number: \( Pe = \frac{U_i \cdot d_c}{D_p} \)
- Particle diffusion coefficient: \( D_p = \frac{k_B \cdot T}{3\pi \cdot \mu \cdot d_p} \cdot SCF \)
- "Pore" velocity: \( U_i = \frac{u_w}{\varepsilon} \)
- Single collector collection efficiency by diffusion: \( \eta_D = 3.5 \cdot g(\varepsilon) \cdot Pe^{-2/3} \)

**Interception**

- Interception parameter: \( N_R = \frac{d_p}{d_c} \)
- Exponent: \( s = \frac{3 - 2\varepsilon}{3\varepsilon} \)
- Single collector collection efficiency by interception: \( \eta_R = 1.5 \cdot N_R^2 \cdot \frac{[g(\varepsilon)]^3}{(1 + N_R)^s} \)

**Inertial impaction**

**Single grain combined collection efficiency** \( \eta = \eta_D + \eta_R - \eta_D \cdot \eta_R \)

Lee and Gieseke (1978)
Konstandopoulos and Johnson (1989)
Filtration mechanisms in fibrous DPFs

Single collector collection efficiency by diffusion

\[ \eta_D = 2.7 \cdot Pe^{-\frac{2}{3}} \left( 1 + 0.39 \cdot h(\varepsilon, Kn)^{-\frac{1}{3}} \cdot Pe^{\frac{1}{3}} \cdot Kn \right) + 0.624 \cdot Pe^{-1} \]

Single collector collection efficiency by interception

\[ \eta_R = \frac{1}{2h(\varepsilon, Kn)} \left[ \frac{1}{(1 + N_R)} - (1 + N_R) + 2(1 + N_R)\ln(1 + N_R) + 2.86 \cdot Kn \frac{(2 + N_R)N_R}{(1 + N_R)} \right] \]

Single collector collection efficiency by inertial impaction

\[ \eta_I = 0.16 \left[ N_R + \left( \frac{1}{2} + \frac{4}{5} N_R \right) Stk - 0.105 \cdot N_R \cdot Stk^2 \right] \]

\[ Stk = \frac{\rho_p \cdot d_p^2 \cdot U_i }{(18 \mu \cdot d_f)^{\frac{1}{1.1}}} \cdot SCF \]

\[ SCF = 1 + Kn \cdot (1.257 + 0.4e^{\frac{-1}{Kn}}) \]

Interaction term Diffusion and Interception

\[ \eta_{DR} = \frac{1.24 \cdot N_R^{\frac{2}{3}}}{\sqrt{h(\varepsilon, Kn) \cdot Pe}} \]

Single fiber combined collection efficiency

\[ \eta = \eta_D + \eta_R + \eta_I + \eta_{DR} \]

Kirsch and Stechina (1978)
Interception diameter of fractal aggregates

- Mobility diameter correlates with radius of gyration $R_g$
- For modelling particle capture by interception, a larger particle size is needed
- Better to consider sphere that is inscribed by the fractal aggregate
- Interception $N_R$ parameter modified to account for this.
Transient filtration model: Unit cell/collector concept

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**Clean unit cell**

- **Clean collector diameter**
  \[ d_{c0} = \frac{3}{2} \cdot \frac{(1 - \varepsilon_0)}{\varepsilon_0} \cdot d_{pore} \]

- **Clean unit cell diameter**
  \[ \frac{d_{c0}^3}{b^3} = (1 - \varepsilon_0) \]

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**Partially loaded unit cell**

- **Loaded collector diameter**
  \[ d_{c}(t) = 2 \cdot \left[ \frac{3}{4\pi} \cdot \frac{m_c(t)}{\rho_{soot,w}} + \left( \frac{d_{c0}}{2} \right)^3 \right]^{1/3} \]

- **Loaded porosity**
  \[ \varepsilon(t) = 1 - \left( \frac{d_{c}(t)}{d_{c0}} \right)^3 \cdot (1 - \varepsilon_0) \]

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**Completely loaded unit cell**

- **Permeability of loaded medium**
  \[ \frac{k(t)}{k_0} = \left( \frac{d_c(t)}{d_{c0}} \right)^2 \cdot \frac{f(\varepsilon(t))}{f(\varepsilon_0)} \]

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Deep Bed filtration to cake filtration transition

Distribution of particulate mass deposited in the filter

\[ m_{in} = \Phi m_{in} + (1-\Phi)m_{in} \]

\[
\Phi(t) = \begin{cases} 
\frac{(d_c(1,t))^2 - d_{c0}^2}{(\psi \cdot b)^2 - d_{c0}^2} & \text{Spherical} \\
\frac{(d_c(1,t)) - d_{c0}}{(\psi \cdot b) - d_{c0}} & \text{Cylindrical}
\end{cases}
\]

Partition coefficient


\( d_{c0} \) diameter of clean unit collector
\( d_c \): diameter of loaded unit collector
\( b \): diameter of unit cell
\( \varepsilon_0 \): clean filter wall porosity
\( \varepsilon \): loaded filter wall porosity
\( m_c \): particulate mass deposited on unit collector
\( \psi \): dimensionless percolation constant
\( \Phi \): particulate mass partition coefficient
\( \rho_{soot,w} \): particulate density inside filter wall
Transient filtration numerical algorithm

Particulate mass transport equations

\[ \frac{\partial m_p}{\partial x} + \frac{\partial m_c}{\partial t} = 0 \quad \frac{\partial m_p}{\partial x} = -e_f(m_c)\dot{m}_p \]

Local collection efficiency

\[ E(i, t) = \int_{x_i}^{x_{i+1}} e_f(m_c(x, t))dx = \begin{cases} 1 - \exp \left[ -\frac{3\eta(i, t) \cdot (1 - \varepsilon(i, t)) \cdot (x_{i+1} - x_i)}{2\varepsilon(i, t)d_c(i, t)} \right] \\ 1 - \exp \left[ -\frac{4\eta(i, t) \cdot (1 - \varepsilon(i, t)) \cdot (x_{i+1} - x_i)}{\pi\varepsilon(i, t)d_c(i, t)} \right] \end{cases} \]

Filter wall discretization

- **Spherical**
- **Cylindrical**
Transient filtration numerical algorithm-2

START
Read input file

Calculate $u_w$, $\mu$, $\rho$ of the gas

Calculate $d_{of}$, $b$, $w/x$

TEMPORAL LOOP
Calculate $k$, $w_{sot}$, $\Delta P$

SPATIAL LOOP
Calculate $f(\epsilon)$, $g(\epsilon)$ functions

PARTICLE SIZE LOOP

INNER SPATIAL LOOP
Calculate $Pe$, $\eta_d$, $\eta_{re}$, $\eta_{dr}$

Spatial loop: repeat inner loops, recalculating collector properties as particulate matter accumulates in the layers.

Particle size loop: calculate collected mass from each layer for given time-step.

Inner spatial loop: calculation of flow parameters, unit collector properties and $E$ for each layer.

Print results
STOP
Transient Loading Model Validation

Cordierite Filters (Exper. Murtagh et al. 1994)

EX-47

EX-54

EX-66

EX-80

Konstandopoulos et al 1999
Cordierite wall-flow DPF – collection efficiency

- Experimental upstream
- Experimental downstream
- Theoretical downstream

**Graph Details:**
- **Y-axis:** Number concentration (#/cm³)
- **X-axis:** Particle size (nm)
- **Legend:**
  - Experimental upstream
  - Experimental downstream
  - Theoretical downstream
Cordierite wall-flow DPF – transient pressure drop

Onset of cake formation

2400 rpm, 50% Load

TIME (sec)
PRESSURE DROP (Pa)

experimental
simulation
Silicon carbide DPF – collection efficiency

![Graph showing the collection efficiency of silicon carbide DPF with comparison between experimental and simulation data.](image-url)
Silicon carbide DPF – transient pressure drop

Onset of cake formation

2400 rpm, 50% Load

Experimental
Simulation
Fibrous filters – woven fiber filter collection efficiency

![Graph showing particle size distribution](image)

- **Experimental Upstream**
- **Experimental Downstream**
- **Simulation Downstream**
Fibrous filters – woven fiber filter pressure drop

**Onset of cake formation**
Fibrous filters – non-woven fiber filter

Collection Efficiency

- Experimental upstream
- Experimental downstream
- Simulation downstream

Pressure Drop

- Experiment
- Simulation
Fibrous filters – gradient porosity filter

Collection Efficiency

Pressure Drop

- Experimental upstream
- Experimental downstream
- Simulation downstream

PARTICLE SIZE (nm)

NUMBER CONCENTRATION (#/cm³)

PRESSURE DROP (Pa)

TIME (sec)
Soot Cake Formation Mechanism

DIFFUSION (Diffusion Limited deposition)

\[
\text{Pe} = \frac{u_w \cdot d_{\text{primary}}}{D_p}
\]

\[
D_p = \frac{k_B \cdot T}{3\pi \cdot \mu \cdot d_{\text{aggregate}}} \cdot SCF
\]

CONVECTION (Ballistic deposition)

Low Pe

High Pe
Discrete Particle Dynamics Simulation


The graph shows a plot of normalized porosity versus Peclet number, with data points indicating different dimensionless mean free paths labeled as 1, 3, and 4. The high Peclet asymptote is indicated on the graph.
Pressure Drop of Cake Wall Flow Filters

- \( m_{\text{soot}} \): particulate mass collected in DPF
- \( N_{\text{cells}} \): number of inlet cells of wall-flow filter
- \( \alpha \): cell density
- \( Q \): exhaust volumetric flow rate
- \( V_{\text{trap}} \): filter volume
- \( L \): filter length
- \( a \): channel width
- \( w \): particulate layer thickness
- \( w_s \): filter wall thickness
- \( k_0 \): filter wall permeability
- \( k_{\text{soot}} \): particulate layer permeability
- \( \rho_{\text{soot, c}} \): particulate packing density in cake deposit
- \( \mu \): exhaust dynamic viscosity
- \( F \): factor equal to 28.454
- \( l_p \): plug length
- \( \beta \): Forchheimer losses coefficient
- \( \zeta \): contraction/expansion losses coefficient
- \( \rho \): air density
Pressure Drop of Cake Wall Flow Filters-2

Konstandopoulos et al. 1989-2001

\[ \Delta P_{\text{loaded}} = \frac{\mu Q}{2V_{\text{trap}}} (a + w_s)^2 \left[ \frac{w_s}{k_o a} + \frac{1}{2k_{\text{soot}}} \ln \left( \frac{a}{a - 2w} \right) + \frac{4F_L^2}{3} \left( \frac{1}{(a - 2w)^4} + \frac{1}{a^4} \right) + \frac{4L_p^2}{a^4} \right] + \frac{Q^2}{4V_{\text{trap}}} (a + w_s)^4 \beta \rho \frac{w_s}{a^2} + \frac{1}{2} \zeta \rho u_{\text{inlet}}^2 \]

where

\[ w = \sqrt{\frac{\alpha^2 - \frac{m_{\text{soot}}}{N_{\text{cells}} L \rho_{\text{soot, c}}}}{2}} \]

\[ u_{\text{inlet}} = \frac{8Q}{\pi \sigma D^2 a^2} \]
Validation of Cake $\Delta P$ model

10 filters in 31 experimental runs with light and heavy duty engines

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Min-Max. value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Filter size (diam.xlength)</strong></td>
<td>4.66x6 – 12x15</td>
<td>in x in</td>
</tr>
<tr>
<td>Filter cell density</td>
<td>100 – 200</td>
<td>cpsi</td>
</tr>
<tr>
<td>Filter wall thickness</td>
<td>12- 17</td>
<td>mil</td>
</tr>
<tr>
<td>Filter geometry</td>
<td>Round, Oval</td>
<td>-</td>
</tr>
<tr>
<td>Engine flow rate</td>
<td>97.5 – 790</td>
<td>kg/hr</td>
</tr>
<tr>
<td>Engine flow temperature</td>
<td>240 – 370</td>
<td>°C</td>
</tr>
<tr>
<td>Particulate emission rate</td>
<td>1.45 – 20.8</td>
<td>gr/hr</td>
</tr>
<tr>
<td><strong>Loading duration</strong></td>
<td>1.3 – 118</td>
<td>hr</td>
</tr>
</tbody>
</table>

Masoudi et al (2001)
Soot Cake Microstructural Descriptors

In-situ measurement of soot cake permeability and packing density (or equivalently primary particle size and porosity)

\[ \rho_{soot} = \rho_{solid} \times (1 - \varepsilon) \]

\[ f(\varepsilon) = \frac{2}{9} \left[ \frac{2 - \frac{9}{5} \cdot (1 - \varepsilon)^{1/3} - \varepsilon - \frac{1}{5} \cdot (1 - \varepsilon)^2}{(1 - \varepsilon)} \right] \]

\[ SCF = 1 + Kn \left( 1.257 + 0.4e^{-1.1/Kn} \right) \]

\[ Kn = \frac{2\lambda}{d_{primary}} \]

Simulation vs. Experiment

7.5”X8” 100 cpsl/17 mil
Soot Primary Particle Size

COMPUTED FROM PERMEABILITY

Soot mass, primary particle size ($d_0$) (hence surface area) and soot cake porosity have been linked with a first principles predictive model to system pressure drop.

mean: 32 nm
Particle concentration measured with RES (mg/cm$^3$)

$y = 2339.1x$

Slope = primary particle density (kg/m$^3$)
Soot Cake Porosity Variation with Pe number

Soot Packing Density and Porosity were for the first time measured in-situ and are found as power laws of Peclet number in agreement with discrete particle dynamics calculations [Tassopoulos, 1991, Konstandopoulos, 1991].

\[ \varepsilon = A \cdot Pe^{-B} + C \]

\( Pe = \frac{U_w d_c}{D_p} \)
Soot Cake Porosity Variation with Pe number

31 FILTER RUNS

Diffusion limited deposition of spheres

Ballistic deposition of spheres

Porosity

Konstandopoulos et al
SAE 2002-01-1015

light duty

heavy duty

Pe
Soot Cake Density Variation with Pe number

Computes From Porosity

From photos of Nagata et al (2002)
Otto et al (1980) @ low Pe
Soot cake shaken from trap
Soot cake from electr. precipitator
Kladopoulou (2002)
Catalyzed trap
Konstandopoulos et al SAE 2002-01-1015
Soot Cake Thickness Variation with Pe number

At similar soot loads (24 gr in trap)

Low Peclet Deposit
“Thicker” = less dense

High Peclet Deposit
“Thiner” = denser

Nagata et al. SAE 2002-01-1013
Unrealistic permeabilities (by a factor of 10 or more) are employed in many modelling studies!

Konstandopoulos et al. SAE 2002-01-1015

**Soot cake permeability variation with Pe**

**THEORY vs. EXPERIMENT**

- light duty
- heavy duty

Temperature settings:
- $T = 200 ^\circ C$
- $T = 250 ^\circ C$
- $T = 300 ^\circ C$
- $T = 350 ^\circ C$
- $T = 400 ^\circ C$
On-Board Soot Sensing

FUTURE EMISSION CONTROL SYSTEMS: Assemblies of reactors, hardware and virtual sensors

ENGINE

ECU

CAN bus

T, P, ∆P Soot, NOx sensor inputs

SENSOR A/D INTERFACE

DOC

DPF

DeNOx

HC, CO removal

Soot removal

NOx removal

tailpipe
Estimation of Trap Soot Load (st. state)

Experimental data Johnson et al (1987)
SiC filter 9”x12” 60cps/31mil

Heavy duty engine
350 kg/hr
310 C
Experimental data CPERI, light duty 1.9 L engine
SiC filter 5.66”x7” 70cpsi/31mil
Model estimation of trap soot load (transient)

ACCUMULATED MASS ESTIMATION = 17.4 gr
MEASURED MASS = 15.2 gr
NEXT STEP: Microscale Flow Modelling

Kikkinides, Vlachos & Konstandopoulos (2002, in preparation)

Flow simulation

SEM picture

Reconstruction computational engine matching:
- porosity, pore size
- autocorrelation function

Binary representation of porous wall

- Microstructure simulation
- Explore variations around a particular design
- Connected vs. non-connected porosity etc.
- Design desired material picture before making it

Permeability Prediction
Permeability Design from first principles
Monte Carlo Diffusion-Convection Filtration Simulator
Monte Carlo Diffusion-Convection Filtration Simulator

Flow

Soot cake

Soot inside the wall
Conclusions

- Understanding the structure of the soot cake is a prerequisite for the intelligent operation of Diesel filters and the practical estimation of their pressure drop for field applications.
- A key parameter that determines the resulting microstructure of the soot cake is the Peclet number for mass transfer.
- A non-destructive methodology has been developed for the measurement of soot packing density and permeability and their correlation to the prevailing Peclet number. The correlation is self-consistent permitting the estimation of soot cake permeability from a knowledge of the soot primary particle size and vice-versa.
- The developed methodology can be adapted for on-board estimation of the trap soot load in real time.
Thank You For Your Attention