Model-based analysis of TWC-coated filters performance aspects

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How different is (c)GPF from (c)DPF modeling?

- Pressure drop
- Filtration efficiency
- Catalytic functions
- Soot oxidation
- Ash effects
- Durability
- OBD
Experiments
Measurement setup and test protocol

Transient engine dyno at LAT/Aristotle University

2.0 l turbocharged engine EURO 6 (gasoline)
Modeling
Mass & momentum balance equations

Channel scale
\[ \frac{\partial}{\partial z} (d_i^2 \rho_i v_i) = (-1)^i \cdot 4d \rho_w v_w \]
\[ \frac{\partial p_i}{\partial z} + \frac{\partial}{\partial z} (\rho_i v_i^2) = -\alpha_1 \mu v_i / d_i^2 \]

Wall scale
\[ \frac{dP}{dw} = \frac{\mu \cdot v(w)}{k_p} \]

Contraction/expansion losses
\[ \Delta P_{\text{contraction}} = \left[ 1.1 - 0.4 \left( \frac{d - 2w_p}{2(d + w_w)} \right)^2 \right] \rho_1 v_1^2 |_{z=0} \]
\[ \Delta P_{\text{expansion}} = \left[ 1 - \frac{d^2}{2(d + w_w)^2} \right] \rho_2 v_2^2 |_{z=L} \]
Once the wall permeability is tuned, the model is predictive with respect to changes in wall thickness and cell density.
The calibrated model for soot loaded filter is predictive in a wide range of flow rates and temperatures.
Effect of accumulated soot on filtration efficiency

Semi-empirical equation for soot loaded wall filtration efficiency: $E_{\text{wall}} = f(m_{\text{wall}}) \cdot E_{\text{wall},0}$

- Wall filtration
- Transition
- Cake filtration

300 kg/h, 550°C, $\lambda=0.89$
8 mils/200 cpsi

Big challenge to correlate PM with PN for proper model feed

<table>
<thead>
<tr>
<th>MSS</th>
<th>APC</th>
<th>CPC</th>
<th>SMPS</th>
<th>EEPS</th>
</tr>
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<tbody>
<tr>
<td>Transient PM</td>
<td>Transient PN $&gt;23$nm</td>
<td>Transient PN $&gt;10$nm</td>
<td>Steady state size-resolved PN</td>
<td>Transient size-resolved PN</td>
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</table>
Soot loading with GPFs of different cell structures

165 kg/h, 360°C, λ=0.9

HP & Large MPS

- Model tuning becomes less trivial. Interaction with filtration model.
- Semi empirical modeling of soot-in-the-wall effect on permeability
- Cell structure effect on soot loaded filter deltaP is predictable

Uncoated GPFs

12mils/300cpsi
10mils/300cpsi
9mils/240cpsi
Application example
Filtration efficiency vs deltaP trade-off

Thin-wall GPF achieves lower pressure drop but lower filtration performance.
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Fundamentals are same. Main differences/ challenges identified:

- Operation in the depth-filtration regime is much more challenging in terms of predictive modeling.
- Measurement of very low emissions and correlation between mass and number.
- Soot properties generated in accelerated loading modes.
- Gasoline engine(er)s are more sensitive to deltaP. Higher simulation accuracy requirements.
- Catalyst coating can be used as filtration efficiency enhancer.
\[ \frac{\partial}{\partial z} (d_i^2 \rho_i v_i) = (-1)^i \cdot 4 d \rho_w v_w \]

\[ \frac{\partial p_i}{\partial z} + \frac{\partial}{\partial z} (\rho_i v_i^2) = -\alpha_1 \mu v_i / d_i^2 \]

\[ C_{p,g} \rho_1 v_1 \left|_{\frac{\partial T_1}{\partial z}} = h_1 \frac{4}{d_1} (T_s - T_1) \right. \]

\[ C_{p,g} \rho_2 v_2 \left|_{\frac{\partial T_2}{\partial z}} = (h_2 + C_{p,g} \rho_w v_w) \frac{4}{d} (T_s - T_2) \right. \]

\[ \frac{\partial (v_1 y_{1,j})}{\partial z} = - \frac{4}{d} \cdot f_w v_w y_{1,j} + \frac{4}{d} \cdot f_w k_{1,j} (y_{1s,j} - y_{1,j}) \]

\[ \frac{\partial (v_2 y_{2,j})}{\partial z} = \frac{4}{d} \cdot f_w v_w y_{2,j} + \frac{4}{d} \cdot f_w k_{2,j} (y_{2s,j} - y_{2,j}) \]

**Channel scale**

**Wall scale**

\[ \frac{dP}{dw} = \frac{\mu \cdot v(w)}{k_p} \]

\[ \frac{d\tilde{m}_p}{dt} = -\tilde{m}_p \sum_k R_k + S_p \rho_w v_w \mu_p \]

\[ v_w \frac{\partial y_j}{\partial w} - D_{w,j} \frac{\partial}{\partial w} \left( f_w \frac{\partial y_j}{\partial w} \right) = \frac{f_w}{c_m} \sum_k n_{j,k} R_k \]

**Filter scale**

\[ \rho_s C_{p,s} \frac{\partial T_s}{\partial t} = \lambda_{s,x} \frac{\partial^2 T_s}{\partial x^2} + \lambda_{s,y} \frac{\partial^2 T_s}{\partial y^2} + \lambda_{s,z} \frac{\partial^2 T_s}{\partial z^2} + S \]

\[ S = H_{\text{conv}} + H_{\text{wall}} + H_{\text{react}} + H_{\text{rad}} \]

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Impact of zoning on flow distribution

Flow preferably directed to the areas of low washcoat \(\rightarrow\) non-uniform profile pattern. Impact on filtration, deltaP and reactions.
More washcoat at the front results in an earlier light-off (~15°C difference).

Self-enhancing effect due to exotherm generation from CO oxidation at the front zone.
Effect of soot on species conversion
Mass transfer limitations in soot layer

The negative effect of soot on the TWC activity is related to the diffusion limitations of species across the soot layer.

Reaction-diffusion equation:

\[ v_w \frac{\partial y_j}{\partial w} - D_{w,j} \frac{\partial}{\partial w} \left( f_w \frac{\partial y_j}{\partial w} \right) = f_w \sum_k c_{j,k} R_k \]

Soot tortuosity:

\[ \frac{1}{D_{w,j}} = \frac{\tau}{\varepsilon_{pore}} \left( \frac{1}{D_{mol,j}} + \frac{1}{D_{knud,j}} \right) \]

T=400°C, Flow 200 kg/h, λ=1.006, CO=0.75%, NO=0.2%, 0.15% HC

Increasing soot loading with \( \tau=2 \)
Transient cycle simulation: species conversion with clean and soot loaded GPFs

CO concentration [clean]

CO concentration [6 g/l]
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A coated GPF may replace a rear TWC. The coating amount and zoning schemes can be optimized in terms of filtration and catalytic activity.
Effect of soot-borne ash on soot oxidation

240 kg/h, 530°C, λ=0.9

Possibility to perform long-term simulations where soot oxidation is time dependent according to the local ash content
Soot oxidation
O₂ competition (forward diffusion) effect

Configurations

- TWC ➔ GPF
- TWC ➔ cGPF

GPF & cGPF: V=1.5l, 300/12

Boundary conditions

- Soot loading: 1 g/l
- Lambda: 1.01
- Temperature: 600°C
- Flow-rate: 100 kg/h

Intralayer O₂ profiles at filter entrance (z=10mm)

O₂ concentration [%]
0 0.01 0.02 0.03 0.04 0.05

Soot

Wall

O₂ consumption by TWC reactions
O₂ consumption by soot oxidation

Forward O₂ diffusion in cGPF due to lower concentrations in the wall → O₂ availability within the soot cake is less compared to the bare GPF → soot oxidation rate will be affected
Soot oxidation: $O_2$ competition under realistic lean/rich cycling operation

Configurations

1. TWC - GPF
2. TWC - cGPF

GPF & cGPF: $V=1.5l$, 300/12

In the coated GPF, $O_2$ is competitively consumed between soot and TWC reactions. Strong concentration gradients in the axial and intra wall direction $\rightarrow$ Soot oxidation rate is lower compared to bare GPF.
Soot oxidation uncoated vs coated GPF in a transient cycle

Normal operation

Fuel-cut events

Part of US06 cycle

Coating positive effect:
Higher temperature as cGPF is closer to the engine.

Coating negative effect:
Competitive O2 consumption, TWC vs soot.

Coating positive effect:
Higher temperature due to TWC reactions exotherm.
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• The ash/soot ratio emitted from gasoline engines is higher compared to Diesel engines, apparently affecting oxidation reactivity.
• Apart from fuel cutoff events, $O_2$ availability is less and can become even lesser due to ‘forward diffusion’.
• Temperatures are higher on average in GPFs.
Soot mass limit (SML) investigation
Worst case scenario: fuel cut-off event

GPF exposed to either too low ($\lambda=1$) or too high (fuel cut-off mode) $O_2$ concentrations

Q1: What is the safe soot mass assuming that the filter temperature should not exceed 1100°C?
Q2: How does accumulated ash affect the soot mass limit?
Effect of layer ash on soot mass limit

The layer ash effectively increases the thermal mass of the filter, therefore reduces generated exotherms and increases the soot mass limit.
The plug ash effectively increases the local soot loading, therefore increases generated exotherms and decreases the soot mass limit.
1. Change the boundary condition here.

2. Apply the change to selected damaged regions

\[
\frac{\partial}{\partial z} \left( d_i^2 \rho_i v_i \right) = (-1)^i \cdot 4 \rho_w v_w \\
\frac{\partial p_i}{\partial z} + \frac{\partial}{\partial z} \left( \rho_i v_i^2 \right) = - \alpha_1 \mu v_i / d_i^2
\]
OBD applications
Simulation of damaged filters

cGPF: V=1.5l, 300/12
Inlet scenario: WLTC

Damaged filter

ANIMATION...

Time: 50sec

Damaged filter

ANIMATION...

Mass Flux (kg.s.m²)

Soot loading (g/l)
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• Worst-case events may be more severe in GPFs due to higher inlet temperatures
• Ash may have multiple effects. Better understanding needed for predictive modeling. Correlation with ‘real-world’ ash.
• GPF OBD is a challenge. Modelers are expected to support…
Acknowledgements

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Thank you very much!