Exothermia
modeling efficiency

Model-based analysis of TWC-coated filters performance aspects

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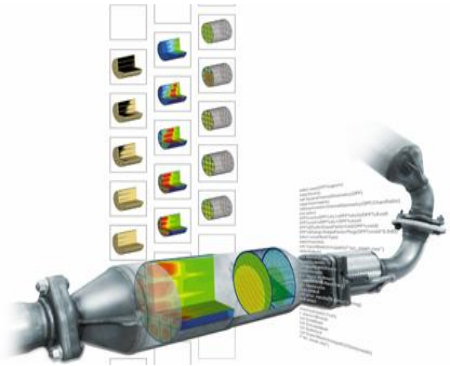


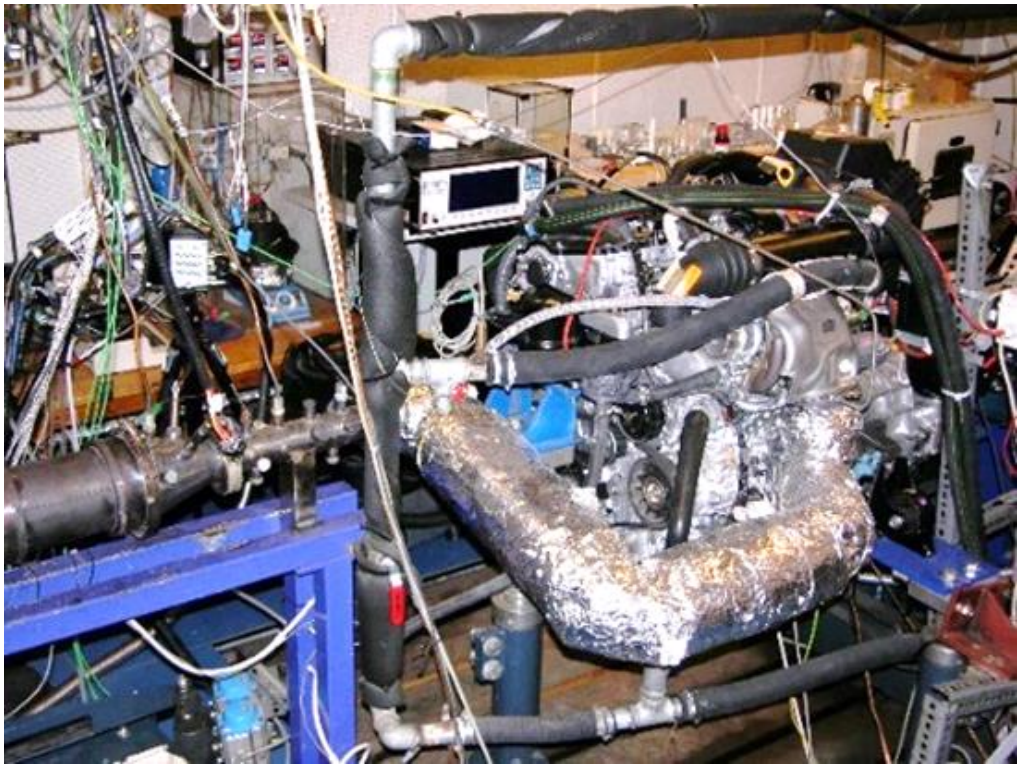
LAT

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

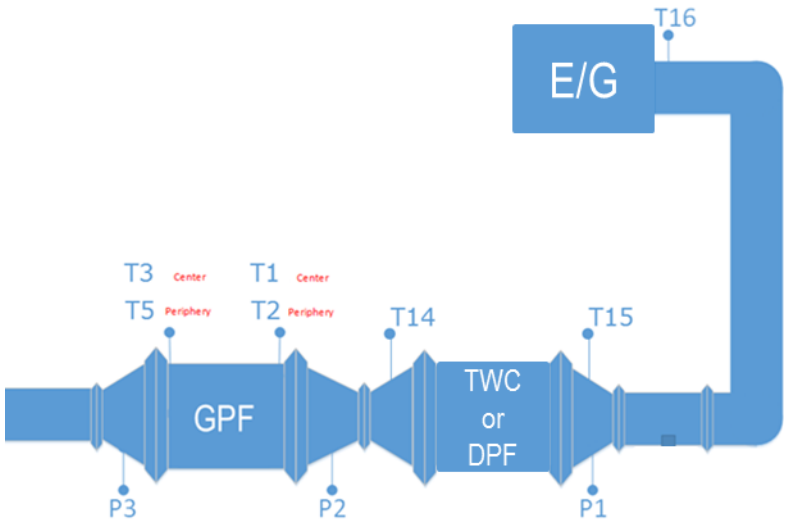
- Pressure drop
- Filtration efficiency
- Catalytic functions
- Soot oxidation
- Ash effects
- Durability
- OBD

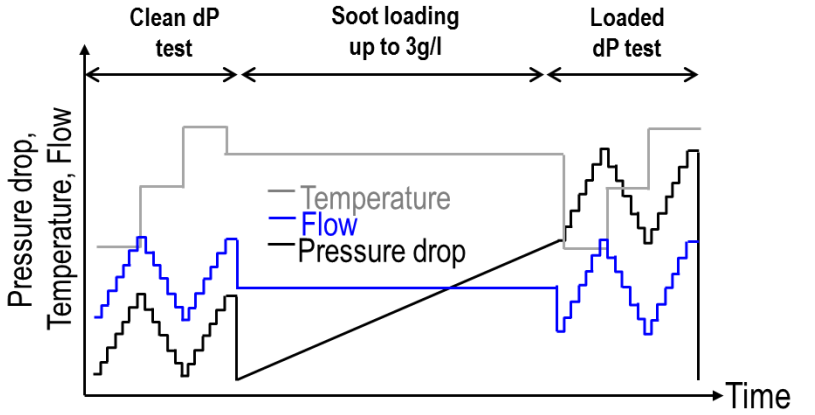
Experiments
Measurement setup and test protocol

Transient engine dyno at LAT/Aristotle University

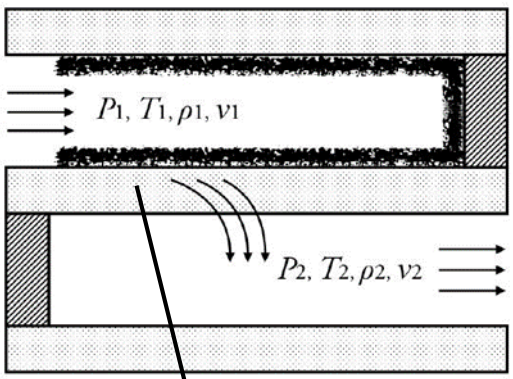


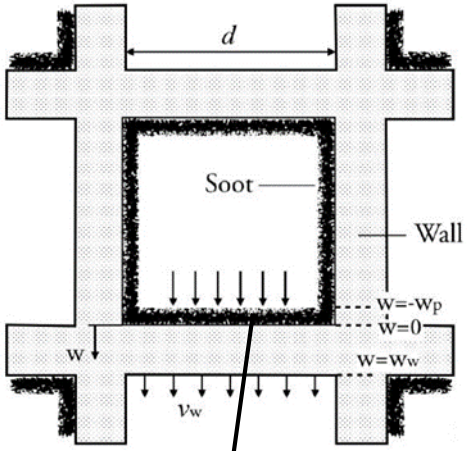
2.0 l turbocharged engine EURO 6 (gasoline)





Modeling
Mass & momentum balance equations





Channel scale

$$\frac{\partial}{\partial z}\left(d_i^2 \rho_i v_i\right) = (-1)^i \cdot 4 d \rho_w v_w$$

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

Wall scale

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

Contraction/expansion losses

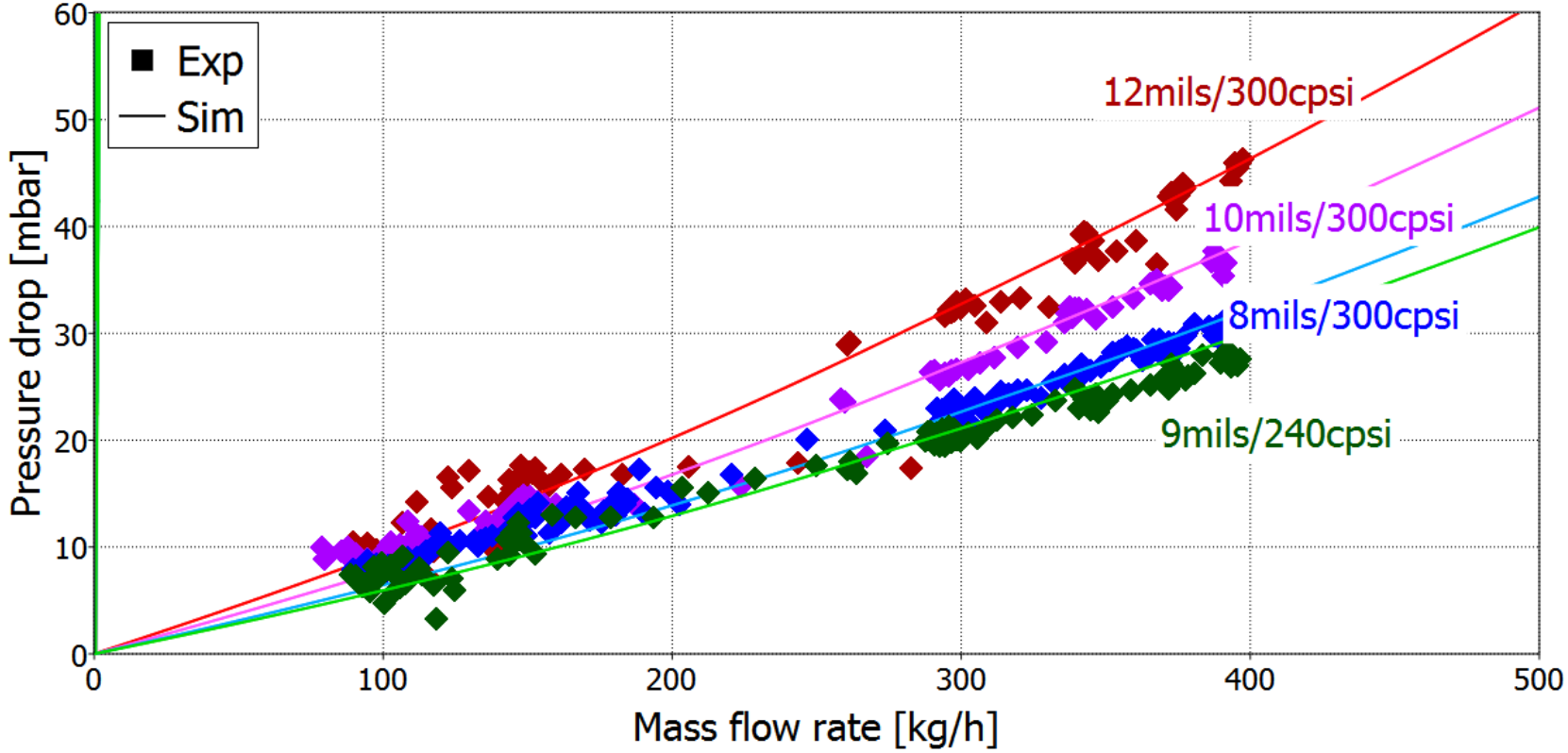
$$\Delta P_{contraction} = \left[1.1 - 0.4\frac{\left(d - 2w_p\right)^2}{2(d + w_w)^2}\right]\frac{\rho_1 v_1^2\big|_{z=0}}{2}$$

$$\Delta P_{expansion} = \left[1 - \frac{d^2}{2(d + w_w)^2}\right]^2 \frac{\rho_2 v_2^2\big|_{z=L}}{2}$$

Cell structure effect on pressure drop

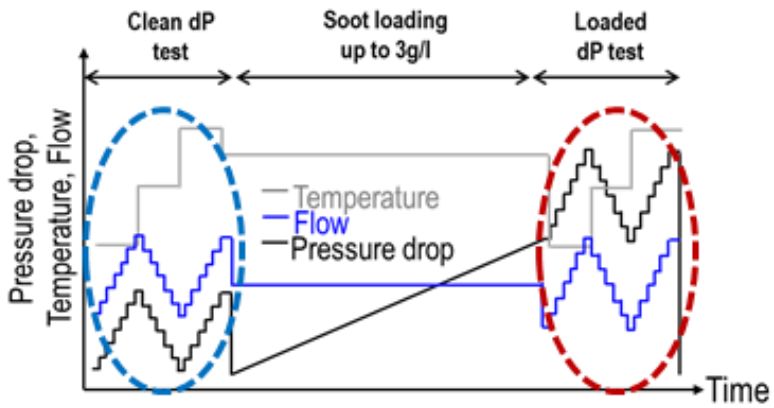
Uncoated GPFs

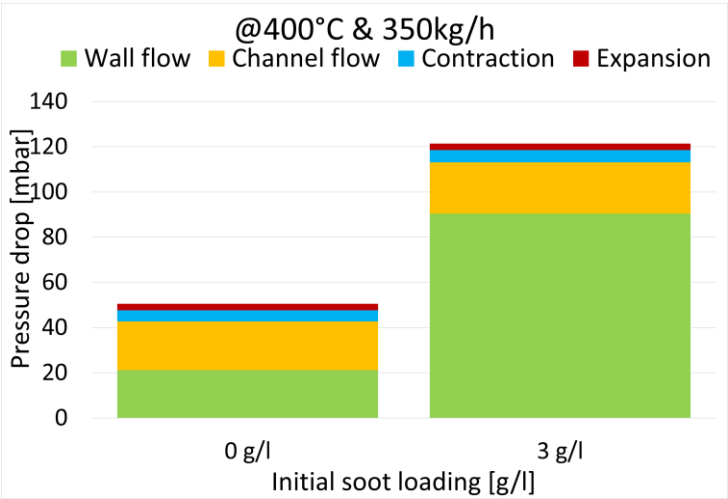
High porosity and large mean pore size. Results @ 300+/-10 degC



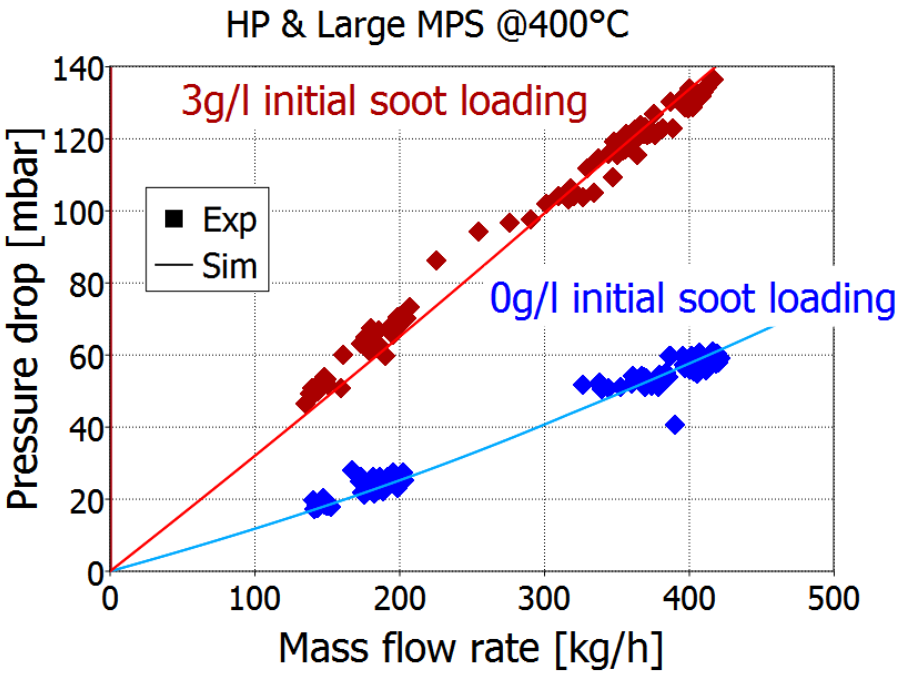
- Once the wall permeability is tuned, the model is predictive with respect to changes in wall thickness and cell density

Soot loading effect on deltaP



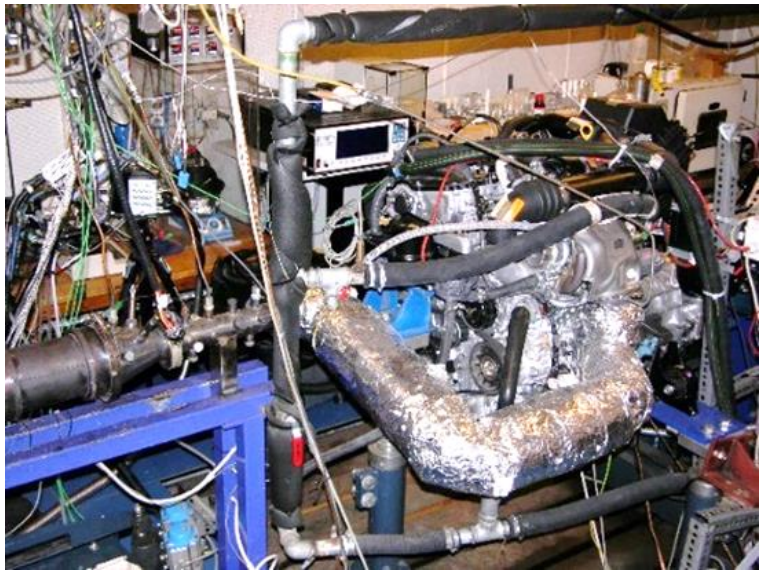


Uncoated GPF, 12mils/300cpsi, DxL 118x127mm

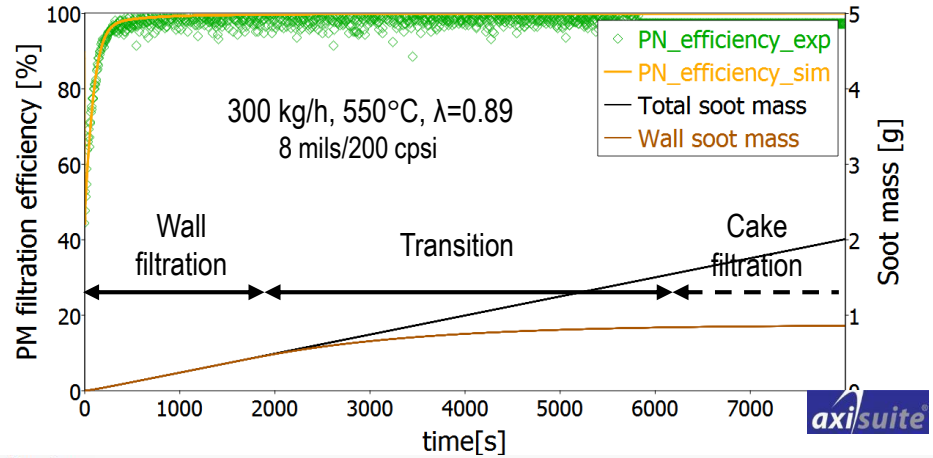


- The calibrated model for soot loaded filter is predictive in a wide range of flow rates and temperatures

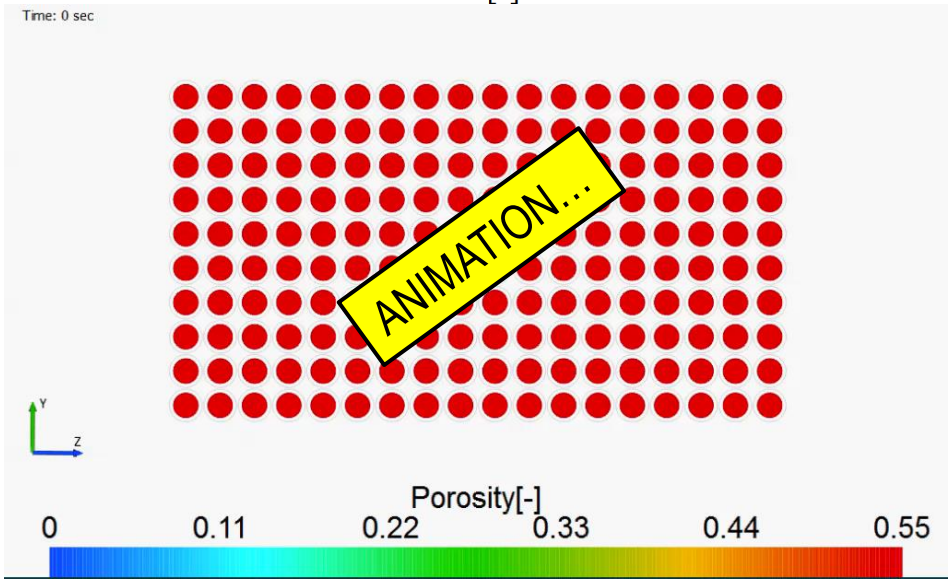
Effect of accumulated soot on filtration efficiency



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



MSS	APC	CPC	SMPS	EEPS
Transient PM	Transient PN >23nm	Transient PN >10nm	Steady state size-resolved PN	Transient size-resolved PN

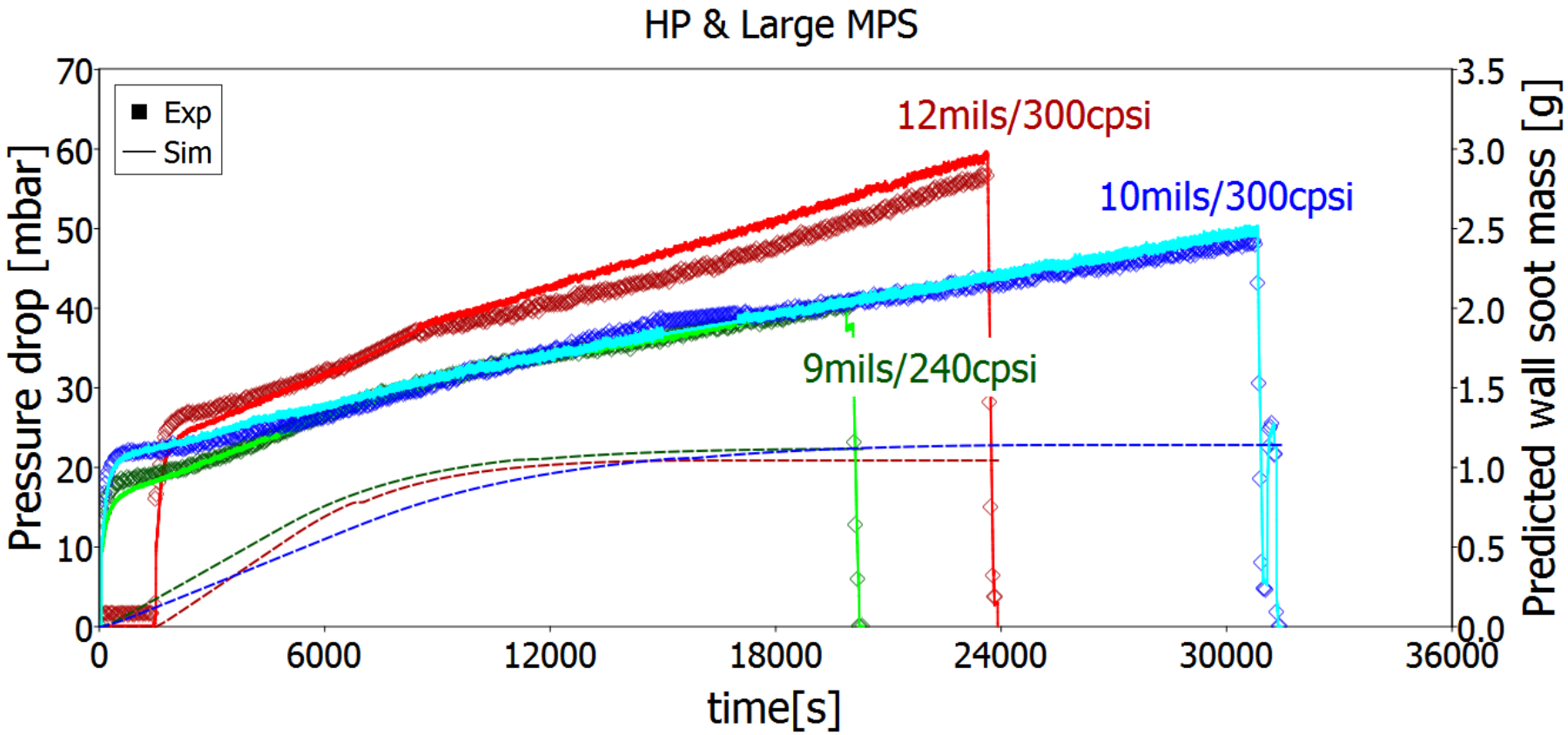


Big challenge to correlate PM with PN for proper model feed

Soot loading with GPFs of different cell structures

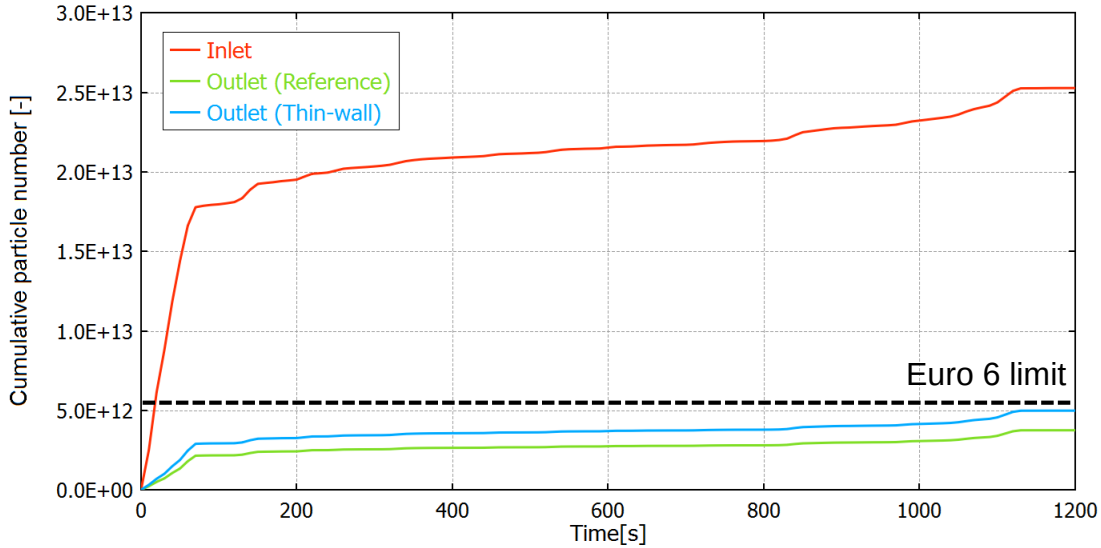
165 kg/h, 360°C, λ=0.9

Uncoated GPFs

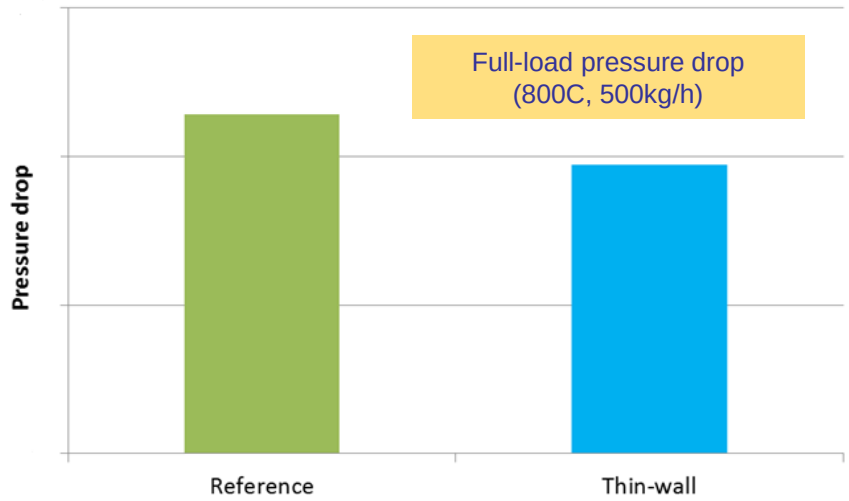


- Model tuning becomes less trivial. Interaction with filtration model.
- Semi empirical modeling of soot-in-the-wall effect on permeability
- Cell structure effect on soot loaded filter deltaP is predictable

Application example
Filtration efficiency vs deltaP trade-off



Reference	Thin-wall
Un-coated	
200 cpsi	
8 mils	5 mils
Ø 120mm, ℓ 130mm	
50% porosity	40% porosity



Thin-wall GPF achieves lower pressure drop but lower filtration performance.

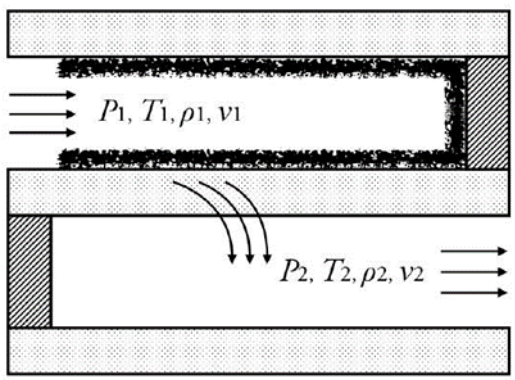
How different is (c)GPF from (c)DPF modeling?

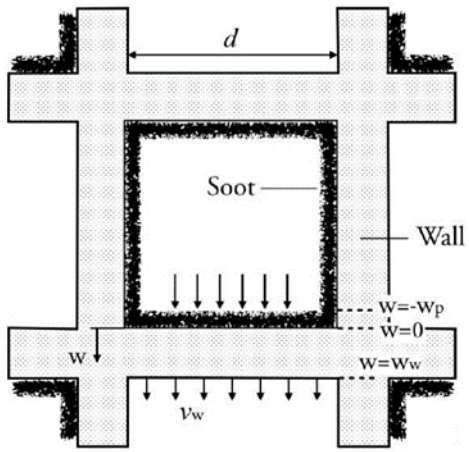
- Pressure drop
- Filtration efficiency
- Catalytic functions
- Soot oxidation
- Ash effects
- Durability
- OBD

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

TWC reactions
Transport, reaction equations





CO + 1/2 O2 --> CO2
H2 + 1/2 O2 --> H2O
CH4 + 2 O2 --> CO2 + 2 H2O
C3H6 + 9/2 O2 --> 3 CO2 + 3 H2O

C3H6 + 9 NO --> 3 CO2 +3 H2O + 9/2 N2
CO + 2 NO --> CO2 + N2O
H2 + 2 NO --> H2O + N2O
NO + 5/2 H2 --> NH3 + H2O

NO + 5/2 CO +3/2 H2O --> NH3 + 5/2 CO2
N2O + CO --> N2 + CO2
N2O + H2 --> N2 + H2O
NH3 + 3/2 NO --> 5/4 N2 + 3/2 H2O

fCe2O3 + 1/2 O2 --> 2 fCeO2
fCe2O3 + NO --> 2 fCeO2 + 1/2 N2
2 fCeO2 + CO <--> fCe2O3 + CO2
2 fCeO2 + H2 <--> fCe2O3 + H2O
2 fCeO2 + 1/6 C3H6 --> fCe2O3 + 1/2 CO + 1/2 H2O
Ce2O3 + 1/2 O2 --> 2 CeO2
Ce2O3 + NO --> 2 CeO2 + 1/2 N2
2 CeO2 + CO --> Ce2O3 + CO2
2 CeO2 + H2 --> Ce2O3 + H2O
2 CeO2 + 1/6 C3H6 --> Ce2O3 + 1/2 CO + 1/2 H2O

Channel scale

$$\frac{\partial}{\partial z}\left(d_i^2 \rho_i v_i\right) = (-1)^i \cdot 4 d \rho_\mathrm{w} v_\mathrm{w}$$

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

$$C_{\mathrm{p,g}} \rho_1 v_1 \Big|_z \frac{\partial T_1}{\partial z} = h_1 \frac{4}{d_1}\left(T_\mathrm{s} - T_1\right)$$

$$C_{\mathrm{p,g}} \rho_2 v_2 \Big|_z \frac{\partial T_2}{\partial z} = \left(h_2 + C_{\mathrm{p,g}} \rho_\mathrm{w} v_\mathrm{w}\right) \frac{4}{d}\left(T_\mathrm{s} - T_2\right)$$

$$\frac{\partial\left(v_1 y_{1,j}\right)}{\partial z} = -\frac{4}{d \cdot {f_\mathrm{w}}^2} v_\mathrm{w} y_{1,j} + \frac{4}{d \cdot f_\mathrm{w}} k_{1,j}\left(y_{1\mathrm{s},j} - y_{1,j}\right)$$

$$\frac{\partial\left(v_2 y_{2,j}\right)}{\partial z} = \frac{4}{d \cdot {f_\mathrm{w}}^2} v_\mathrm{w} y_{2\mathrm{s},j} + \frac{4}{d \cdot f_\mathrm{w}} k_{2,j}\left(y_{2\mathrm{s},j} - y_{2,j}\right)$$

Wall scale

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

$$\frac{d\hat{m}_p}{dt} = -\hat{m}_p \sum_\mathrm{k} R_\mathrm{k} + S_F \rho_w v_\mathrm{w} \mu_\mathrm{p}$$

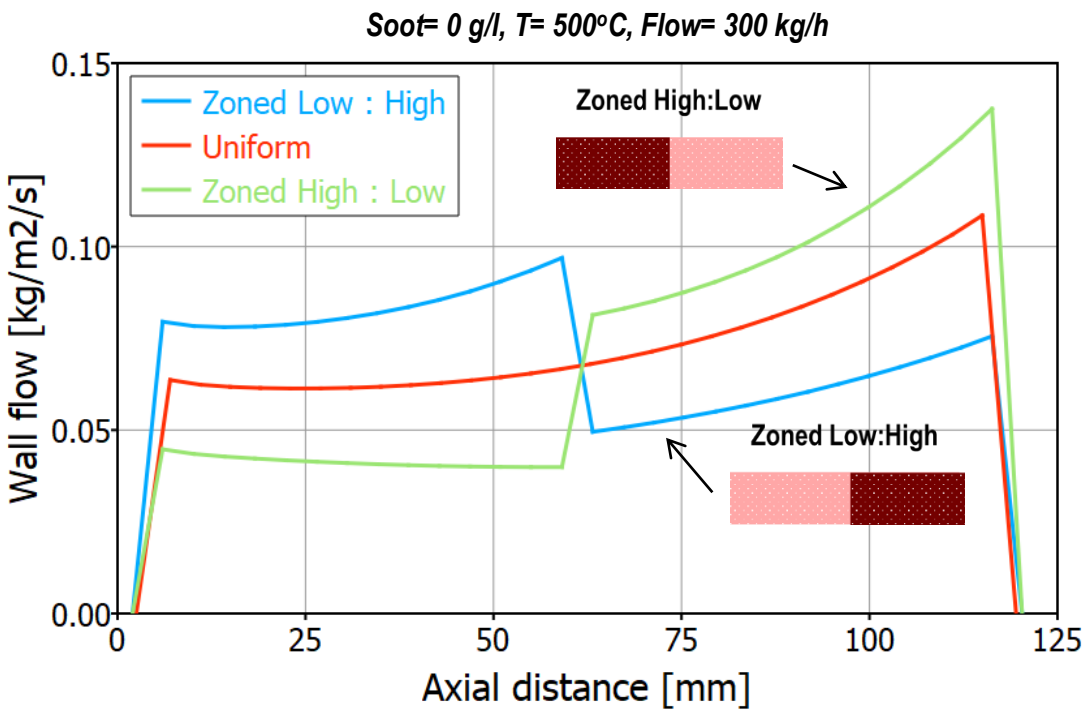
$$v_\mathrm{w} \frac{\partial y_j}{\partial w} - D_{\mathrm{w},j} \frac{\partial}{\partial w}\left(f_\mathrm{w} \frac{\partial y_j}{\partial w}\right) = \frac{f_\mathrm{w}}{c_\mathrm{m}} \sum_\mathrm{k} n_{j,\mathrm{k}} R_\mathrm{k}$$

Filter scale

$$\rho_\mathrm{s} C_{\mathrm{p,s}} \frac{\partial T_\mathrm{s}}{\partial t} = \lambda_{\mathrm{s},x} \frac{\partial^2 T_\mathrm{s}}{\partial x^2} + \lambda_{\mathrm{s},y} \frac{\partial^2 T_\mathrm{s}}{\partial y^2} + \lambda_{\mathrm{s},z} \frac{\partial^2 T_\mathrm{s}}{\partial z^2} + S$$

$$S = H_\mathrm{conv} + H_\mathrm{wall} + H_\mathrm{react} + +H_\mathrm{rad}$$

Impact of zoning on flow distribution

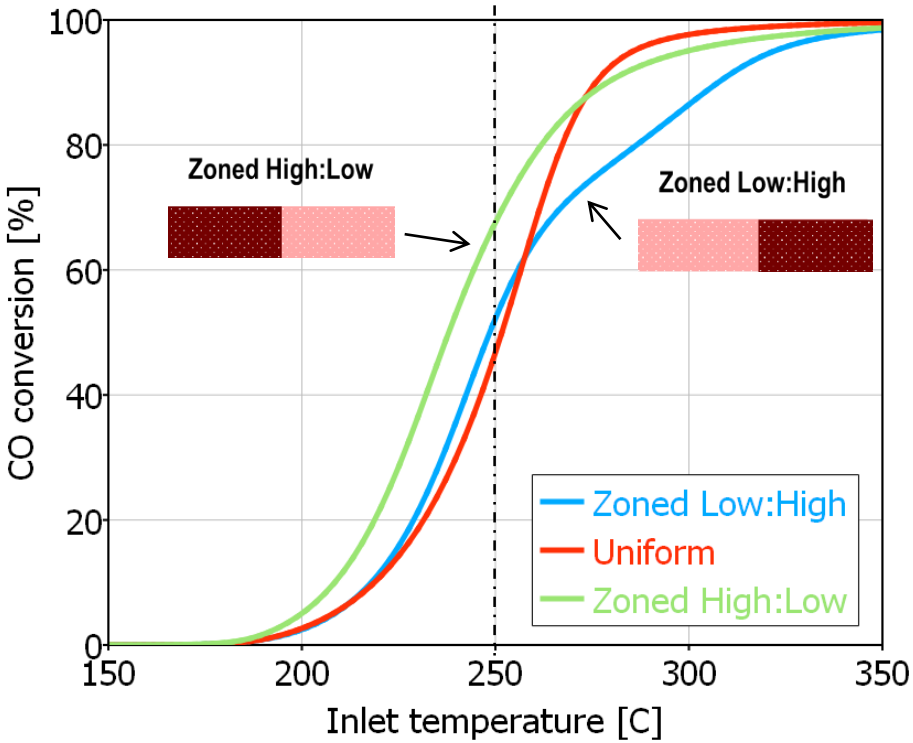


Flow preferably directed to the areas of low washcoat → non-uniform profile pattern.

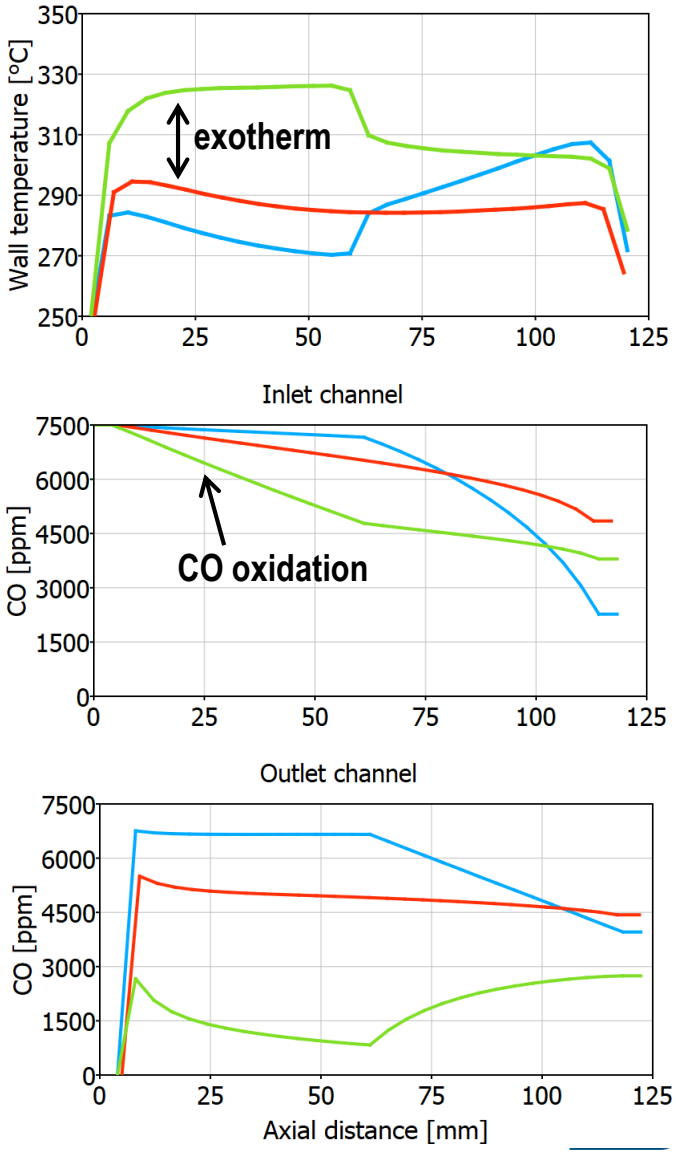
Impact on filtration, deltaP and reactions.

Impact of zoning on species conversion

Flow rate 300 kg/h, λ=1.006, CO=0.75%, NO=0.2%, 0.15% HC, T increase rate: 2°C/s

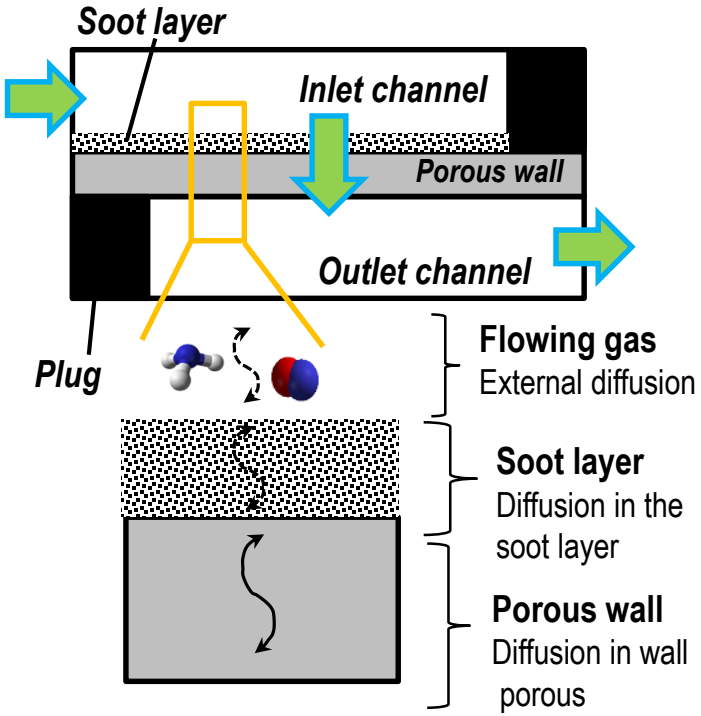


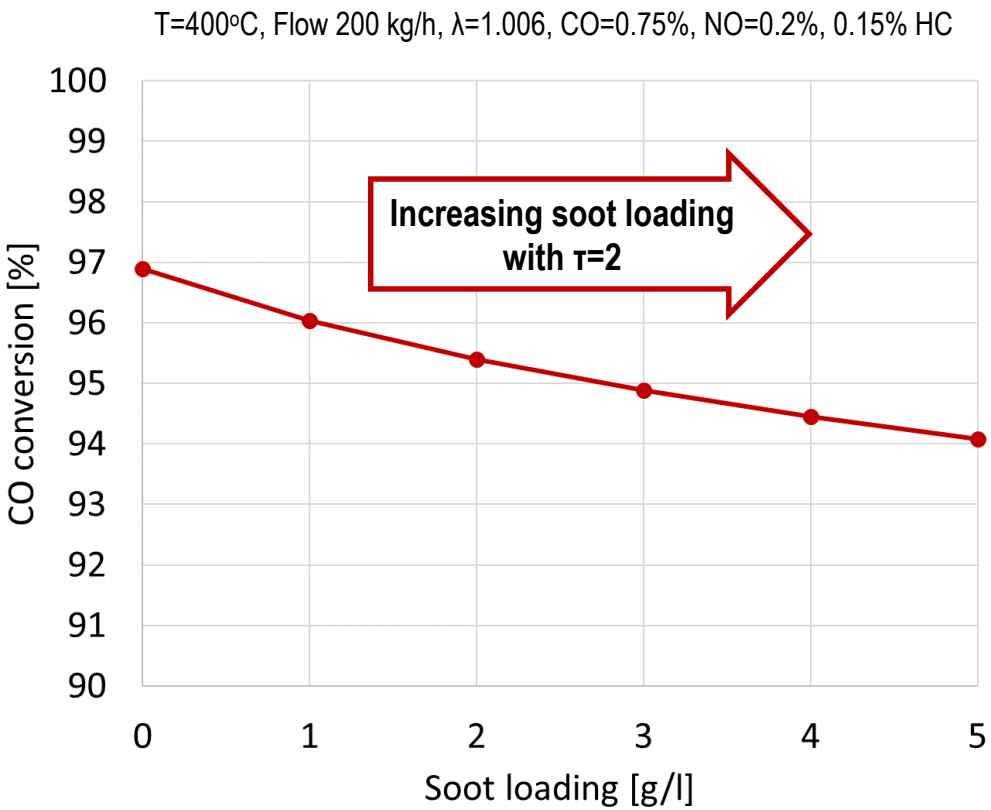
250°C



- 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





Reaction-diffusion equation

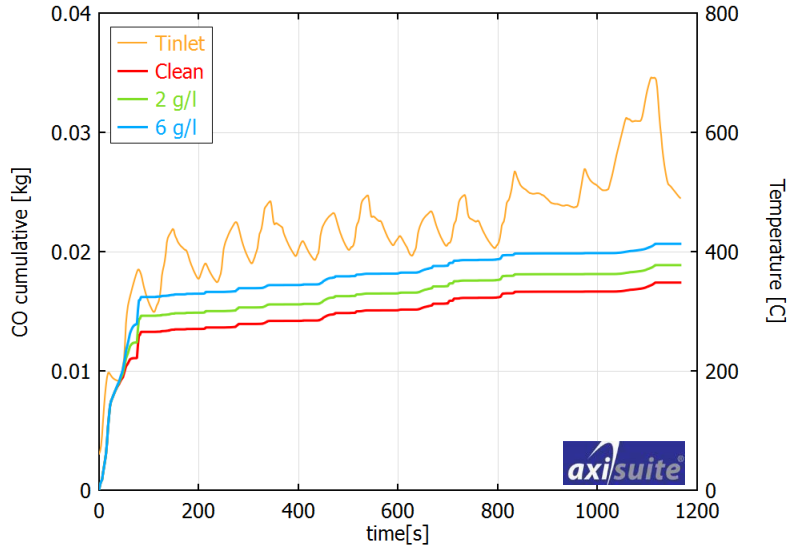
$$v_w \frac{\partial y_j}{\partial w} - D_{w,j} \frac{\partial}{\partial w}\left(f_w \frac{\partial y_j}{\partial w} \right) = \frac{f_w}{c_m} \sum_k c_{j,k} R_k$$

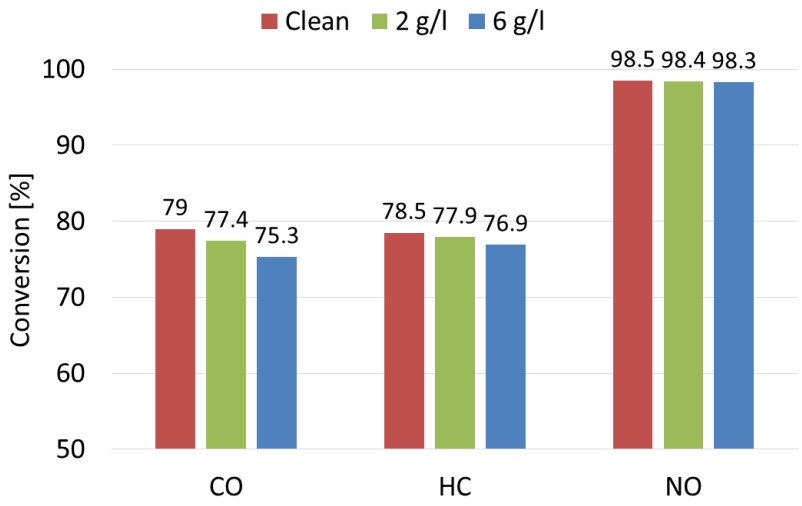
Soot tortuosity

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

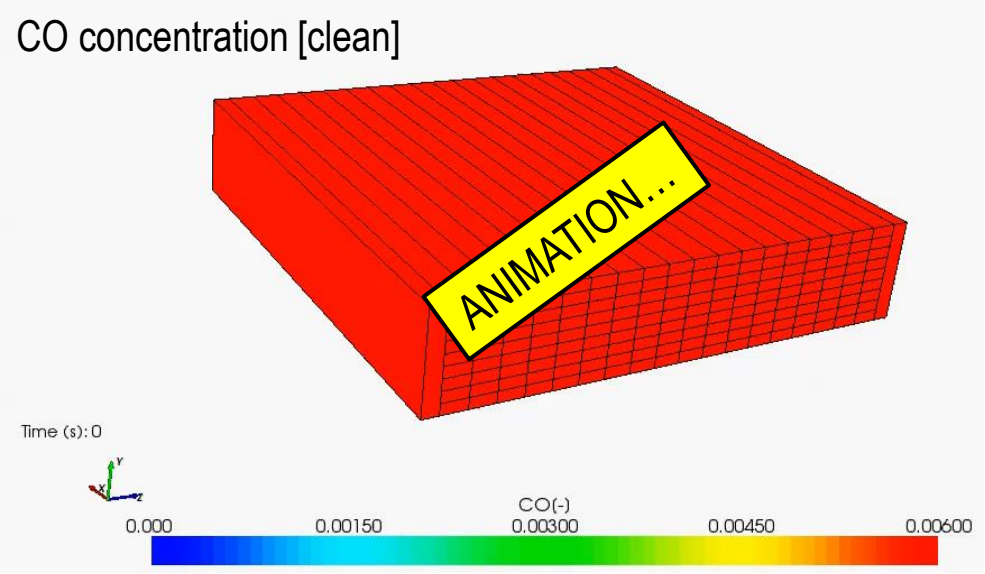
The negative effect of soot on the TWC activity is related to the diffusion limitations of species across the soot layer.

Transient cycle simulation: species conversion with clean and soot loaded GPFs

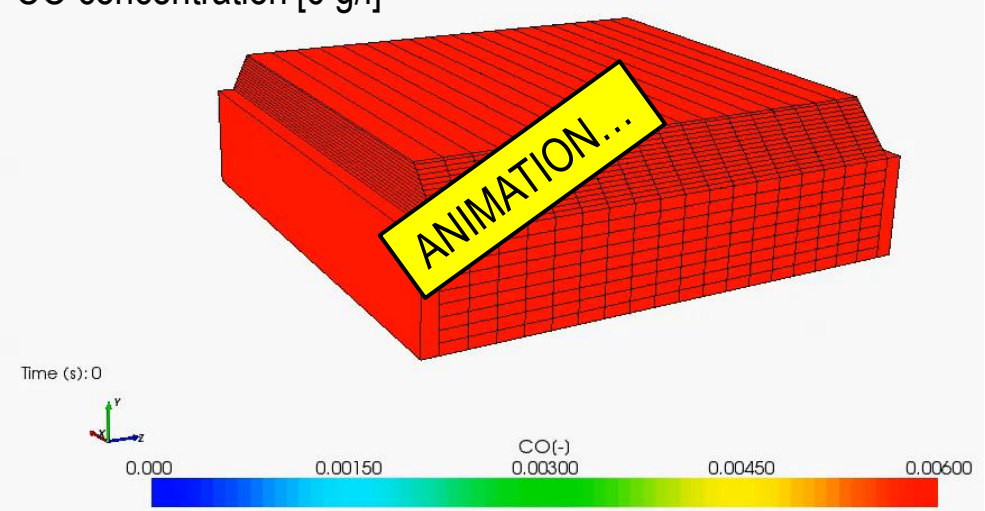




CO concentration [clean]



CO concentration [6 g/l]



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

- Pressure drop
- Filtration efficiency
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- Soot oxidation
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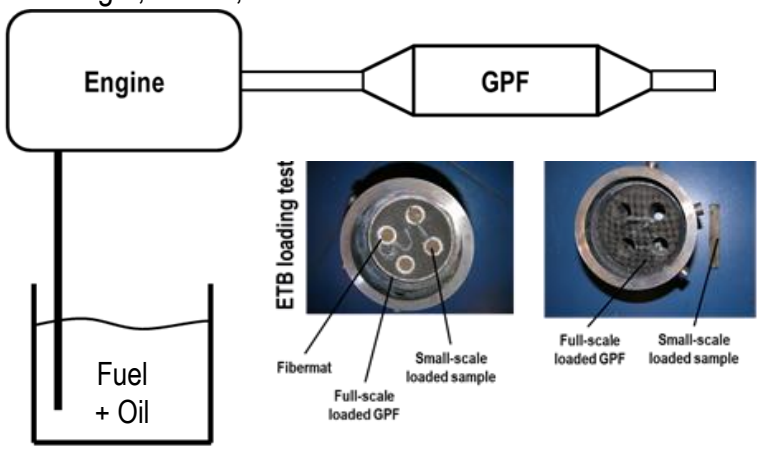
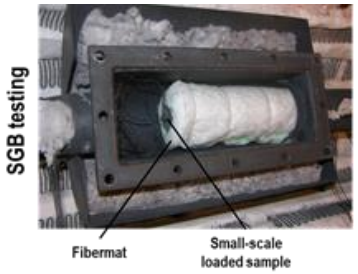
A coated GPF may replace a rear TWC. The coating amount and zoning schemes can be optimized in terms of filtration and catalytic activity.

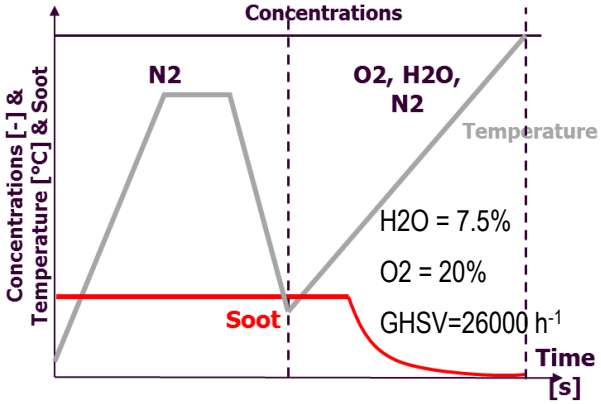
Effect of soot-borne ash on soot oxidation

240 kg/h, 530°C, λ=0.9



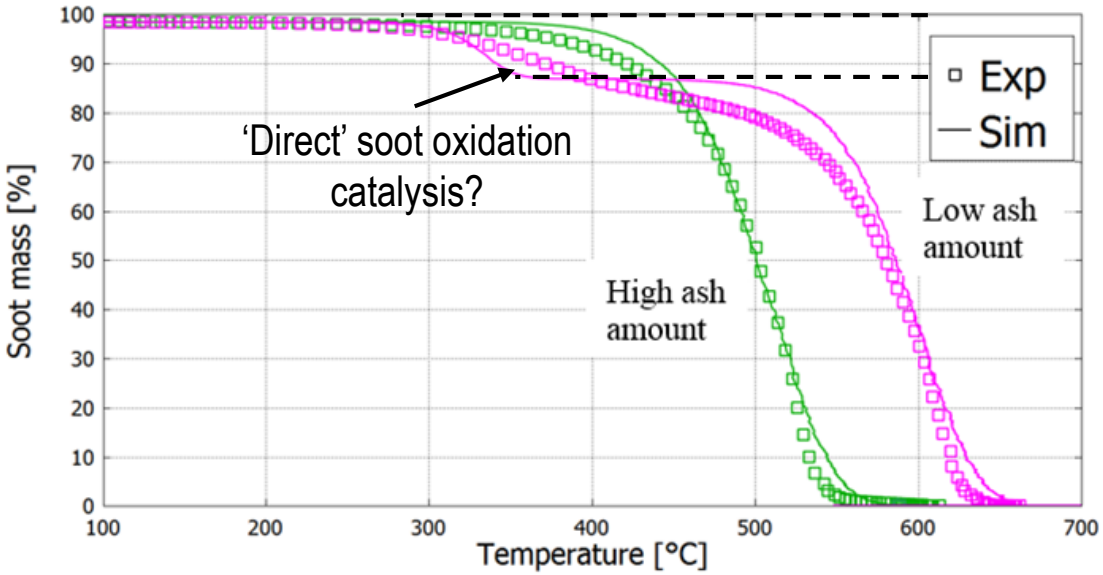


soot oxidation protocol



Reaction	
$C + O_2 \rightarrow CO_2$	Non-catalyzed
$C + {}^1/_2\, O_2 \rightarrow CO$	
$C + O_2 \rightarrow CO_2$	Direct soot catalysis (wall region only)
$C + {}^1/_2\, O_2 \rightarrow CO$	
$C + 4aMeO_2 \rightarrow 2aMe_2O_3 + 2(a-0.5)CO_2 + 2(1-a)CO$	Additive-promoted

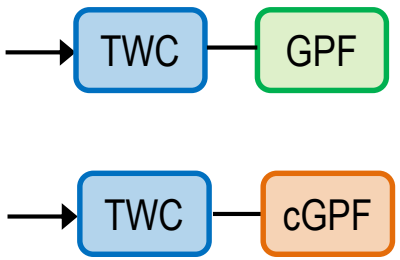
Possibility to perform long-term simulations where soot oxidation is time dependent according to the local ash content



Soot oxidation
O_2 competition (forward diffusion) effect

Exothermia

Configurations

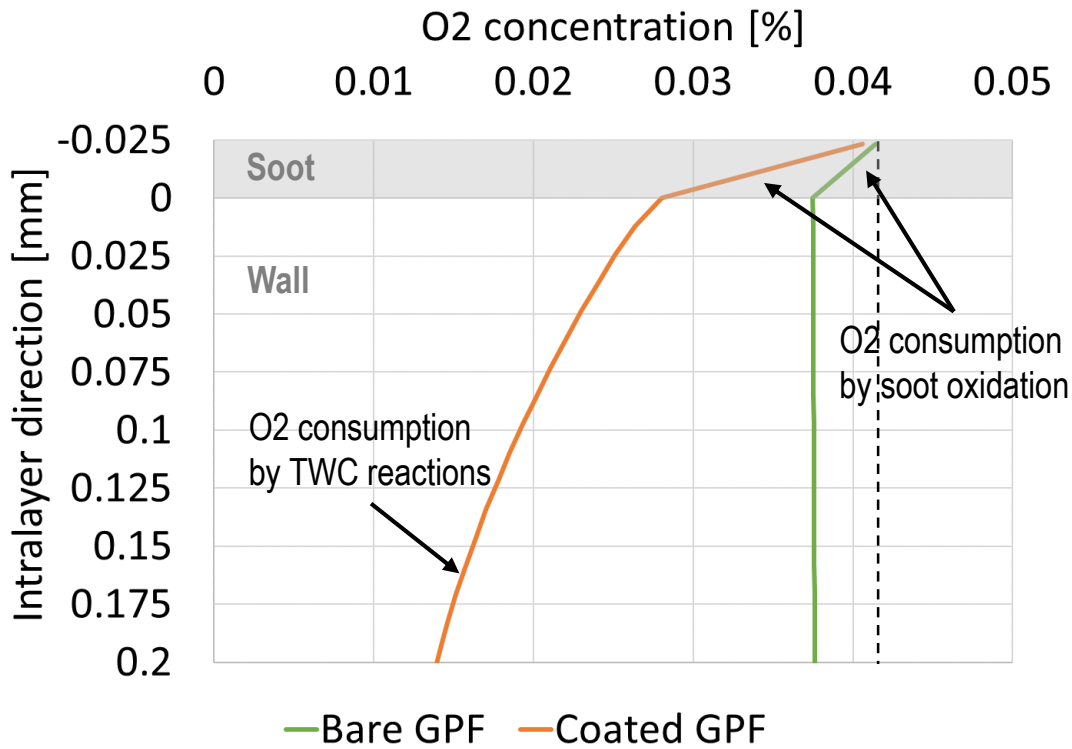


GPF & cGPF: V=1.5l, 300/12

Boundary conditions

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

Intralayer O_2 profiles at filter entrance (z=10mm)



- Forward O_2 diffusion in cGPF due to lower concentrations in the wall → O_2 availability within the soot cake is less compared to the bare GPF → soot oxidation rate will be affected

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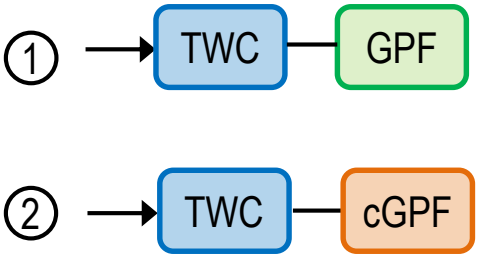
Soot oxidation: O_2 competition under realistic lean/rich cycling operation

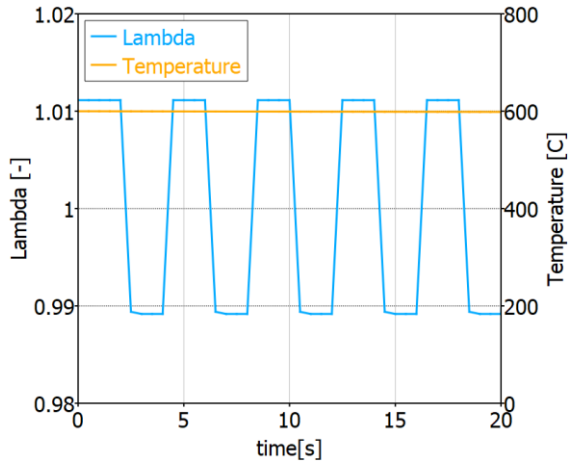
Exothermia

Configurations

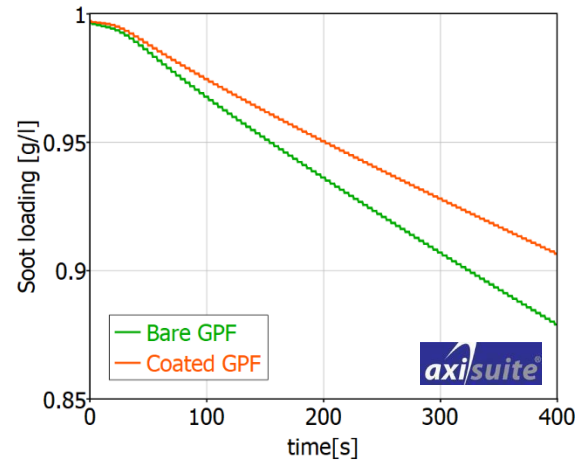


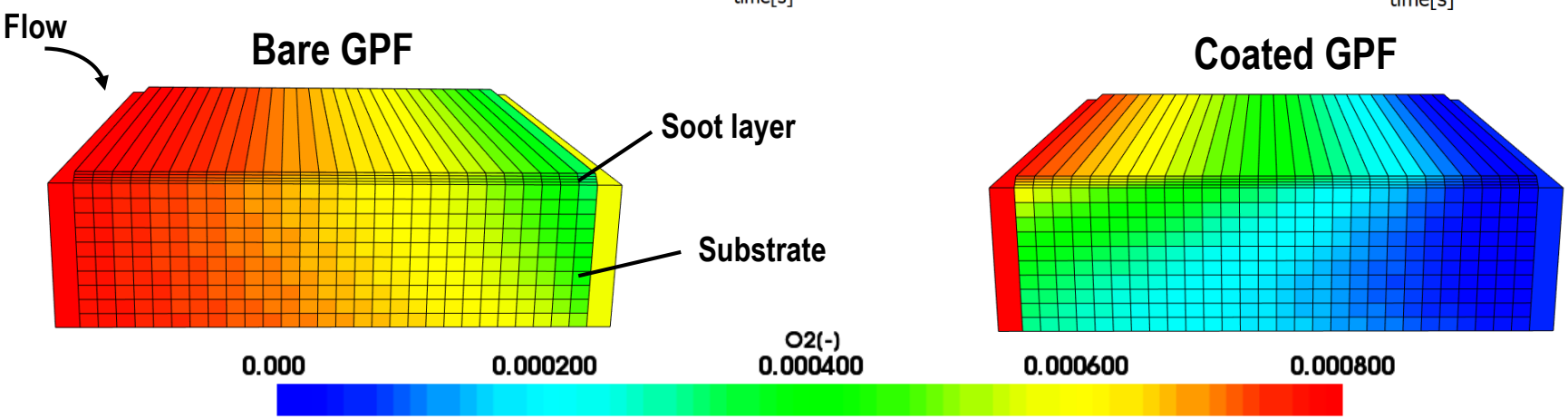
GPF & cGPF: V=1.5l, 300/12

Inlet scenario



Soot oxidation rate





- In the coated GPF, O_2 is competitively consumed between soot and TWC reactions. Strong concentration gradients in the axial and intra wall direction → Soot oxidation rate is lower compared to bare GPF

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Soot oxidation
uncoated vs coated GPF in a transient cycle

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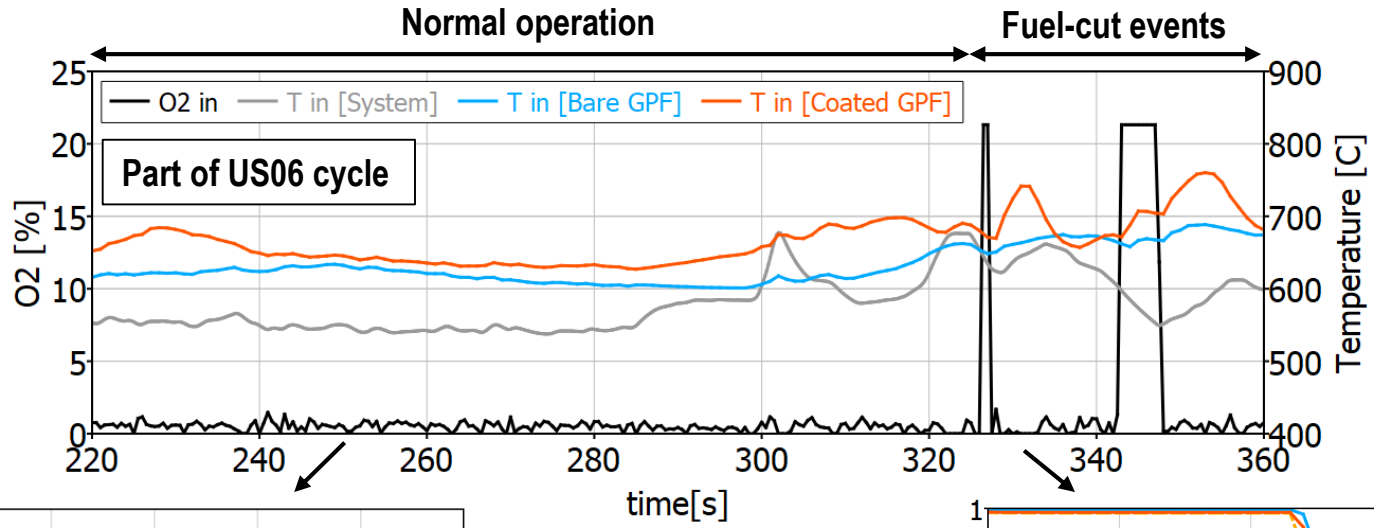
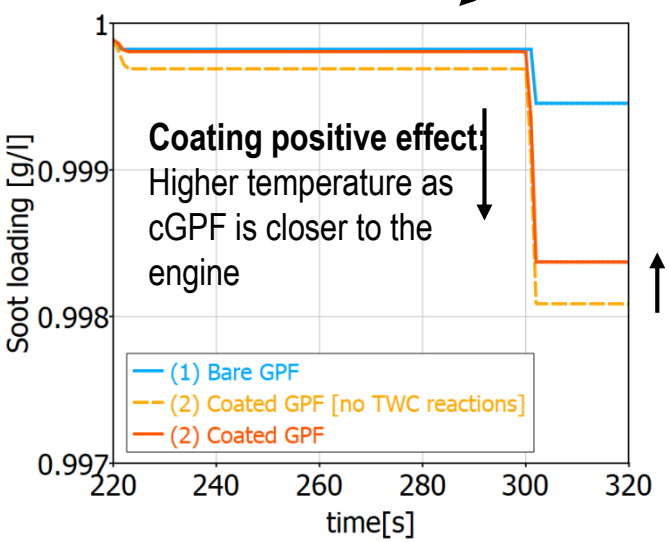
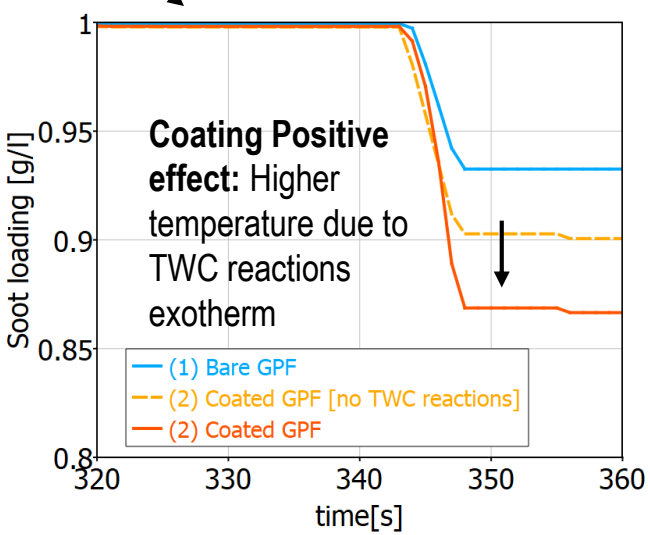
① → TWC — TWC — GPF

② → TWC — cGPF





Coating negative effect: Competitive O2 consumption, TWC vs soot



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

- Pressure drop
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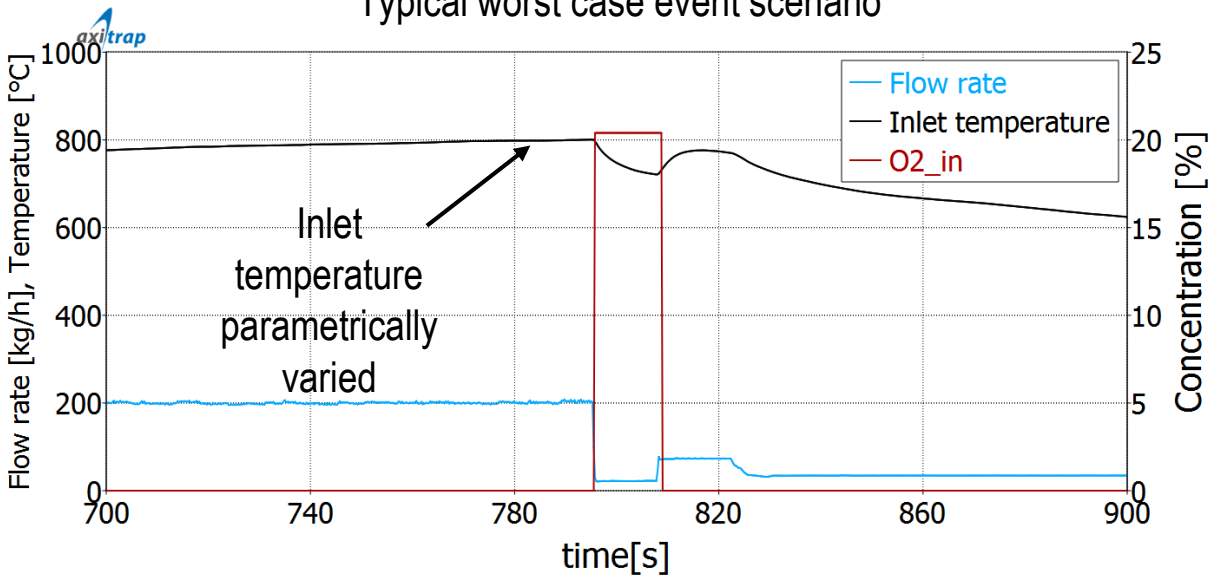
- The ash/soot ratio emitted from gasoline engines is higher compared to Diesel engines, apparently affecting oxidation reactivity.
- Apart from fuel cutoff events, O_2 availability is less and can become even lesser due to 'forward diffusion'.
- Temperatures are higher on average in GPFs.

Soot mass limit (SML) investigation
Worst case scenario: fuel cut-off event

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

Typical worst case event scenario

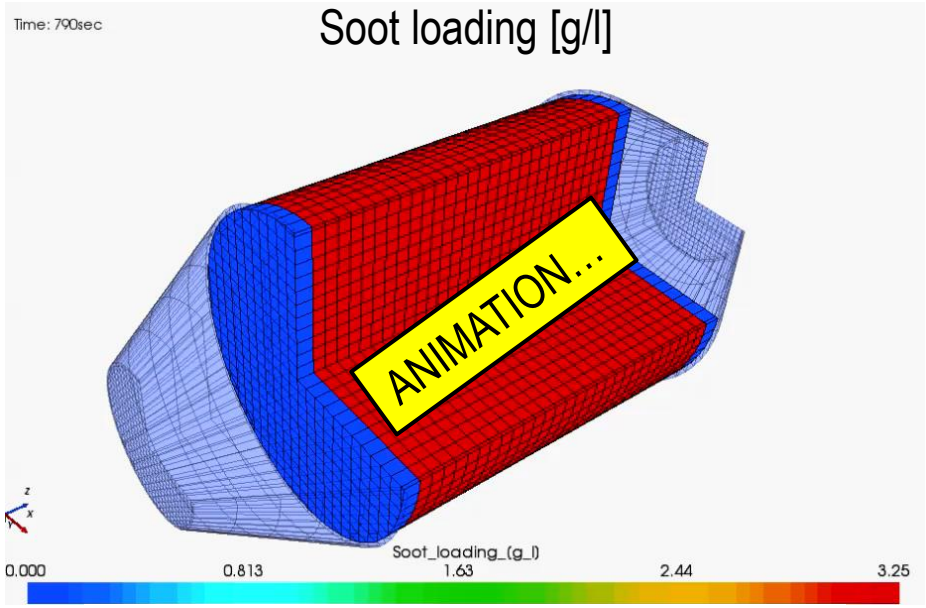


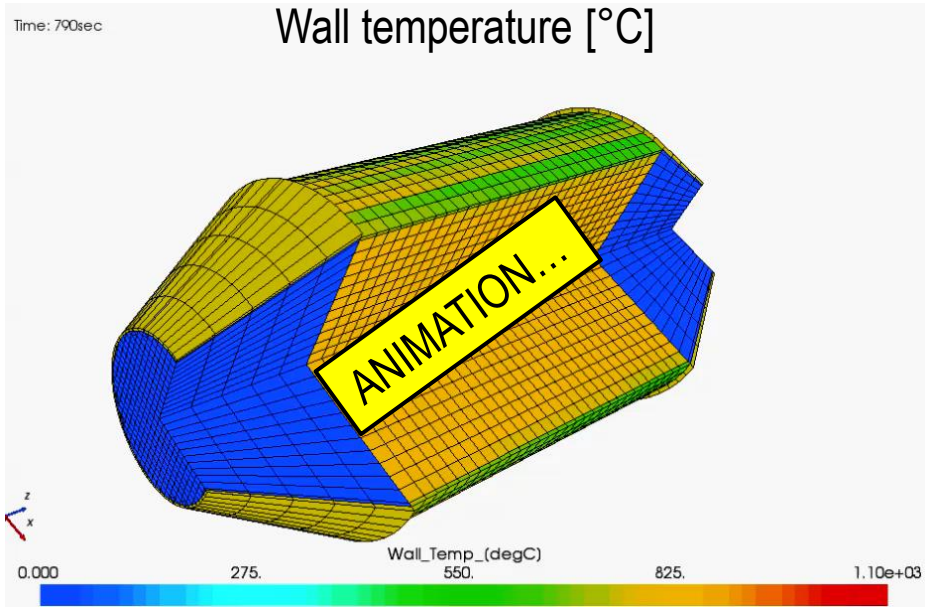
GPF: Diameter: 132 mm, Length: 163 mm, Cell structure: 300cpsi / 12mils, square

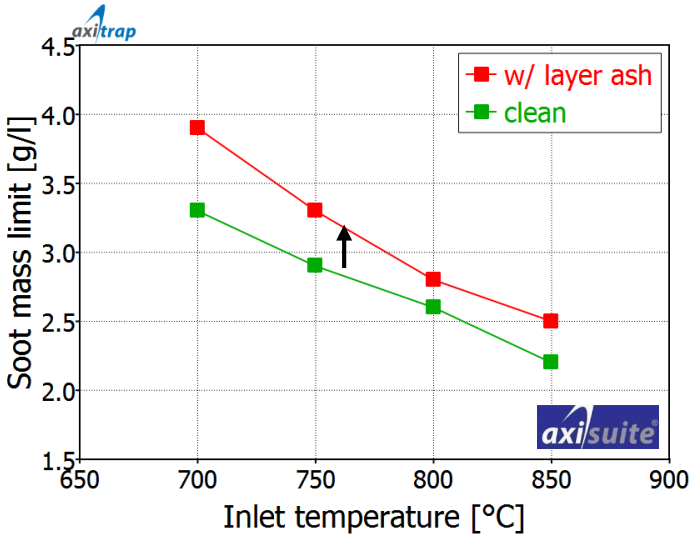
Q1: What is the safe soot mass assuming that the filter temperature should not exceed 1100°C?

Q2: How does accumulated ash affect the soot mass limit?

Effect of layer ash on soot mass limit

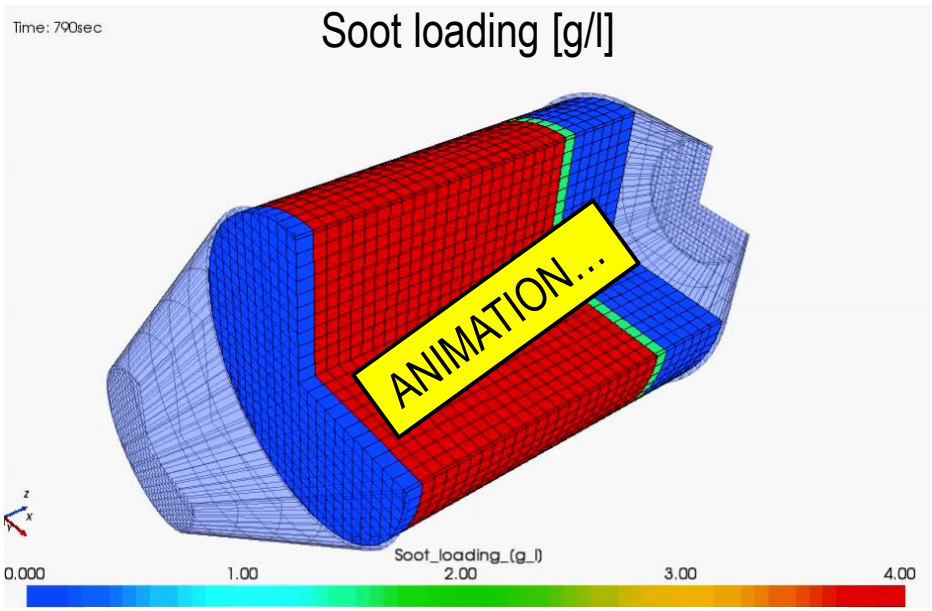


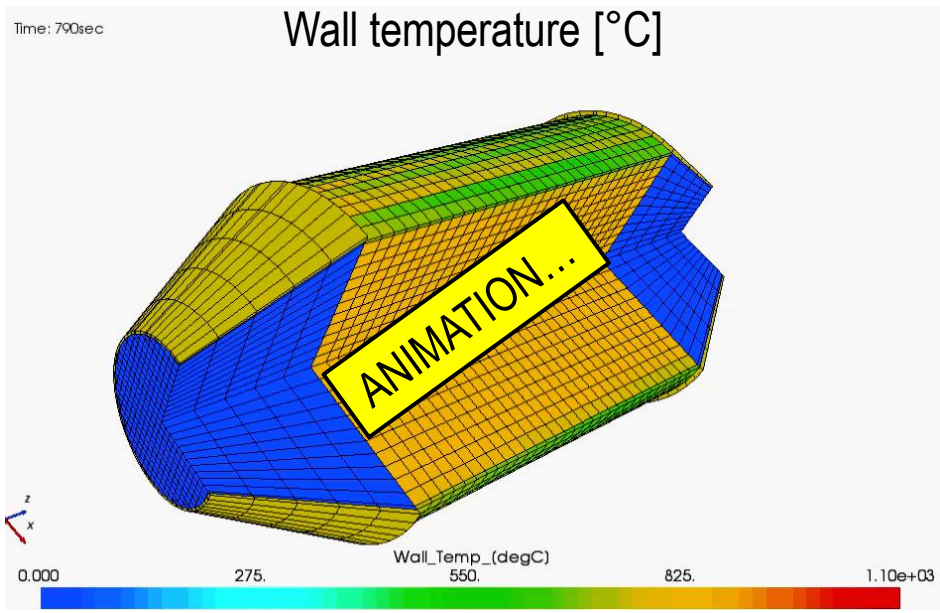


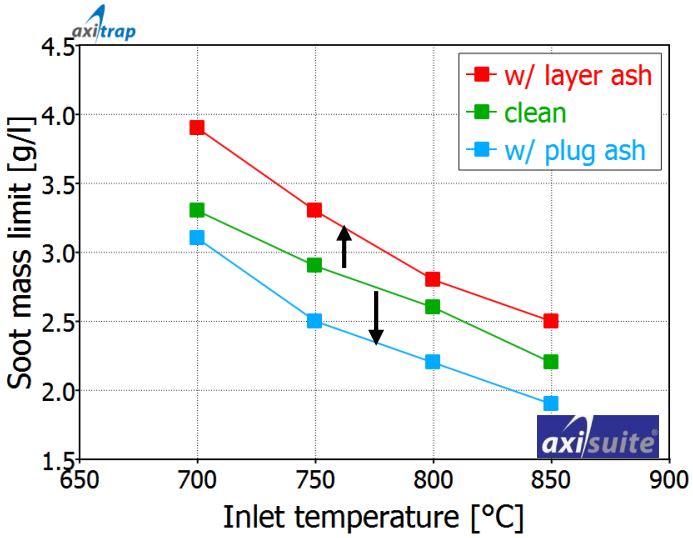


The layer ash effectively increases the thermal mass of the filter, therefore reduces generated exotherms and increases the soot mass limit

Effect of plug ash on soot mass limit



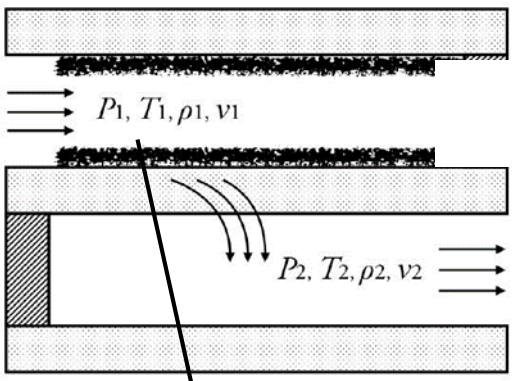




The plug ash effectively increases the local soot loading, therefore increases generated exotherms and decreases the soot mass limit

OBD applications: How to model a partial damage

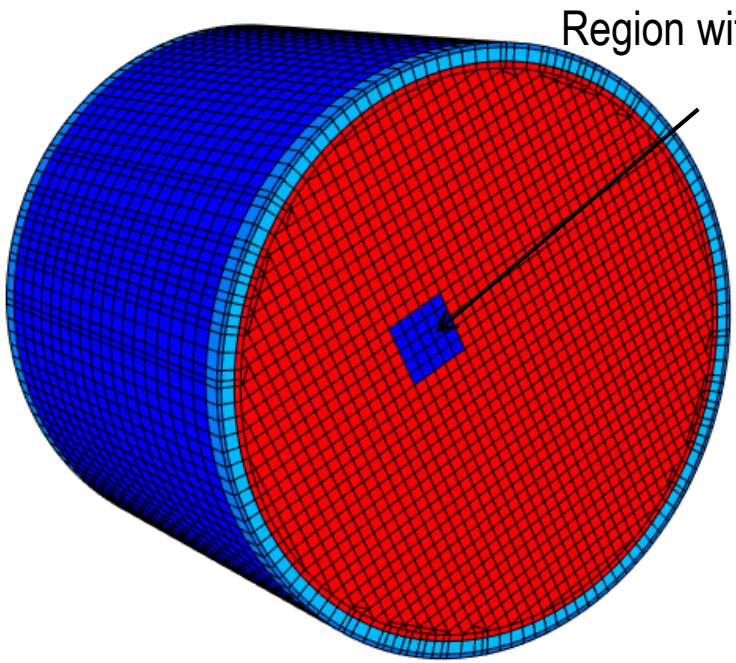
1. Change the boundary condition here.



$$\frac{\partial}{\partial z}\left(d_i^2 \rho_i v_i\right) = (-1)^i \cdot 4 d \rho_w v_w$$

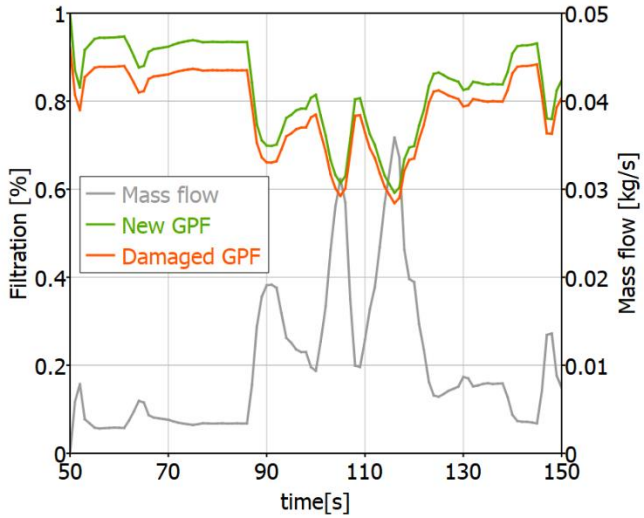
$$\frac{\partial p_i}{\partial z} + \frac{\partial}{\partial z}\left(\rho_i v_i^2\right) = -\alpha_1 \mu v_i / d_i^2$$

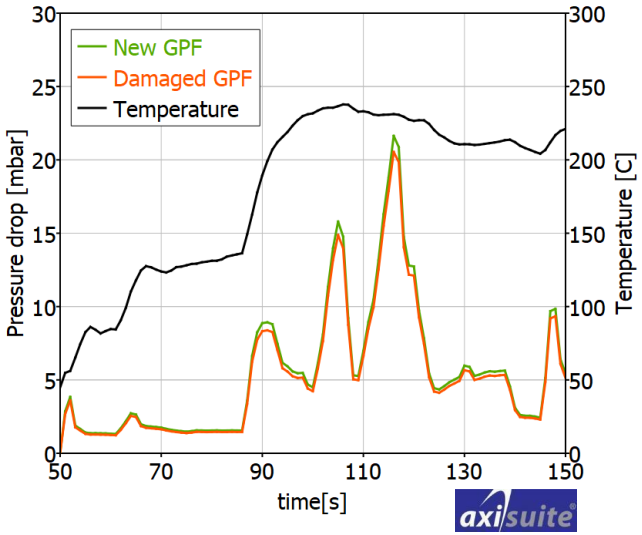
2. Apply the change to selected damaged regions

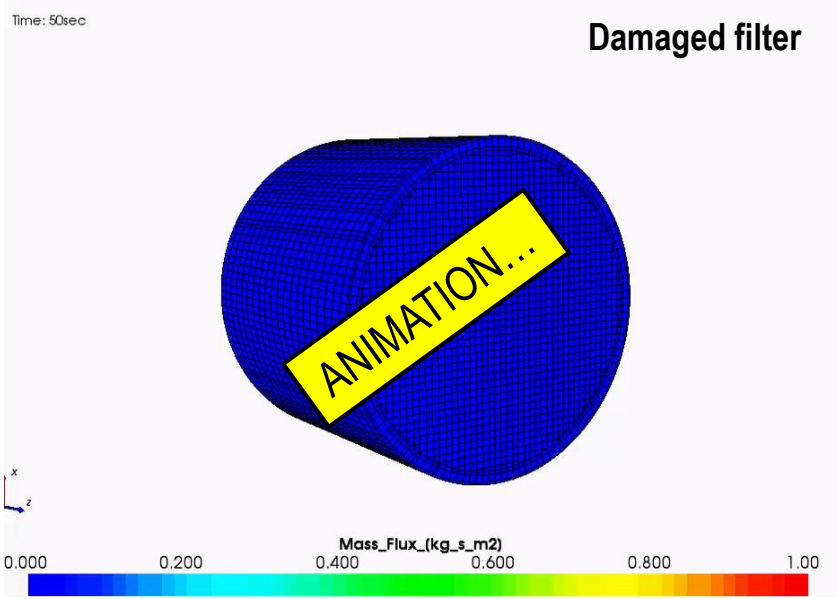


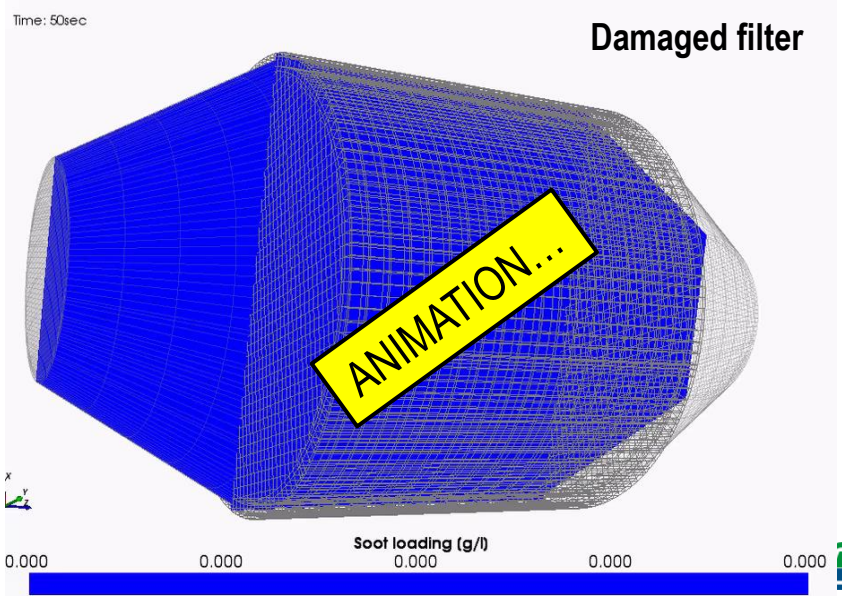
OBD applications
Simulation of damaged filters

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









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

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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

Part of the results presented here were obtained within the project UPGRADE. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 724036.

Thank you very much!