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ExhAUST: SOOT MODEL FOR ADVANCED DESIGN AND CONTROL OF DIESEL ENGINE AFTERTREATMENT SYSTEMS

Diesel Particulate Filters (DPFs) are well assessed aftertreatment devices, equipping almost every modern diesel engine on the market to comply with today's stringent emission standards. However, an accurate estimation of soot loading, instrumental to get an optimal behavior of the whole engine-after-treatment assembly, is still a major challenge.
This challenge may be faced with models characterized by different degrees of detail (0-D to 3-D) depending on the specific application. System design, control issues and OBD model-based sensor development may be successfully approached with 1D modeling. However, high degree of detail and physical consistence in the model formulation are primarily important to increase model predictive capabilities.
This paper addresses DPF modeling issues with special regard to key parameter settings, by using the 1D code ExhAUST (Exhaust Aftertreatment Unified Simulation Tool), developed jointly by the University of Rome Tor Vergata and West Virginia University. ExhAUST is characterized by a novel and unique full analytical treatment of the wall, which allows for a highly detailed representation of the evolution of soot loading inside the porous matrix. In its current version, ExhAUST is composed by different submodels, devoted to DOC and DPF representation, according to Figure 1 schematic. Special attention is devoted to the treatment of particle filtration depending on particle size.

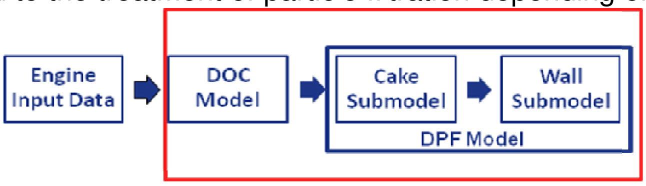

Figure 1: Schematic of ExhAUST Structure for DOC+CDPF Modeling

The main innovations of ExhAUST lie in the 1D treatment of the DPF, that is schematized in Figure 2.

Figure 2: Schematic of Particle Deposition on a CDPF Channel

Conservation equations of particulate deposition and regeneration are in fact treated analytically. Thus, the code presents particularly high computational speed, accuracy and robustness. Analytical treatment of filtration into the wall is possible by representing mass deposition over wall thickness by means of the following formula based on deposition function f(x)

$$\frac{d\dot{m}_p}{dx} = \frac{dC}{dx} \cdot Q_{side} = f(x) \cdot C(x) \cdot Q_{side}$$

Particle concentration over wall thickness can be expressed instead by the following integral formula

$$C(x) = C_0 \cdot e^{-\int_0^x f(t,m)dt}$$

where f(x) takes into account the effects of wall filtration, that may be defined starting from the average efficiency over 32 diameter classes and then by varying filtration regime (namely diffusion and interception), according to Figure 3.

$$\eta(x)_{mass} = \frac{\sum_{i=1}^{32} \eta_{DR}(x) \cdot N_i(x) \cdot dlogD_p \cdot D_i^3}{\sum_{i=1}^{32} N_i(x) \cdot dlogD_p \cdot D_i^3} \quad \Rightarrow \quad f_{mass}(x) = \frac{3}{2}\frac{\eta_{mass}(x)[(1-e(x))]}{d_C(x)\, e(x)}$$

Figure 3: Mass Based Filtration Efficiency (left) and f(x) deposition function.

By this way, discretization over the wall thickness is avoided and thus accuracy and computational efficiency are increased.
Another main innovation presented by ExhAUST consists of the treatment of the regeneration process in the wall, by means of the $\partial w / \partial x$ function that represents the equivalent soot thickness in the wall per cake unit length. Thus, O_2 and NO_2 consumption over wall thickness may be expressed by the formulas described in Figure 4.

$$\begin{cases} \frac{\partial}{\partial x}(\rho_g v_w Y_{O_2}) = -S_p \rho_g Y_{O_2} \cdot \left(k_{th}\left(1-\frac{f_{co}}{2}\right)(1-\beta) + k_{cat}\left(1-\frac{f_{co'}}{2}\right)\beta\right) \cdot \frac{\partial w}{\partial x} \\ \frac{\partial}{\partial x}(\rho_g v_w Y_{NO_2}) = -S_p \rho_g Y_{NO_2} k_{NO_2}(2-g_{CO}) \cdot \frac{\partial w}{\partial x} \\ \frac{\partial w}{\partial x} = \frac{1}{\rho_{soot,ck}} \cdot \frac{1-\varepsilon_0}{\frac{4}{3}\pi\left(\frac{b}{2}\right)^3} \frac{\partial m_{wall}}{\partial x} \end{cases} \Rightarrow \begin{cases} Y_{O_2}(x) = Y_{O_2,0} \exp\left(\frac{-\int_0^x S_p k_{O_2}\left(\frac{\partial w}{\partial x}\right)dx}{v_w}\right) \\ Y_{NO_2}(x) = Y_{NO_2,0} \exp\left(\frac{-\int_0^x S_p (2-g_{CO}) k_{NO_2}\left(\frac{\partial w}{\partial x}\right)dx}{v_w}\right) \end{cases}$$

Figure 4: Gaseous species conservation equations in the DPF wall (left), and expressions for gas concentration over wall thickness (right).

Numerical results are compared with experimental data gathered at West Virginia University (WVU) Engine and Emissions Research Laboratory using a Mack heavy-duty diesel engine coupled to a Johnson Matthey CCRT (DOC, Diesel Oxidation Catalyst+CDPF, Catalyzed DPF) aftertreatment system. TSI-EEPS 3090 with gravimetric measurements and gaseous emission analyzers have been used to give proper experimental input to the model. A direct weighing procedure has been also used to directly compare model results with soot loading measurements.
Two steady state operating modes have been selected according to Figure 5 (table in the left). As an example, the satisfactory comparison between experimentally weighed and numerically calculated soot load over the two modes are instead reported in Figure 5 (right).

Test Mode	R10	R100
Duration [h]	30	1.5
Eng. Load [ft-lbf]	105	1018
Eng. Speed [rpm]	1800	1800
Fuel Flow Rate	11.64	56.11
C-CRT Inlet	226.5	483.8
Intake Air Flow	256.4	588.1

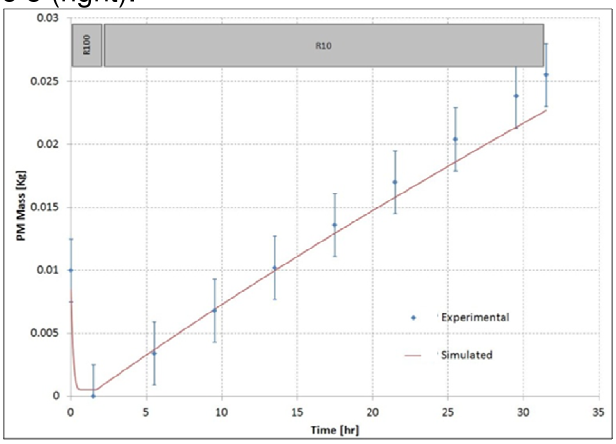

Figure 5: Test Points (left) and comparison between Experimental and Simulated Back Pressure over time (right).

Overall results obtained so far led to the following conclusions: a) wall and washcoat cake layer show different regeneration and collecting dynamics, whose behavior is primarily important to capture back pressure and collected mass evolution during time. b) the model is able to represent the evolution of soot loading during engine operation by varying engine conditions. c) advanced filtration and regeneration process treatment in the wall allow the use of constant wall and cake parameters, so that ExhAUST can be used to track back pressure and mass history of diesel particulate filters under subsequent regeneration and loading processes. d) filtration sub-model results are highly influenced by engine-out particle distribution during deep bed filtration mechanism suggesting a possible implementation in conjunction with soot sensor devices. e) mass trapped estimation performed by DPF sub-model gives the opportunity to use mass loading as direct control parameter for filter diagnostics.

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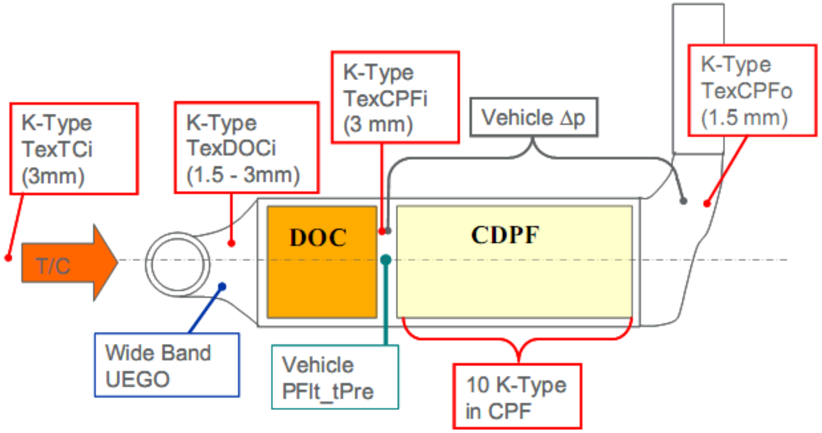
Background

- DPF control strategy is important
  - Fuel consumption and nanoparticle Emission Minimization
  - Preventing engine failures due to DPF clogging
  - Detecting/predicting failures due to DPF malfunction
- Advanced DPF modeling can support both sensors and empirical model-based control strategies
- Soot content (g/l) is the key quantity to predict
  - Back Pressure depends on load history



After treatment sensor schematic for DPF control (Corning, SAE 2009-01-1262)

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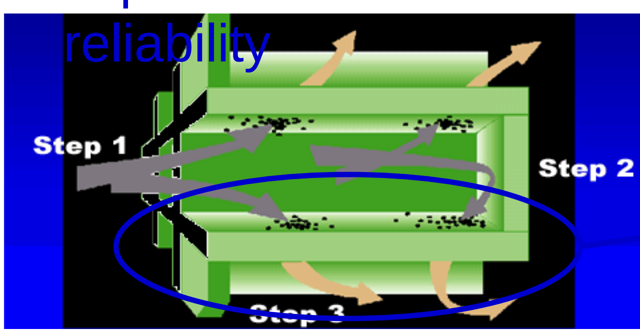
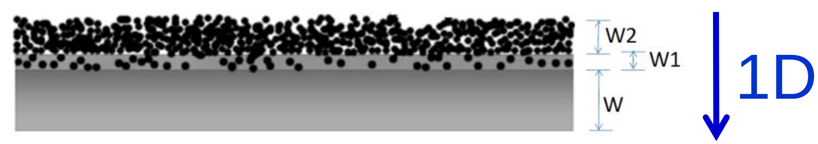
ExhAUST

Engine Input Data ➡ DOC Submodel ➡ Cake Submodel ➡ Wall Submodel

ASME ICEF 2010-35160

- ExhAUST: Exhaust Aftertreatment Unified Simulation Tool (Matlab)
- ExhAUST is characterized by fully analytical 1D representation over wall thickness
  - Increase calculation speed as much as possible
- O2 and NO2 regeneration are taken into account
  - Continuous and Discontinuous regeneration can be represented
- Novel wall filtration and regeneration analytical models have been implemented into the wall (SAE ICEF 2010) to improve prediction reliability





ExhAUST: Equation Set

DOC

DPF-CAKE

DPF-WALL

- 1D Analytical Treatment over channel length

$$u\frac{\partial C_{g,i}}{\partial x} = \left(m_{gas-to-surf}\right)_i = min\left[\left(-k_{m,i}A_{ac,spec}C_{g,i}\right);\left(-R_i^{surf,kin-lim}\right)\right]$$

$$\begin{cases} u\frac{\partial C_{g,i}}{\partial x} = -k_{m,i}A_{ac,spec}C_{g,i} & for\ T > T_{light-off} \\ u\frac{\partial C_{g,i}}{\partial x} = -R_i^{surf,kin-lim} & for\ T < T_{light-off} \end{cases}$$

CO, C3H6, NO, NO2

$$\begin{cases} C_{NO,out} = max\left(C_{NO,out}^{mass-tr};C_{NO,out}^{eq}\right) \\ C_{NO2,out} = max\left(C_{NO2,out}^{mass-tr};C_{NO2,out}^{eq}\right) \end{cases}$$

NO, NO2

$$\rho_g c_{p,g} u\frac{\partial\left(T_g - T_s\right)}{\partial x} = -hA_{ac,spec}\left(T_g - T_s\right)$$

Energy gas phase

$$(1-OFA)\rho_{solid}c_{solid}\frac{\Delta T_s}{\Delta t} = \int_0^L hA_{ac,spec}\left(T_g - T_s\right)dx$$

Energy solid phase

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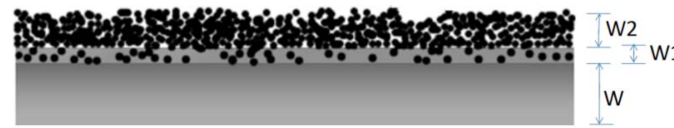
ExhAUST: Equation Set

DOC | DPF-CAKE | DPF-WALL

- Regeneration, 1D Analytical Treatment



$$\begin{cases} \dfrac{\partial}{\partial x}\left(\rho \quad v_w Y_{w,1}\right) = -S_p \rho \quad Y_{w,1}\cdot\left(k_{th}\left(1-\dfrac{f_{co}}{2}\right)(1-\beta) + k_{cat}\left(1-\dfrac{f_{co'}}{2}\right)\beta\right) \\ \dfrac{\partial}{\partial x}\left(\rho_w v \quad Y_{w,2}\right) = -S_p \rho \quad Y_{w,2} k_{th}\left(1-\dfrac{f_{CO}}{2}\right) \\ \dfrac{\partial}{\partial x}\left(\rho_w v_w Y_{NO_2}\right) = -S_p \rho_w Y_{NO_2} k_{NO_2}(2-g_{CO}) \end{cases}$$

$$R_{O_2,total\,,1} = \rho \quad v_w Y_{w,1}\left(1-\exp\left(\frac{-S_p k^* w_1}{v_w}\right)\right)$$

$$\begin{cases} \dfrac{\partial}{\partial t}\left(\rho_{soot\,,ck} w_2\right) = -\left(\dfrac{M_c}{M_{ox}}\left(\dfrac{R_{O_2,2}}{1-\dfrac{f_{CO}}{2}}\right) + \dfrac{M_c}{M_{NO_2}}\left(\dfrac{R_{NO_2,2}}{2-g_{co}}\right)\right) \\ \dfrac{\partial}{\partial t}\left(\rho_{soot\,,ck} w_1\right) = -\left(\dfrac{M_c}{M_{ox}}\left(\dfrac{R_{O_2,th,1}}{1-\dfrac{f_{CO}}{2}}\right) + \dfrac{M_c}{M_{ox}}\left(\dfrac{R_{O_2,cat\,,1}}{1-\dfrac{f_{CO'}}{2}}\right)\right) - \left(\dfrac{M_c}{M_{NO_2}}\left(\dfrac{R_{NO_2,1}}{2-g_{co}}\right)\right) \end{cases}$$

Soot cons I layer

Soot cons II layer

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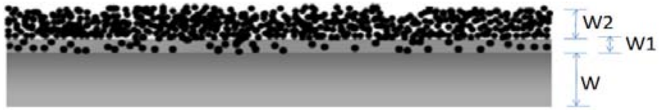
ExhAUST: Equation Set

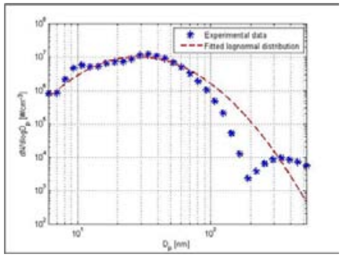
DOC | DPF-CAKE | DPF-WALL



- Filtration, 1D Analytical Treatment

$$\begin{cases} \dfrac{dC_i(x,t)}{dx} = -f_i(x,t) * C_i(x,t) \\ f_i(x,t) = \dfrac{3}{2}\dfrac{\eta_{DR,i}(x,t)\left[\left(1-\varepsilon(x,t)\right)\right]}{d_C(x,t)\ \varepsilon(x,t)} \end{cases}$$

$$\begin{cases} \eta_{DR} = \eta_D + \eta_R - \eta_D \eta_R \\ \eta_D = 3.5 \cdot g(\varepsilon) \cdot Pe^{-2/3} \\ \eta_R = 1.5 \cdot N_R^2 \cdot \dfrac{[g(\varepsilon)]^3}{(1+N_R)^{\frac{3-2\varepsilon}{\varepsilon}}} \end{cases}$$



32 Diameter Classes

$$\begin{cases} \dfrac{dC_{mass}(x,t)}{dx} = -f_{mass}(x,t) * C_{mass}(x,t) \\ \eta_{mass} = \dfrac{\sum_{i=1}^{32} \eta_i N_i d_i^3}{\sum_{i=1}^{32} N_i d_i^3} \end{cases}$$

$$\begin{cases} \dfrac{d\dot{m}_P}{dx} = \dfrac{dC}{dx} \cdot Q_{channel} = f(x) \cdot C(x) \cdot Q_{channel} \\ m_{wall} = \displaystyle\int_0^w f(x) \cdot C(x) \cdot Q_{channel}\ dx \\ d_c(x,t) = 2\left(\dfrac{3}{4\pi}\dfrac{m_{collector}(x,t)}{\rho_{soot,w}} + \left(\dfrac{d_{co}}{2}\right)^3\right)^{1/3} \end{cases}$$

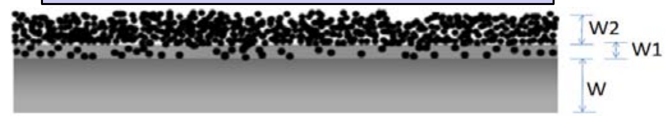
Mass Conc.

ExhAUST: Equation Set

DOC

DPF-CAKE

DPF-WALL



- Filtration, 1D Analytical Treatment

$$\frac{dC_i(x,t)}{dx} = -f_i(x,t) * C_i(x,t)$$

$$C(x) = C_0 \cdot e^{-\int_0^x f(x',n)dx'}$$

$$\frac{dC_{mass}(x,t)}{dx} = -f_{mass}(x,t) * C_{mass}(x,t)$$

f(x,n) polynomial functions
n-th order

$$\phi(0,t) = \left(\frac{\left(d_c(0,t)\right)^2 - d_{c_0}^2}{(\psi \cdot b) - d_{c_0}^2}\right)$$

$$\Delta P_{DPF} = \Delta P_{channels} + \Delta P_{cake} + \Delta P_{wall}$$

Partition coefficient
cake-wall
DPF Back Pressure

ExhAUST: Equation Set

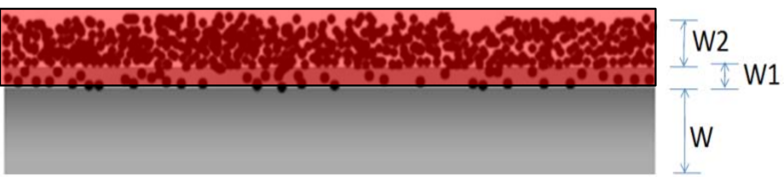
DOC | DPF-CAKE | DPF-WALL

- Wall regeneration1D Analytical Treatment

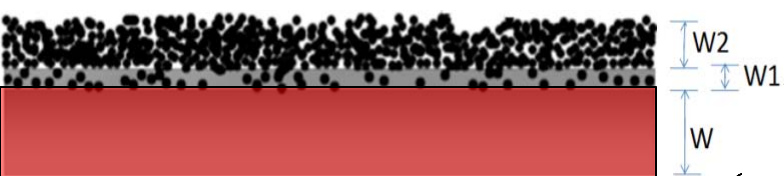
$$\frac{dR_{NO_2,w}(x)}{dx} = -S_p k_{NO_2} \frac{dw}{dx}$$

$$\frac{dR_{O_2,w,total}(x)}{dx} = -S_p k^* \frac{dw}{dx}$$

Reaction rate distribution over wall thickness



$$\frac{dw}{dx} = 1 \qquad Y_{O2}(x) = Y_{O2,inlet} \exp\left(\frac{-\int_0^x dR_{O_2,w,total}(x')}{\rho v_w}\right)$$



$$\frac{dw}{dx} \propto \frac{dm_{wall}}{dx} \qquad Y_{NO2}(x) = Y_{NO2,inlet} \exp\left(\frac{-\int_0^x dR_{NO_2,w}(x')}{\rho v_w}\right)$$

$$\frac{\partial}{\partial t}\left(\rho_{soot,ck} \frac{dw}{dx}(x)\right) = \left\{-\left(\frac{M_c}{M_{ox}}\left(\frac{\frac{\partial}{\partial x}(\rho \ v_w Y_{O2,})}{1-\frac{f_{CO}}{2}}\right) + \frac{M_c}{M_{NO_2}}\left(\frac{\frac{\partial}{\partial x}(\rho \ v_w Y_{NO2,})}{2-g_{co}}\right)\right)\right\}$$

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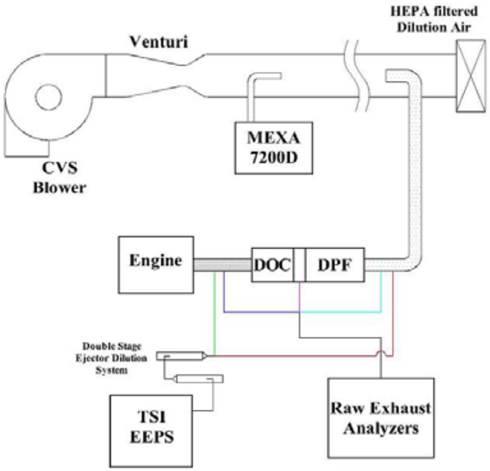
Example: CCRT coupled to Volvo Engine

- Engine testing performed at WVU
- Steady state modes
- Complete particle analysis performed with TSI-EEPS
- DPF has been weighed at high temperature during operation



Parameter	DOC	DPF
Diameter (in)	12	12
Length (in)	5	12
Cell Density (cpsi)	400	100
Wall Thickness (mil)	4	12
Clean wall porosity	-	0.5

Model	MACK MP7-355E
Configuration	6 cylinders, Inline
Aspiration	Sliding Nozzle Variable Turbocharger / Intercooler
Injection System	Dual Solenoid Electronic Unit Injector (EUI)
Maximum Torque	1844 Nm (1360 ft-lbs) @ 1200 RPM
Maximum Power	265 kW (355 bhp) @ 1800 RPM
Displacement, L (cu-in)	11 (659)
Compression Ratio	16.0:1
Bore & Stroke, mm (in)	122.94x151.89 (4.84x5.98)

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Conditions / Modeling Parameters

- Two modes selected
  - R10 and R100 load
  - 2 hrs R10 and 30hrs R100 defining a complete regeneration/loading procedure

Test Mode	R10 (Soot Loading)	R100 (Regeneration)
Duration [h]	30	1.5
Eng. Load [ft-lbf]	105	1018
Eng. Speed [rpm]	1800	1800
Fuel Flow Rate [kg/h]	11.64	56.11
C-CRT Inlet Temp. [C]	226.5	483.8
Intake Air Flow [scfm]	256.4	588.1

R10 Mode	Pre-DOC	Post-DPF
HC [ppm]	118.4*	2.7
CO [ppm]	197*	2.5
NO [ppm]	123.9	52.5
NO_2 [ppm]	40.0	107.4
NO_x [ppm]	163.9	159.9
NO/NO_2 Ratio	3.09	0.49
PM [mg/Sm^3]	2	-

R100 Mode	Pre-DOC	Post-DPF
HC [ppm]	37.7	0
CO [ppm]	N/A	0
NO [ppm]	361.4	335.0
NO_2 [ppm]	116.8	96.6
NO_x [ppm]	478.2	431.6
NO/NO_2 Ratio	3.09	3.47
PM [mg/Sm^3]	13	-

- Model Parameters

Symbol	Description	Value	Units
E_{th,O_2}	O_2 Thermal Activation Energy	2.0E+4	K
E_{cat,O_2}	O_2 Catalytic Activation Energy	1.8E+4	K
E_{NO_2}	NO_2 Activation Energy	1.12E+4	K
A_{th}	O_2 Thermal Rate Constant	25.08	m/sK
A_{cat}	O_2 Catalytic Rate Constant	2.84	m/sK
A_{NO_2}	Catalytic Rate Constant	2.9	m/sK
S_p	Soot Specific Area	5.5E+7	1/m
d_{C_0}	Initial Unit Collector Diameter	16.5	µm
b	Unit Cell Diameter	20.8	µm
$\rho_{soot,w}$	Soot Packing Density in the Wall	6.5	kg/m^3
$\rho_{soot,ck}$	Soot Packing Density in the Cake	40	kg/m^3
k_0	Soot Wall Clean Permeability	3.95E-13	m^2
k_{soot}	Cake Permeability	3.1E-14	m^2
ψ	Wall Filtration Filling Parameter	0.88	-

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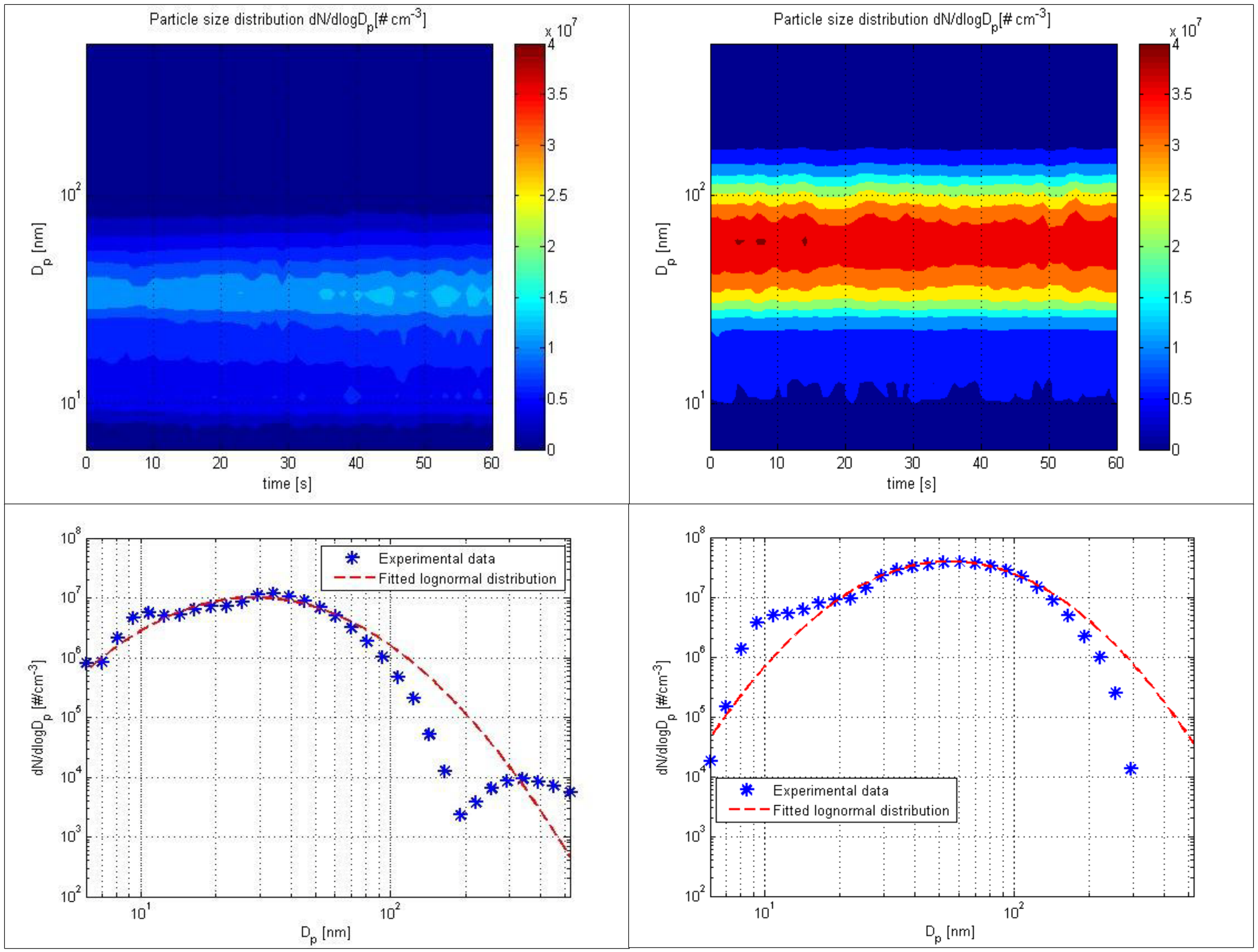
Particle Distribution upstream of the DPF (measured with TSI-EEPS)

Mode R10



Mode R100

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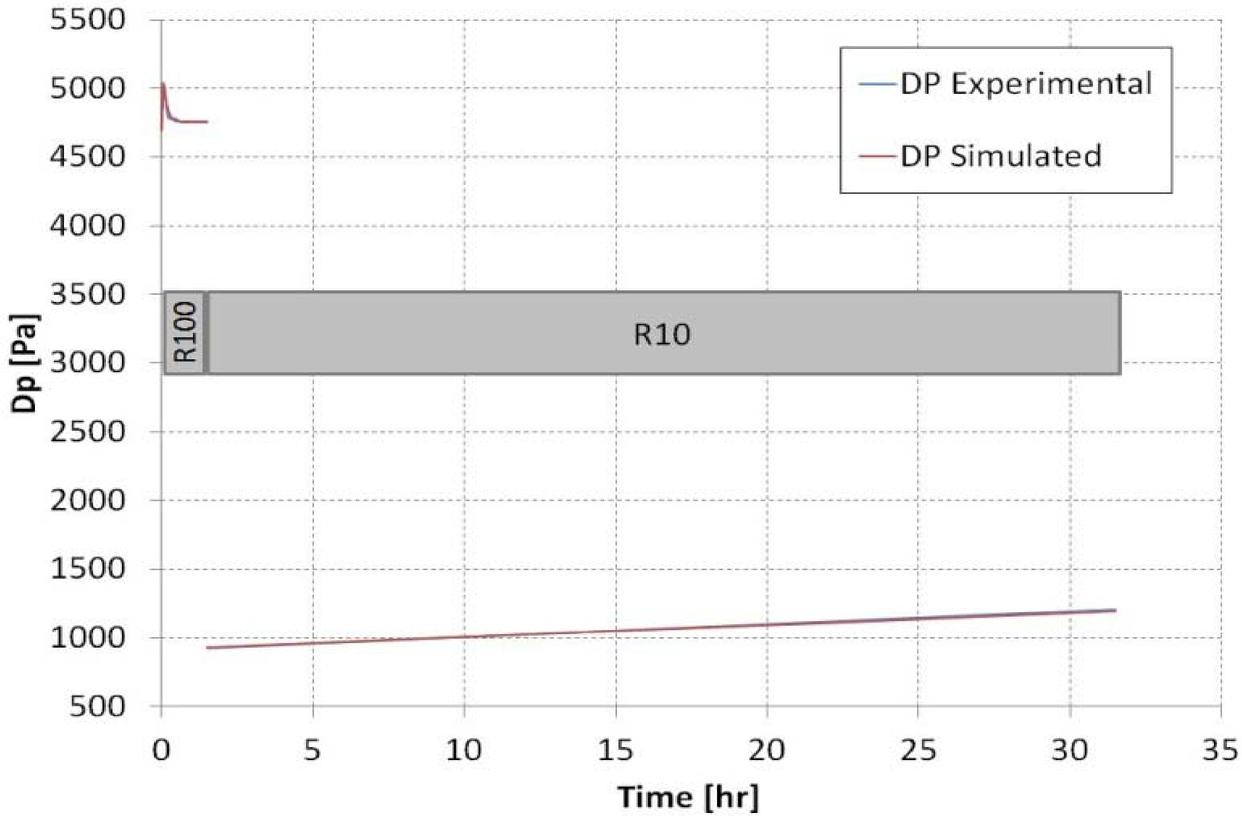
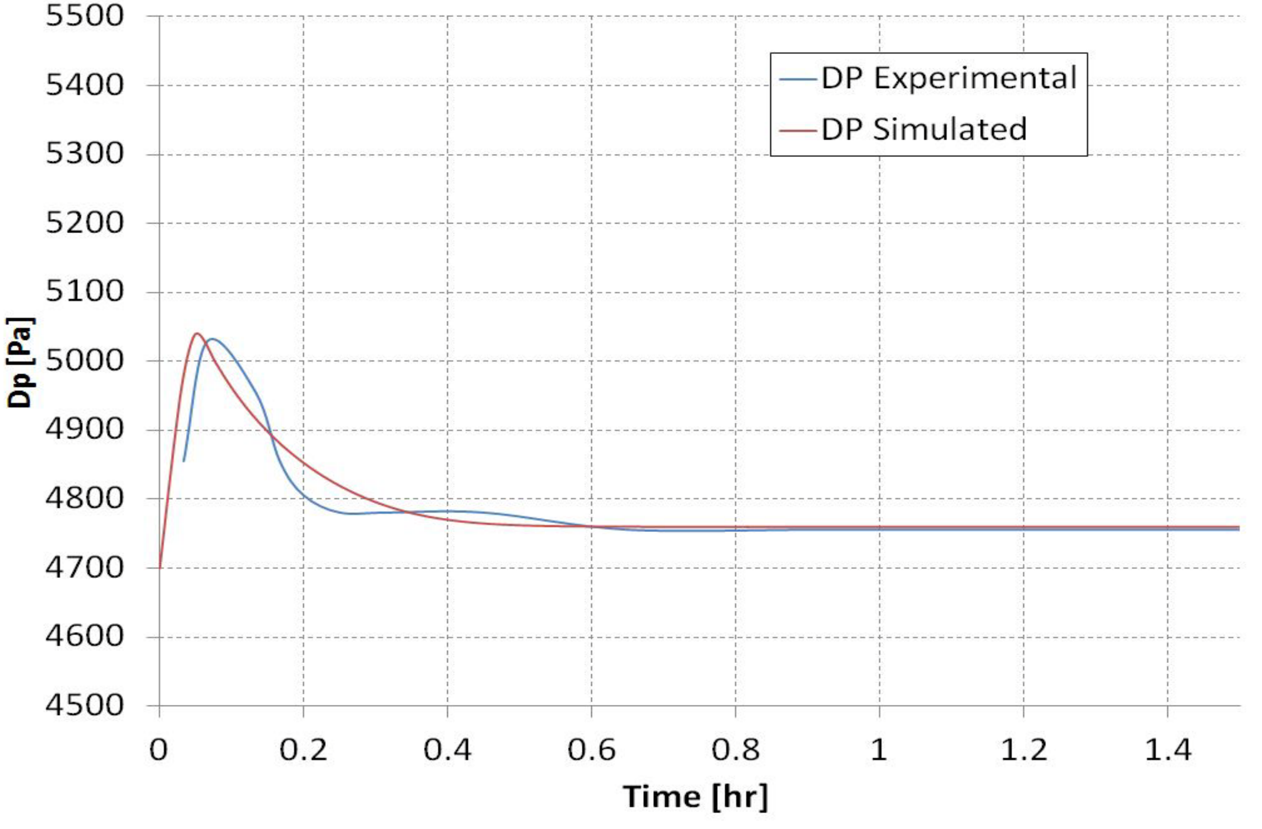
Back pressure (predicted vs simulated) over the whole regeneration/loading procedure



Back pressure (measured vs predicted) detail of R100 mode



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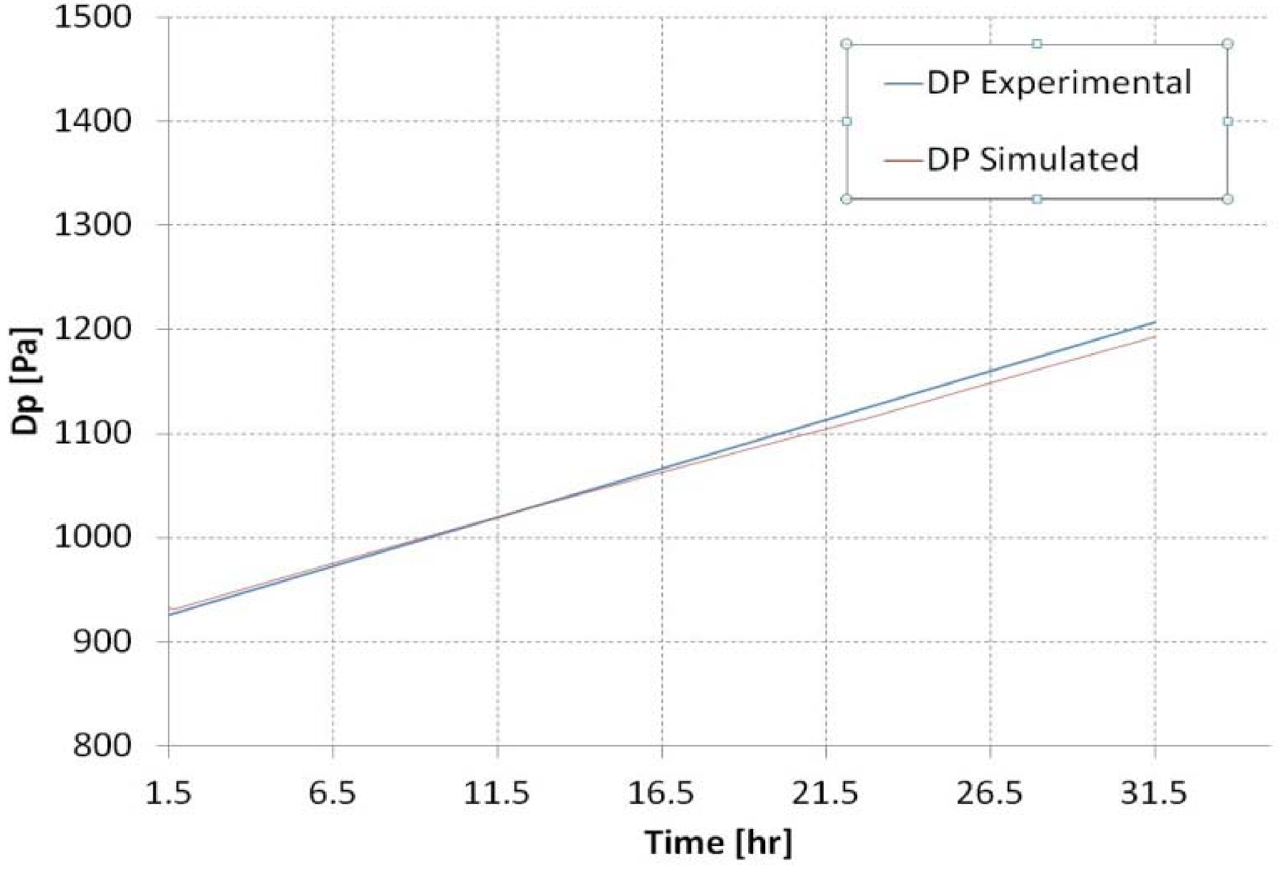
Back pressure (measured vs predicted) R10 mode



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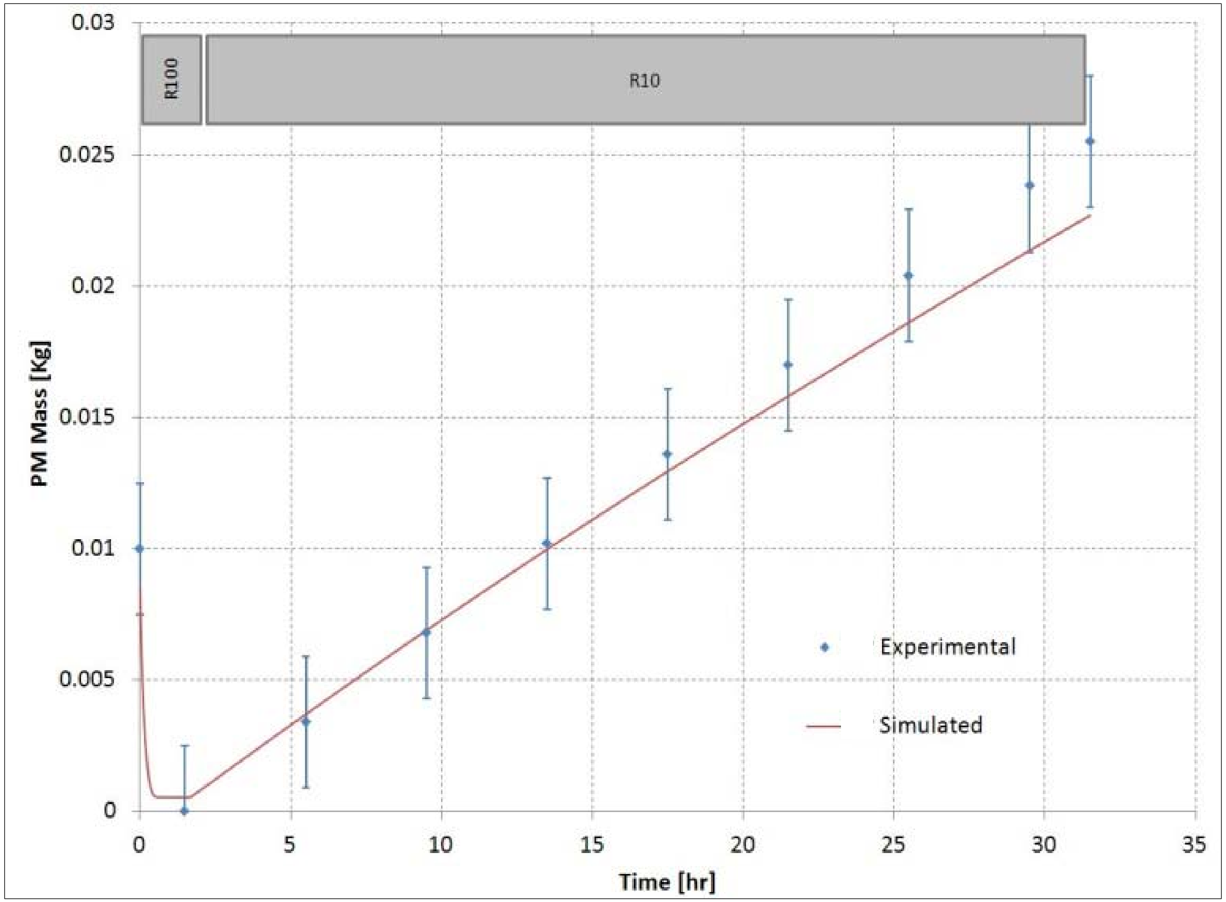
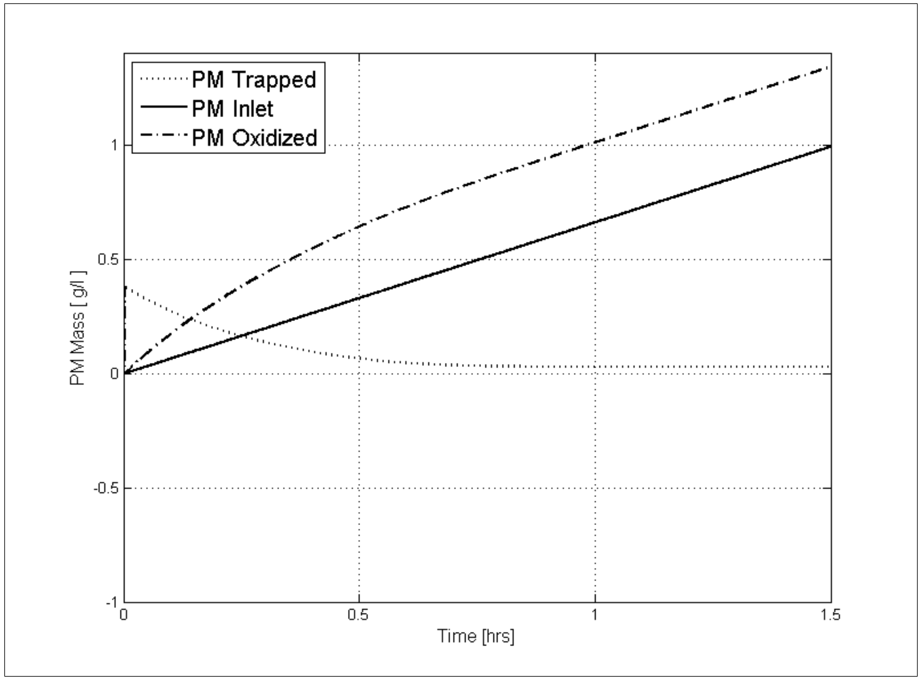
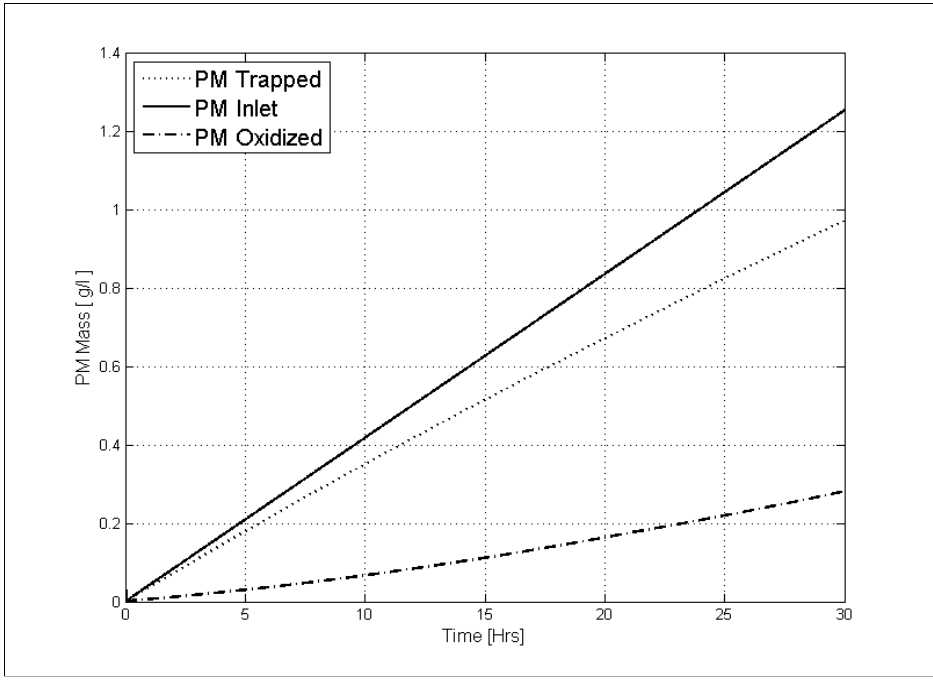
PM Mass (measured vs predicted)



PM inlet vs oxidized

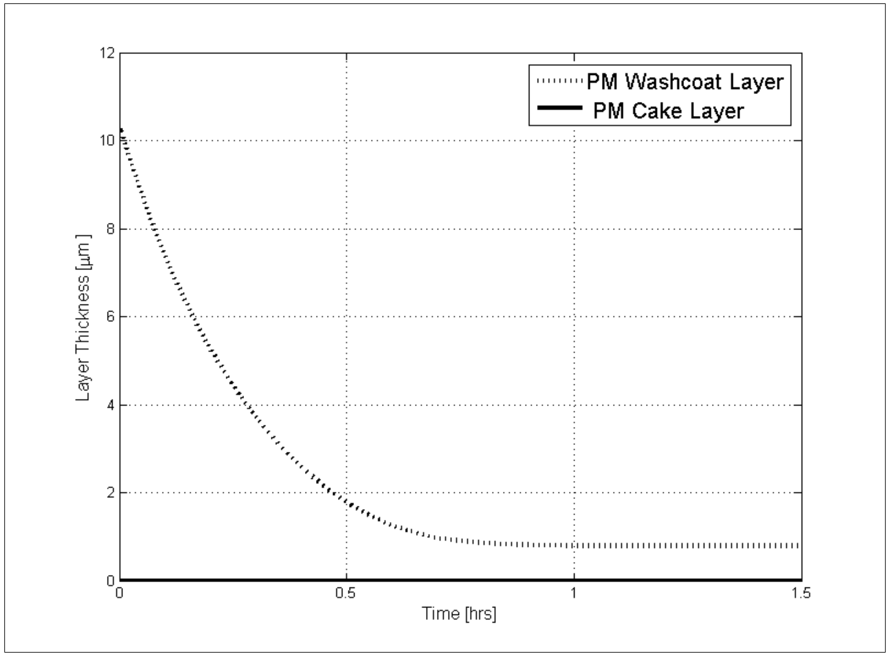


Mode R100

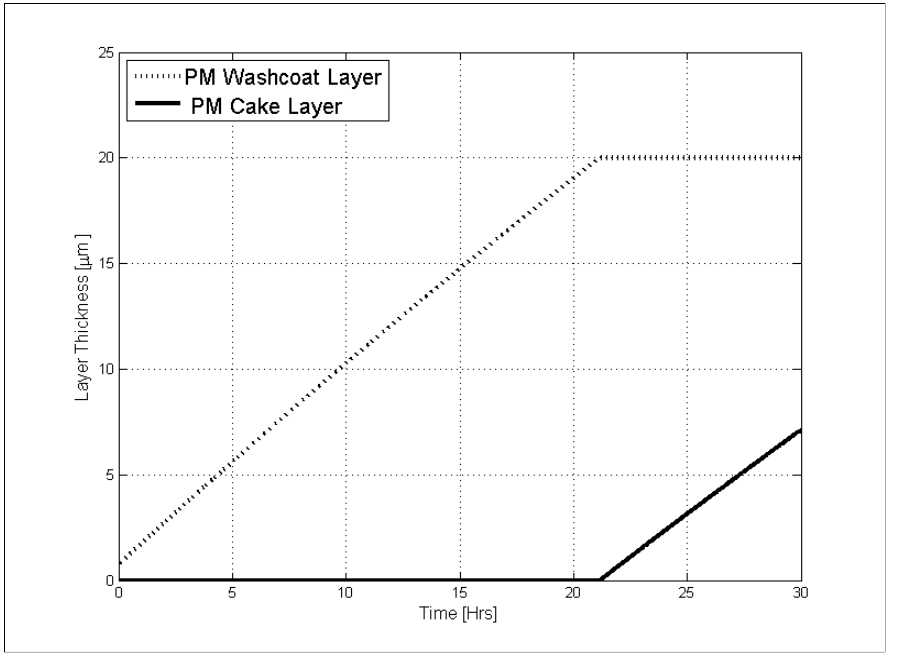


Mode R10

PM in the washcoat vs cake

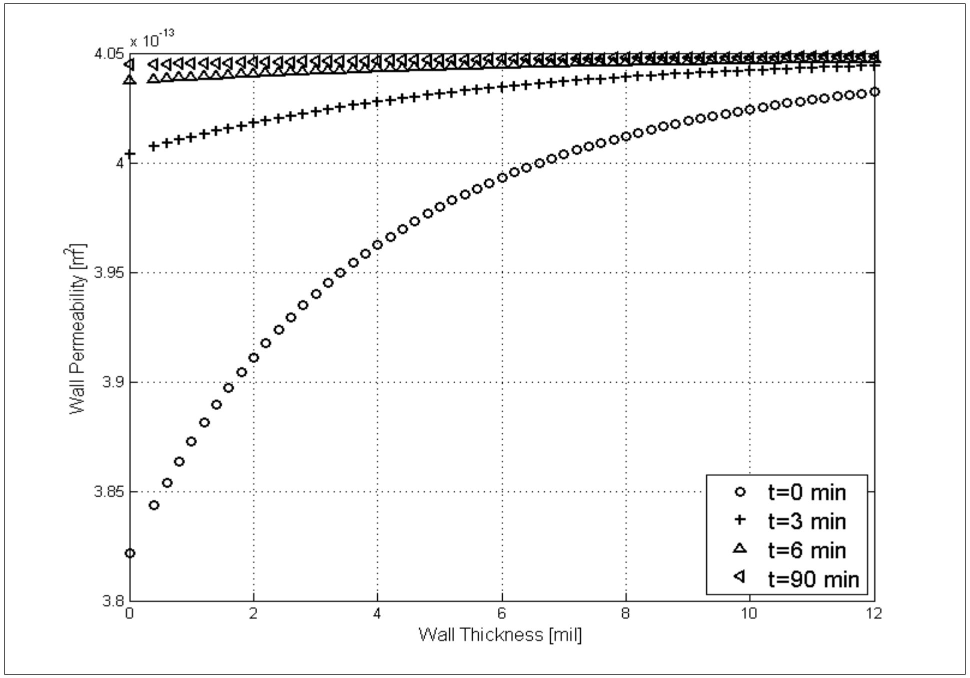


Mode R100

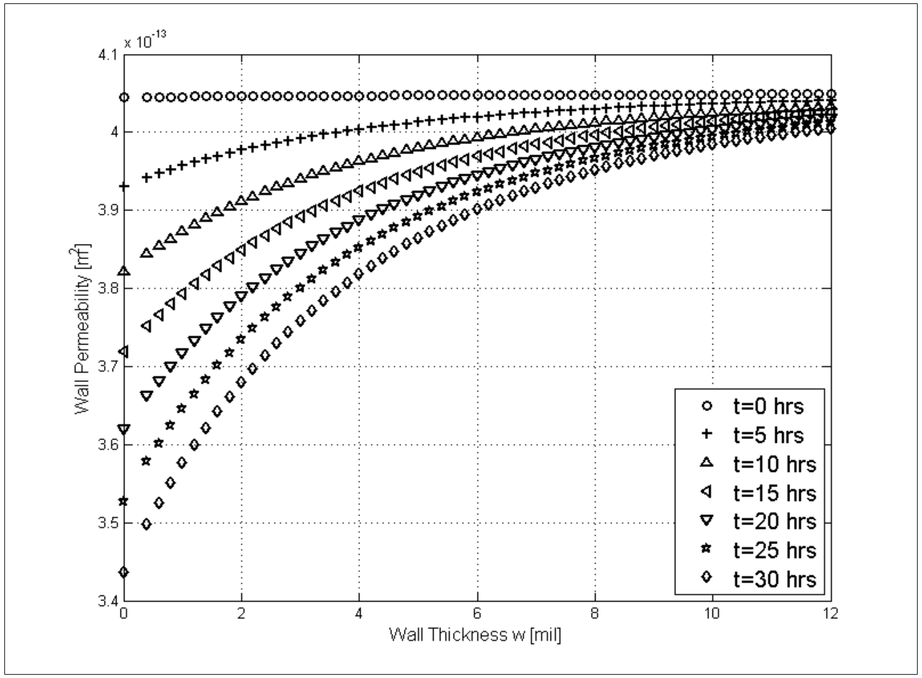


Mode R10

Wall permeability over thickness



Mode R100



Mode R10

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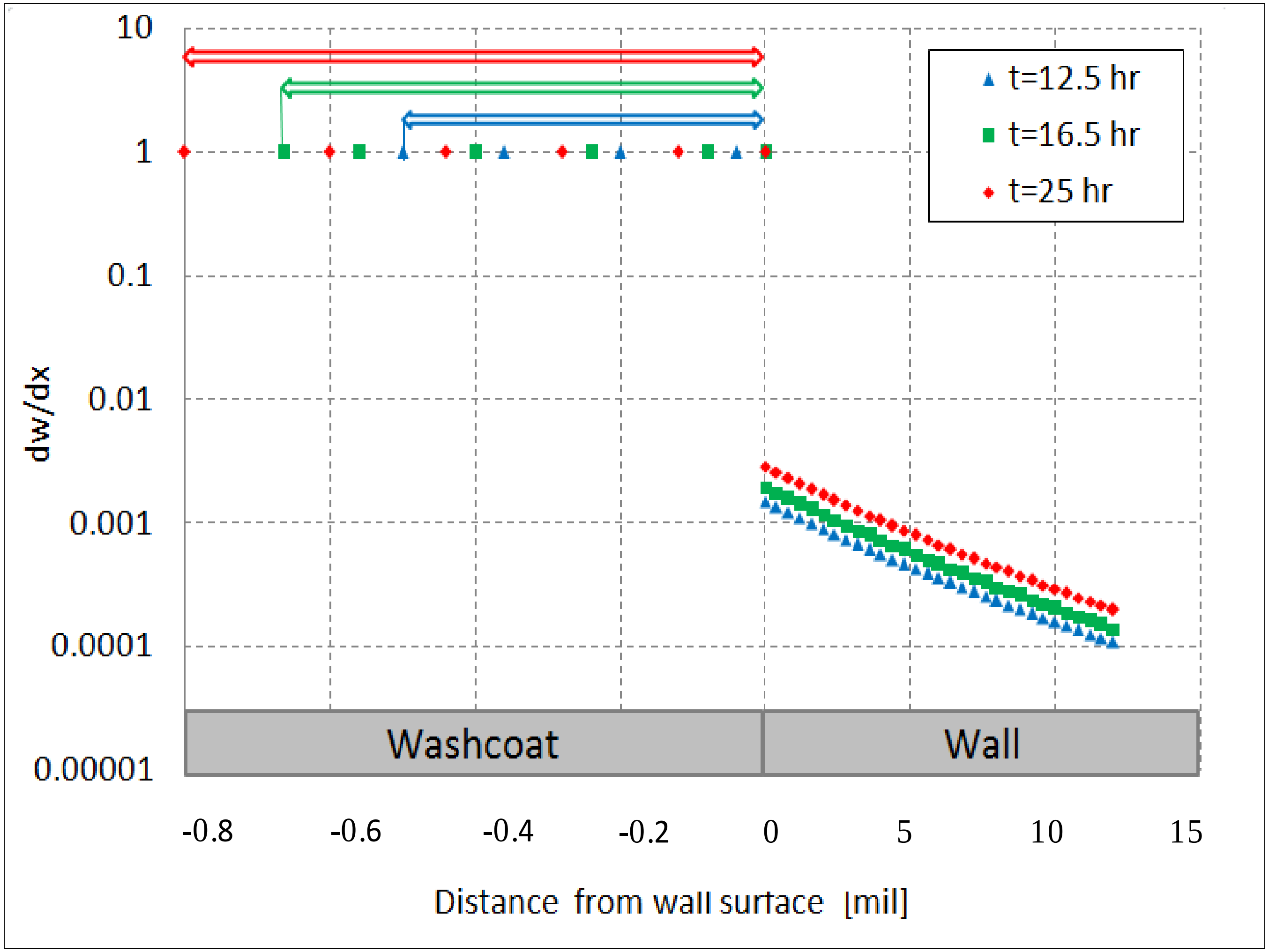
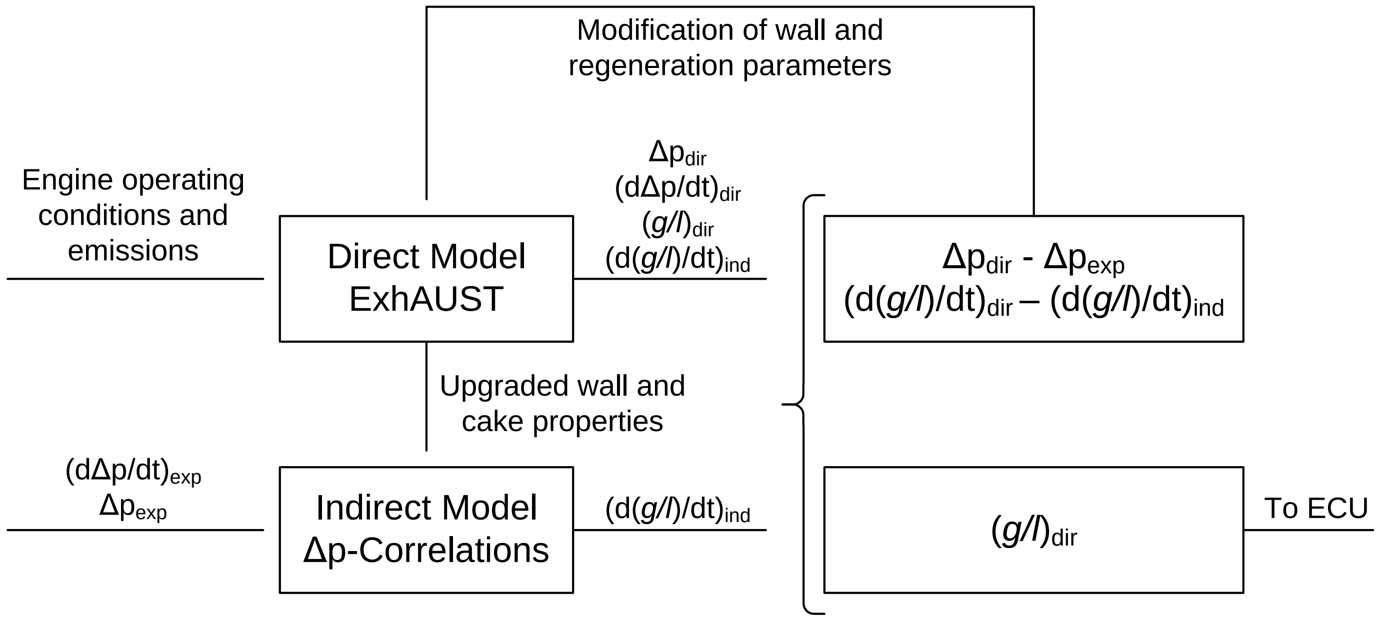
Equivalent cake thickness distribution: trend over R10 mode



Example of model-based control strategy for active regeneration events



- Strategy based on estimated DPF soot loading by real-time implementation of ExhAUST

Conclusions

- ExhAUST: control/design oriented after treatment code
- Full analytical treatment
  - Wall loading
  - Wall regeneration (integrated with cake)
- Satisfactory comparison with steady state HD engine experimental data
  - No different constant set in the two modes
- Next steps
  - Transient tests
  - Real Time
  - Integration with real time PM sensors for OBD

    Besch M. et al., "In-line, Real-time Exhaust PM Emissions Sensor for Emission Control and OBD Applications"

ExhAUST: SOOT MODEL FOR ADVANCED DESIGN AND CONTROL OF DIESEL ENGINE AFTERTREATMENT SYSTEMS

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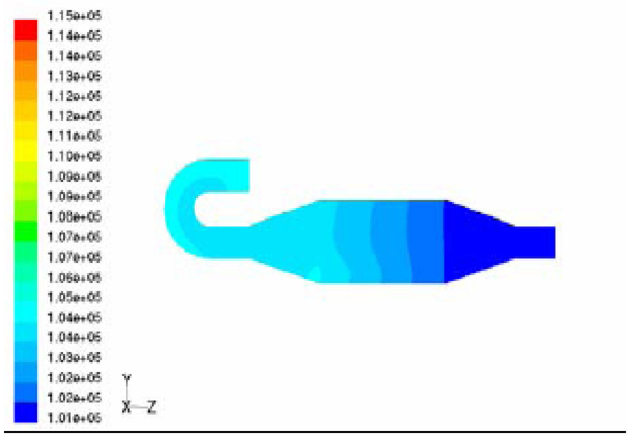
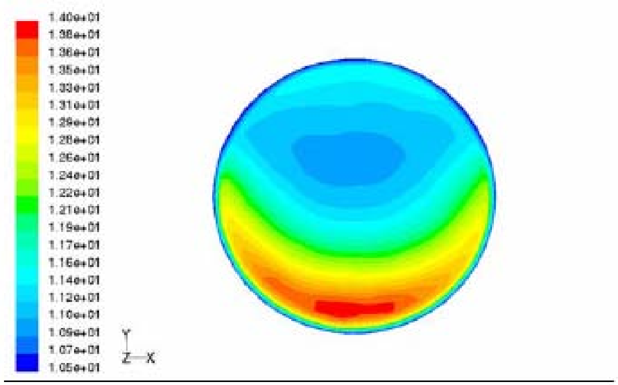
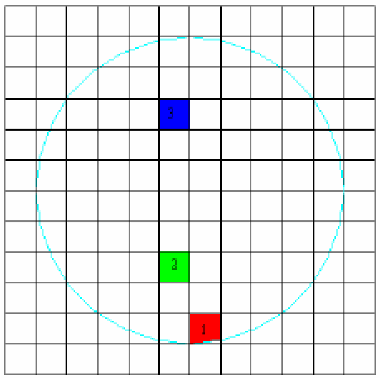
Examples of CFD coupling

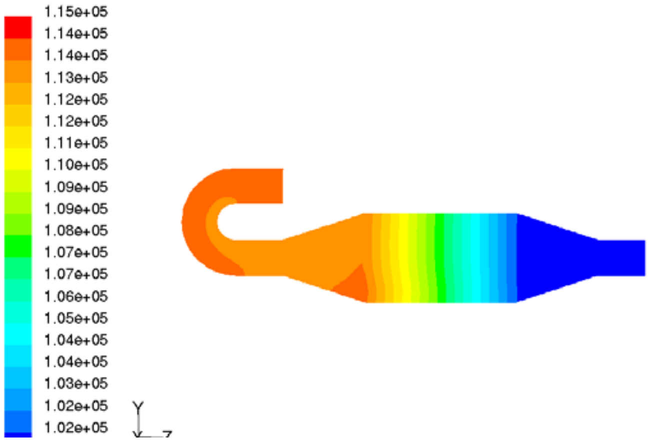


Pressure field (clean)

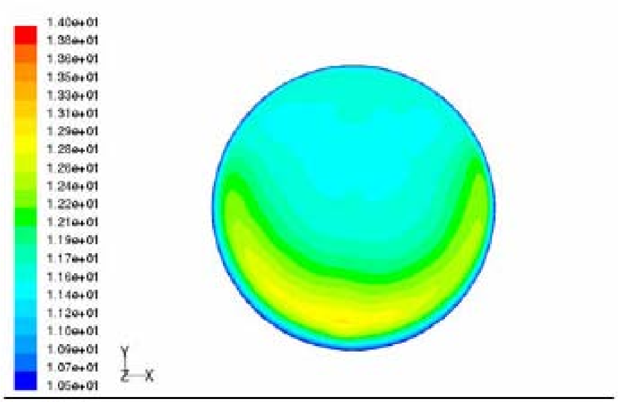


Velocity on the front section (clean)

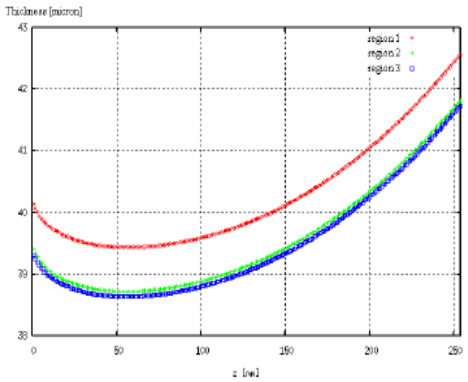




Pressure field (t=16h)



Velocity on the front section (t=16h)



Soot thickness vs DPF length for different regions (1,2,3) after 16h