DPF Modeling and Experimental Data to Support Model Development: Past Research and Future Directions

John H. Johnson
Presidential Professor
Michigan Technological University
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I Acknowledge the Support of:

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GM/DOE

John Deere/DOE

Navistar

Dow Automotive

DDC/DOE

that have supported our (MTU) DPF Research the past 10 years.

Overview of Presentation

- Past Recommendations by National Academies
- 21st Century Truck Partnership Testimony to House
- DOE RFP for Universities
- CLEERS Priorities
- Brief Literature Review
- MTU Early Work on Passive Regeneration and the Effect of Wall PM Mass on Pressure Drop Including a Cake Filtration Model
  - Modeling
  - Experimental Data
- MTU DPF Systems Model Using Lumped Model for Controls
- Using the MTU ID Model to Predict the Effect of Substrate Dimension Changes on Pressure Drop
- MTU Recent Work on Predicting PM Mass in the DPF
- MTU Present Work on Active Regeneration
  - Experimental Data – Approach
  - Activation Energy for Global Oxidation Model
  - Modeling Using I-D MTU Model
  - Results of Post Loading as Compared to Clean Filter Pressure Changes
  - Effect of Active Regeneration Temperature
  - Cake Break – Through
- NGK Membrane Filter Data
- MTU's ID Model for Active Regeneration
- Future Data Needs
- Future Modeling Needs
- From CLEERS Poll – Future Research

Past Recommendations by National Academies

- “Review of the Research and Development Plan for the Office of Advanced Automotive Technologies,” National Academy Press, 1998.
  - Pg. 36, “Recommendation. The OAAT should ensure that its program includes a major engineering effort to integrate particulate traps, reducing and oxidizing catalysts, plasmas, and fuel additives, as well as advanced materials, sensors, and controls, into a complete after-treatment system to control emissions. The program should include both hardware development and modeling.”

Past Recommendations by National Academies

- "Review of the U.S. Department of Energy's Heavy Vehicle Technologies Program," National Academy Press, 2000.
  - "Recommendation 4. The Office of Heavy Vehicle Technologies should place a high priority on integrated emissions-control technology (engine combustion and after-treatment technologies) to meet future emission requirements. Research and Development (R&D) should be focused on sulfur tolerant catalysts, sulfur traps, and selective catalytic reduction, for diesel fuel with sulfur levels of 5 to 50 parts per million. R&D should be focused on both experimental work and modeling related to basic in-cylinder combustion and after-treatment technologies."

Past Recommendations by National Academies

- “Review of the 21st Century Truck Partnership,” National Academy Press, 2008.
  - “Finding 3-16. No specific goals have been outlined for 21CTP diesel engine after-treatment systems but some goals have been set for eliminating after-treatment. However, as discussed in this chapter, the goal of eliminating after-treatment does not appear to be achievable in the foreseeable future.”
  - “Recommendation 3-16. Specific goals should be set for after-treatment systems (improved efficiency, lower fuel consumption, lower cost of substrates, lower cost catalyst, etc).”
  - “Finding 3-17. The CLEERS, DCT, CRADAS have contributed to many successful projects and programs.”
  - “Recommendation 3-17. The 21CTP should continue with the CLEERS, DCT, and CRADA activities for after-treatment systems.”

21st Century Truck Partnership Testimony to House

"Testimony on the R & D Needs for the 21st Century Truck Partnership Program based on the Review of the Program by the National Academies U.S. House Subcommittee on Energy & Environment of the Committee on Science & Technology," March 24, 2009, Dr. John Johnson.

- "In light of the potential fuel economy regulations by NHTSA as required by Section 102 of EISA, it is important that the Federal government fund the DOE program at levels such as $200 million/year with $90 million/year for engine, emission control systems, and biodiesel fuels research. The program should be funded for 5-10 years at this level so that the industry will have the technology in the 2015-2020 timeframe to meet potential fuel economy regulations. Safety is an important part of the program with support in the past from DOE and DOT, with DOT providing the majority of the budget. As crash protection measures have not substantially reduced highway fatalities during the past decade, the main objective going forward will be to prevent crashes using crash avoidance technologies and in-vehicle communications systems. There is need for $25 million per year for safety related research which should be designated for DOT by line item for the 21st Century Truck Partnership."

DOE RFP for Universities – University Research in Advanced Combustion and Emissions Control

- Issue Date: 11/14/08
  Application Due Date: 01/16/09
  Area of Interest 2: Efficient Emission Control Devices
- "Applications submitted under this Area of Interest shall support the overall effort in modeling of emission control (after-treatment) devices as described at www.cleers.org.
- Example research subjects would include but are not limited to:
  - Experiments and/or models to improve understanding of diesel particle filter phenomena at the soot cake layer and filter regeneration for DI gasoline and diesel applications."
    (Only DPF subject listed.)

Major Highlights Of CLEERS Poll Findings Relative To DPF’s(2008)

- DPF’s are still a primary area of recognized need
- OBD for DPF’s are of more concern than before

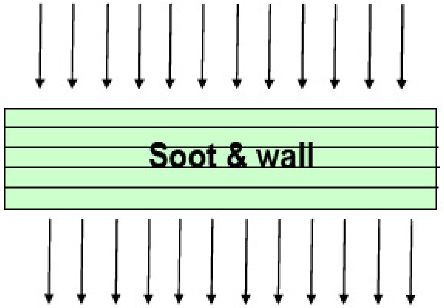
•Diesel Responses – Top Priorities	•Weighted Score (2008)
1. Urea SCR Durability and Poisoning	10
6. Diesel Particulate Filter/Reaction Mechanism	3
7. Diesel Particulate Filter Kinetics/Reaction Mechanism: Reaction Rates for passive and active regeneration of soot	3
8. Diesel Particulate Filter Kinetics/Reaction Mechanism: Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles (including particles from advanced combustion and alternate fuels)	3
9. Diesel Particulate Filter Kinetics/Reaction Mechanism: Capture, generation, and release of nano-particles	3
10. Diesel Particulate Filter OBD and Sensors: Accurate estimation of soot loading and prediction of regeneration exotherm.	3

Brief Literature Review

- Observations by JHJ
  - Experimental and modeling results are complimentary
  - Quality experimental data are needed to support modeling development
  - Both modeling and experimental data have inaccuracies
  - Models can calculate quantities that can not be determined experimentally

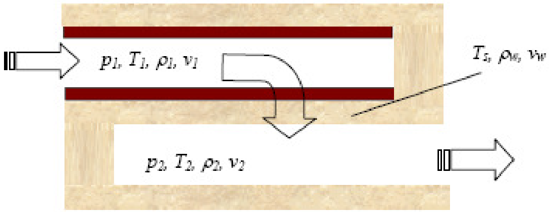
Representations of Filter Geometry

0-d



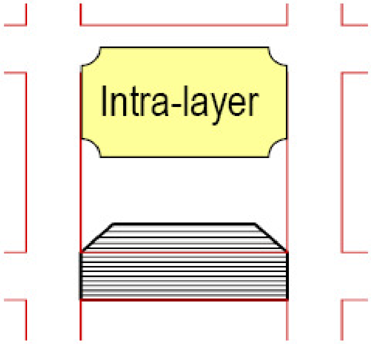
Representative channel
& axial uniformity

1-d



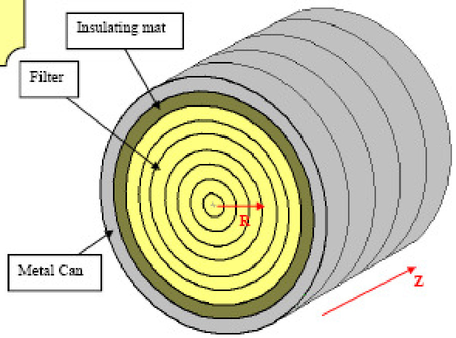
Representative channel
(adiabatic, uniform inlet flow)

Intra-layer



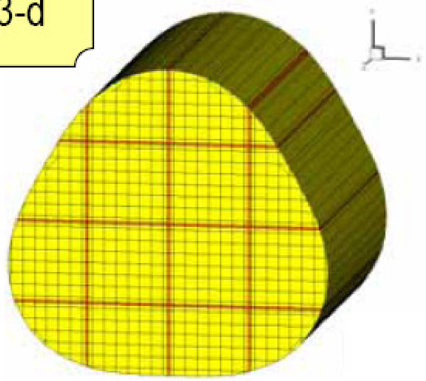
Catalyst effects
soot layer properties

2-d



Axi-symmetric, non-segmented filter
(circular shape, symmetric flow distribution)

3-d



Random shape, segmentation
any flow distribution

** Koltsakis et al – CTI 2008*

Research in Particulate Filter Modeling - 1

1983 (SAE) – Pauli
1984 (Chem. Eng. Sci.) – Bissett
1988 (SAE) – Garner et al
1989 (SAE) – Konstandopoulos/Johnson
1998 (SAE) – Opris/Johnson (2-D)
2001 (SAE) – Konstandopoulos et al (quasi 3-D)
2002 (SAE) – Hunyh et al (MTU CPF 1-D Model)
2003 (SAE) – Konstandopoulos et al (multi-channel/quasi 3-D)
2003 (SAE) – Kladopoulou et al (Lumped)
2003 (SAE) – Haralampous et al (2-D Regeneration Model)
2004 (SAE) – Wangard (3-D CFD)
2005 (Proc. IMechE) – Law et al (2-D)
2005 (SAE) – Koltsakis et al (3-D Regeneration)

Research in Particulate Filter Modeling - 2

2005 (MTU PhD Thesis) – Triana (MTU CPF 1-D Model + NO_2 oxidation)

2005 (SAE) – Singh et al (Lumped Systems)

2005 (SAE) – Law et al (2-D)

2006 (J. Eng. Gas Tur. & Pow.) – Pontikakis et al (SiC DPF 3-D regeneration model)

2006 (SAE) – Yi et al (Fluent 3-D CFD Macroscopic Model)

2006 (SAE) – Mohammed et al (MTU CPF 1-D Model + wall PM oxidation + PM cake filtration + heat addition)

2006 (SAE) – Singh et al (experimental - active regeneration of CPF)

2007 (SAE) – Premchand/Johnson/Yang (MTU CPF 1-D model + data analysis)

2007 (SAE) – Hinterberger et al (ArvinMeritor)

2007 (Top. In Cat.) – Frey et al (2-D regeneration model)

2008 (SAE) – Koltsakis et al (multi-channel quasi 3-D regeneration model)

2009 (SAE) – Premchand et al (MTU 1D 2 Layer Active regeneration model)

MTU Early Work on Passive Regeneration and the Effect of Wall PM Mass on Pressure Drop Including a Cake Filtration Model

An Advanced 1D 2-Layer Catalyzed Diesel Particulate Filter Model to Simulate: Filtration by the Wall and Particulate Cake, Oxidation in the Wall and Particulate Cake by NO2 and O2, and Regeneration by Heat Addition

Hasan Mohammed – Cummins/Michigan Technological University
Antonio Triana – John Deere/Michigan Technological University
S.L. (Jason) Yang – Michigan Technological University
John H Johnson – Michigan Technological University

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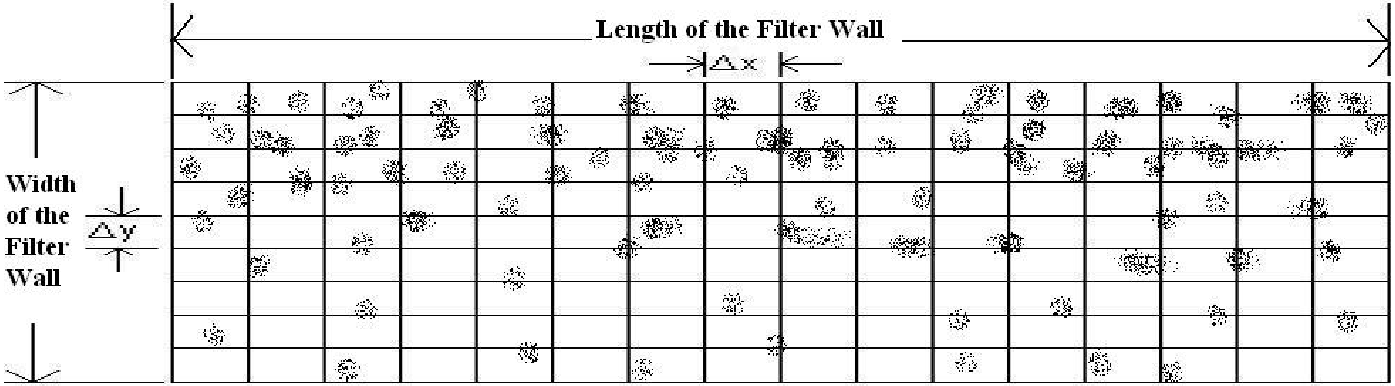
Wall oxidation model

- Modeling accurate PM oxidation in the wall is difficult, because the physical structure is not well defined.
  - Simplifying assumptions have to be made.
  - Should be computationally feasible
  - Numerical solution with small PM mass in wall should not allow numerical errors to propagate.
  - Regeneration framework should be compatible with that of the PM cake layer.

Wall Oxidation Model



- For each axial discretized location, sum all the PM present in each of the 'slabs' of the filter wall and form a 'virtual' wall layer.
- Determine reaction rates in the wall such that if a similar amount of PM were present on the wall under the same conditions, they would both deplete by the same rates.
- Determine the O_2 and NO_2 exiting layer I and entering the filter wall.
- Regeneration equations similar to those in layers I and II, can be applied.

Particulate Cake Layer Filtration Model

- The wall oxidation model does not couple properly with the overall filtration-oxidation model.
- Once the cake forms, it is more natural and useful to describe the filtration by means of PM cake parameters which are separate from the wall.
- In this approach, the PM cake and filter wall are two separate filters in series.
  - Depending on its thickness, oxidation in the PM cake layer can affect filtration by the wall.
  - Oxidation in the wall does not affect filtration by the PM cake layer.
- The PM cake filtration model assumes that the particles it filters increase its thickness while keeping the diameter of the unit collector and the porosity constant.

Particulate Cake Layer Filtration Model

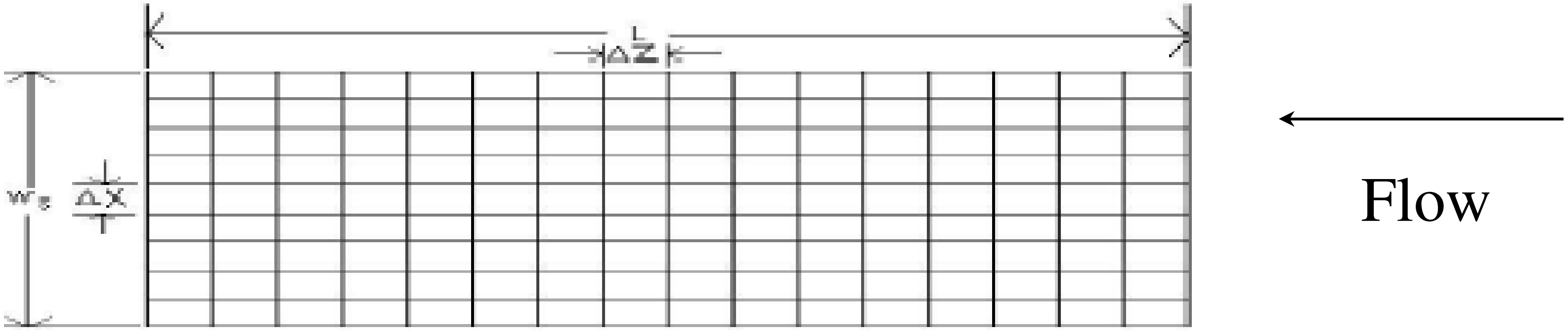
- PM cake filtration is simulated by a parametric equation as shown below, which relates the efficiency of the cake layer to its thickness and collection efficiency of each collector.
- The parameter n_C is related to the collection efficiency of each of the unit collectors in the cake.
- The parameter A_n is used to predict efficiencies less than 100% for cake thicknesses greater than um.

$$\eta_{cake} = A_{\eta} . \left(1 - e^{-\eta_c \cdot \frac{w_{cake}}{dc_{cake}}}\right)$$

CPF Wall Filtration Model

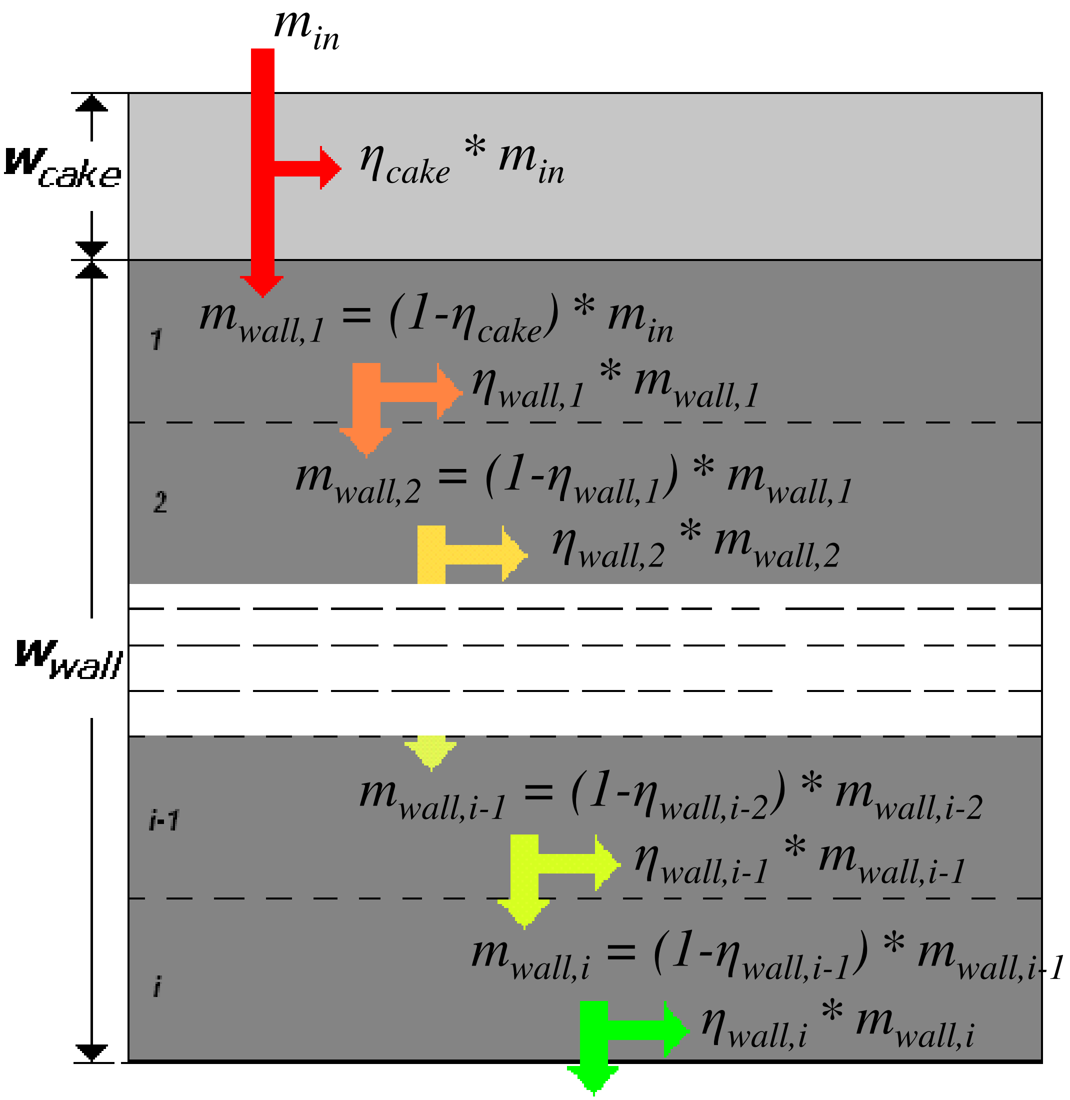
- Wall Filtration model is based on SAE:2000-01-1016 by Konstandopoulos et.al.
- Simulate filtration of PM by ‘unit collectors’ to model depth filtration phenomenon.
- Particles not captured by the PM cake layer, enter the filter wall.
- Particles of relatively small diameters (<100nm) are primarily collected by Brownian diffusion.
- Larger particles are collected by direct interception.

CPF Wall Filtration Model



- For computational purposes, the filter wall is discretized in the axial direction.
- Because the properties of the wall change in the transverse direction due to PM collection, the thickness of the wall is divided into a number of layers as shown above.
- The result is a computational domain as shown above.

PM Filtration – 2 Sequential Filters Approach



m_{in}

$\eta_{cake} * m_{in}$

$m_{wall,1} = (1-\eta_{cake}) * m_{in}$

$\eta_{wall,1} * m_{wall,1}$

$m_{wall,2} = (1-\eta_{wall,1}) * m_{wall,1}$

$\eta_{wall,2} * m_{wall,2}$

$m_{wall,i-1} = (1-\eta_{wall,i-2}) * m_{wall,i-2}$

$\eta_{wall,i-1} * m_{wall,i-1}$

$m_{wall,i} = (1-\eta_{wall,i-1}) * m_{wall,i-1}$

$\eta_{wall,i} * m_{wall,i}$

$m_{out} = (1-\eta_{wall,i}) * m_{wall,i}$

An Experimental and Modeling Study of a Diesel Oxidation Catalyst and a Catalyzed Diesel Particulate Filter Using a 1-D 2-Layer Model

Hasan Mohammed – Cummins/ Michigan Technological University
Venkata Lakkireddy – Cummins/ Michigan Technological University
John H Johnson - Michigan Technological University
Susan T Bagley - Michigan Technological University

MichiganTech

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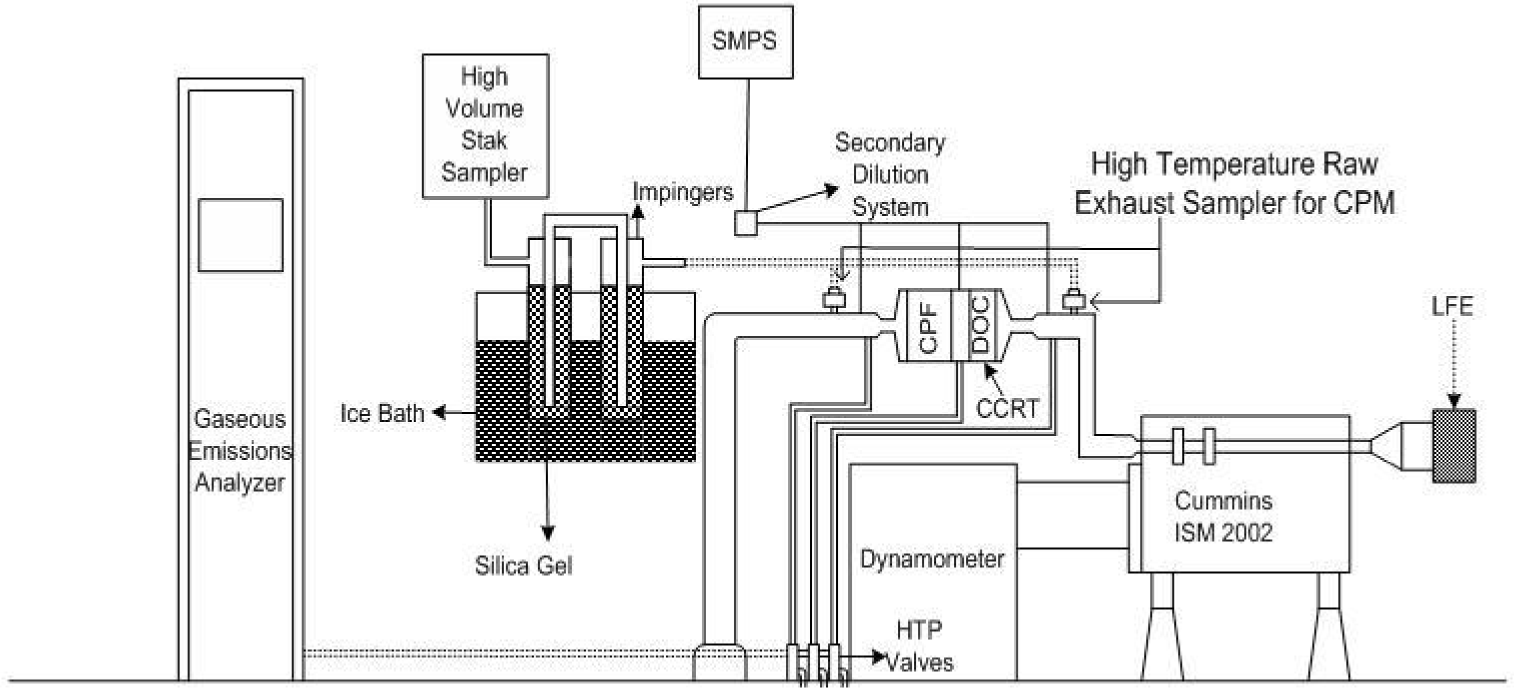
Experimental Test Setup



CCRT: Catalyzed Continuously Regenerating Trap
CPF: Catalyzed Particulate Filter
HTP: High Temperature Pneumatic
CPM: Carbonaceous Particulate Matter

LFE: Laminar Flow Element
DOC: Diesel Oxidation Catalyst
SMPS: Scanning Mobility Particle Sizer

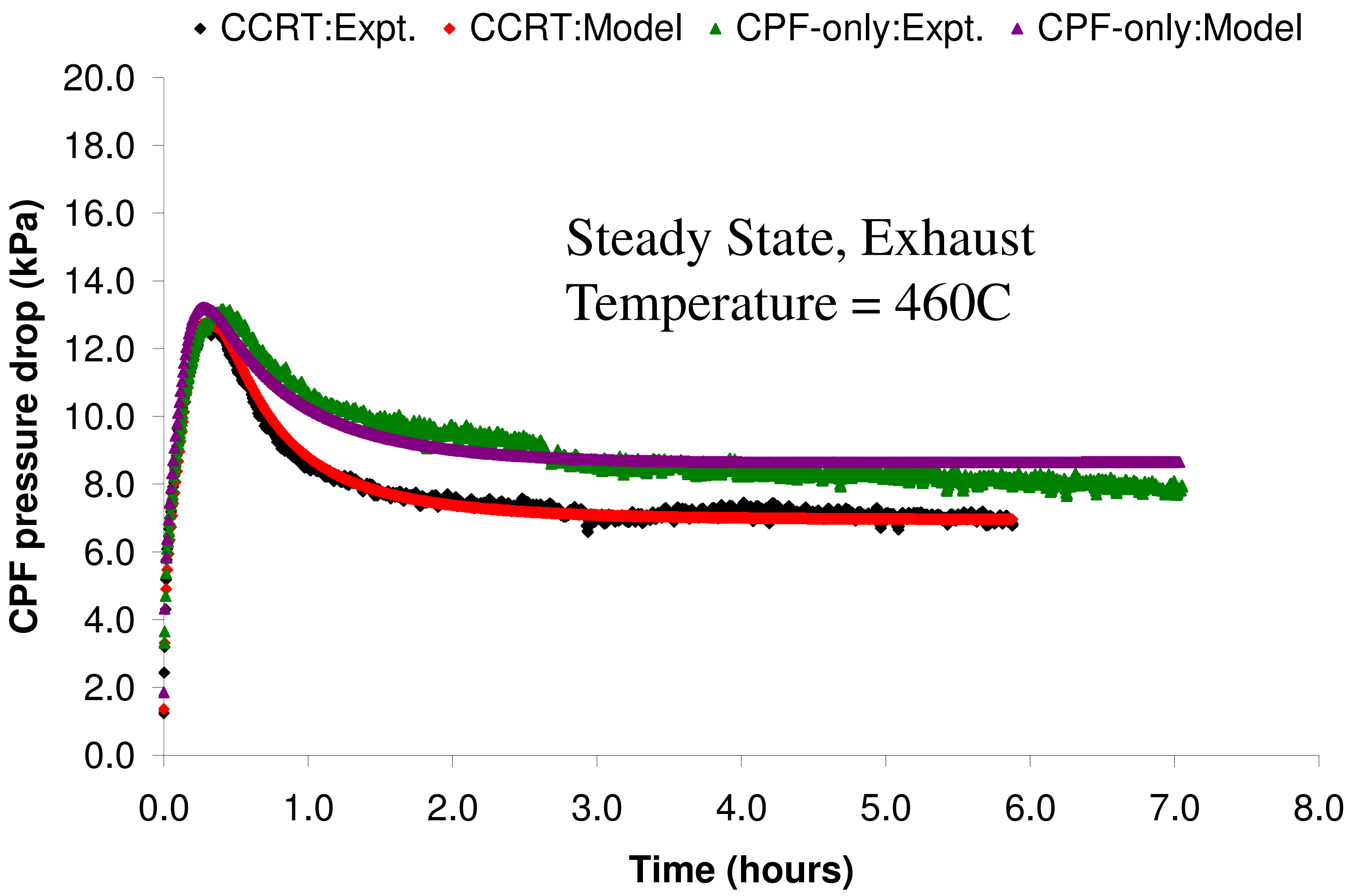
-Fuel was ultra low sulfur fuel with ~0.3 ppmS

Experimental Test Matrix

Description	20% Load	40% Load	60% Load	75% Load
Load (Nm) at 2100 rpm	224	448	672	840
Configurations	CPF-only & CCRT®	CPF-only & CCRT®	CPF-only & CCRT®	CPF-only & CCRT®
Temperature (^oC)	280	340	415	460

- Study the effect of temperature on PM oxidation by performing experiments at different loads
- Study the effect of NO_2 concentrations at each load, by performing the experiments with and without the DOC upstream of the CPF

75% load: CCRT® and CPF-only



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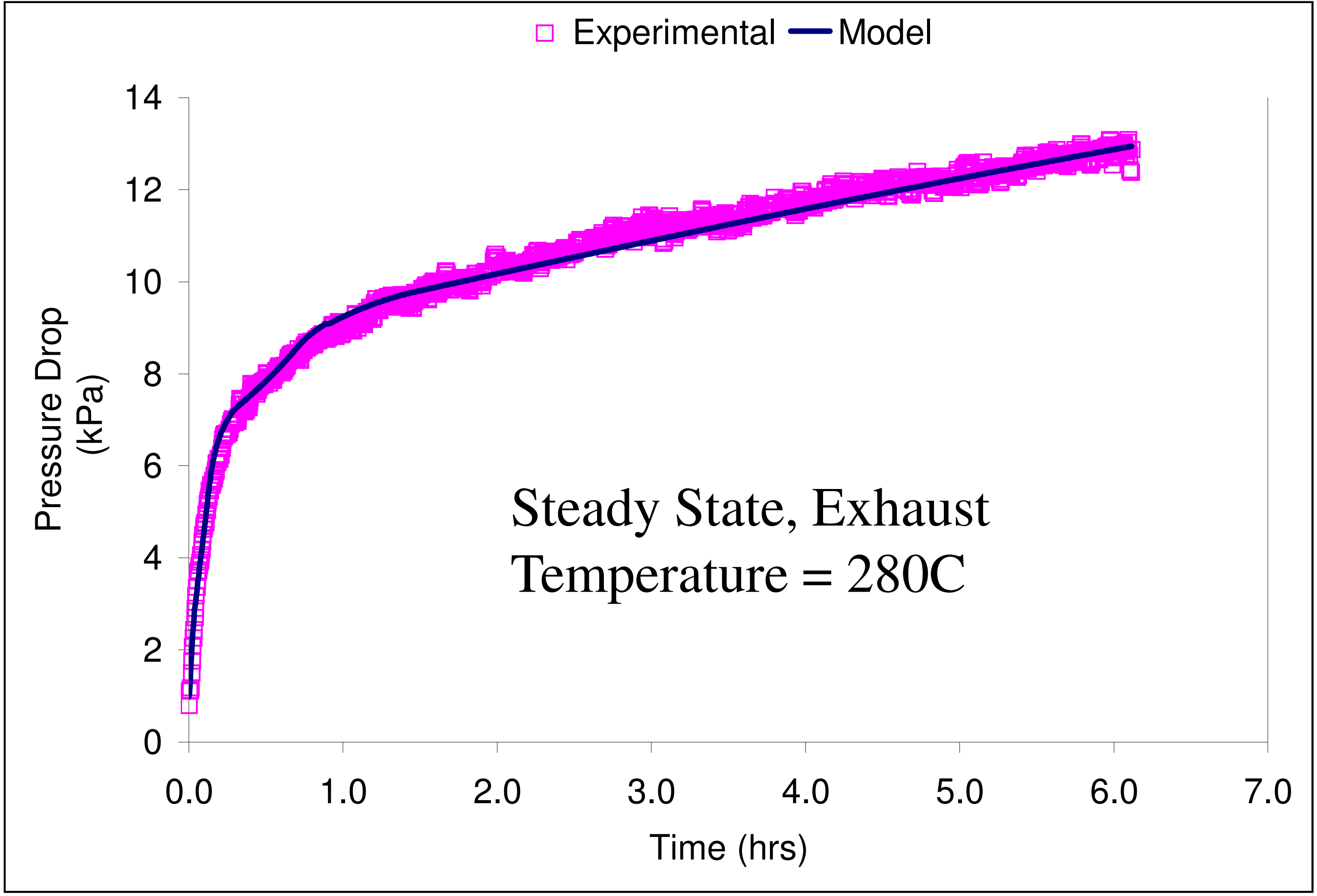
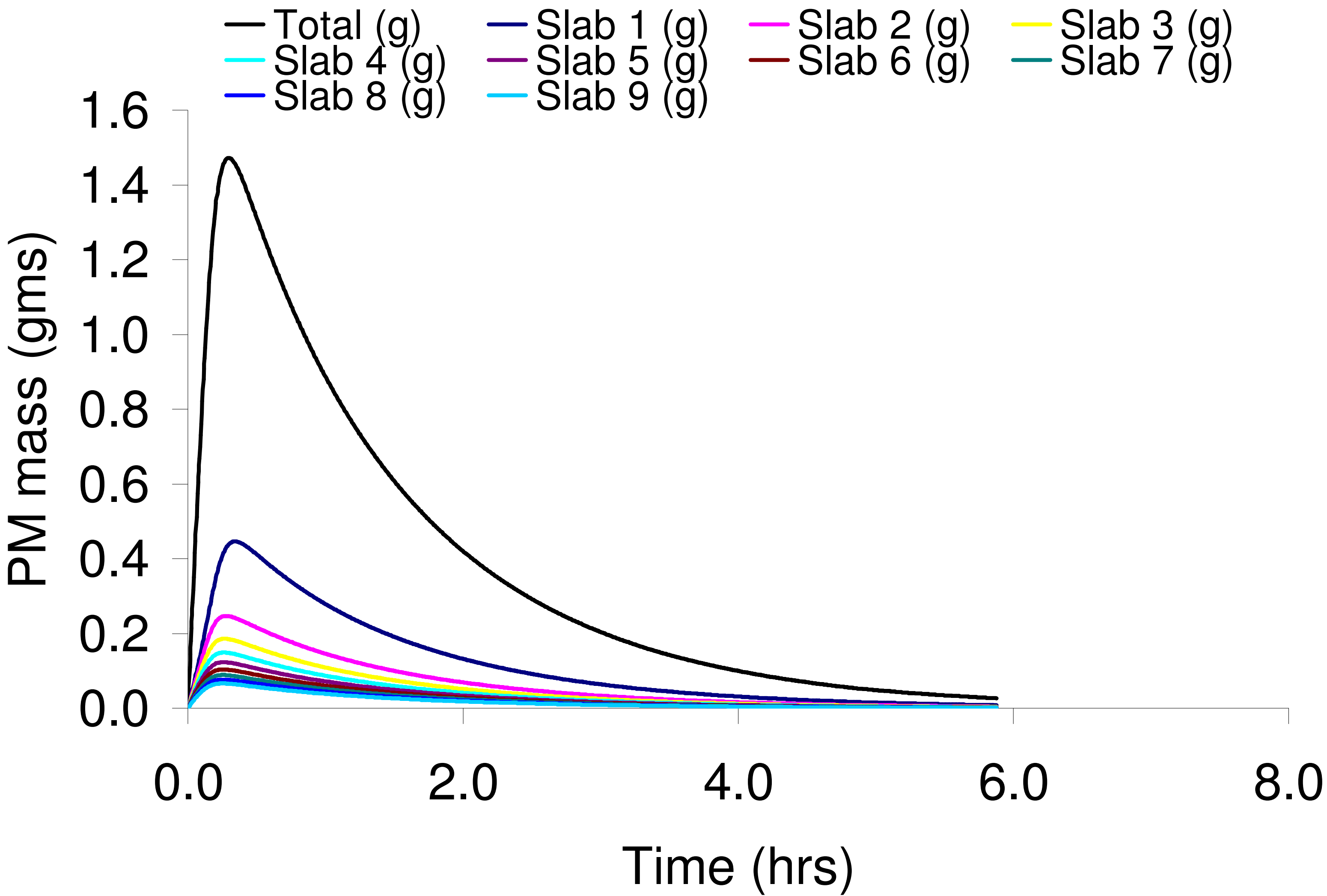
2006-01-0466

20% load: Pressure drop in CCRT® configuration



Oxidation in the wall at 75% CCRT®



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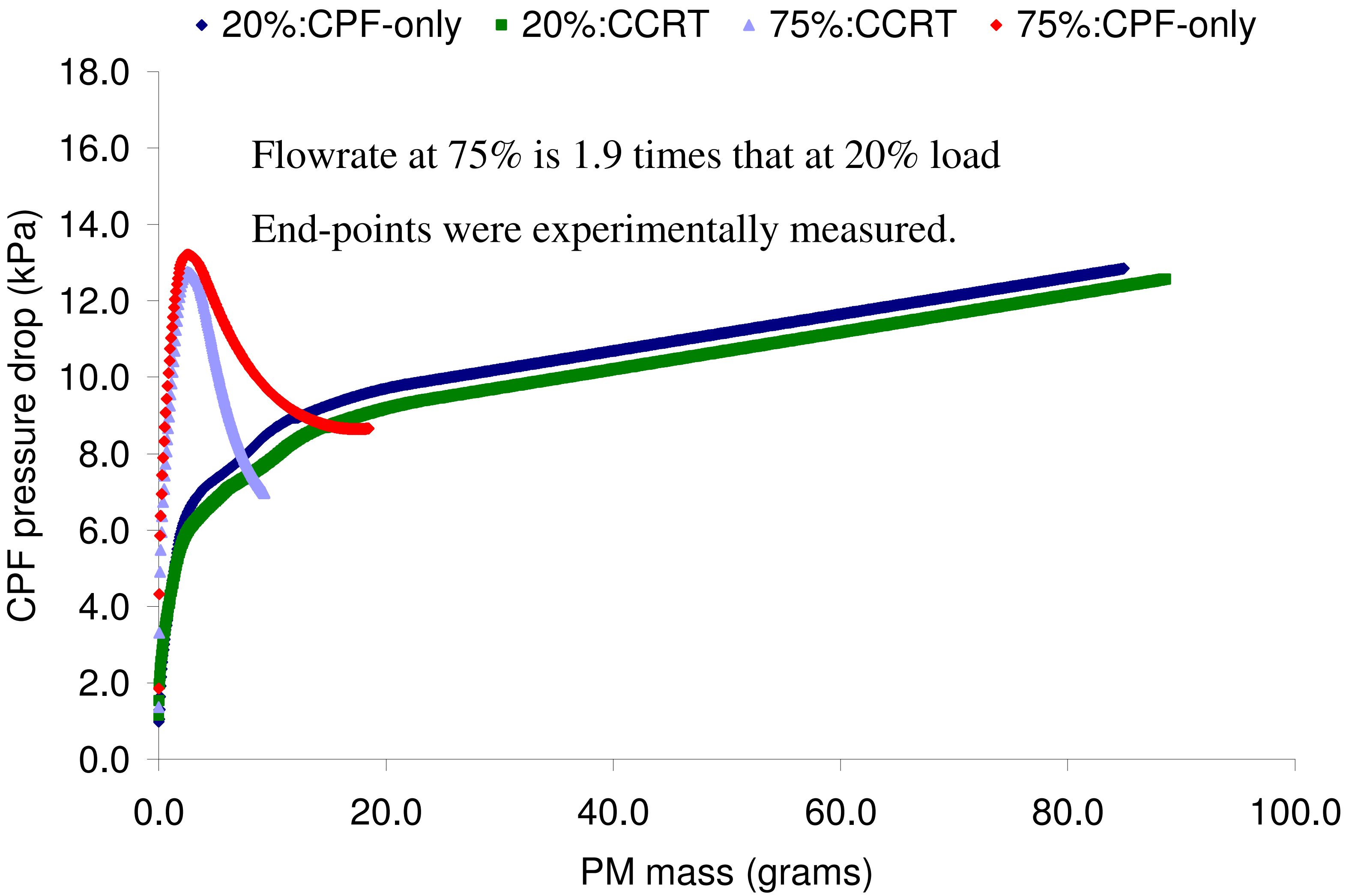
CPF Pressure drop with PM Load



Flowrate at 75% is 1.9 times that at 20% load

End-points were experimentally measured.

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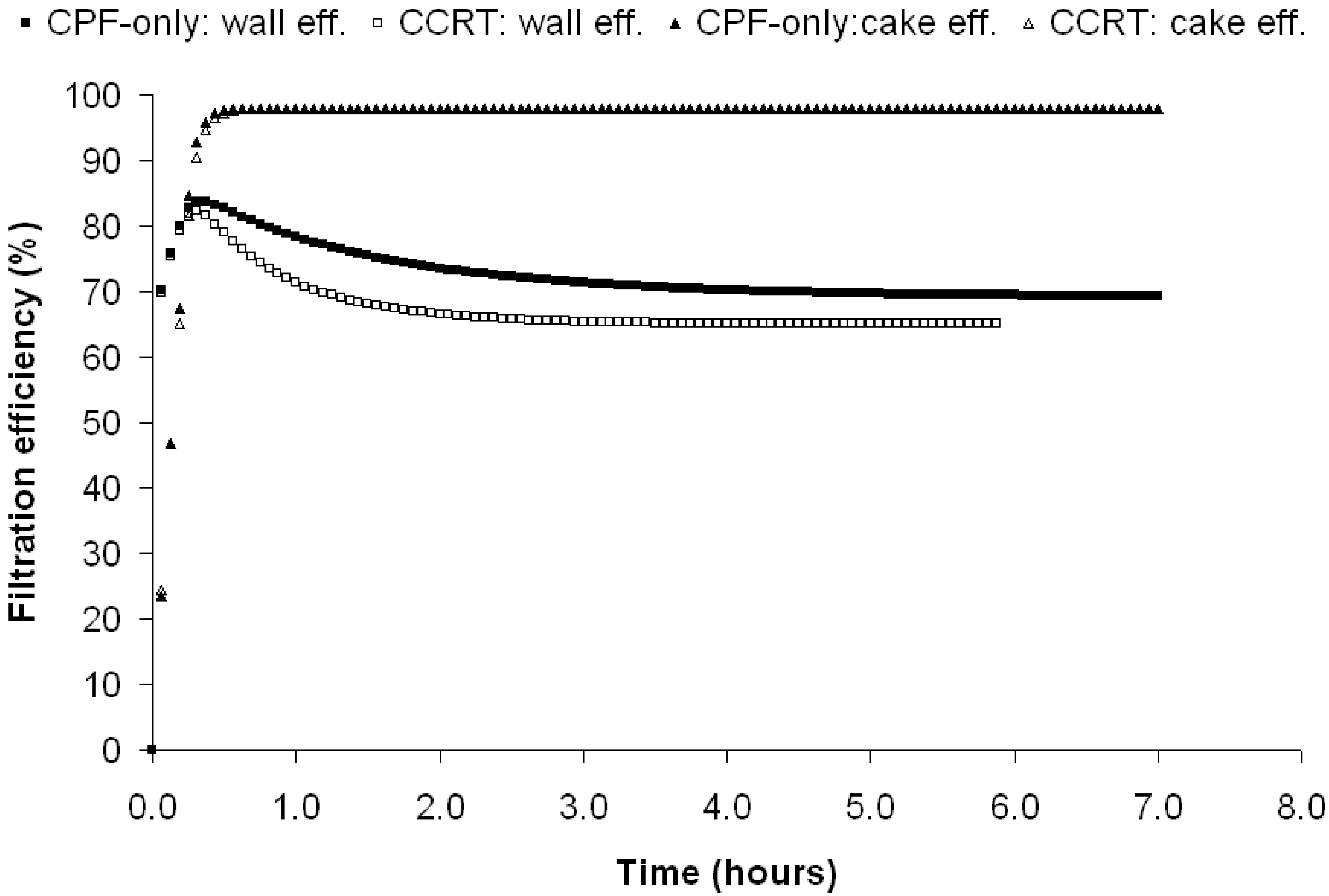
75% load CCRT®: Filtration Efficiency



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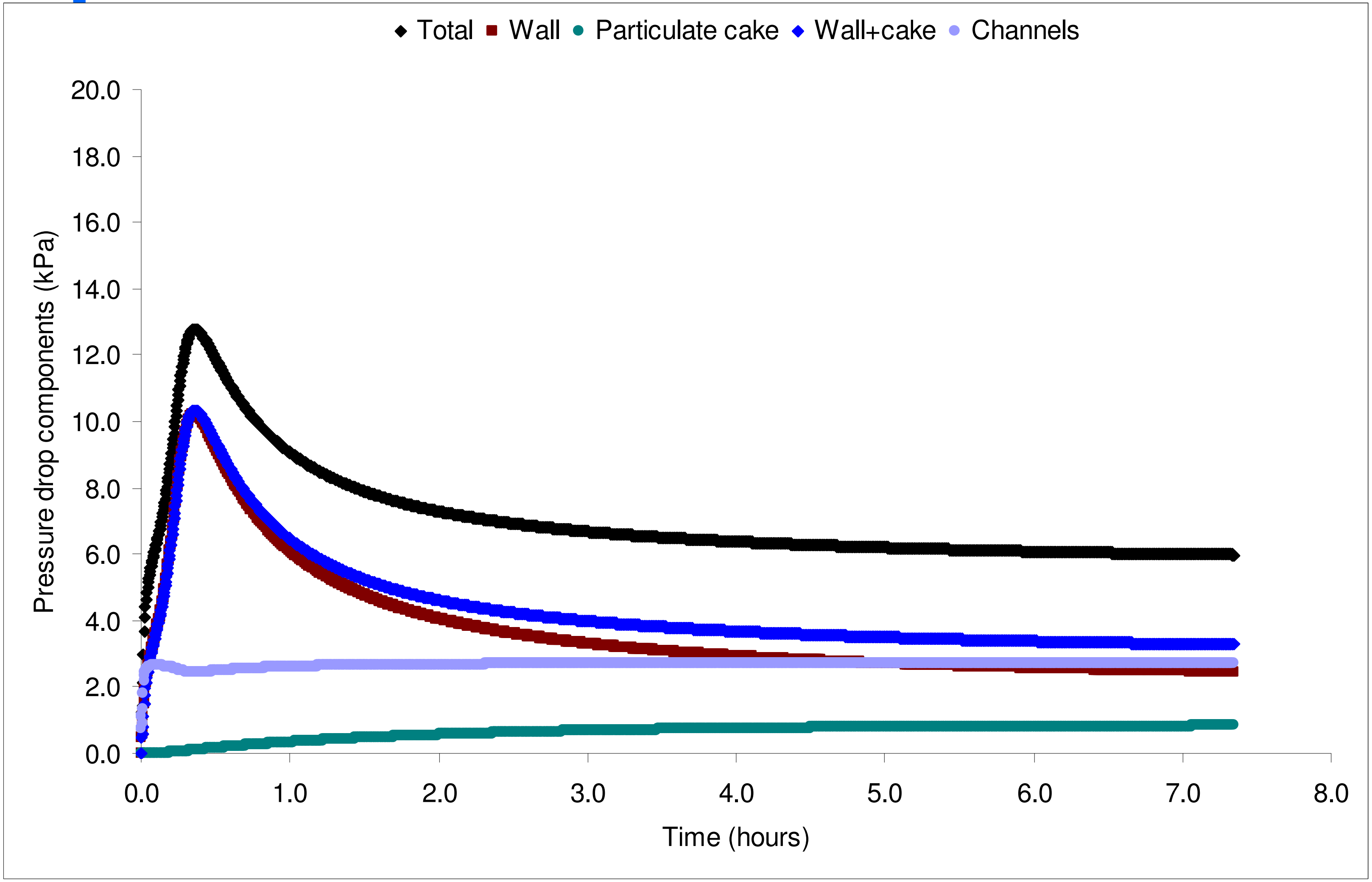
2006-01-0467

60% DOC + CPF: Pressure drop components



Summary and Conclusions

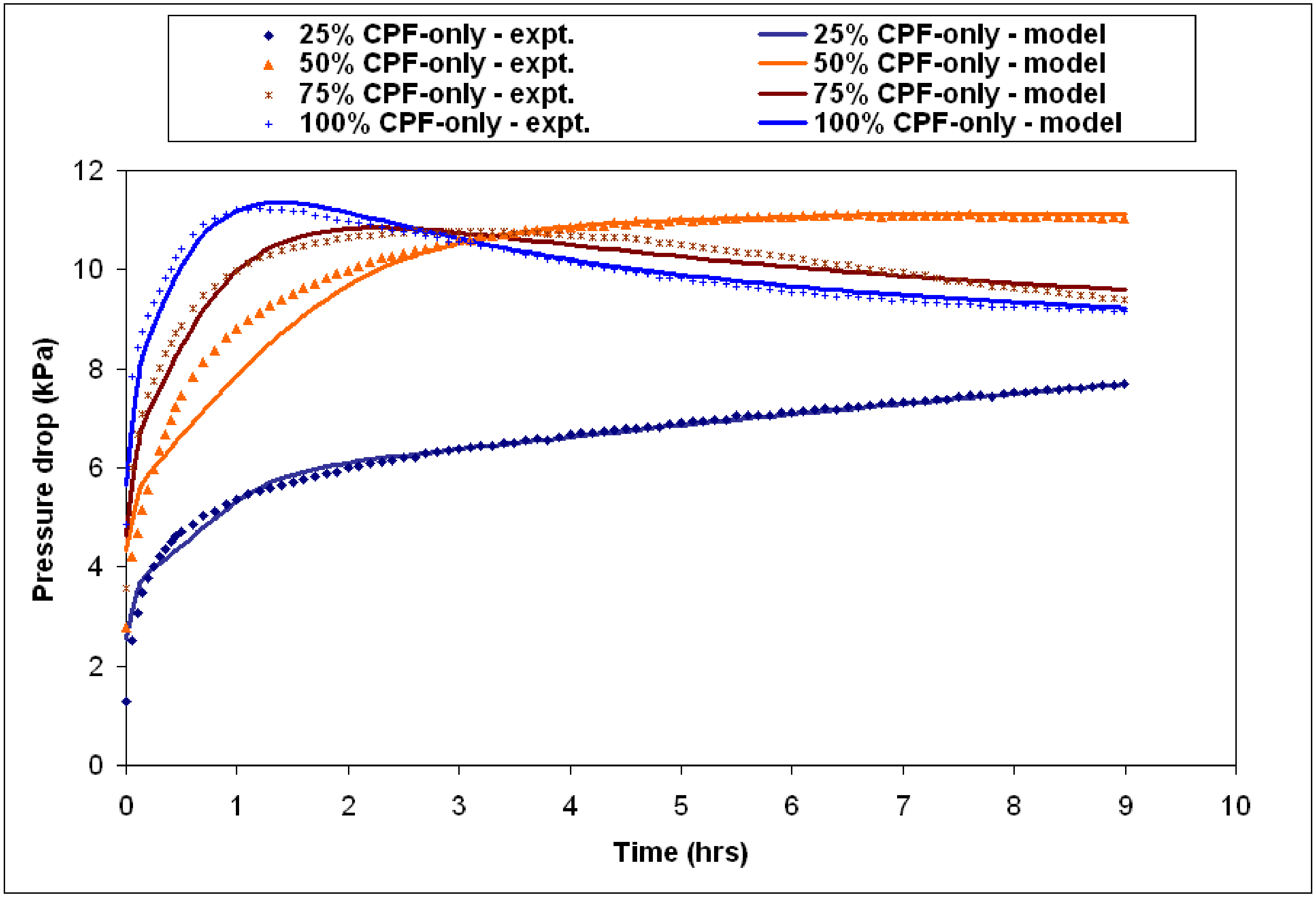
- The model showed that NO_2/Temperature is the dominant means of PM oxidation in the temperature range of 280^{o}C – 460^{o}C. Layer I (first 20um) was the dominant physical location of PM oxidation.
- For the CPF-only configuration, the catalyst in the CPF significantly increases PM oxidation rates.
- For the CCRT® configuration, the CPF catalyst only modestly increased the PM oxidation rates. Hence, the catalyst loading in the CPF could possibly be reduced without significantly decreasing the passive regeneration performance of the CCRT®.

Study of the Filtration and Oxidation Characteristics of a Diesel Oxidation Catalyst and a Catalyzed Particulate Filter

Kiran C Premchand, John H Johnson and Song-Lin Yang
Michigan Technological University

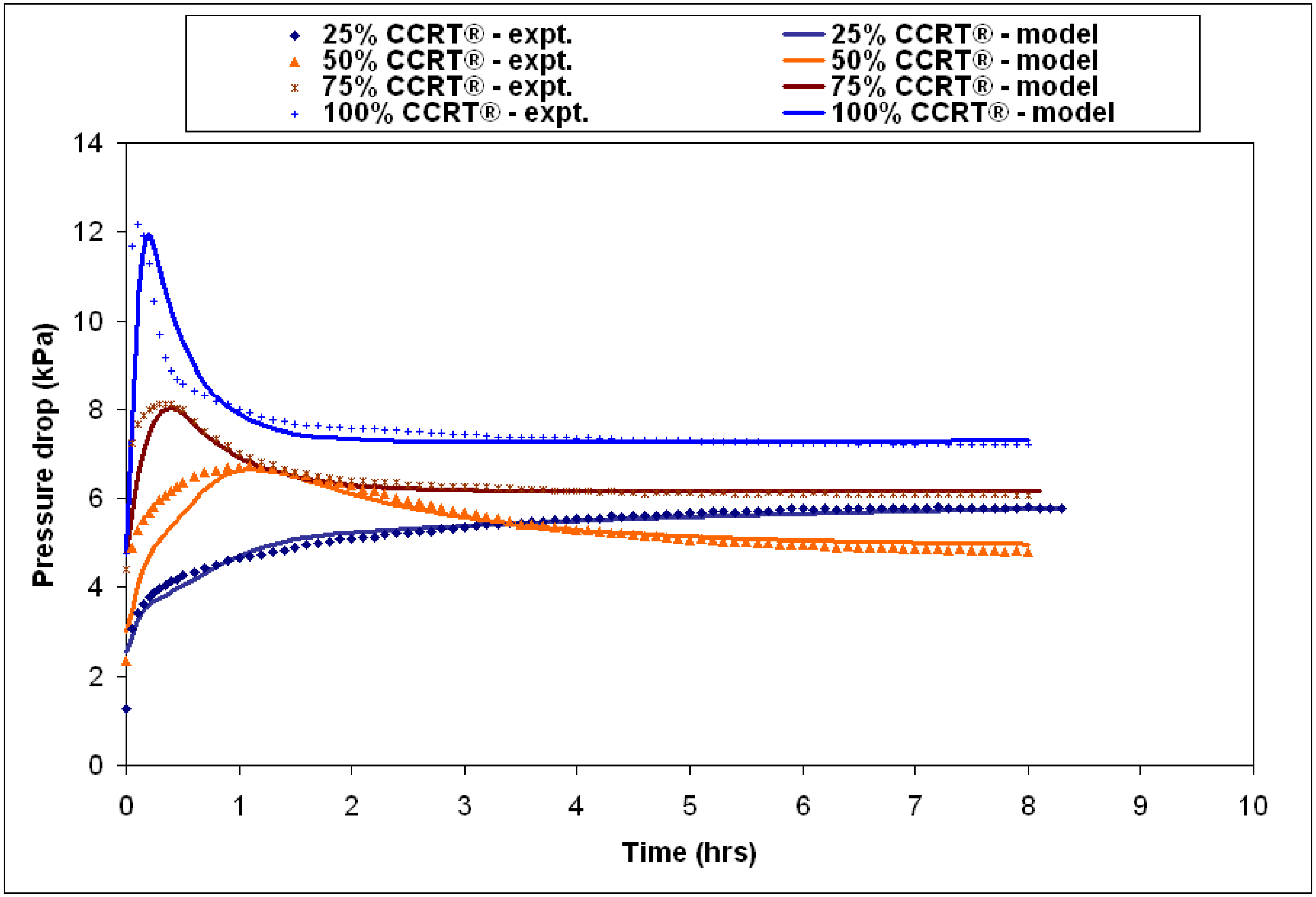
Antonio P Triana and Kirby J Baumgard
John Deere Product Engineering Center

CPF model calibration results – Model vs. Experimental pressure drop profiles in CPF-only configuration



2007-01-1123

CPF model calibration results – Model vs. Experimental pressure drop profiles in CCRT® configuration



MTU DPF Systems Model Using Lumped Model for Controls

Vehicle Engine Aftertreatment System Simulation (VEASS) Model: Application to a Controls Design Strategy for Active Regeneration of a Catalyzed Particulate Filter

Nishant Singh Michigan Technological University
John H. Johnson Michigan Technological University
Gordon G. Parker Michigan Technological University
Song-Lin Yang Michigan Technological University

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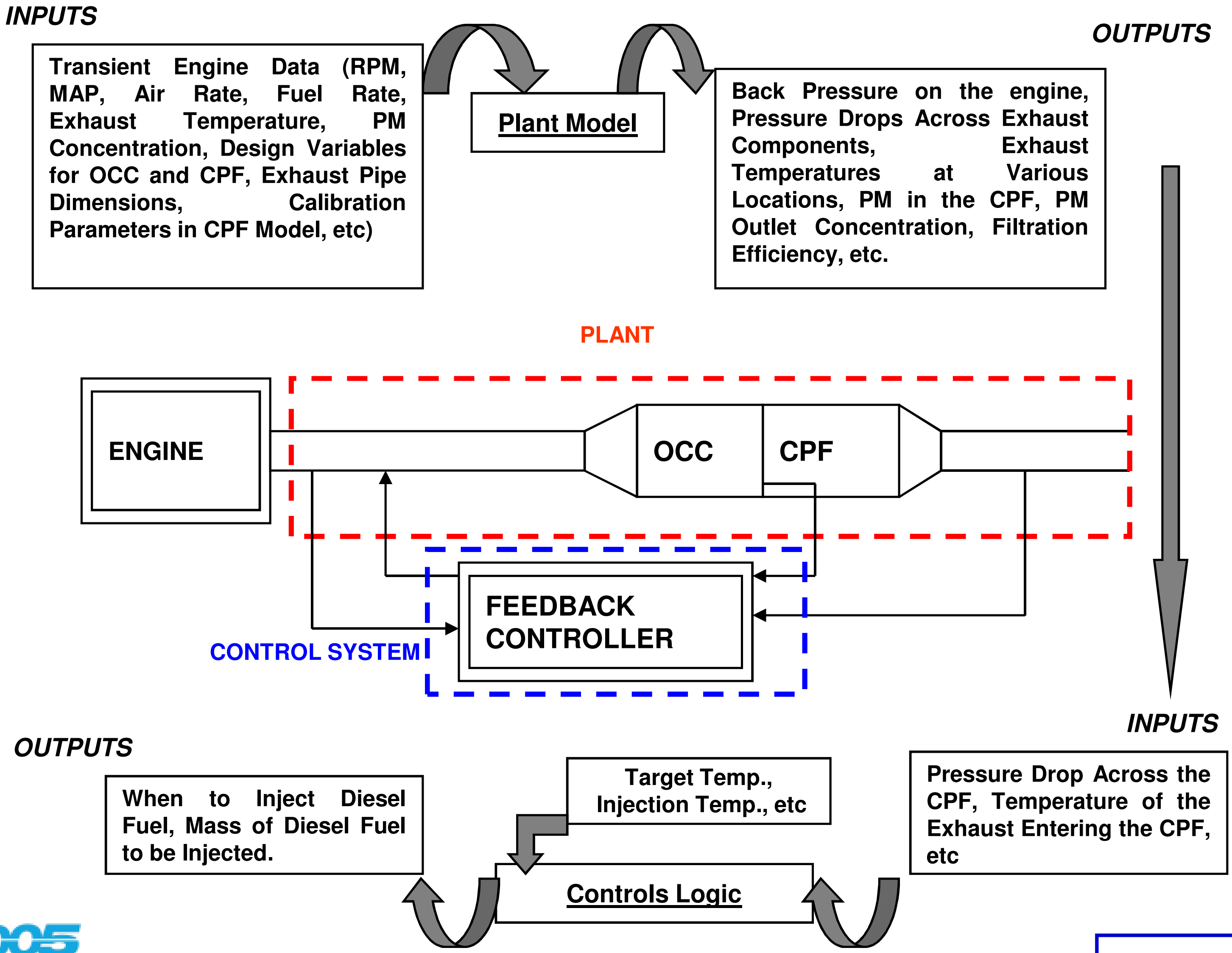
The Integrated Plant & Controls Model



INPUTS

Transient Engine Data (RPM, MAP, Air Rate, Fuel Rate, Exhaust Temperature, PM Concentration, Design Variables for OCC and CPF, Exhaust Pipe Dimensions, Calibration Parameters in CPF Model, etc)

Plant Model

OUTPUTS

Back Pressure on the engine, Pressure Drops Across Exhaust Components, Exhaust Temperatures at Various Locations, PM in the CPF, PM Outlet Concentration, Filtration Efficiency, etc.

INPUTS

Pressure Drop Across the CPF, Temperature of the Exhaust Entering the CPF, etc

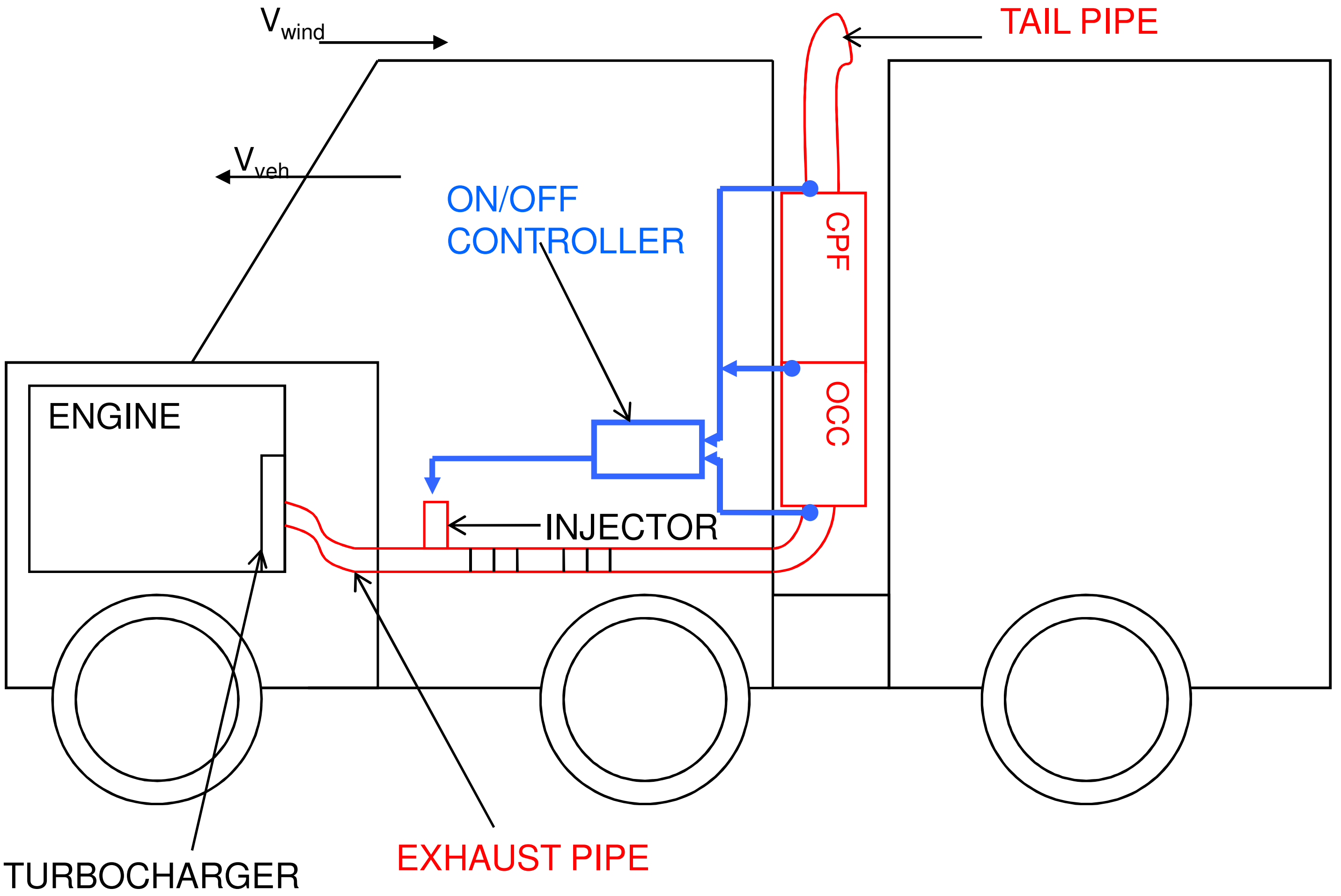
Target Temp., Injection Temp., etc

Controls Logic

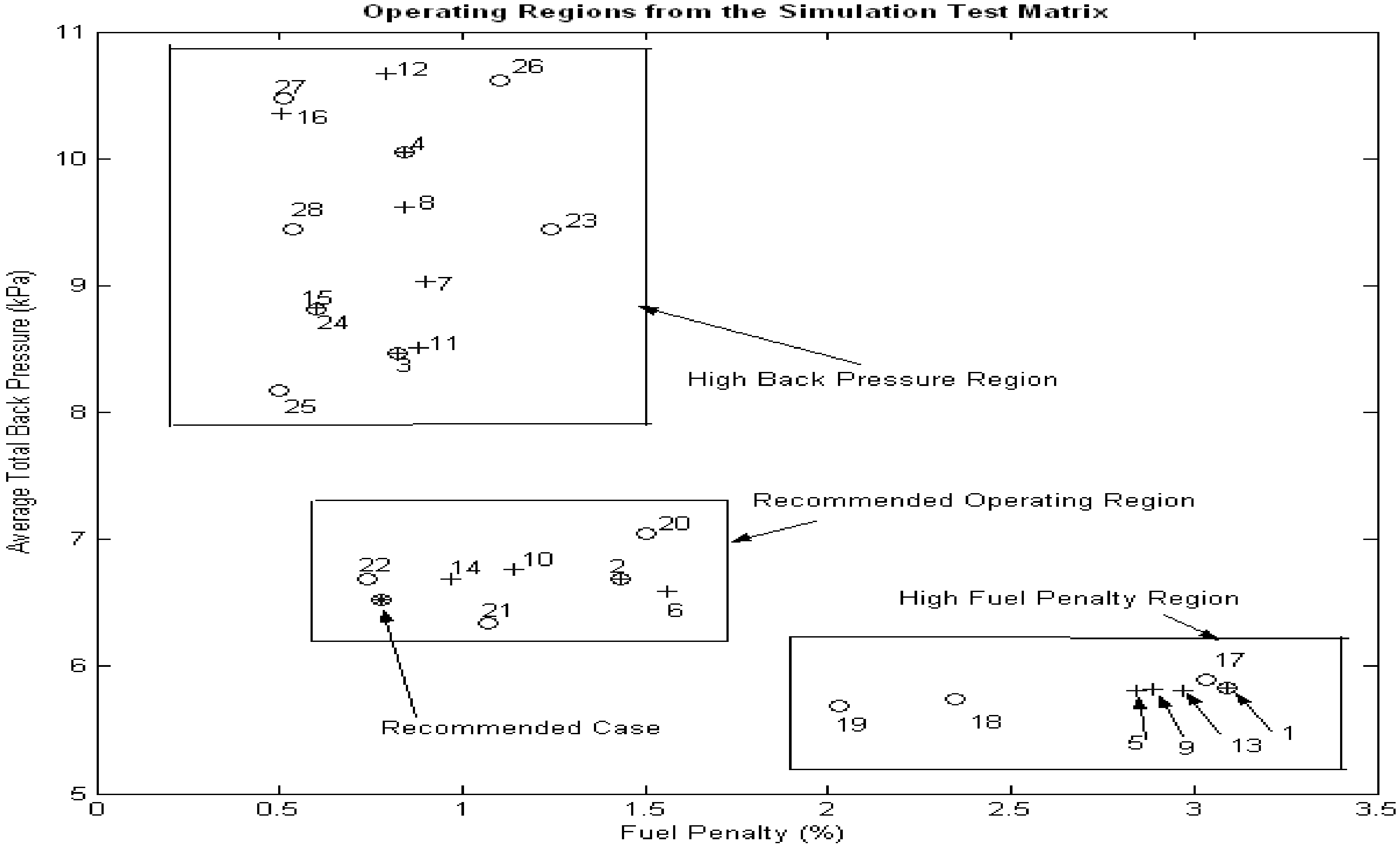
OUTPUTS

When to Inject Diesel Fuel, Mass of Diesel Fuel to be Injected.

Exhaust System Layout Schematic



Operating Regions



Conclusions

- The most favorable operating range for the maximum allowed loading in the CPF before starting regeneration is approximately 2.7 g/m2. The regeneration occurs frequently enough to keep the back pressures on the engine below 6.5 kPa for the driving cycle studied. Regenerating the CPF with loadings lower than 2.7 g/m2 result in higher fuel penalties, whereas regenerating the CPF with loadings significantly greater than 2.7 g/m2 lead to increased engine back pressures.
- Target temperatures at the inlet to the CPF should be about 550 oC. Operating at temperatures lower than this result in higher fuel penalties.
- The time constant for the OCC inlet temperature low pass filter should be approximately 16 seconds. Lower time constants lead to higher fuel penalties, whereas higher time constants result in increased fuel being injected when the actual OCC inlet temperature is less than 300 oC.

Using the MTU ID Model to Predict the Effect of Substrate Dimension Changes on Pressure Drop

Experimental Studies of an Advanced Ceramic Diesel Particulate Filter

Saurabh Mathur – Michigan Tech/Cummins
John H Johnson – Michigan Tech
Jeffrey D Naber – Michigan Tech
Susan T Bagley – Michigan Tech
Anand S. Shende – Michigan Tech/Cummins

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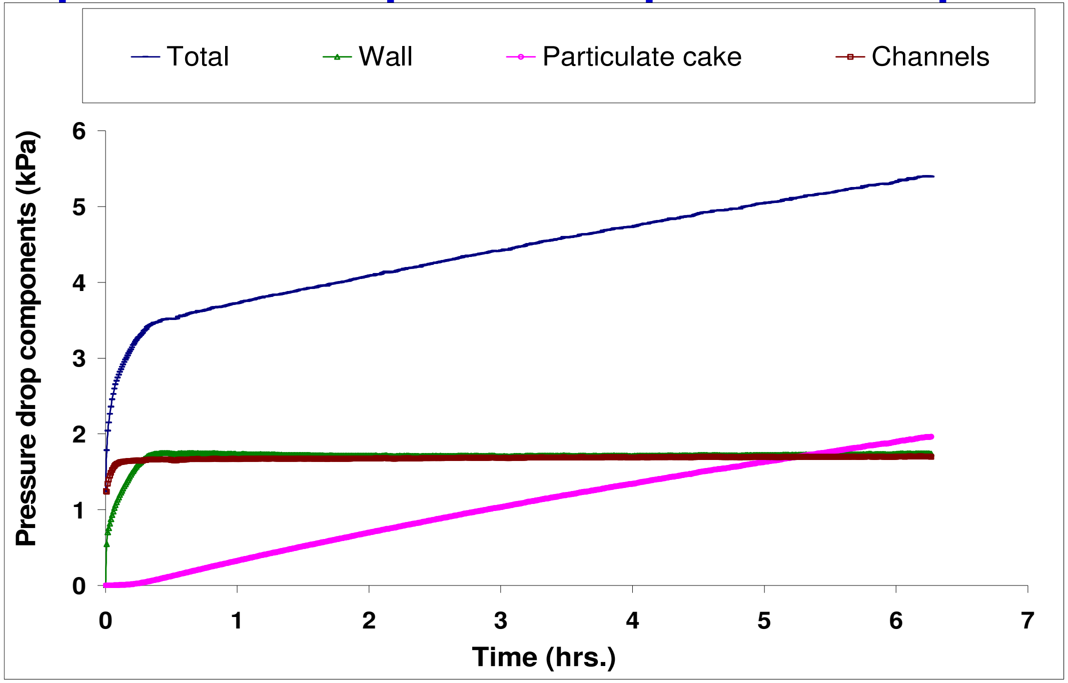
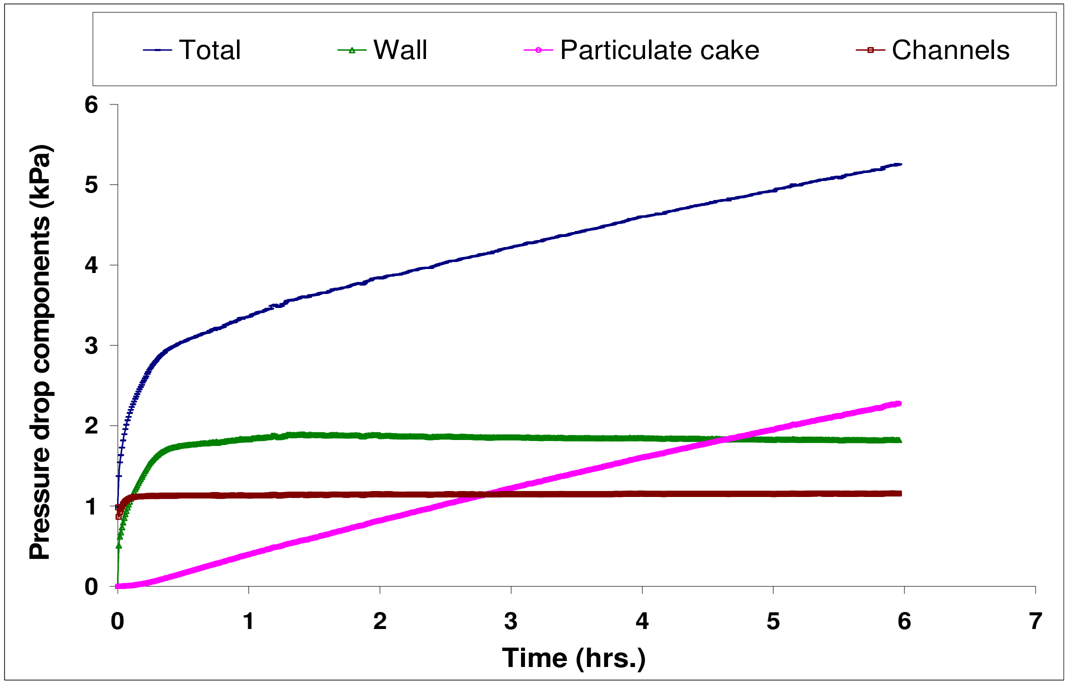
Model predicted components of pressure drop at 40% load

ACM



Cordierite

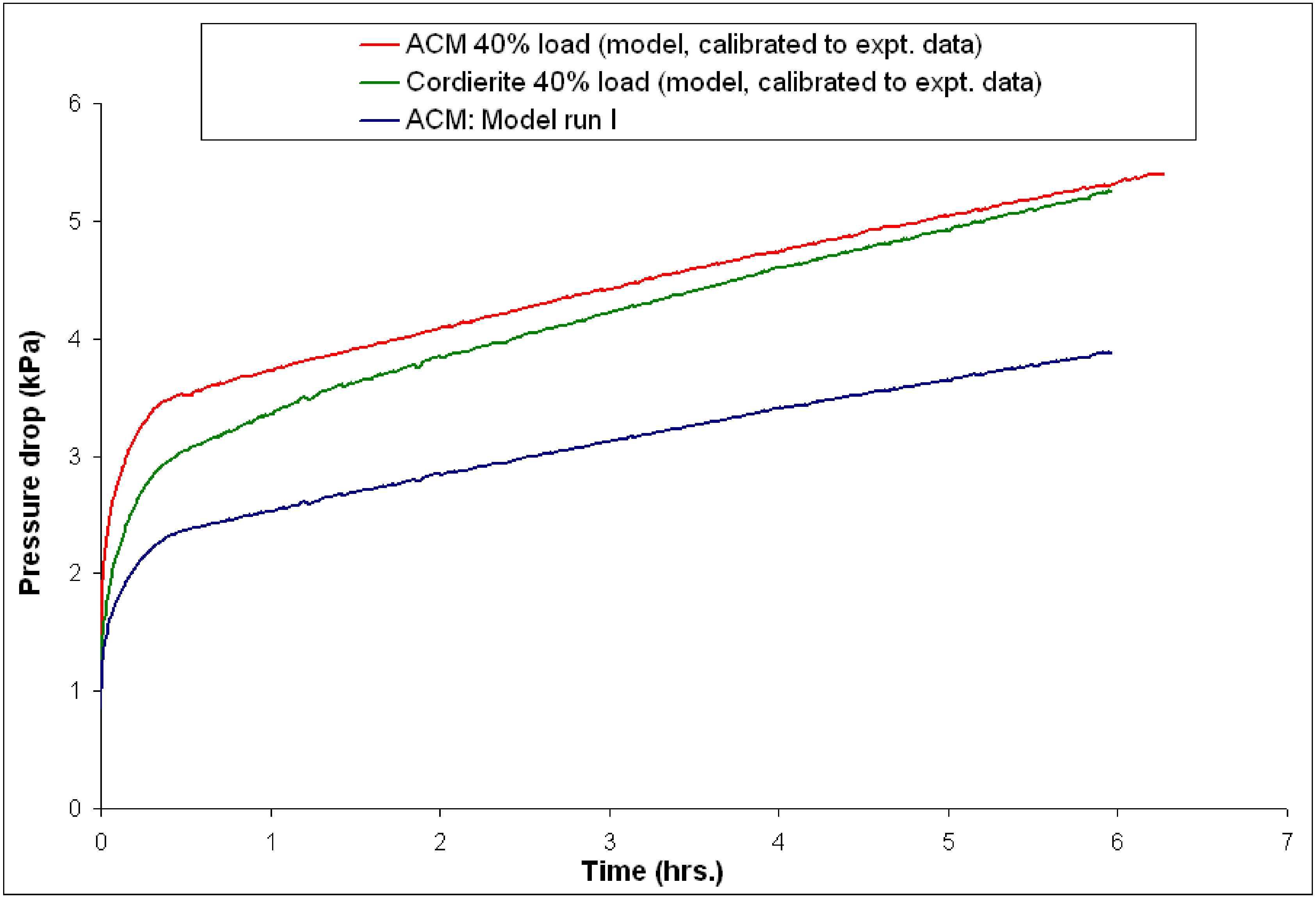


Model run I: Model predicted pressure drops of ACM using matched dimensions

Model was run for ACM using the same channel wall thickness, channel width, diameter and number of inlet cells as cordierite. The substrate wall and PM cake input parameters of ACM are not changed. Exhaust properties from the steady state experiment of cordierite at 40% load are used.

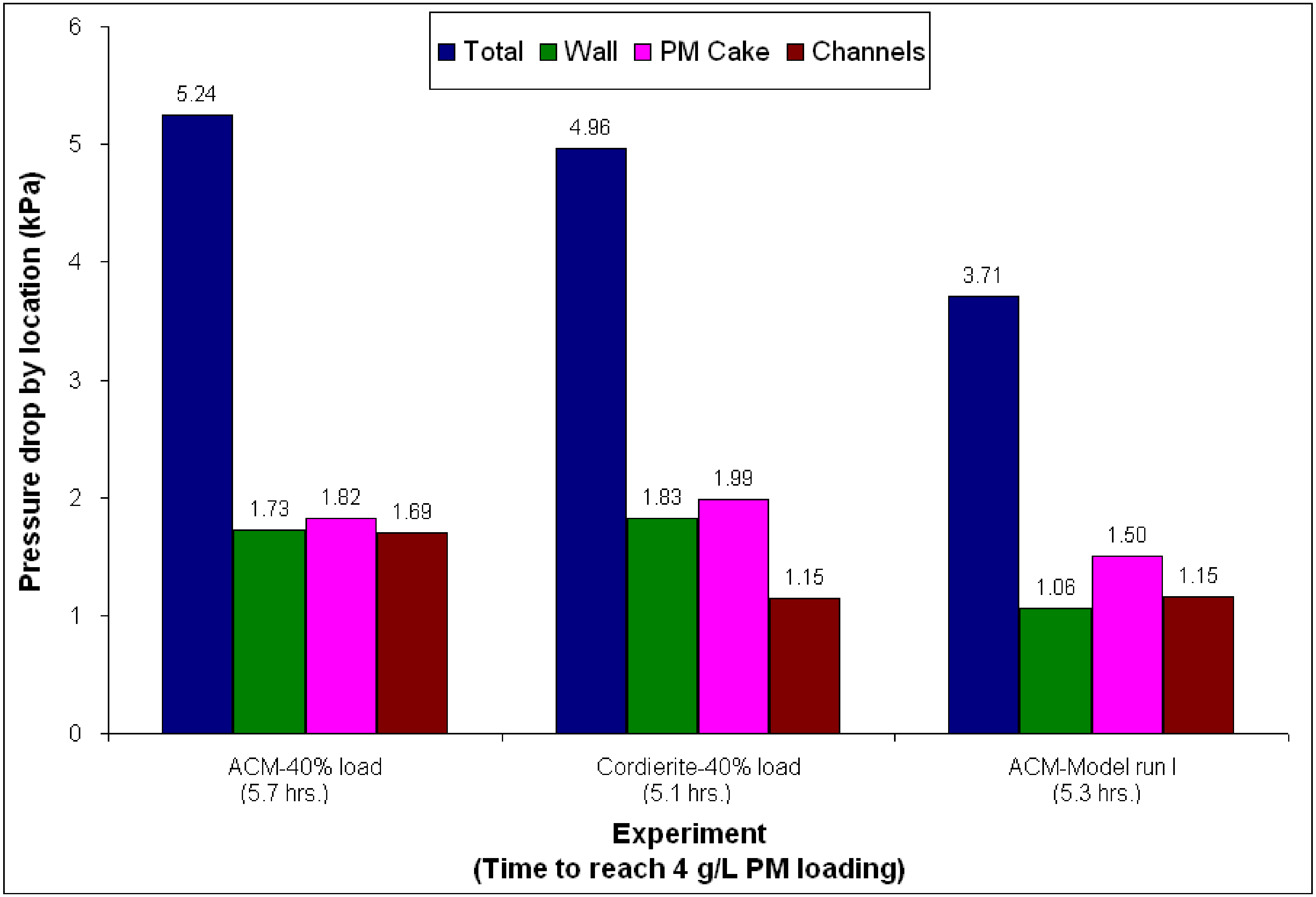
	ACM dimensions		Cordierite dimensions
Specifications	**Original**	**Used for model run I**	**Original**
Channel wall thickness (mm)	0.494	0.311	0.311
Channel width (mm)	1.362	1.520	1.520
Channel length (mm)	305	305	305
Diameter (mm)	235	229	229
Number of inlet cells	6296	6121	6121
Actual Cell Density (cells/in^2)	187	192	192
Clean wall porosity (%)	61	61	50
Mean Pore Size (µm)	23	23	11
Bulk density of wall (kg/m^3)	520	520	500
Specific heat capacity of wall (J/kg-K)	770	770	1000
Wall thermal conductivity (W/m-K)	1.3	1.3	1.0

Model predicted pressure drops of ACM using matched dimensions



Comparison of model predicted pressure drops by location

4 g/L PM loading



MTU Recent Work on Predicting PM Mass in the DPF

A Methodology to Estimate the Mass of Particulate Matter Retained in a Catalyzed Particulate Filter as Applied to Active Regeneration and Onboard Diagnostics to Detect Filter Failures

Rayomand H. Dabhoiwala, Dr. John H. Johnson,
Dr. Jeffrey D. Naber and Dr. Susan T. Bagley

Michigan Technological University

SAE 2008 World Congress

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Motivation Behind Development of this Method

- Accurate estimation of the PM mass retained in the CPF is important in order to determine the time to carry out the active regeneration in an operating vehicle or other stationary diesel engine installation.

- But out of the total PM mass in the CPF, 98% of the mass is in the cake and rest 2% in the wall. However the wall contributes more than 50% to the total pressure drop even with 2% of the total PM mass in it (except at low loads).

- Hasan et. al (2006-01-0466) and Kiran et al. (2007-01-1123) have shown that the mass in the wall oxidizes as a function of time, exhaust gas temperature and NO_2 concentration. This results in change in the wall permeability and in turn the wall pressure drop.

- Thus estimation of the mass retained in the CPF based on the calculated cake and wall pressure drop (accounting for the variable wall permeability) and the measured total pressure drop would give accurate results compared to estimations based on the total pressure drop and empirical relations.

Equation Developed to Estimate Cake Mass (1 of 4)

$$\Delta P_{total} = \Delta P_{wall} + \Delta P_{cake} + \Delta P_{friction/channel} \qquad \ldots (1)$$

- Konstandapoulos et al (2000-01-1016) used the approach in equation (1) to derive the following equation (2) relating the total pressure drop across the filter

$$\Delta P_{total} = \frac{\mu Q}{2\left(\frac{\pi D^2 L}{4}\right)}(a+w_s)^2\left[\frac{w_s}{k_0 a} + \frac{1}{2k_p}\ln\left(\frac{a}{a-2w}\right) + \frac{4FL^2}{3}\left(\frac{1}{(a-2w)^4} + \frac{1}{a^4}\right)\right] \qquad \ldots (2)$$

- Equation (2) was developed taking into account the effect of the particulate cake layer on the inlet channel and cake pressure drops.

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Equation Developed to Estimate Cake Mass (2 of 4)

- Singh et al.(2005-01-0970) used this pressure drop model in the vehicle engine aftertreatment system simulation (VEASS) to solve for cake layer thickness using Newtons method for root solving as a function of time. The mass of the cake was then estimated using equation (3)

$$m_{cake} = 4\left(\frac{a + (a - 2w)}{2}\right) w \; Ln\, \rho_{p} \qquad \ldots (3)$$

- This approach assumes that the permeability of the wall is a constant and equals to the clean wall permeability. It does not take into account that the PM mass in the wall changes.

- Various research and published literature from MTU has shown that mass in the wall changes with time (2006-01-0466 and 2007-01-1123) .

- This results in a change in the wall permeability and in turn the pressure drop across the substrate wall varies as a function of time, exhaust gas temperature and NO_2 concentration.

Equation Developed to Estimate Cake Mass (4 of 4)

- Simplifying equation (7) we get

$$m_{cake} = \left[\frac{\Delta P_{total}}{\mu Q} - \frac{C_2}{k_t} - C_3\right] * \frac{k_p}{C_1} \qquad \ldots (8)$$

where

$$C_1 = \frac{1}{\rho_p} \frac{1}{16 n^2 a^2 L^2} \qquad \ldots (8a)$$

$$C_2 = \frac{w_s}{4 naL} \qquad \ldots (8b)$$

$$C_3 = \frac{2}{3} \frac{LF}{na^4} \qquad \ldots (8c)$$

K_t = Permeability of wall

K_p = Permeability of cake

MTU Present Work on Active Regeneration

An Experimental Study of Particulate Thermal Oxidation in a Catalyzed Filter during Active Regeneration

Krishna Pradeep Chilumukuru
Dr. John H. Johnson
Dr. Jeffrey D. Naber

Michigan Technological University

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Introduction

Literature reported activation energies varied between each study.

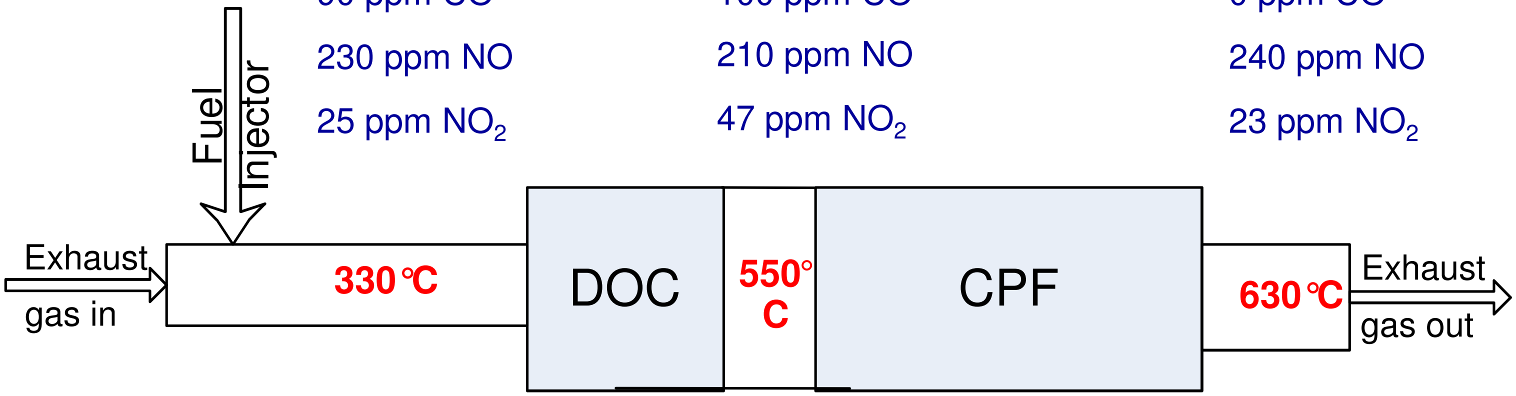
Reference	Arrhenius Model used	Activation Energy (kJ/gmol)	Condition / PM Type
Singh et al. (2006)	S	122	Catalyzed filter; Engine Test Cell
Yezerets et al. (2003)	S	126±3	Un-catalyzed ; Flow Reactor;Diesel Exhaust sample
Yezerets et al. (2003)	S	146±3	Un-catalyzed; Flow reactor;Diesel Exhaust sample
Yezerets et al. (2003)	S	45-65	Applicable for first 10-25% of reactive soot sample
Yezerets et al. (2003)	S	95±5	0-10%(vol) of water; Flow Reactor; Diesel PM
Edgar et al (2000)	S	38	Catalyzed filter; Flow Reactor; Diesel PM samples
Edgar et al (2000)	S	85	Un-catalyzed filter; Flow Reactor; Diesel PM
Neeft et al. (1997)	S	168	Un-Catlyzed; Flow reactor; Printex-U PM
Awara et al. (1997)	S	118	Fuel Additive - Cu; Engine test cell
Pauli et al. (1983)	S	111	Un-Catalyzed; Engine Test Cell
Otto et al. (1980)	S	142	Un-Catalyzed; Engine Test Cell
Field et al. (1967)	M	149	Un-catalyzed; Pulverized Coal

S: Standard Arrhenius Behavior

M: Modified Arrhenius Behavior

Aftertreatment Setup

Cummins 2007 RPF system



16300 ppmC HC	3700 ppmC HC	8 ppmC HC
90 ppm CO	100 ppm CO	0 ppm CO
230 ppm NO	210 ppm NO	240 ppm NO
25 ppm NO_2	47 ppm NO_2	23 ppm NO_2

Fuel Injector

Exhaust gas in

330 °C

DOC

550° C

CPF

630 °C

Exhaust gas out

$HC + O_2 \rightarrow CO_2 + H_2O + CO$

$CO + \frac{1}{2}O_2 \rightarrow CO_2$

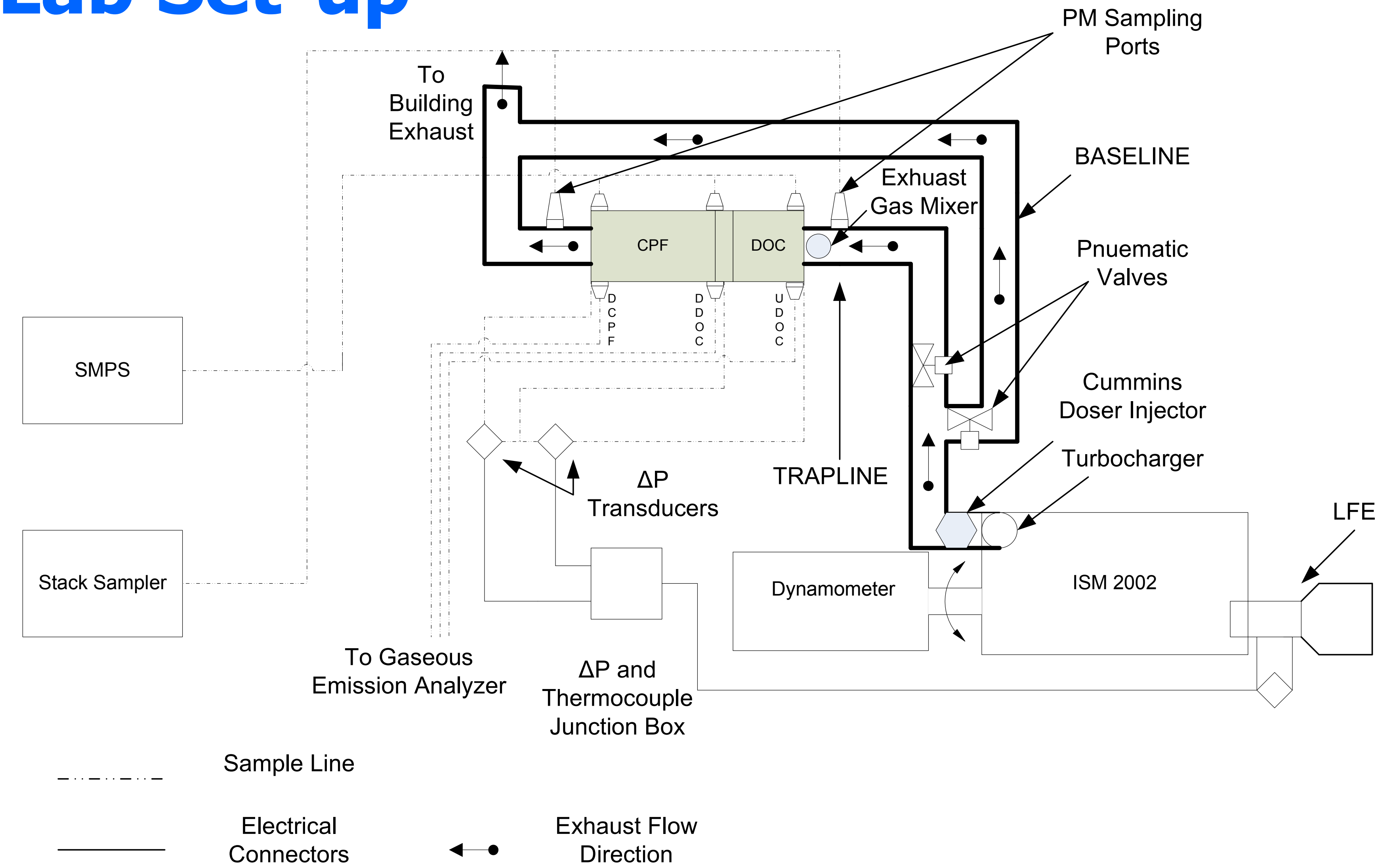
$NO + \frac{1}{2}O_2 \rightarrow NO_2$

$C + NO_2 \rightarrow CO_2 + NO$

$C + O_2 \rightarrow CO + CO_2$

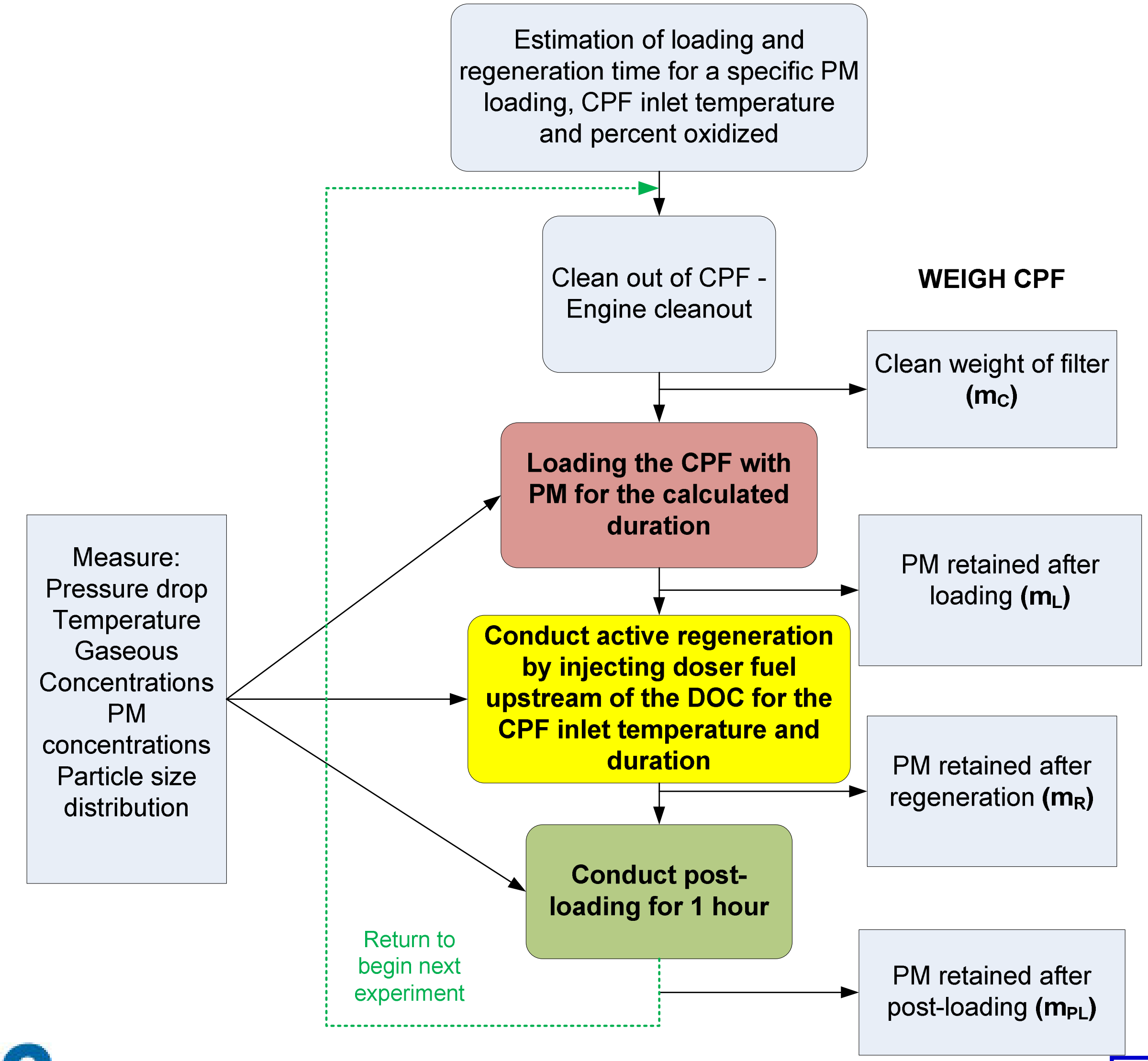
RPF: Regenerative Particulate Filter

Lab Set-up



PM Sampling Ports
To Building Exhaust
BASELINE
Exhuast Gas Mixer
CPF
DOC
Pnuematic Valves
Cummins Doser Injector
Turbocharger
D C P F
D D O C
U D O C
SMPS
Stack Sampler
ΔP Transducers
TRAPLINE
LFE
Dynamometer
ISM 2002
To Gaseous Emission Analyzer
ΔP and Thermocouple Junction Box
Sample Line
Electrical Connectors
Exhaust Flow Direction

Test Procedure



Estimation of loading and regeneration time for a specific PM loading, CPF inlet temperature and percent oxidized

Clean out of CPF - Engine cleanout

WEIGH CPF

Clean weight of filter **(m_C)**

Loading the CPF with PM for the calculated duration

PM retained after loading **(m_L)**

Measure:
Pressure drop
Temperature
Gaseous Concentrations
PM concentrations
Particle size distribution

Conduct active regeneration by injecting doser fuel upstream of the DOC for the CPF inlet temperature and duration

PM retained after regeneration **(m_R)**

Conduct post-loading for 1 hour

Return to begin next experiment

PM retained after post-loading **(m_{PL})**

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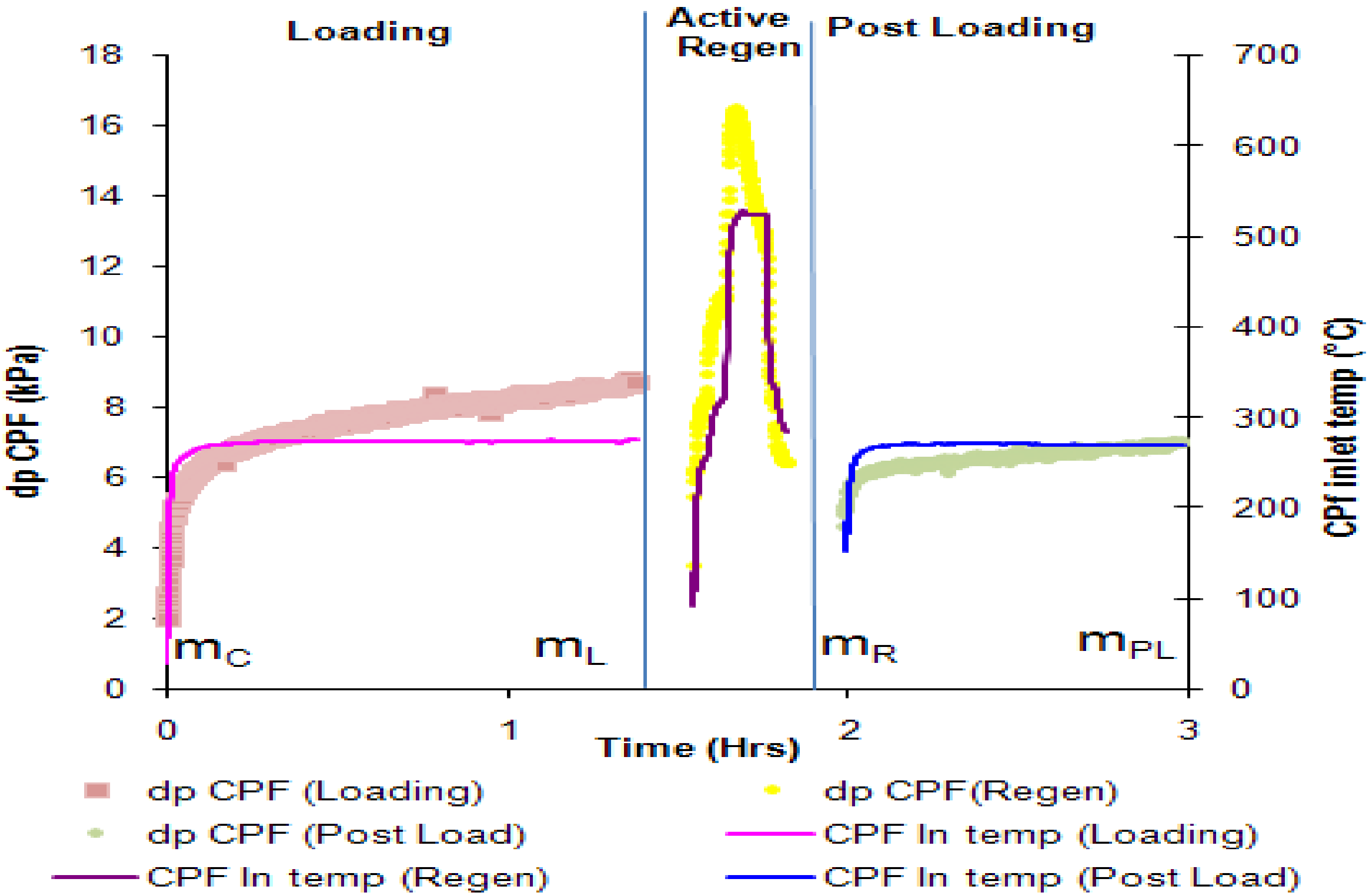
Test Procedure - Schematic



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Estimation of Regeneration Times

An Arrhenius based lumped model was used to determine the RR_O from experimental data acquired in 2006 [1].

$$m_{R1} = \frac{Q \cdot C_{in} \cdot \eta_f}{RR_O \cdot 1000}\left[1 - e^{\left(-RR_O \cdot t_{eff}\right)}\right] + m_{L1} \cdot e^{\left(-RR_O \cdot t_{eff}\right)} \quad [2] \qquad \text{(eqn. 1)}$$

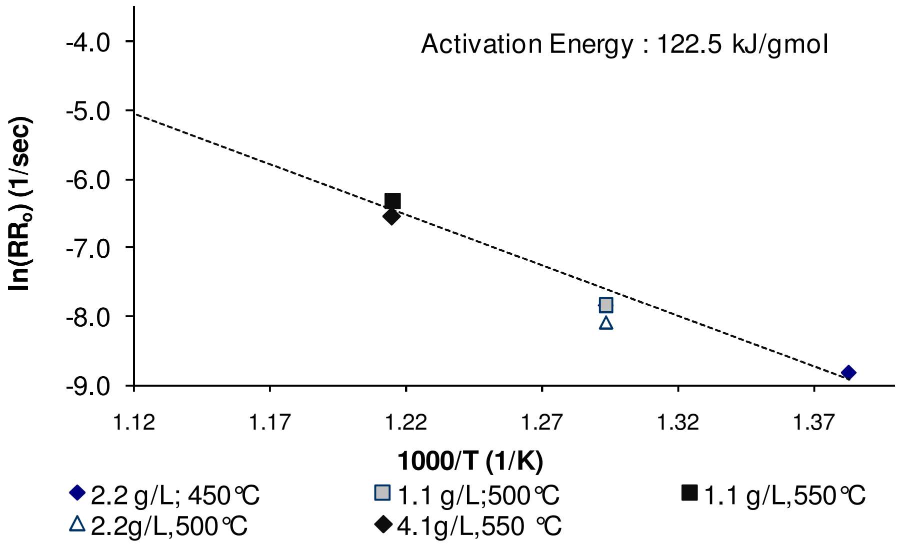
Q= Exhaust volumetric flow rate in std. m3/sec.
C_{in}= Engine out PM concentration in mg/std.m3
η_f= Filtration efficiency of the filter, %
RR_O= Global thermal reaction rate for PM oxidation, s-1
t_{eff} = Effective time of active regeneration, min
m_{R1} = Mass retained in the CPF at time teff, g
m_{L1} = Mass in CPF before start of active regeneration, g

[1]: Singh et al., SAE Paper No.: 2006-01-0879
[2]: Awara et al. SAE Paper No.: 970188

Estimation of Regeneration Times

Standard Arrhenius equation: $\ln(RR_U) = \ln(A) + \left(\frac{-E_a}{R}\right)\cdot\left(\frac{1}{T_R}\right)$ (eqn. 2)

The Arrhenius Plot



* Data from Singh et al., SAE Paper No.: 2006-01-0879

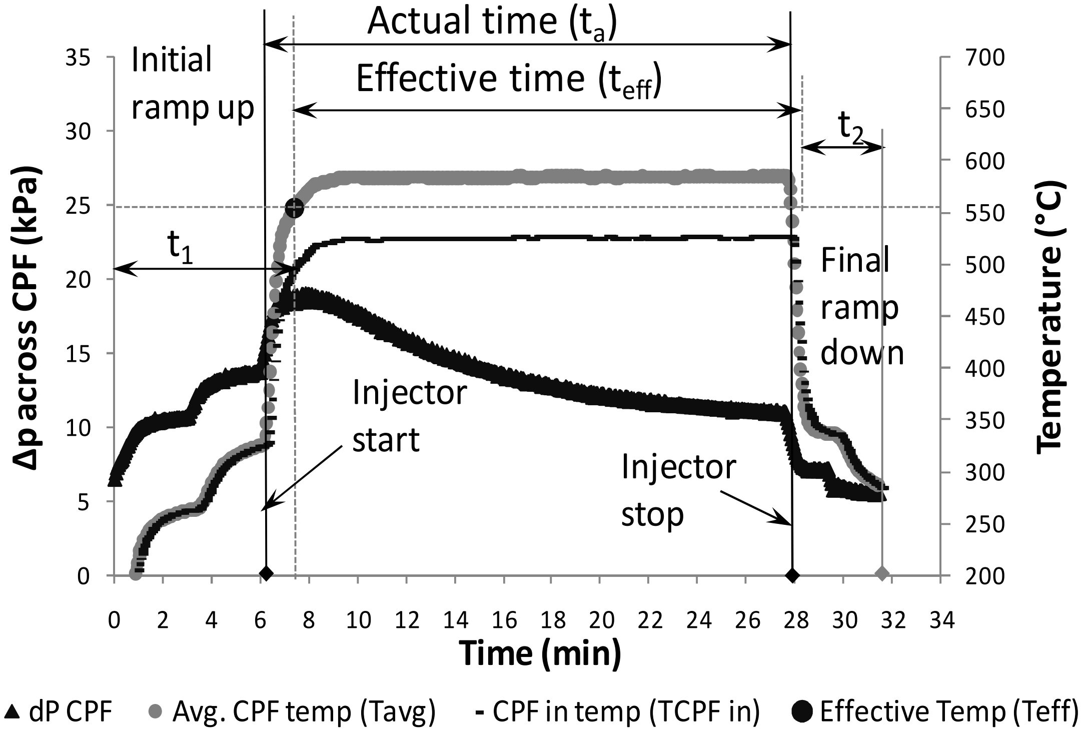
- A least squares fit is used for calculating the Ea and A
- RR_O is plotted on the log scale of a semi-log plot and $1/T_R$ is plotted on the linear (X-axis)

Test Matrix

RUN No.	Target CPF In Temp	Target PM Loading	Target % PM Oxidized	Regeneration Times (min)	
	°C	g/L	Estimated	Actual	Estimated*
1	525	1.1	30%	9.8	10.0
2	525	2.2	60%	20.5	22.0
3	525	4.1	60%	18.1	19.5
4	550	2.2	60%	11.0	11.5
5	550	1.1	60%	6.2	6.5
6^	525	2.2	60%	21.0	22.0
7	525	1.1	40%	6.6	7.0
8	600	2.2	70%	4.0	4.5
9	550	4.1	40%	6.4	6.5
10^	525	2.2	60%	21.5	22.0
11	550	2.2	40%	5.3	6.0
12	550	1.1	40%	4.3	3.5
13^	525	2.2	60%	21.5	22.0
14	600	1.1	70%	3.7	2.6
15	525	2.2	40%	8.1	8.5
16	525	4.1	40%	7.5	8.0
17	600	4.1	70%	5.0	5.0
18	550	4.1	70%	13.9	14.5
19	550	2.2	94%	48.7	50.0

^ These experiments are repeats of RUN 2 – repeated for statistical analysis

Data Correction: Time & Temperature



Effective Temperature

$$T_{eff\,i} = \frac{-\left(\frac{E_a}{R}\right)}{\ln\left(\frac{RR_{ui}}{2}\right) - \ln(A_i)}$$

Regeneration Temperature (T_R)

$$T_R = \frac{1}{n}\sum_{i=1}^{n} T_{avg_i}(t)$$

n is the number of 3 second intervals

T_R is calculated for the period where T_{avg} > T_{eff}

T_{avg} (t) is the average radial channel temperature at 152.25 mm at time, t.

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Activation Energy and Pre-exponential Factors

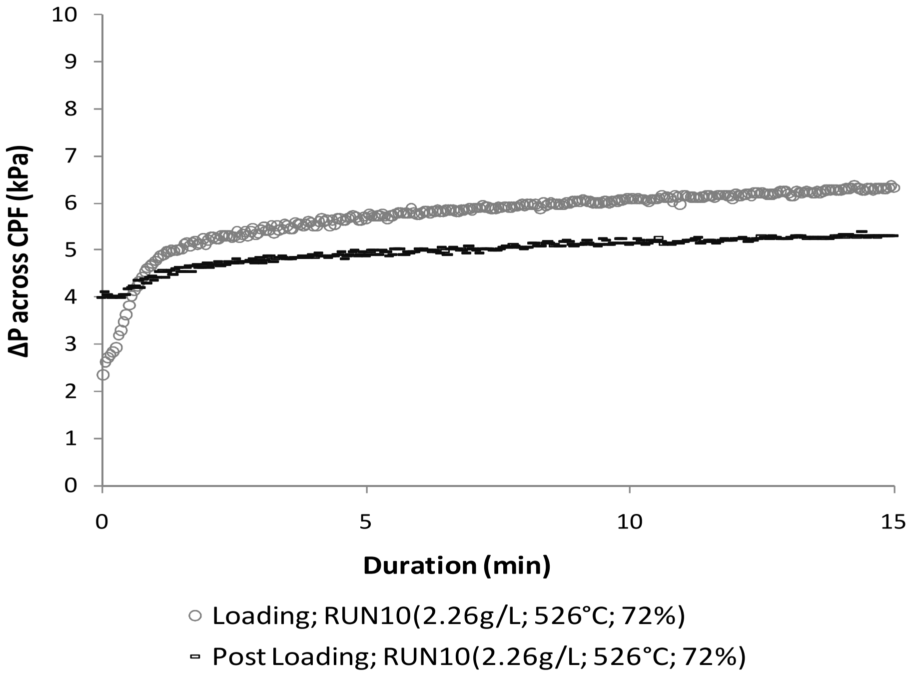
	Std. Arrhenius			Mod. Arrhenius		
Data Set	Pre exp. Factor	Activation Energy	R^2	Pre exp. Factor	Activation Energy	R^2
	s^{-1}	kJ/gmol		$s^{-1}K^{-1}$	kJ/gmol	
1.1 g/L	8.59.E+01	75.9	0.96	0.035	68.5	0.95
2.2 g/L	2.10.E+05	135.9	0.98	86.6	128.5	0.98
4.1 g/L	4.95.E+04	125.3	0.98	20.5	117.9	0.98
2.2+4.1 g/L	1.24.E+05	132.0	0.98	51.0	124.6	0.98
All	1.79.E+04	117.1	0.84	7.37	109.7	0.82

- Calculated activation energies for 2.2 and 4.1 g/L tests lie within the reported activation energies of 85[4] – 150[5] kJ/gmol for un-catalyzed diesel PM
- Activation energy calculated for 1.1 g/L tests is close to reported values of 45 – 65[6] kJ/gmol for the initial 10 -25 % of PM oxidation.
- Both approaches result in activation energies within a range of ±8 kJ/gmol and the R^2 values are similar using either fit.

[4]: Edgar et al., SAE Paper No.: 2000-01-3087
[5]: Koltaskis et al., Ind. Chem Res. 36, pg: 4155 -4165, 1997
[6]: Yezerets et al., SAE Paper NO.: 2003-01-0833

Experimental Results (Contd.)

Post-Loading



- It was observed that during post-loading the ΔP across the CPF was consistently lower as compared to loading from a clean filter
- Deep bed filtration regime is not present resulting in a lower overall ΔP since wall of the CPF is nearly clean and the cake layer is intact after partial-regeneration, thus no PM mass enters the wall [3].

[3]: Arasappa et al., SAE Paper No.: 2009-01-1274

Modeling the Filtration, Oxidation and Pressure Drop Characteristics of a Catalyzed Particulate Filter during Active Regeneration

Rohith Arasappa, Kiran Premchand, Krishna Chilumukuru, Dr. John H. Johnson, Dr. Jeffrey D. Naber, Dr. Song-Lin Yang

Michigan Technological University

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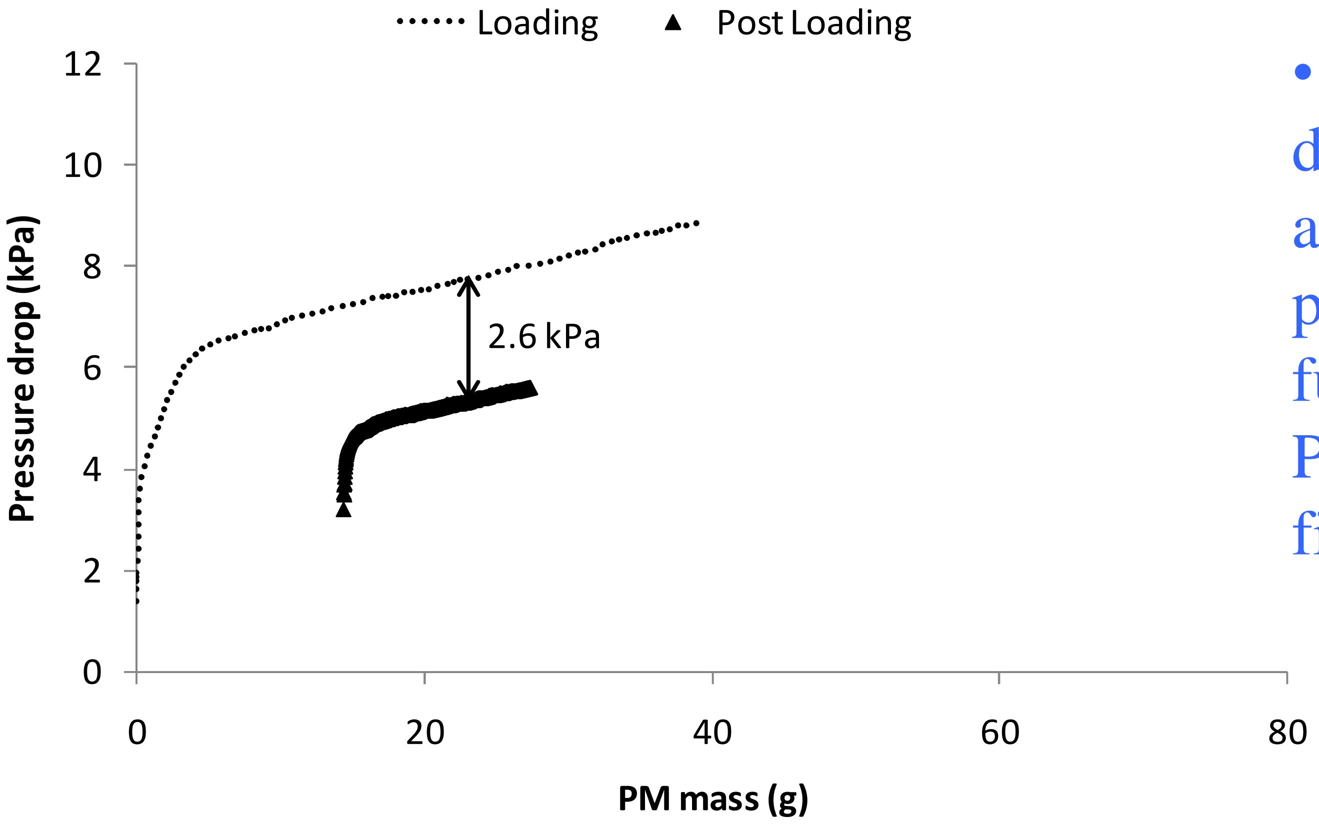
Comparison between Loading and Post Loading Pressure Drop



- Total pressure drop for loading and post loading plotted as a function of total PM mass in the filter

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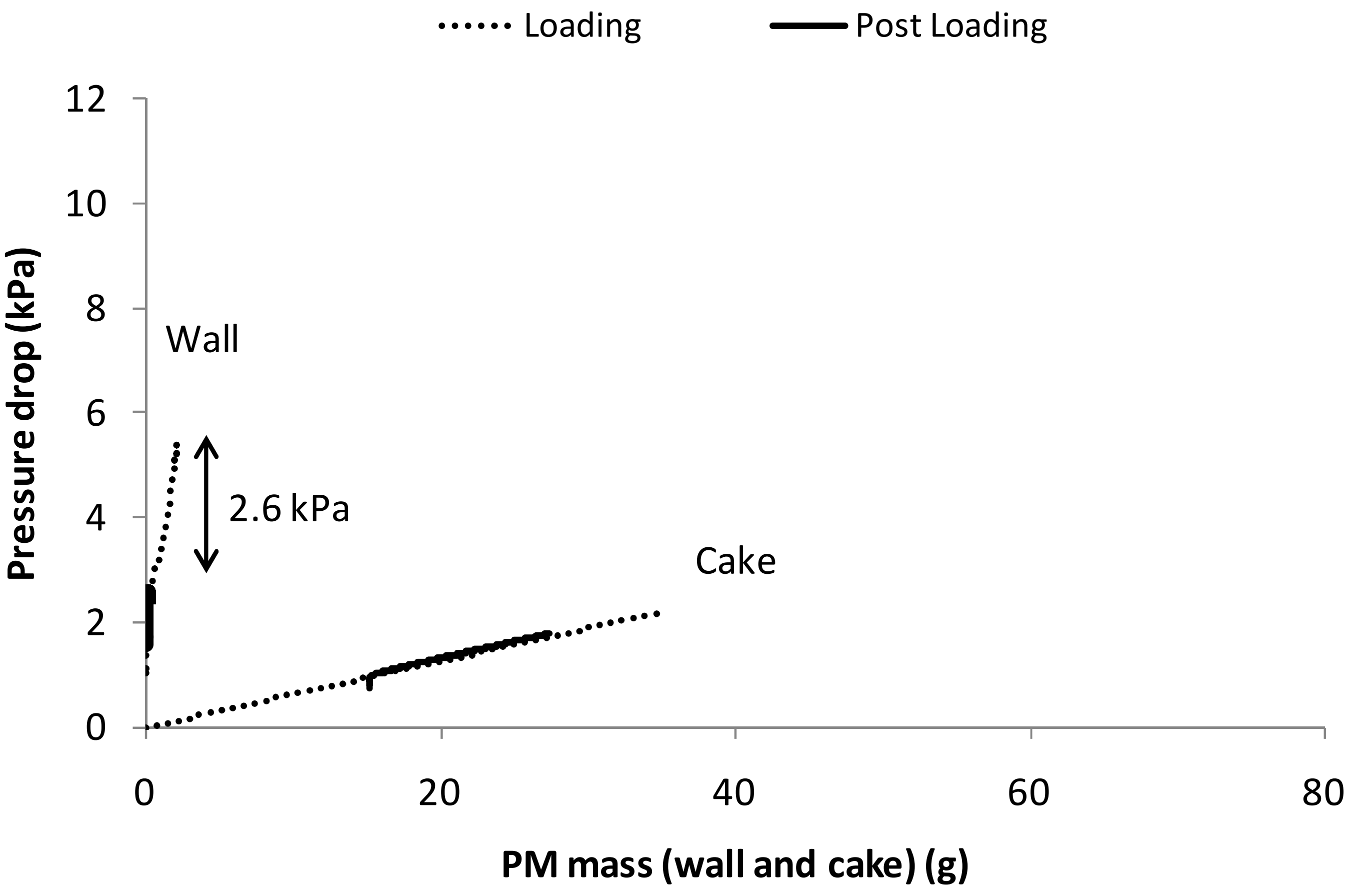
Run 10 (525 C, 2.2 g/L, 60%)



- Wall pressure drop as a function of wall mass and cake pressure drop as a function of cake mass
- Cake pressure drop is comparable
- Wall pressure drop has a 2.6 kPa difference

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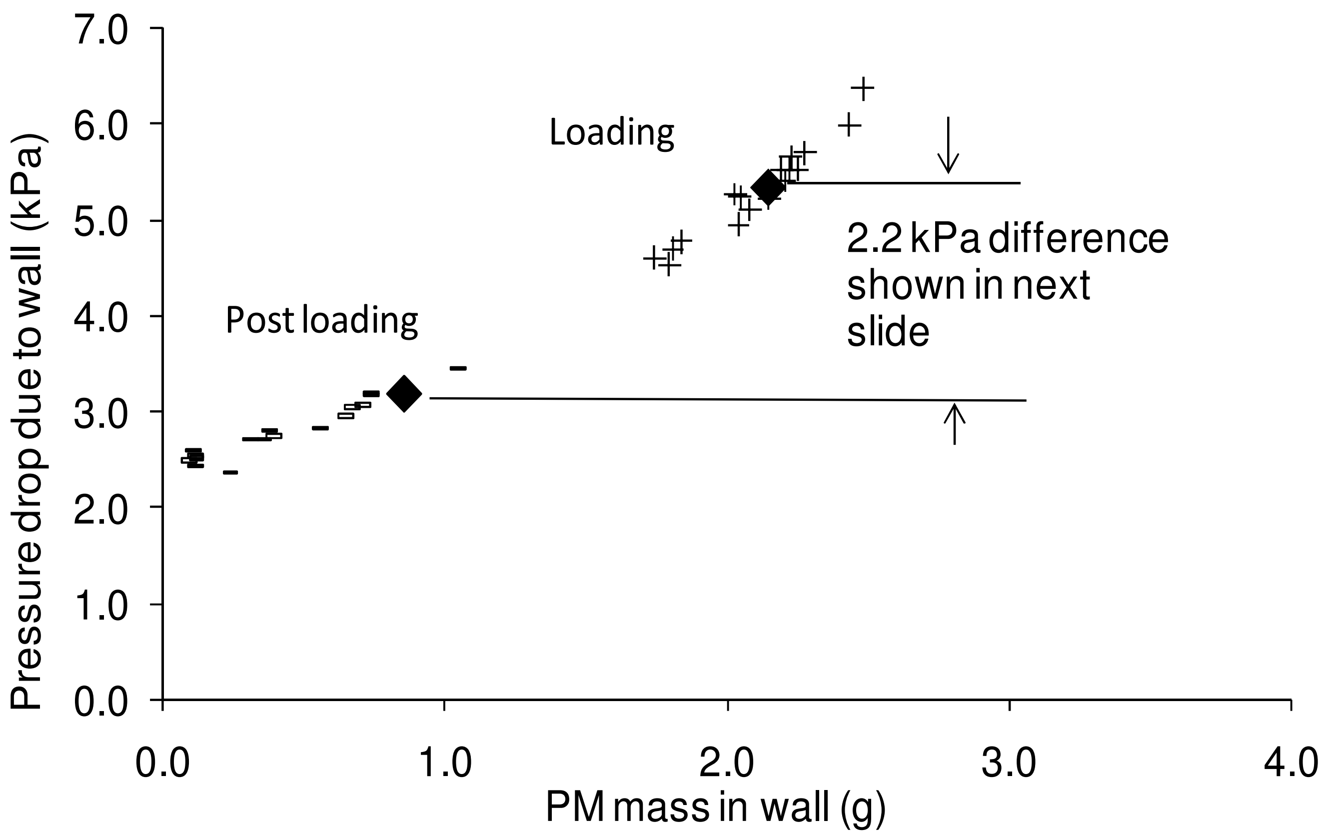
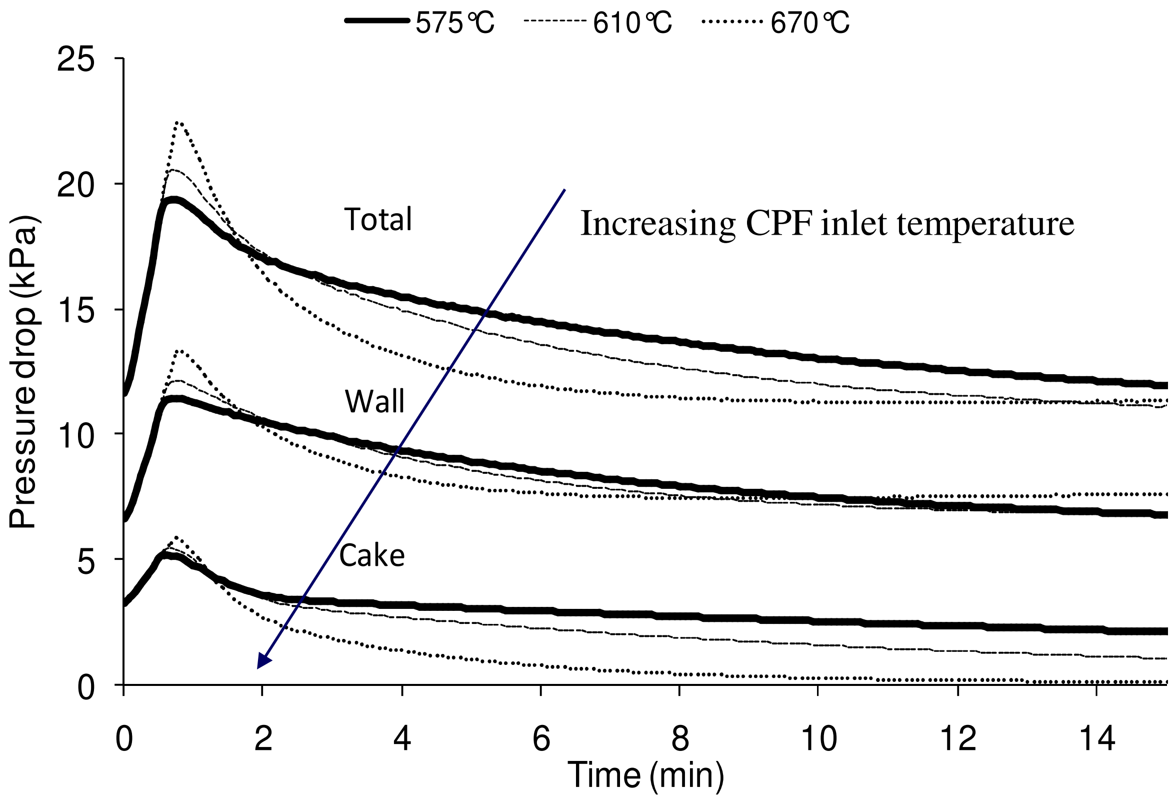
Pressure Drop vs. Wall Mass - All the Runs



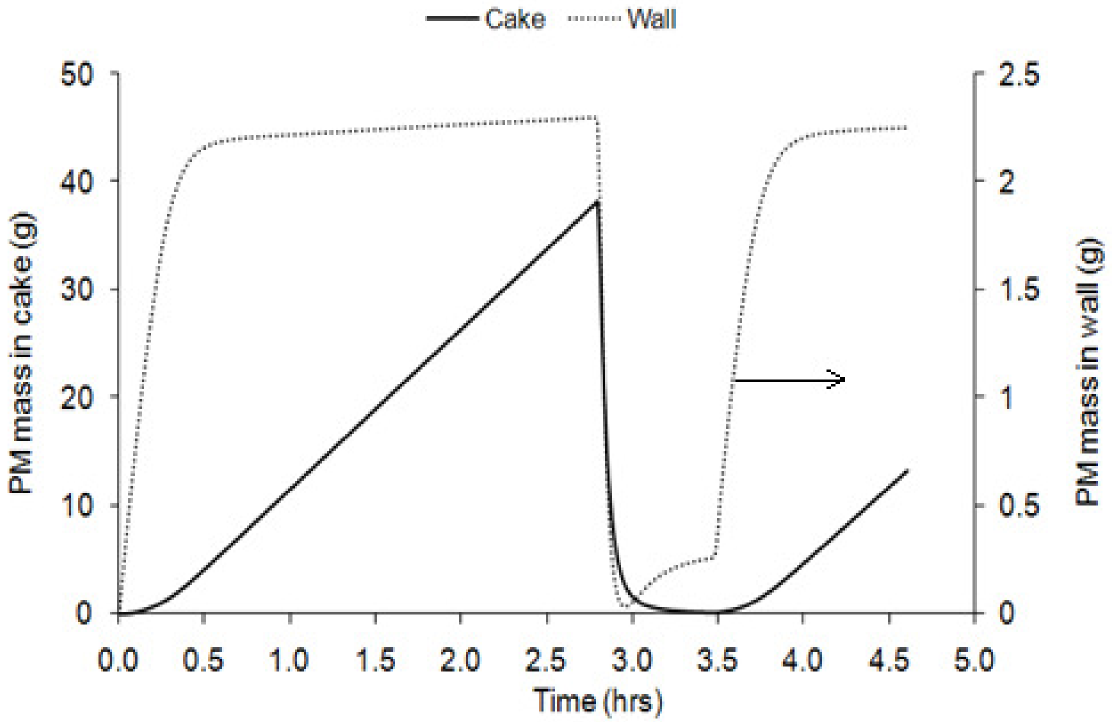
- Difference between loading and post loading primarily due to differences in wall pressure drop
- Wall mass for post loading is low due to oxidation during regeneration

Ramp-Up at 8°C/sec – Pressure Drop Results



- 575, 610 and 670°C represent the temperature inside the filter for 2.2 g/l PM loading and CPF inlet temperature of 525, 550 and 600°C
- Higher peak pressure drop for higher CPF inlet temperature at constant ramp-up to target temperature

Cake Layer Breakthrough - PM Mass Retained - 2.2 g/L, 670°C

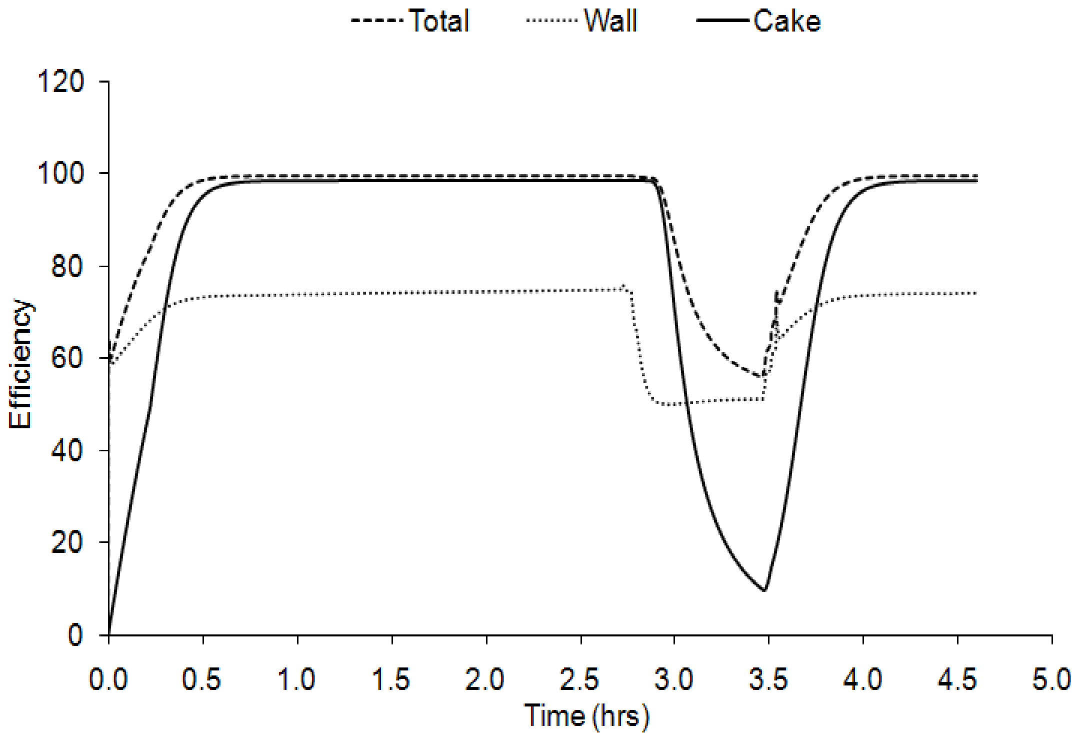


η_c/d_c =0.17 (changed from 0.2 used for all other runs)

- Simulation to show deep bed filtration for post loading
- Cake layer is oxidized completely at the end of 3.5 hr
- Wall mass after 3.5 hr rises to the same value as during loading

2009-01-1274

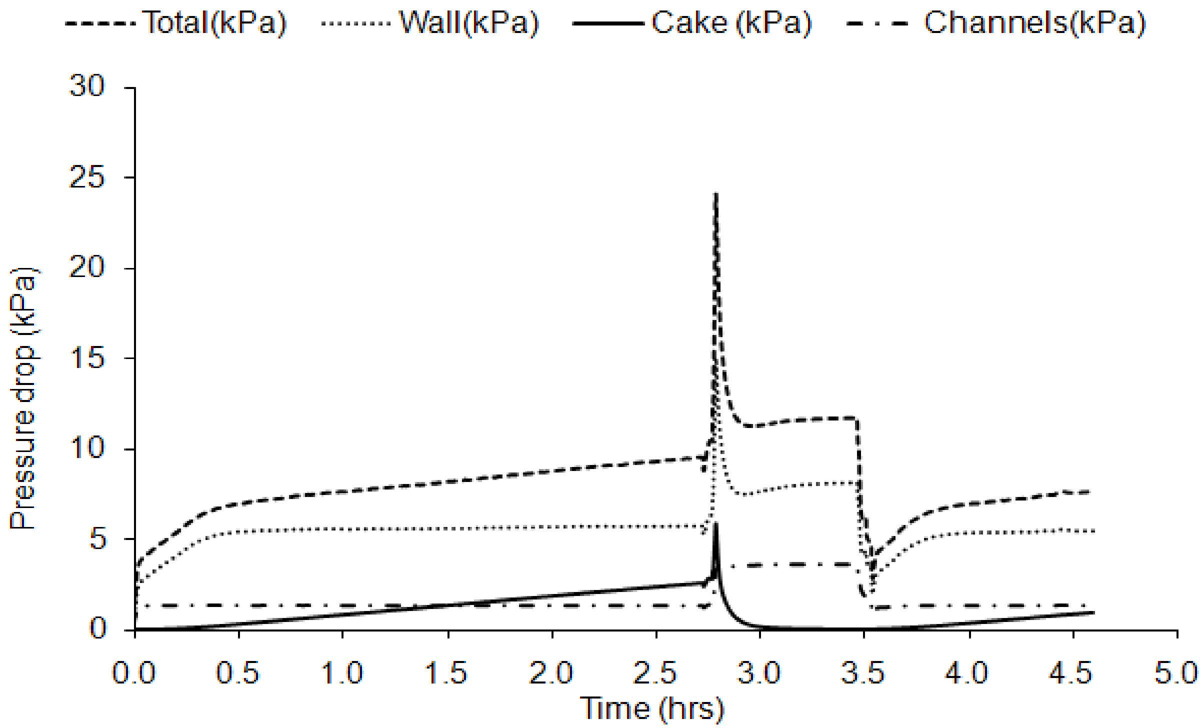
Cake Layer Breakthrough - Filtration Efficiency - 2.2 g/L, 670°C



η_c/d_c =0.17 (changed from 0.2 used for all other runs)

- The value of η_c/d_c was changed (from 0.2 to 0.17) causing the cake layer efficiency to be initiated at a later stage
- The cake filtration efficiency at the end of 3.5 hr is 10% and rises to 98% as post loading begins meanwhile allowing PM mass to get deposited in the wall giving rise to deep-bed filtration regime

Cake Layer Breakthrough -Pressure Drop Components - 2.2 g/L, 670°C



- The pressure drop during post loading is comparable to that during loading because of deep bed filtration for post loading

η_c/d_c =0.17 (changed from 0.2 used for all other runs)

NGK Membrane Filter Data

Yasuyuki Furuta,
Takashi Mizutani,
Yukio Miyairi,
Kazuya Yuki
and Hiroshi Kurachi
NGK Insulators, Ltd.

Illustrated PM Loading Observations.

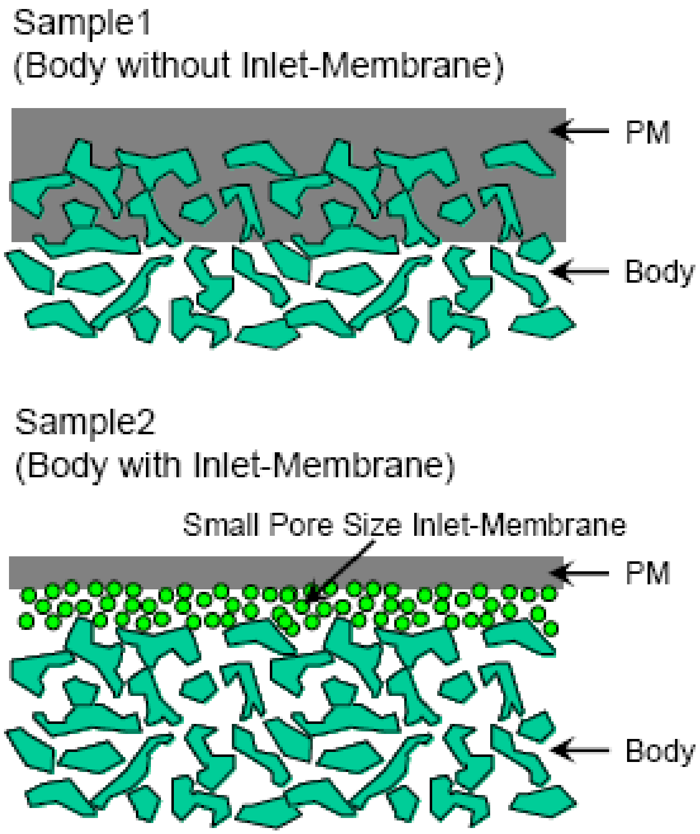


Fig. 6: Illustrated PM Loading Observations.

PM Amount vs. Pressure Drop (Honeycomb Structure).

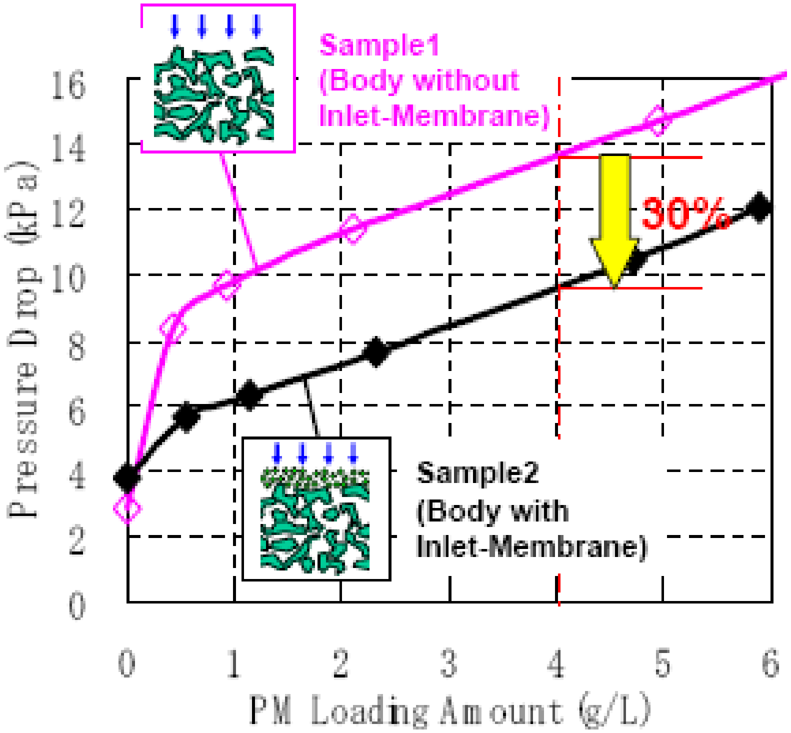


Fig. 9: PM Amount vs. Pressure Drop (Honeycomb Structure).

PM Amount vs. Filtration Efficiency (Honeycomb Structure).

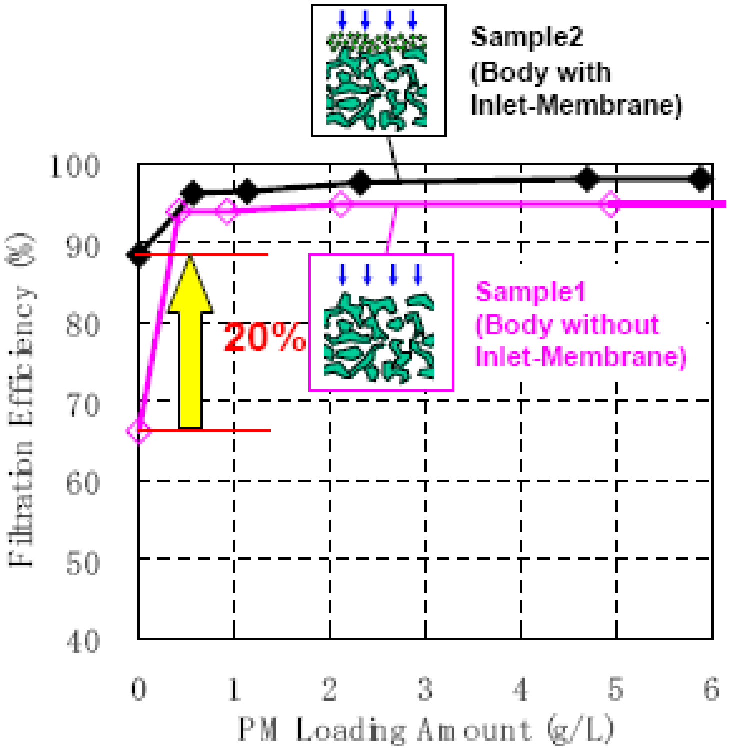


Fig. 10: PM Amount vs. Filtration Efficiency (Honeycomb Structure).

MTU’s ID Model for Active Regeneration

Development of a 1-D CPF Model to Simulate Active Regeneration of a Diesel Particulate Filter

Kiran C Premchand,
Dr. John H Johnson, and
Dr. Song-Lin Yang

Michigan Technological University

Kiran Premchand et al CLEERS Presentation

SAE 2009
World Congress

2009-01-1283

Research Objectives

Develop a Model (version 3.0; SAE:2009-01-1283) by improving an existing 1-D model developed at MTU (version 1; SAE:2006-01-0467):

- *Change & improve numerical techniques used previously in order to model step changes in temperature as a result of active regeneration:*
    - *Adaptive time-step*
    - *Convergence check*
- *Add species conservation solution for gaseous species concentrations,*
- *Account for additional energy release due to exothermic oxidation reactions of gaseous species (HC's, CO, NO) in gaseous energy balance*
- *Include gas-solid mass transport to substrate wall and couple reactions in wall to mass transport (to be included in MTU CPF Model version 4.0)*

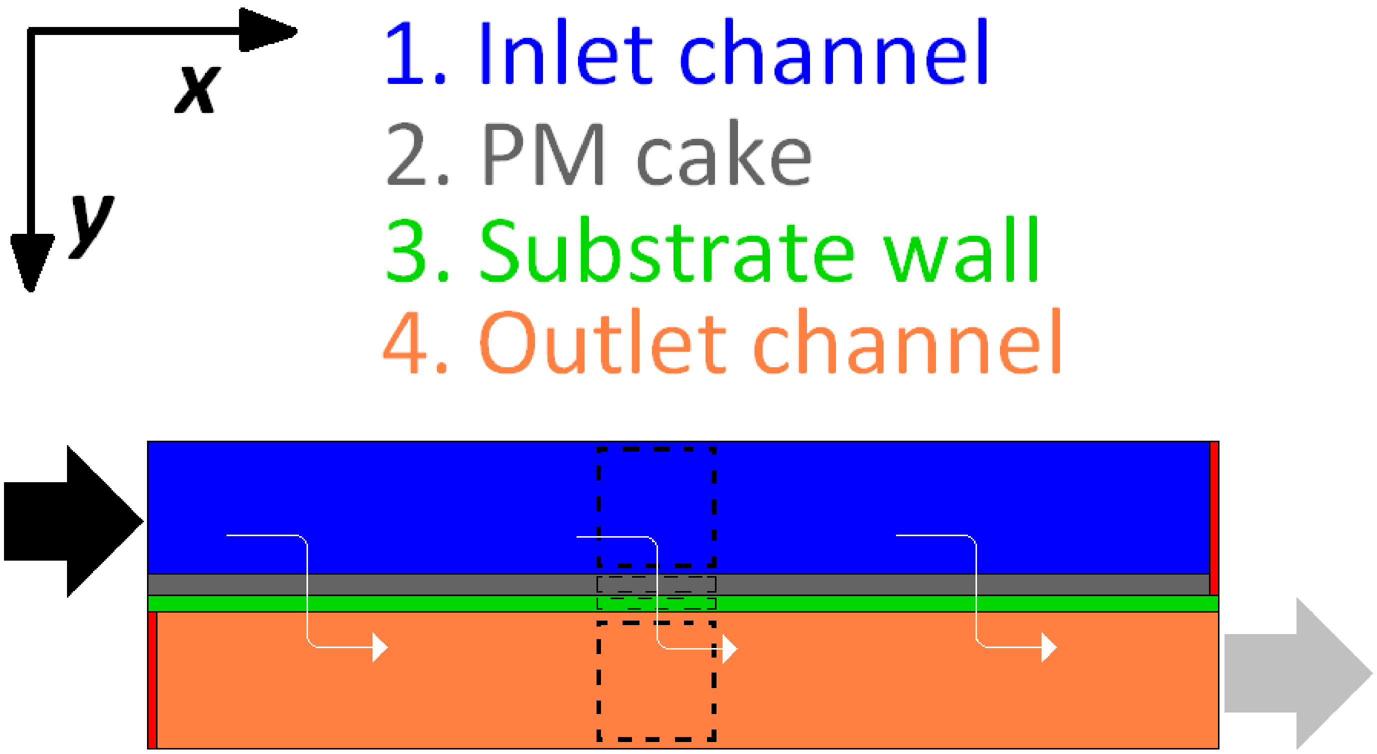
<u>MTU 1-D CPF Model version 3.5</u>

1-D quasi-steady model that includes:

- *Flow Processes,*
- *Filtration Processes,*
- *Gaseous Energy Balance,*
- *PM Oxidation Kinetics,*
- *Gaseous-Phase Reaction Kinetics; and*
- *Improved Convergence Rate,*
- *More Efficient Computations and Data Storage, and*
- *More Output Variables being Written Out*

* Kiran Premchand et al CLEERS Presentation

Representation of Filter Geometry



1. Inlet channel
2. PM cake
3. Substrate wall
4. Outlet channel

Chemical Species Concentrations Solver

- Separate (FORTRAN) sub-routines solve for concentrations of all gaseous species in:
  - ☐ *Inlet channel,*
  - ☐ *(across) PM cake,*
  - ☐ *(across) Substrate wall, and*
  - ☐ *Outlet channel*
- Axial length of DPF divided into 100 individual cells
- 9 chemical species used – $C_{12}H_{24}$, O_2, N_2, CO_2, H_2O, C, CO, NO *and* NO_2
- Finite Difference approach used to solve for species concentrations
- Depletion rates of species are functions of local temperature
- Solvers also calculate energy release due to consumption/production of species
- Gas – Solid phase transport not considered in current model (v3.5 – will be included in v4.0)

Future Data Needs

- Biodiesel Fuels and Effect on DPF’s – PM Oxidation Rates
- Cooperative data collection on a 2007 HD DPF system on: chassis, dyno-FTP and under actual driving conditions – Extensive data that can be used by modelers to compare experimental data to model results – will help in controls, sensors and OBD and whether models work on a real production system
- Experimental data on variables that affect cake permeability and fundamental relations
- Experimental data on oxidation rates versus time on full scale DPF’s during active regeneration (including first 25% of oxidation)

Future Modeling Needs

Models for cake permeability as a function of temperature and other fundamental variables

Simple wall PM oxidation models that can be used in a ECU

Multi-Channel DPF models with heat transfer that run on PC (not computational intensive 3D models) and can solve active regeneration simulations and transient cycles

From CLEERS Poll – Future Research

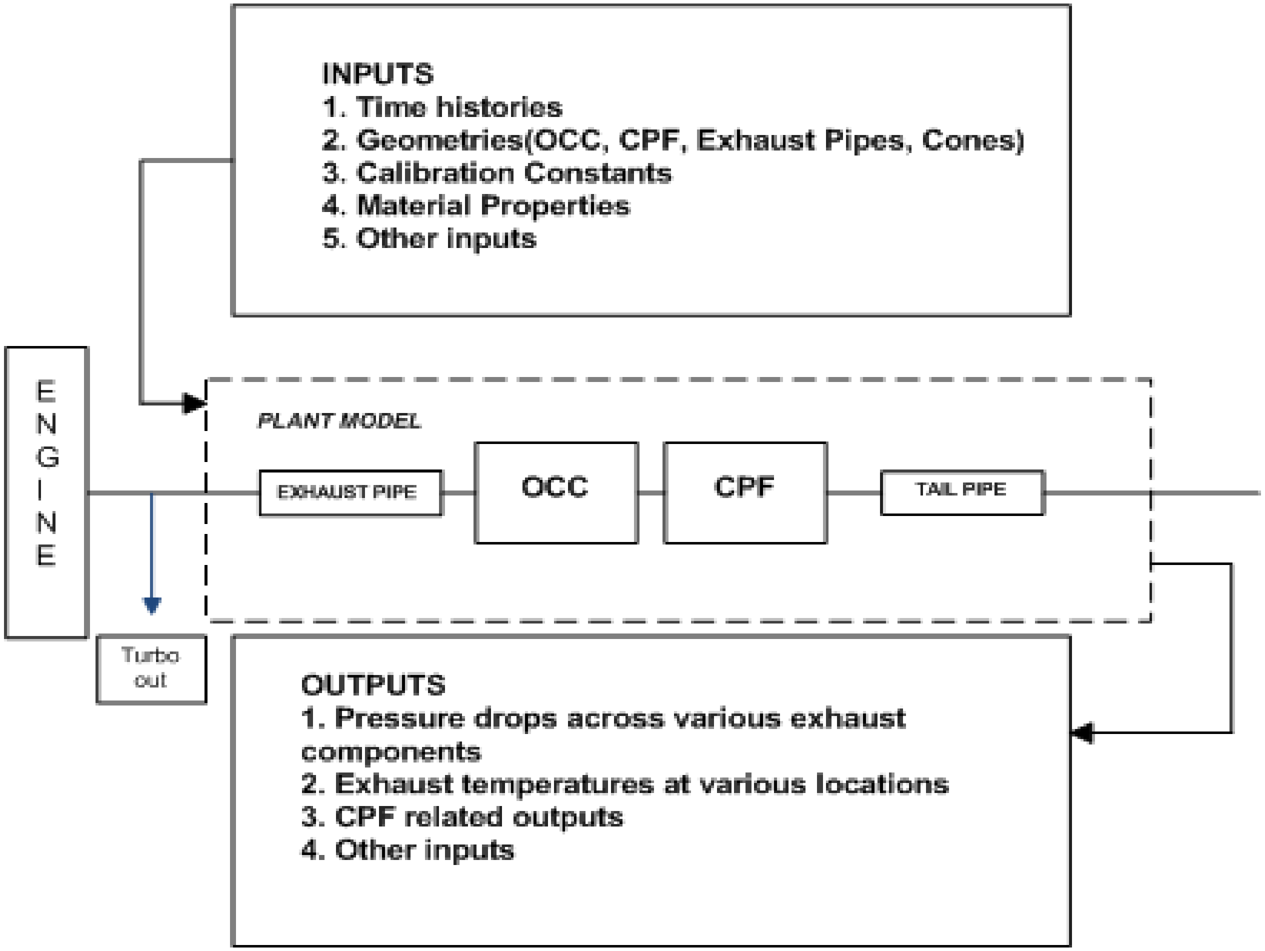
- DPF (OBD and Sensors): Accurate estimation of soot loading and prediction of regeneration exotherm
- DPF (OBD and Sensors): Multiple, combined sensor utilization (both existing and new sensors) for loading assessment beyond simple back pressure
- DPF (Kinetics/Reaction Mechanisms): Relationship between soot oxidation kinetics and chemical/morphological properties of soot particles
- DPF (Kinetics/Reaction Mechanisms): Role of precious metals in soot oxidation (e.g., other than NO oxidation)

Experimental data collected	***Model parameters calibrated***
Pressure drop across CPF	Filtration parameters of CPF model (PM cake permeability and substrate wall & PM cake PM oxidation)
PM concentrations into CPF	Input to CPF model & for PM mass into CPF
Volumetric flow rate into CPF	Input to CPF model and for PM mass into CPF
Gas temperature into CPF	Input to CPF model
Gaseous concentrations upstream and downstream of CPF	Gaseous kinetic parameters of CPF model
PM mass retained at the end of loading	Passive regeneration PM oxidation kinetics of CPF model
PM mass retained at the end of active regeneration	Active regeneration PM oxidation kinetics of CPF model
Particle Size Distribution upstream and downstream of CPF at specific time-points	Filtration efficiency-related parameters of CPF model
Temperature distribution (axial and radial) of CPF and temperature out of the CPF	Ambient heat transfer parameters of multi-channel CPF HT model and gaseous kinetic parameters of 1-D CPF model

CPF Models – Feature Comparison

Feature	*AGK et al*	*Koltsakis*	*Hinterberger*	*Yi*	*Hasan et al – MTU (2006)*	*Premchand et al – MTU (2009)[1]*
Filter geometry	quasi 3-D	quasi 3-D	3-D	3-D	1-D	quasi 3-D
Filtration of PM cake layer	No	No	No	No	Yes	Yes
Filtration of substrate wall	Yes	Yes	Yes	Yes	Yes	Yes
CPF Pressure drop components include channels	Yes	Yes	No	No	Yes	Yes
Passive regeneration	Yes	Yes	Yes	Yes	Yes	Yes
Active regeneration	Yes	Yes	Yes	Yes	No	Yes
PM oxidation in the PM cake layer	Yes	Yes	Yes	Yes	Yes	Yes
PM cake 2-layer concept	Yes	No	No	No	Yes	Yes
PM oxidation in the substrate wall	Yes	Yes	Yes	No	Yes	Yes
PM oxidation in the inlet channel and outlet channel	No	No	No	No	No	Yes
Gaseous species kinetics	Yes	Yes	No	No	No	Yes [2]
Radial variations in CPF inlet temperature	Yes	Yes	Yes	Yes	No	TBD[3]
Radial variations in CPF inlet velocity	Yes	Yes	Yes	Yes	No	TBD
Radial heat transfer between channels during active regeneration	Yes	Yes	Yes	Yes	No	TBD

[1] Current research
[2] Included; needs modeling of gas-solid phase mass transport
[3] Future work



INPUTS
1. Time histories
2. Geometries(OCC, CPF, Exhaust Pipes, Cones)
3. Calibration Constants
4. Material Properties
5. Other inputs

ENGINE

Turbo out

PLANT MODEL

EXHAUST PIPE

OCC

CPF

TAIL PIPE

OUTPUTS
1. Pressure drops across various exhaust components
2. Exhaust temperatures at various locations
3. CPF related outputs
4. Other inputs

Figure 3- Inputs and Outputs (Plant Model).

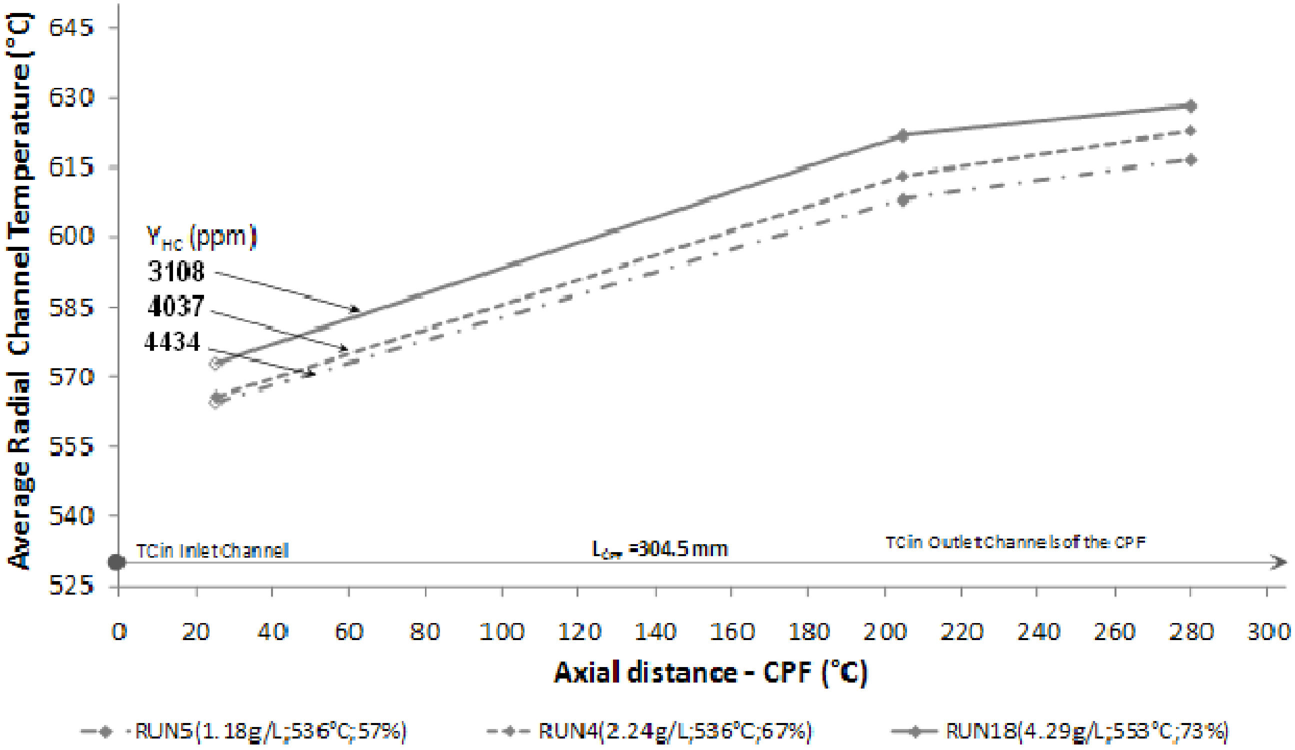
Equation Developed to Estimate Cake Mass (3 of 4)

- In this work, equation (3) describing the mass of PM in the cake equation has been simplified by neglecting the effect of the PM cake layer on the inlet channel and including the effect of variable wall permeability.

- Neglecting the effect of the PM cake layer on the inlet channel and the wall pressure drop results in underestimating the cake mass by 7% at 20% engine load at 4.0 hrs and 4 g/L of filter loading. At the other engine loads (40, 60 and 75%) the cake mass estimation is within 2%.

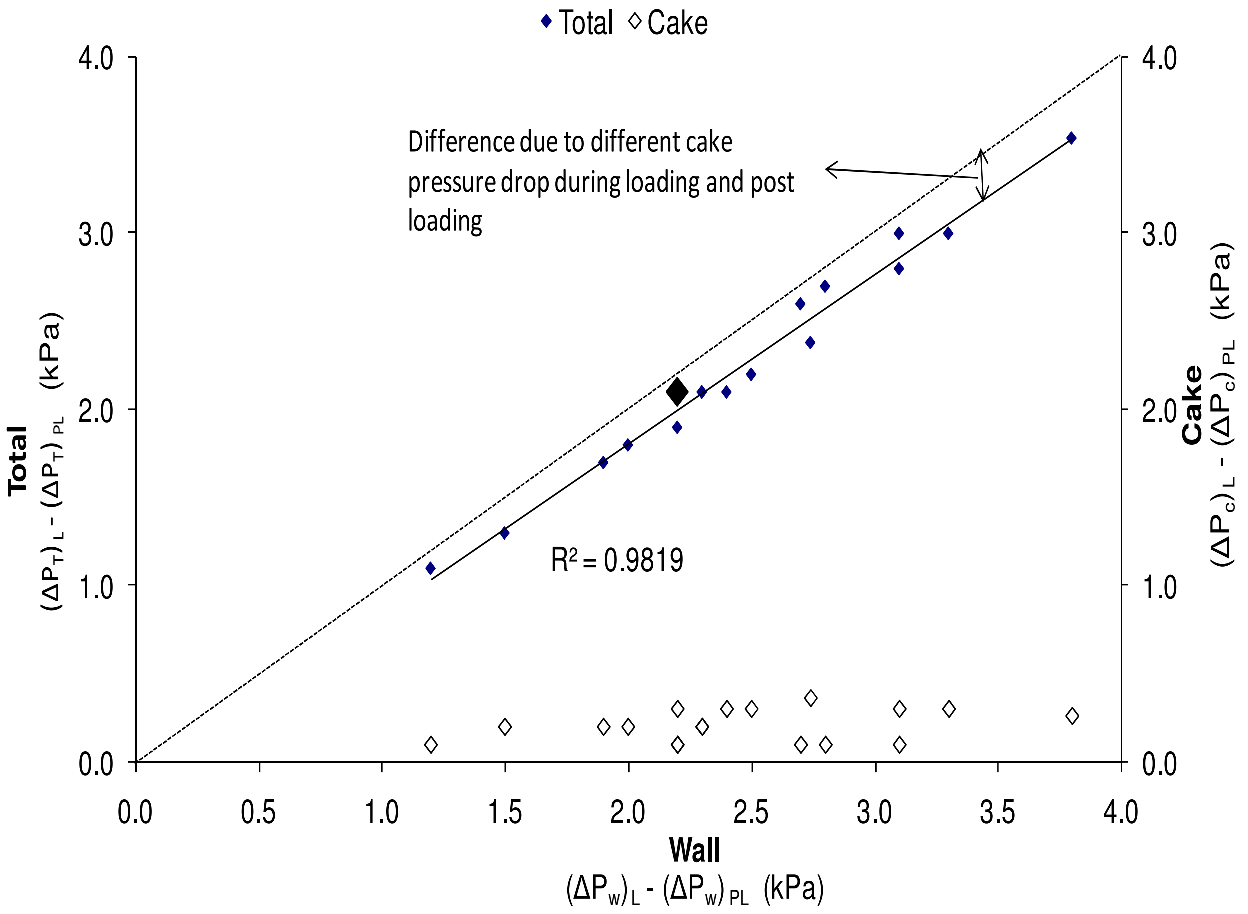
- If the effect of the PM cake layer on the inlet channel pressure drop are found to be significant for other substrate designs or operating conditions, then the effects described in Equations (2) and (3) can be solved with a simple iterative solver for real time applications using a cake mass equation including these effects.

Axial Temperature Profile during Active Regeneration



- Increase in temperature is indicative of oxidation of HC, CO and PM along the CPF channels
- Rate of oxidation of HC, CO and PM and inlet exhaust temperature is constant along the channel length introducing a linear rise of temperature

Comparison between Loading and Post Loading Pressure Drop



- Shows differences between loading and post loading pressure drop in terms of total, cake and wall
- Wall pressure drop is linearly related to total pressure drop which means wall pressure drop is the main reason for difference in pressure drop between loading and post loading

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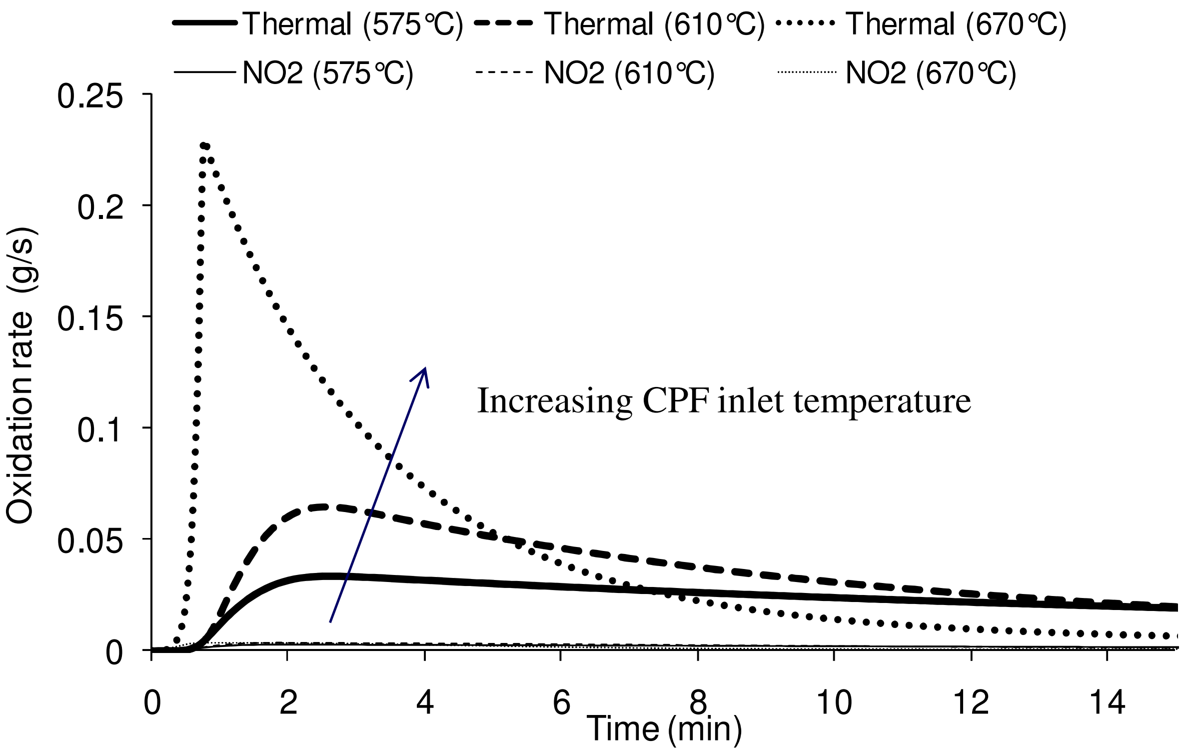
Ramp-Up at 8°C/sec –Mass Oxidation Results



- Thermal oxidation rate for 670°C case is three times that of 610°C and six times that at 575°C
- NO_2 oxidation rate is negligible because of low concentration during active regeneration

Inlet-Membrane DPF.

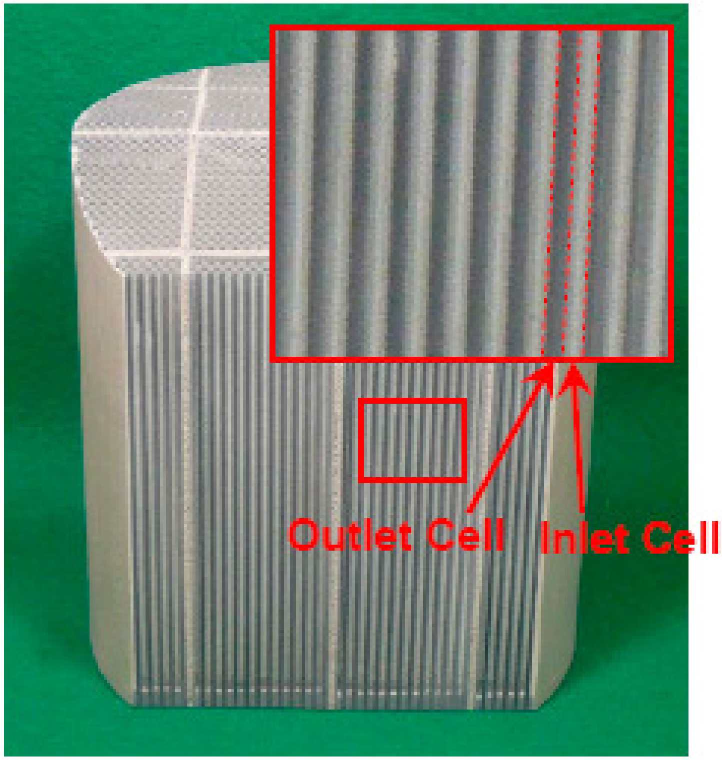


Fig. 8: Example of the Inlet-Membrane DPF.