The Development of the MTU 1-D 2-Layer Model to Simulate a Johnson Matthey CCRT®

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Overview of Presentation

- Introduction and Objectives of Research
- Design of the Experiments
- Description and Development of CPF Model
- CPF Modeling Results
- Summary and Conclusions

- Research sponsored by Cummins Inc.

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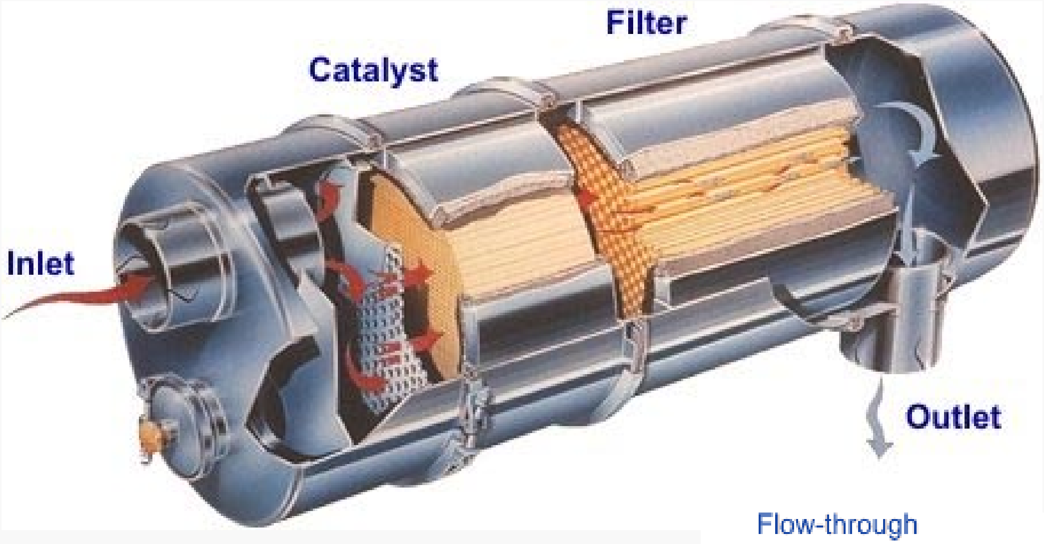
Introduction and Objectives of Research

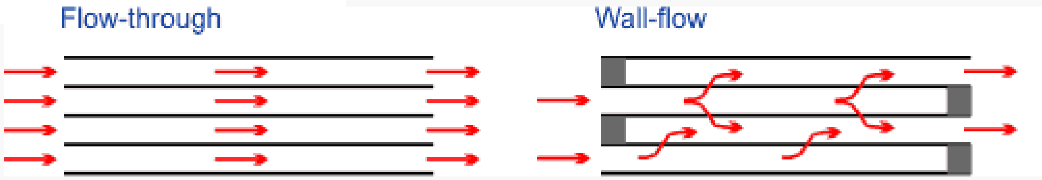
Catalyzed Continuously Regenerating Trap, CCRT®

- Patented by Johnson Matthey -- NO_2 can oxidize particulate at temperatures of 275°C and higher.
- DOC upstream of the CPF increases the NO_2 entering the CPF. Particulate oxidation in CPF is enhanced by a catalyst washcoat in the CPF which promotes the oxidation of NO NO_2



DOC – 400 cpsi, 10.5X 6 in

CPF – 200 cpsi, 10.5 X 12 in

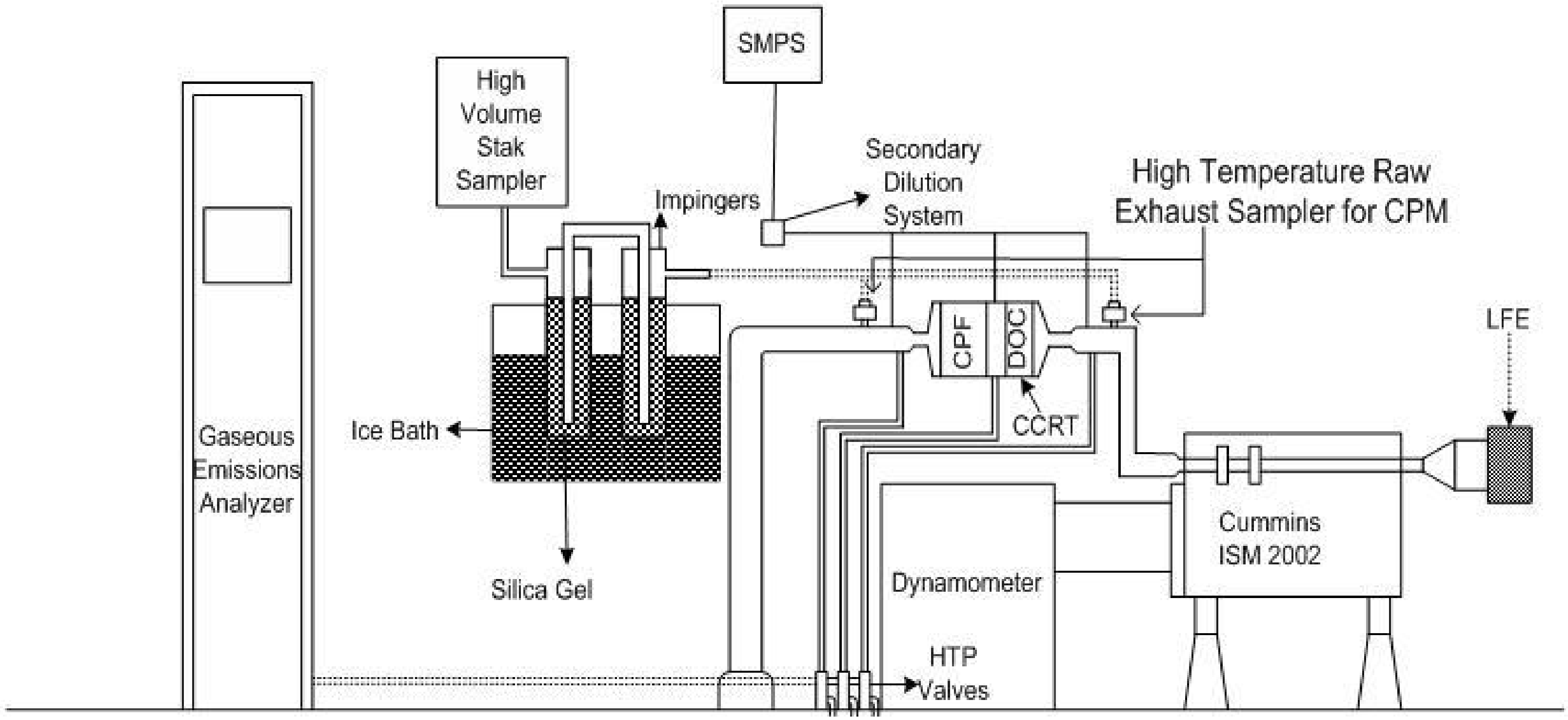


Objectives of Research

- Design and perform experiments with the CCRT® to obtain data to calibrate the CPF model.
- CPF model development to simulate the CCRT®
  - Particulate oxidation in the filter wall
  - Particulate cake layer filtration model
  - Model the NO_2 produced in the CPF catalyst washcoat
- Calibrate the CPF model to study the filtration, loading and oxidation characteristics of the CCRT®. Use the model to better understand the internal performance of the CCRT®.

Design of the Experiments

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

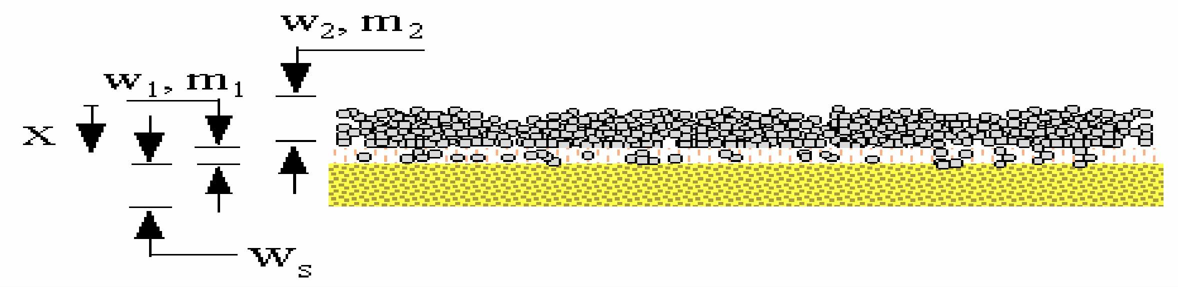
Experimental Test Matrix

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 (^{o}C)	280	340	415	460

- Study the effect of temperature on particulate 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

Description and Development of CPF Model

Overview of the Earlier MTU 1-D 2-Layer* CPF Model



- One-dimensional transient filtration-oxidation model of the CPF, predicts the pressure drop across the filter, particulate mass deposited in and on the wall, particulate mass oxidized and downstream particle size distribution.
- Solves the continuity, momentum, energy and heat transfer equations along the length of the CPF.
- Models filtration by the CPF wall, based on Brownian diffusion and flow-line interception.
- Oxidation in particulate cake layer by the following:
  - Thermal means - Layer I & II
  - Catalytic means - Layer I
  - Oxidation of particulate by NO_2 entering the filter.

*: 2-Layer approach proposed by Konstandopoulos et.al. in SAE Paper 1999-01-0469. Figure from same paper.

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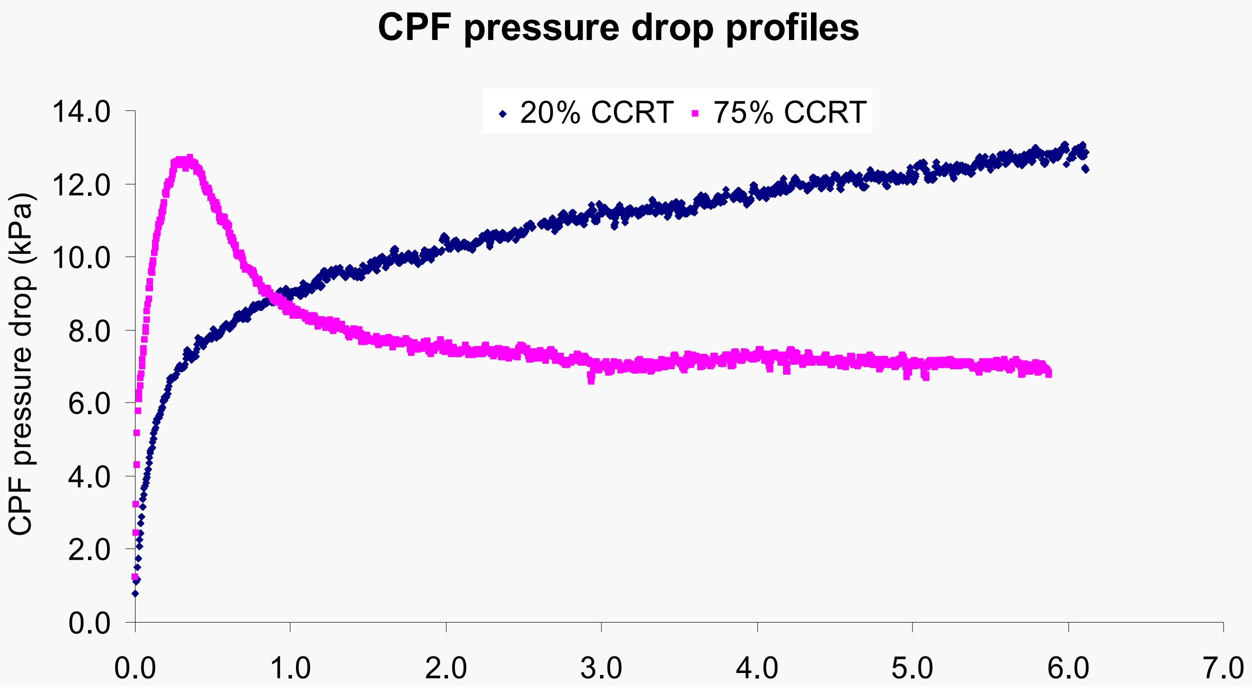
Need for CPF Model Development


CPF pressure drop profiles

Increase in NO_2 concentrations across the CPF

	CCRT® configuration, Mean (S.D)		CPF-only configuration, Mean (S.D)	
% Load	US-CPF	DS-CPF	US-CPF	DS-CPF
20	105 (2)	113 (2)	35 (3)	71 (2)
40	136 (3)	132 (3)	22 (3)	96 (10)
60	103 (4)	113 (4)	24 (3)	111 (5)
75	63 (10)	86 (6)	13 (5)	90 (4)

Improvements to 1-D CPF Model

- Oxidation inside the pores of the filter wall by thermal and by NO_2/Temperature assisted oxidation..
- Particulate cake filtration model — model the porous cake layer like the filter wall and couple the filtration and oxidation models of the filter wall and particulate cake layer.
- Oxidation of particulate by NO_2 produced in the catalyst washcoat of the CPF.

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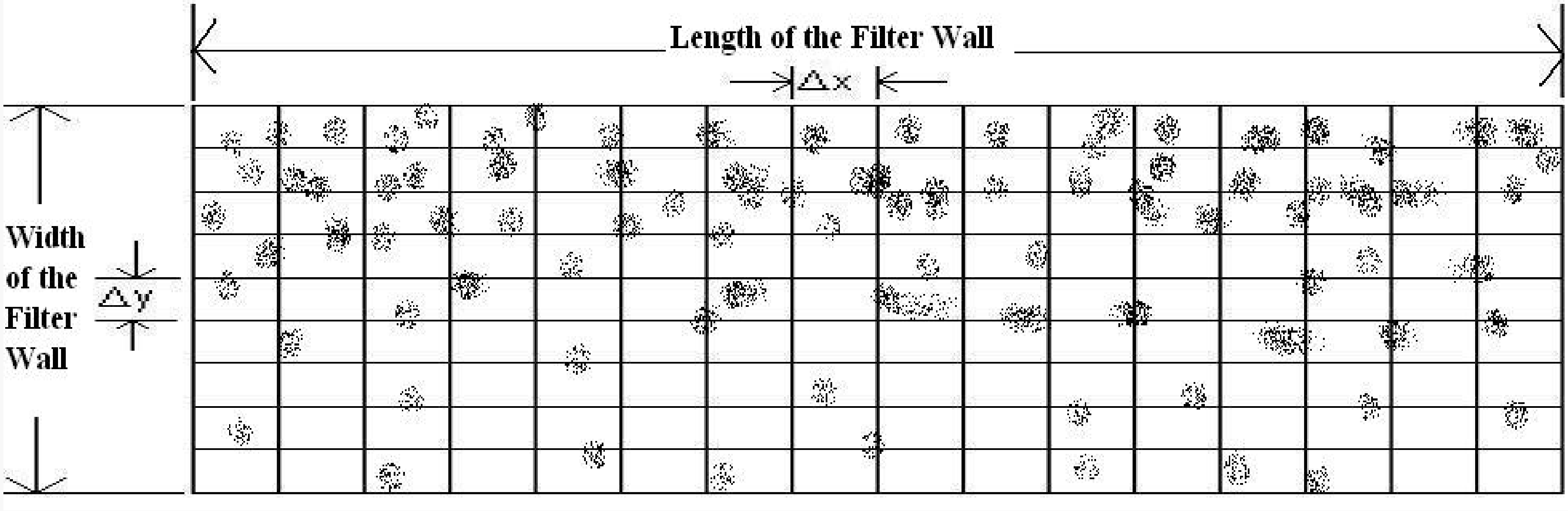
Particulate Oxidation in the Wall

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

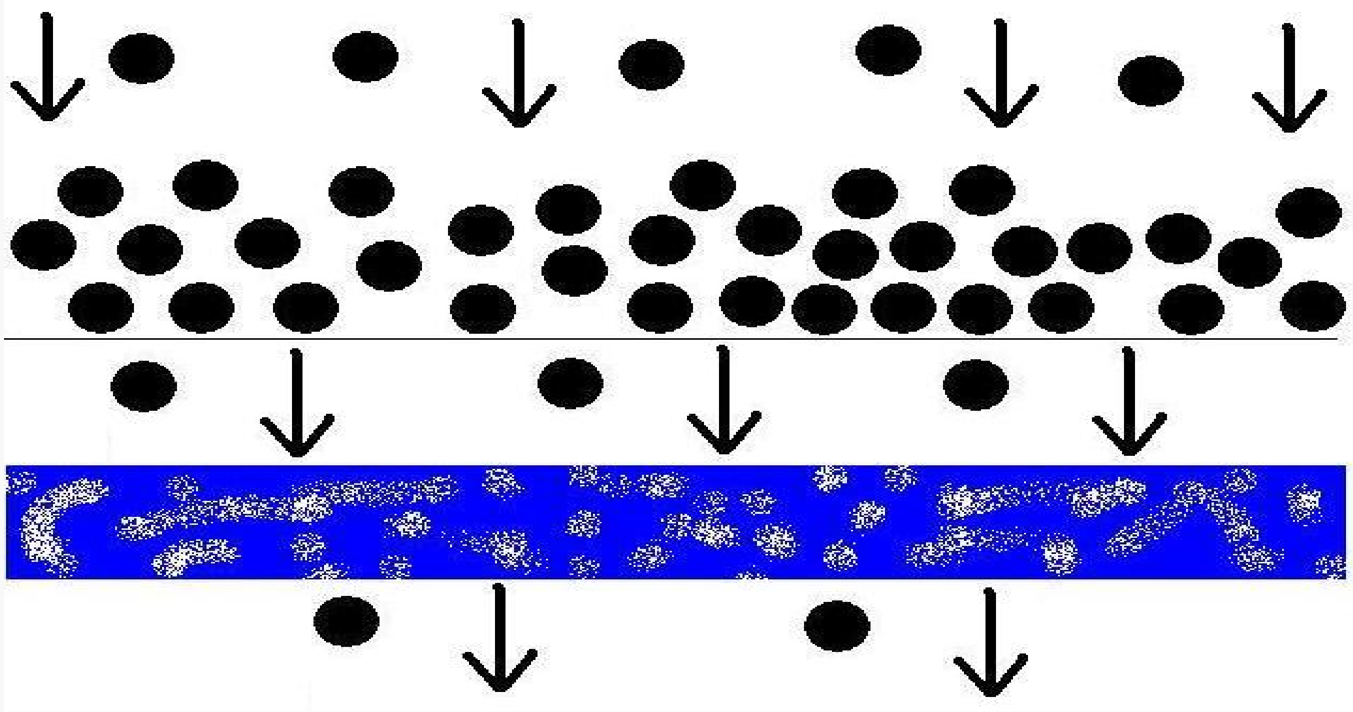


Particulate Oxidation in the Wall (Contd.)

- Determine reaction rates in the wall such that if a similar amount of particulate 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.
  - Sum up all the particulate mass present in the wall to form a ‘virtual’ layer.
  - Regeneration equations similar to those in layers I and II, can be applied.

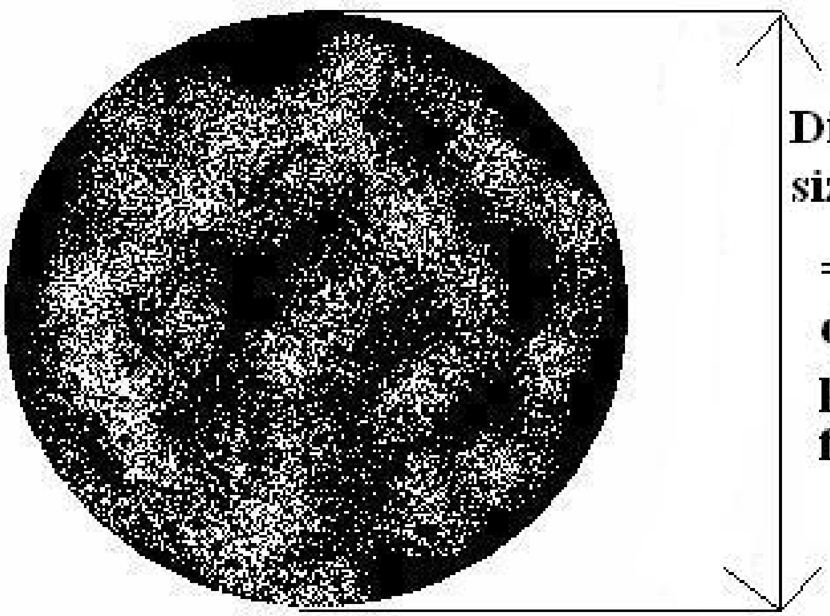
Particulate Cake Filtration Model

- The wall oxidation model does not couple properly with the overall filtration model.
- Once the cake forms, it is more natural and useful to describe the filtration by means of particulate cake parameters which are separate from the wall.
- This is the equivalent of separately simulating filtration by cake sieving as shown in the picture, followed by wall filtration.



Particulate Cake Filtration Model (Contd.)

- Filtration by the particulate cake is modeled like the wall – by the application of unit collector theory.
- Studies of diesel particulate cakes show that it consists of aggregate particles with an approximate diameter of 0.1 um.
- The aggregate particle size can thus be a unit collector which filters other similar sized particles in the exhaust.



Diesel aggregate particle size = 0.1 um

= Unit collector diameter for particulate cake filtration model

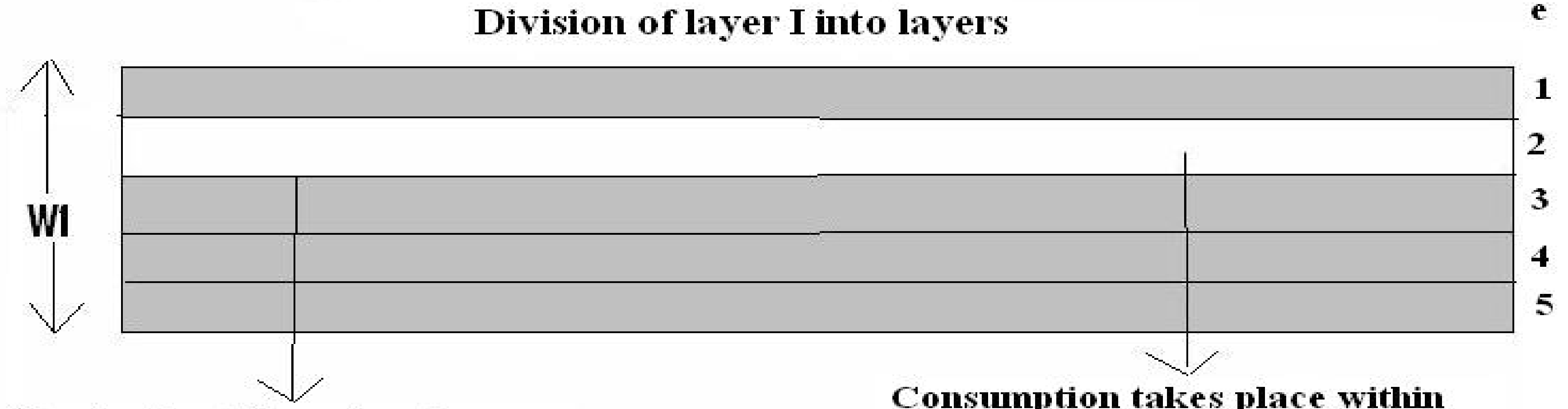
Oxidation in Layer I by NO_2

- A catalyst in the CPF washcoat of the CCRT® promotes the oxidation of NO NO_2 which results in increased particulate oxidation rates.
- Oxidation in Layer I thus has two facets: consumption of NO_2 by particulate oxidation, and generation of NO_2 from NO in the catalyst washcoat. Thus in a CCRT®, reaction rates in layer I will also depend on availability of NO.
- Oxidation of NO NO_2 in the CPF washcoat also changes the O_2 concentrations – NO, NO_2 and O_2 concentrations must be properly handled
- Same frequency factors in layer I and II -- increased reaction rates are due to increased NO_2 concentrations.

Oxidation in Layer I by NO_2 (Contd.)

- To model the simultaneous consumption and production of NO_2, Layer I is divided into 5-10 layers (depending on layer I thickness), with consumption of NO_2 within these layers, and oxidation of oxidation of NO NO_2 in between these layers.

Division of layer I into layers



Production takes place in between the layers

Consumption takes place within the layers

$$\frac{dy_{NO_2}}{dt} = k_{NO} y_{O_2}^{\gamma} y_{NO}^{n}$$

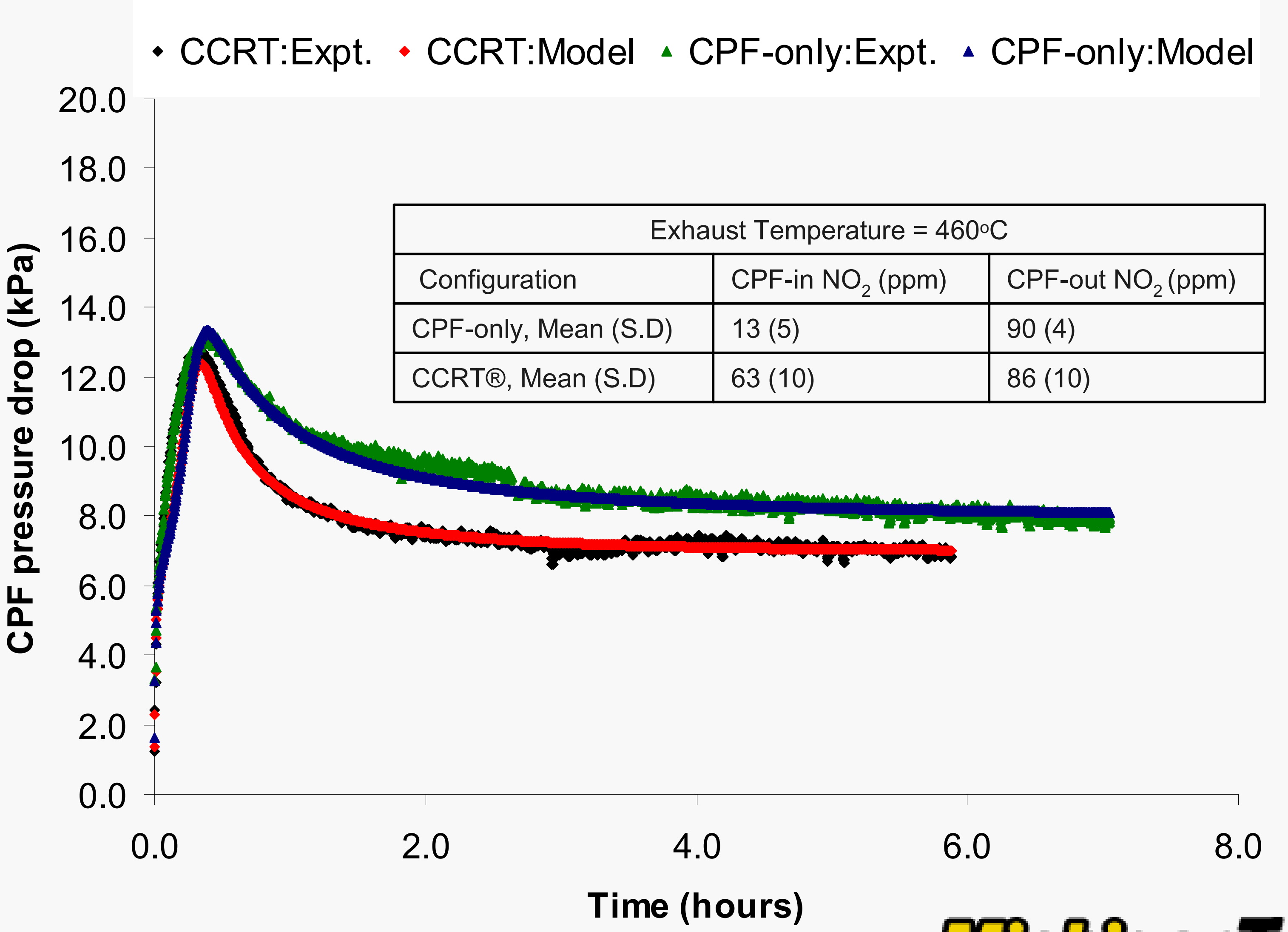
$$Y_{NO_2,e} = Y_{NO_2,1}\left(1 - exp\left(\frac{-S_p k_{NO_2}(2 - g_{CO})w_e}{v_w}\right)\right)$$

– From Cooper et.al. in SAE Paper No. 890404

– Proposed by Konstandopoulos et.al. in SAE Paper No. 2000-01-1016 to take into account oxidation of NO in CPF

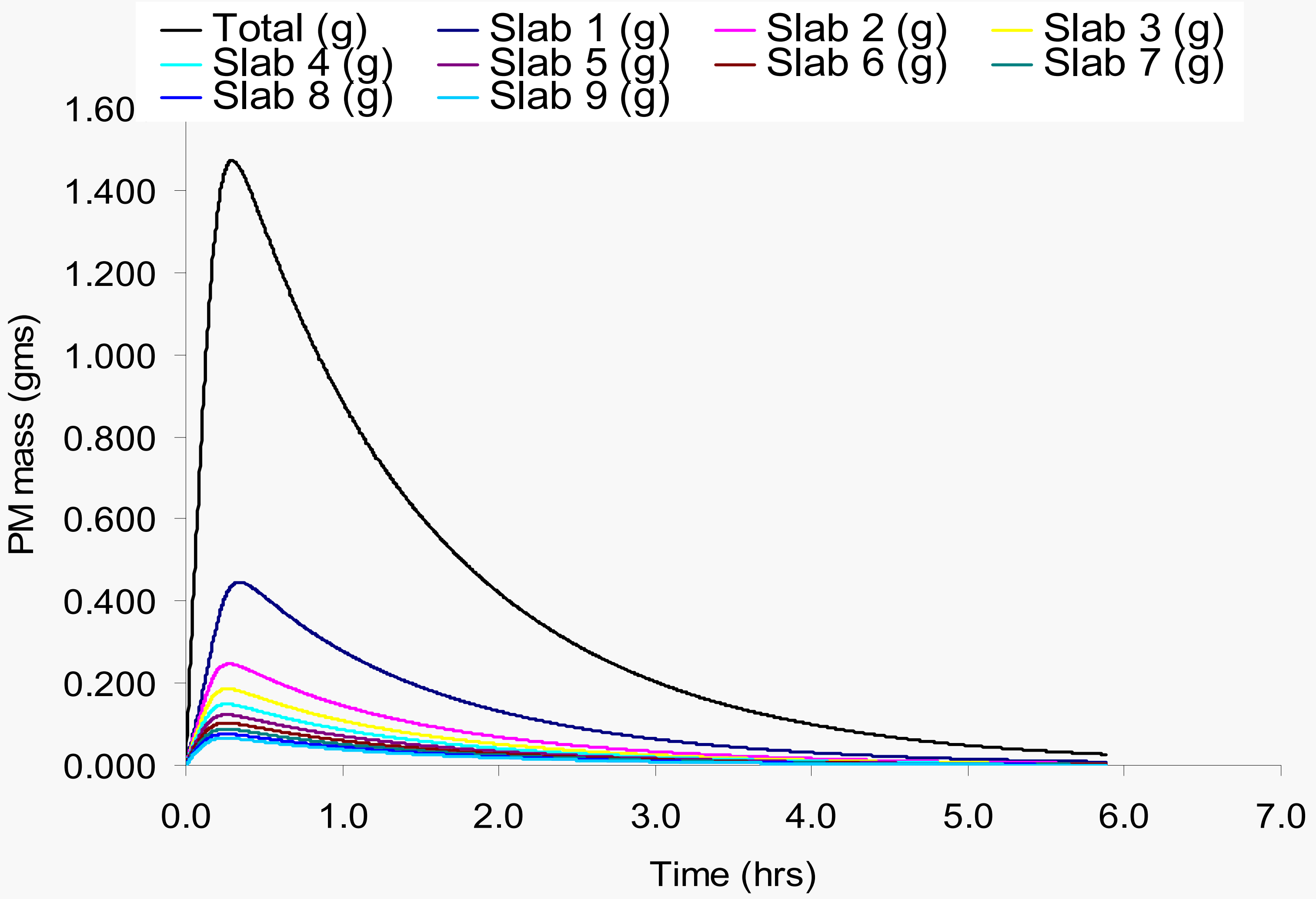
CPF Modeling Results

75% load: Pressure Drop Calibration

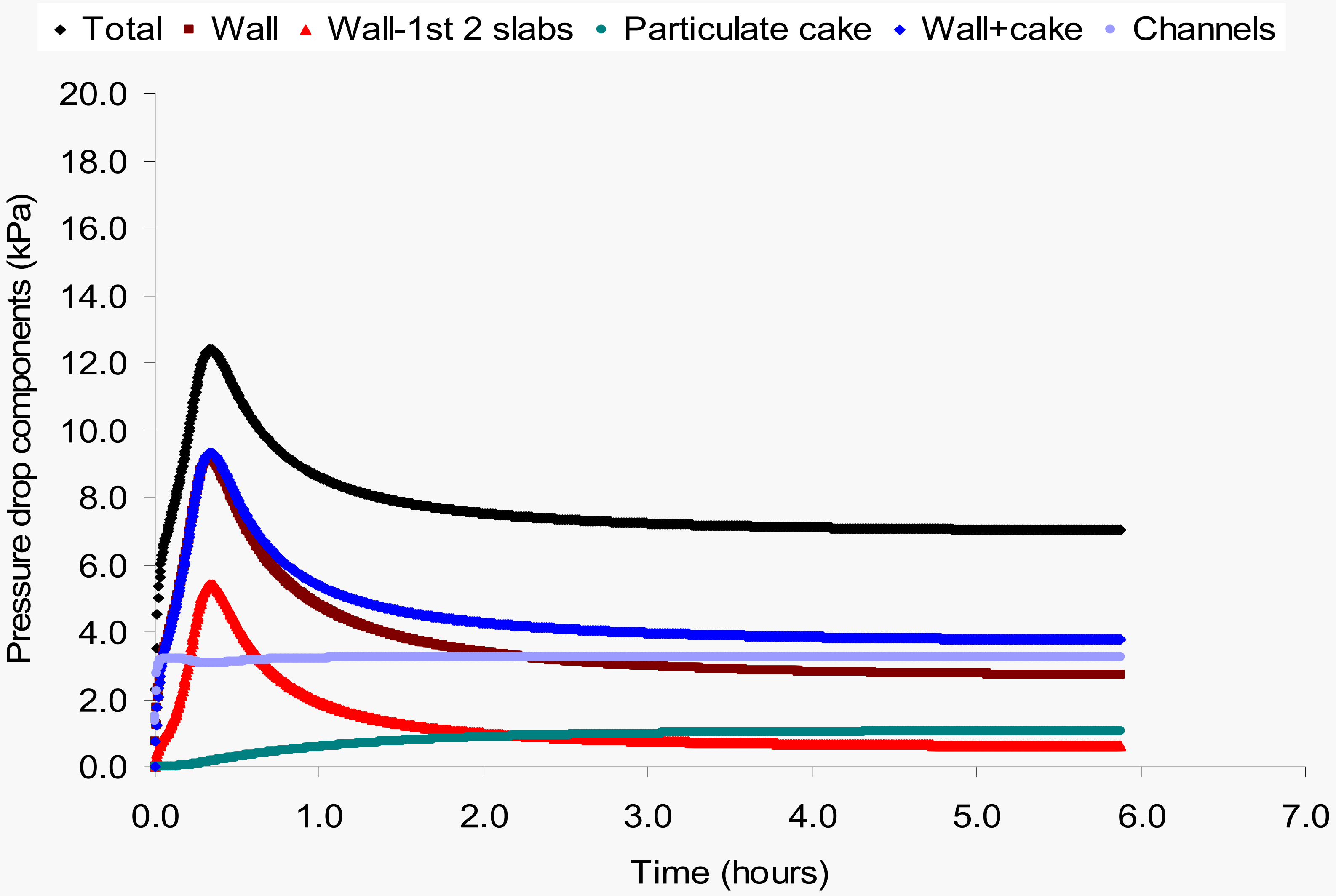


Exhaust Temperature = 460°C		
Configuration	CPF-in NO_2 (ppm)	CPF-out NO_2 (ppm)
CPF-only, Mean (S.D)	13 (5)	90 (4)
CCRT®, Mean (S.D)	63 (10)	86 (10)

75% CCRT®: Mass in Filter Wall with Time



75% CCRT®: Pressure Drop Components



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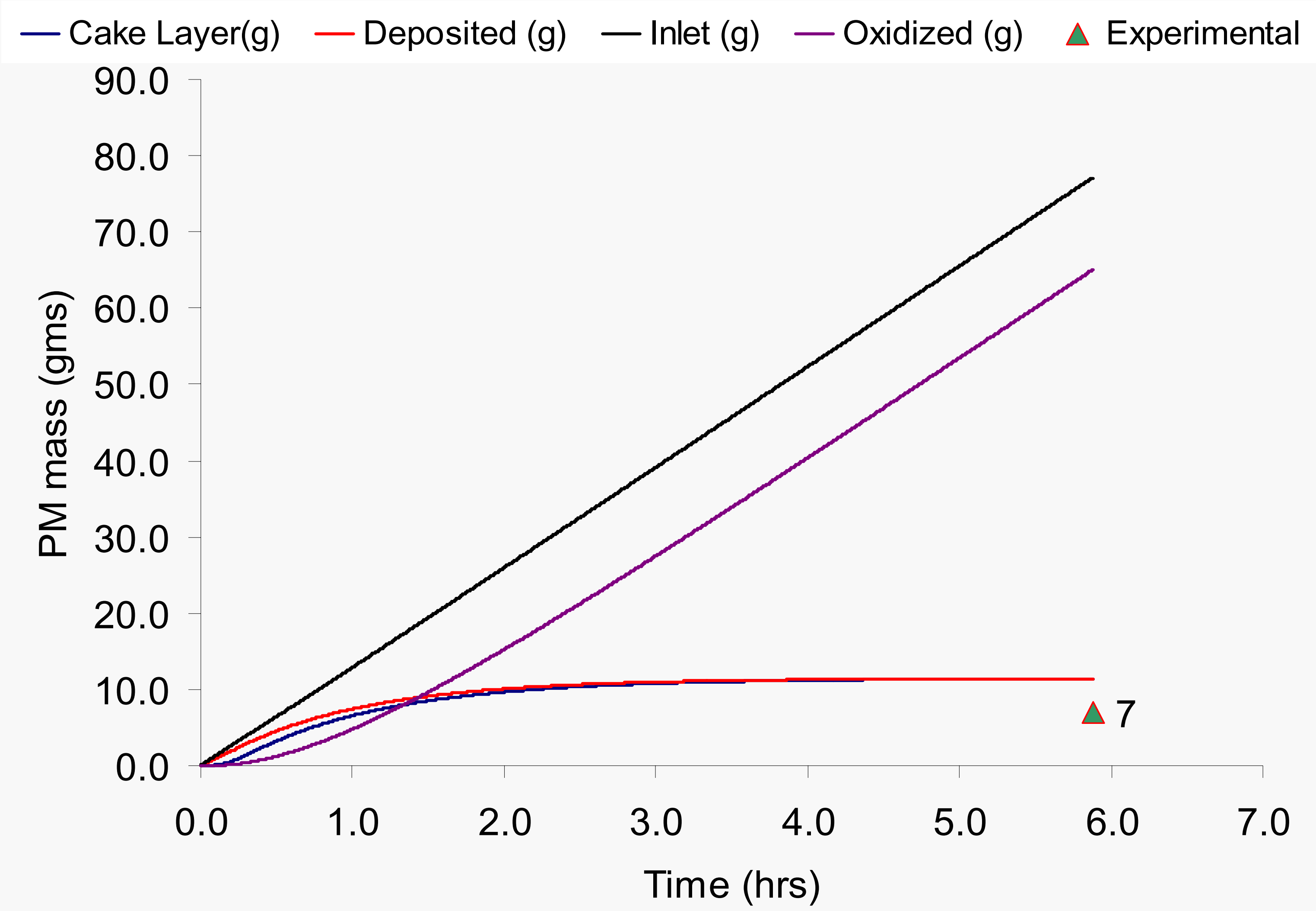
75% CCRT®: Particulate Mass with Time



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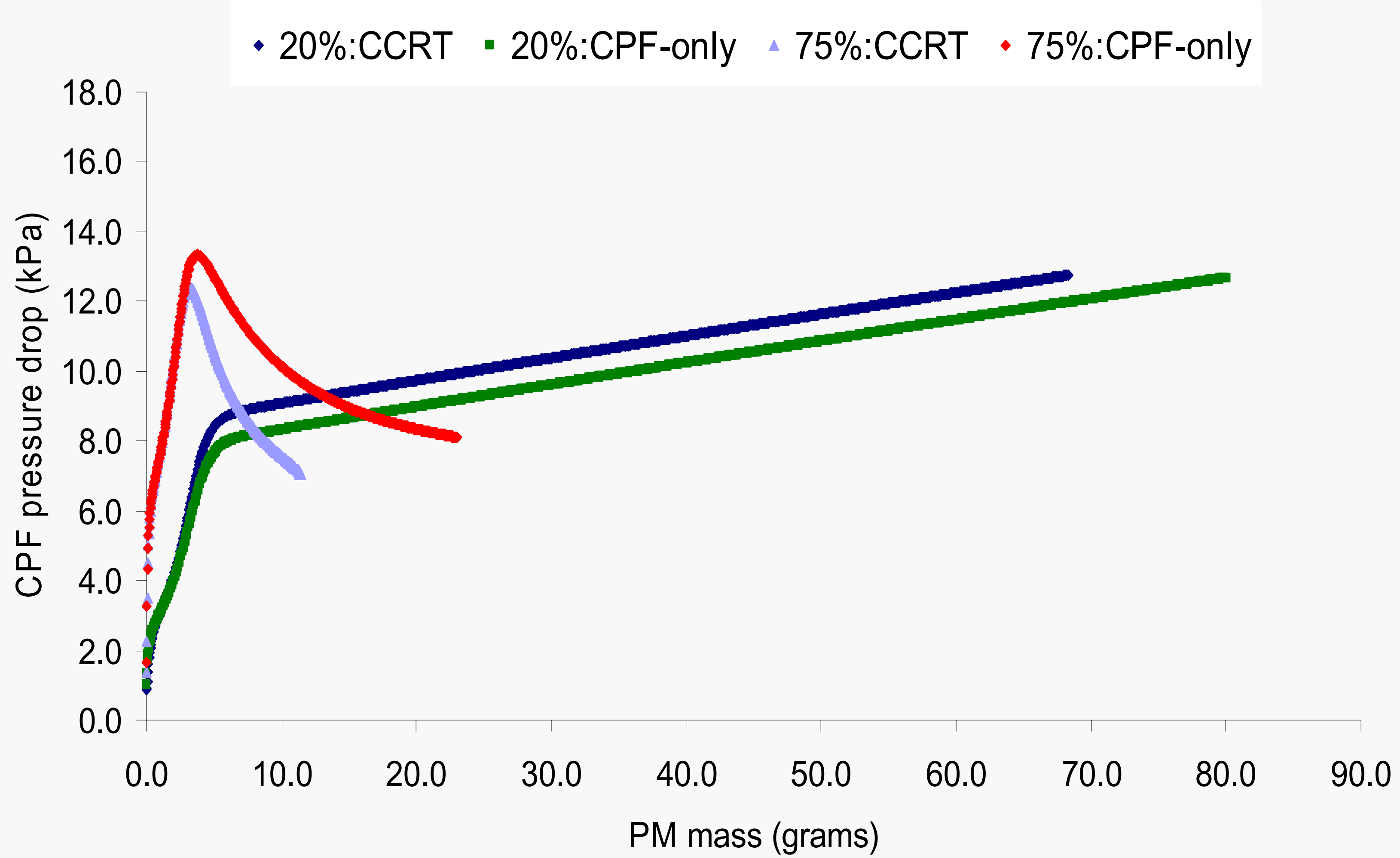
20 and 75% load: Pressure Drop vs. Particulate Mass



-Oxidation in the filter wall results in different pressure drops for the same amount of particulate mass in the filter.

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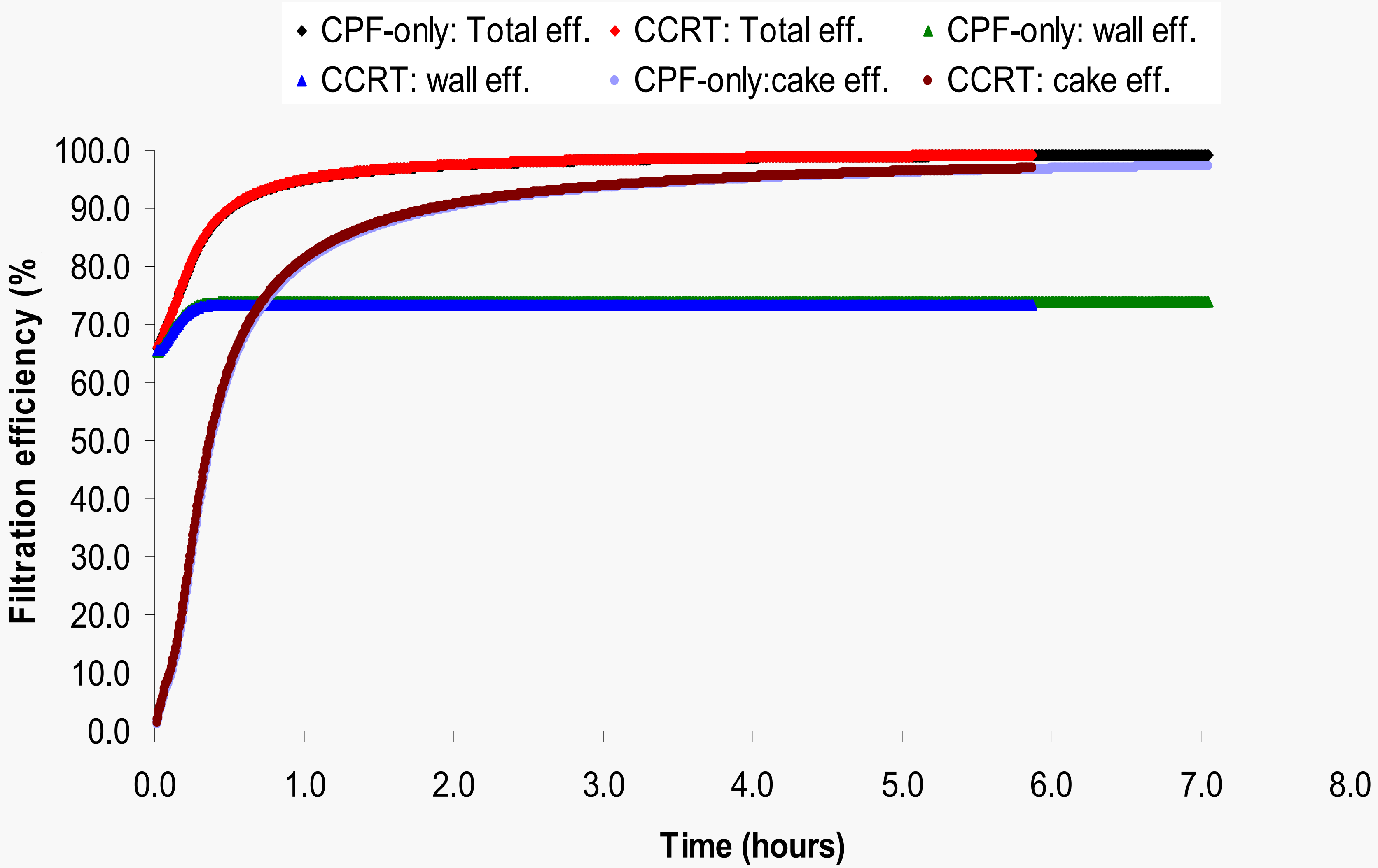
75% load: Comparison of Filtration Efficiencies



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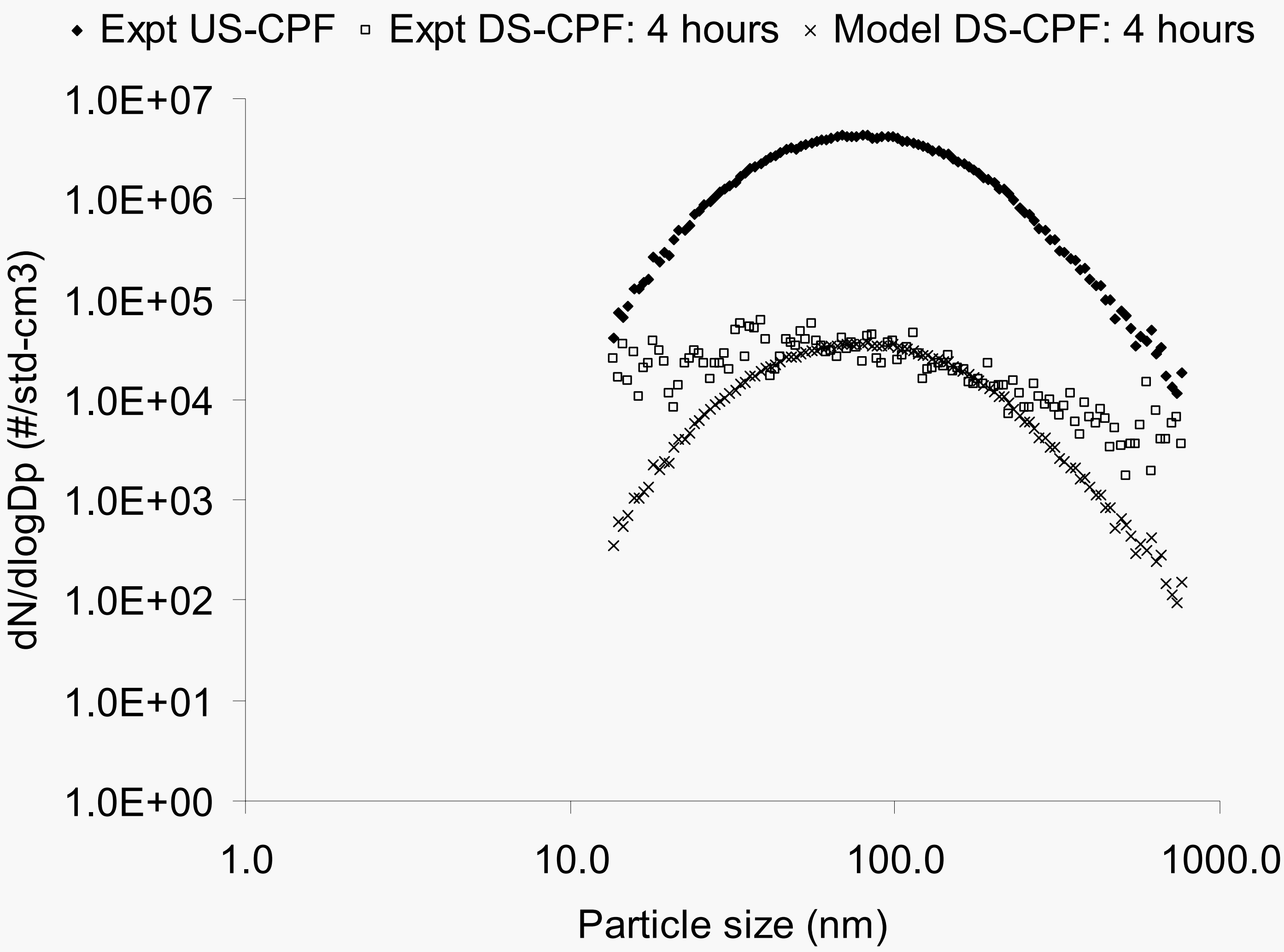
75% CCRT®: DS CPF Particle Size Distribution



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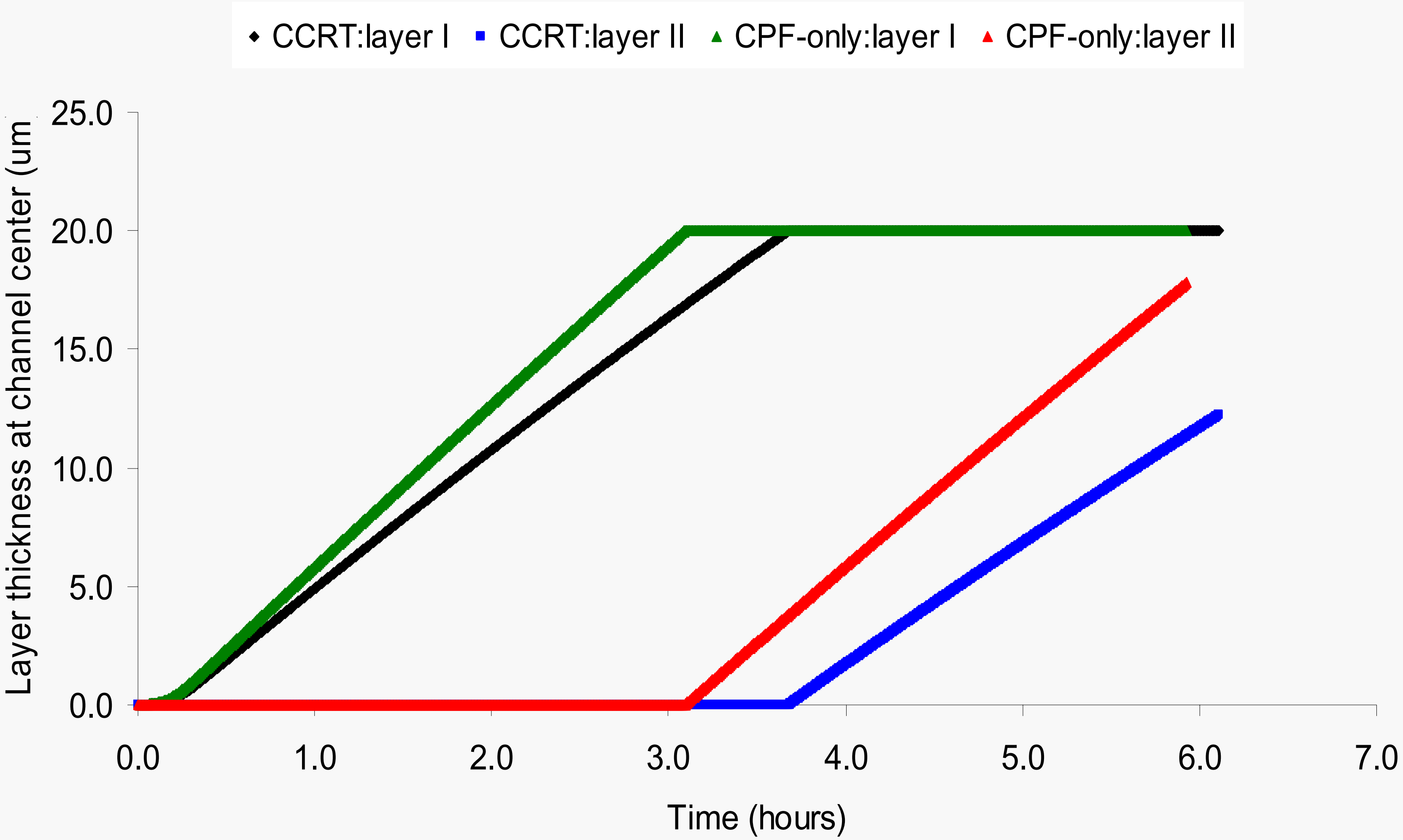
20% load: Layer Thicknesses with Time



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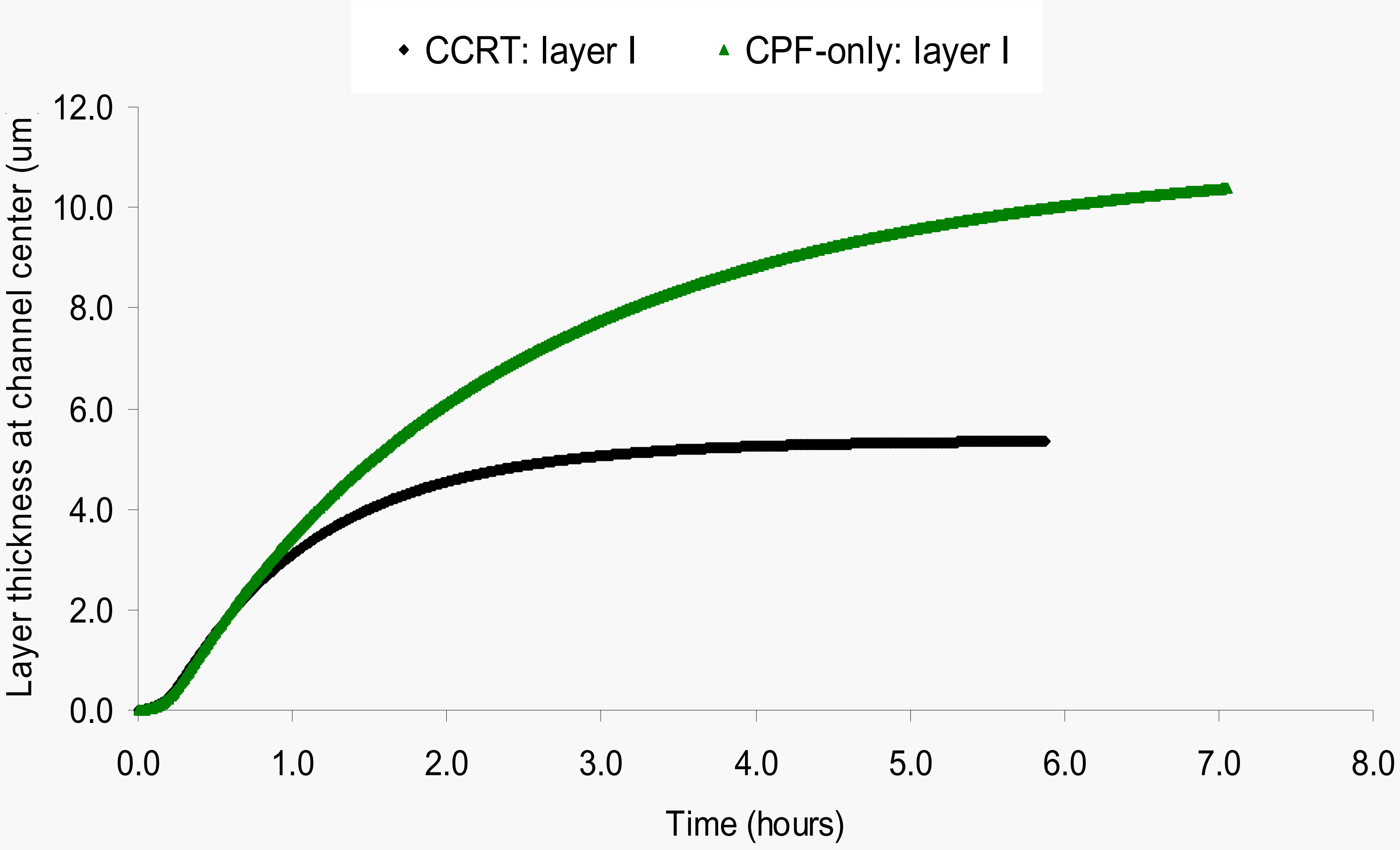
75% load: Layer Thicknesses with Time



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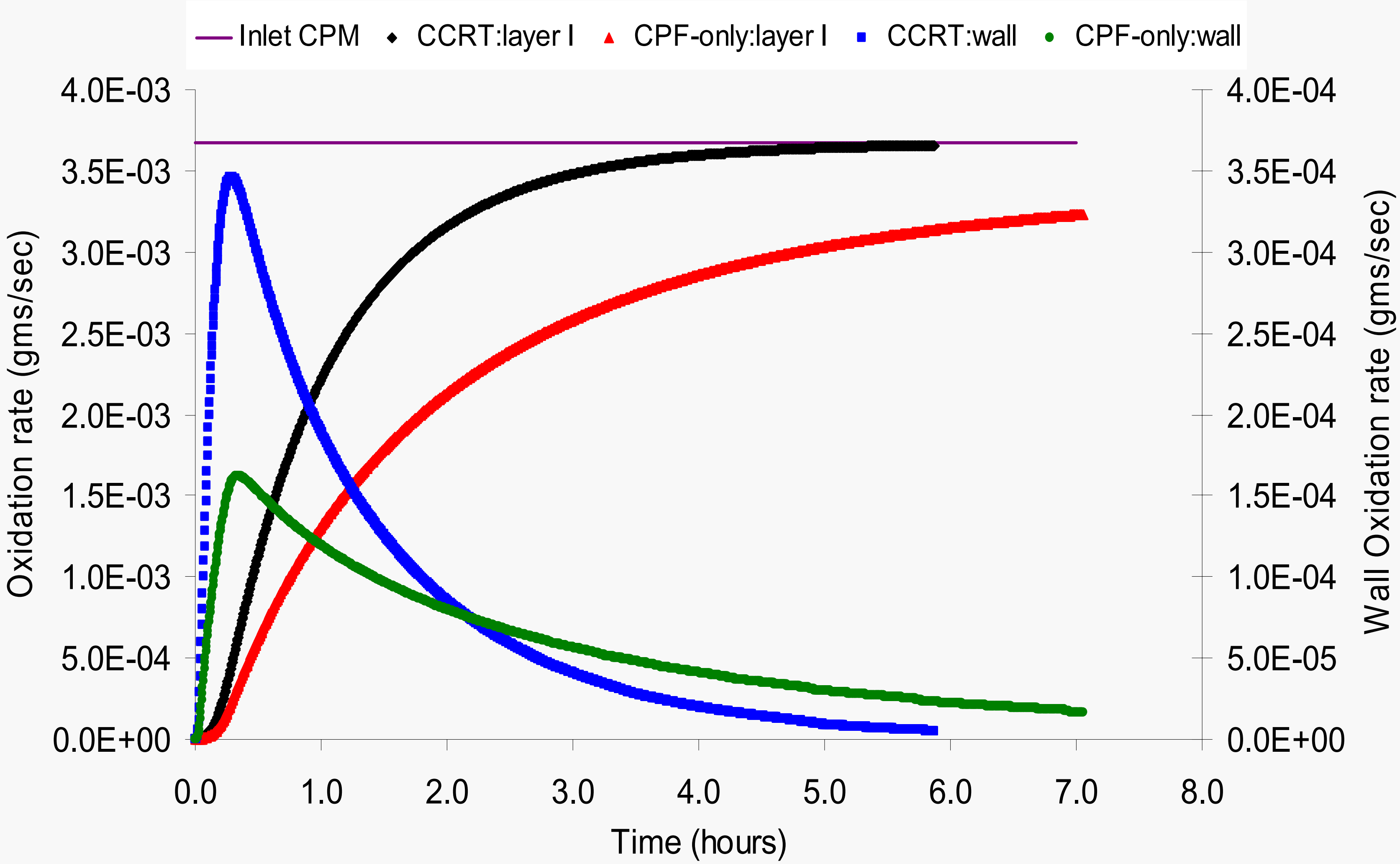
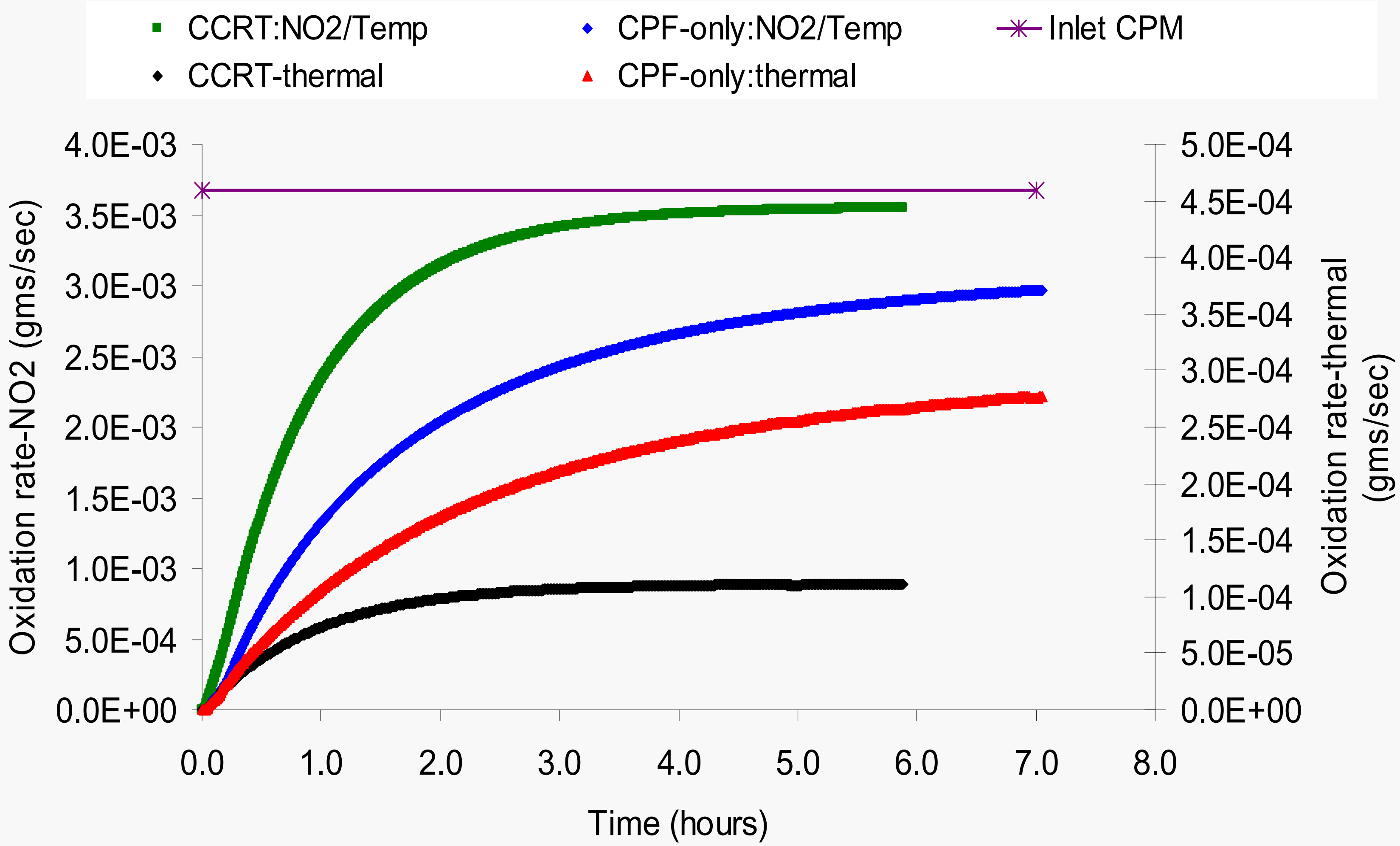
75% load: Oxidation Rates by Physical Location



75% load: Oxidation Rates by Mechanism



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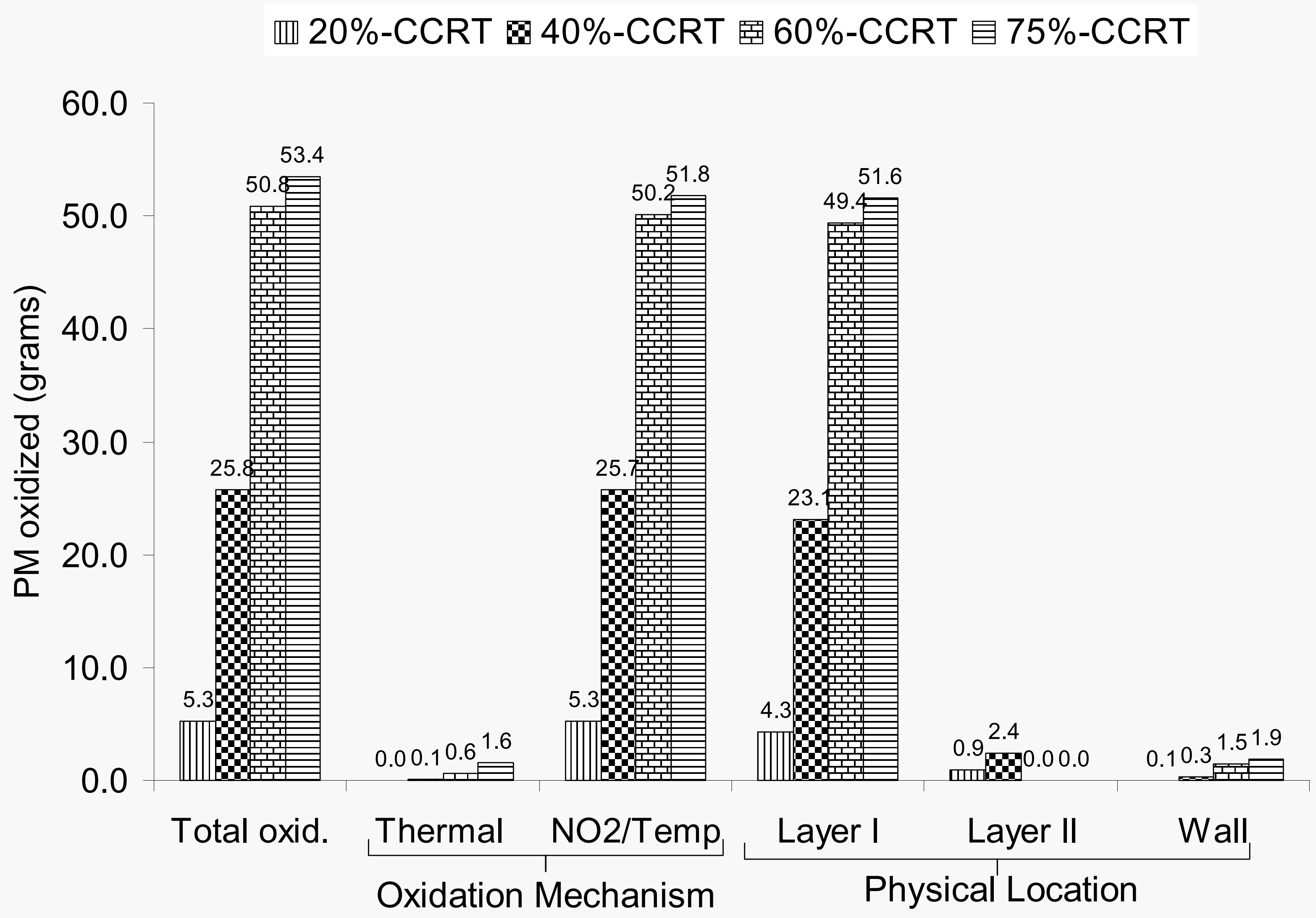
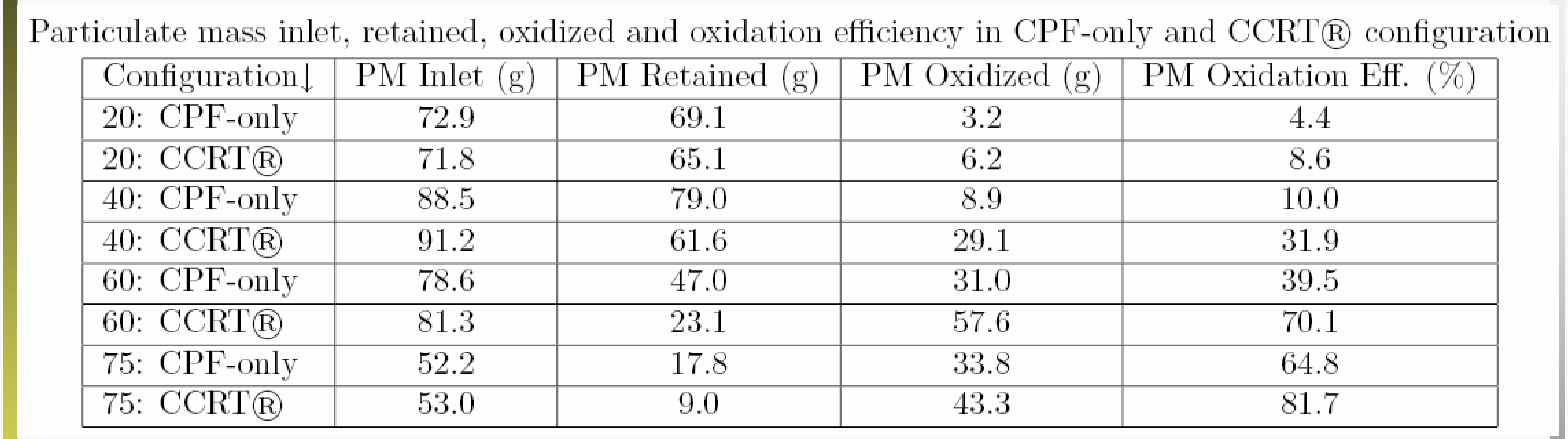
CCRT®: Summary of Particulate Mass Oxidized After 5 Hours



CCRT® and CPF-only: Particulate matter Oxidation Efficiency Comparison After 5 hours



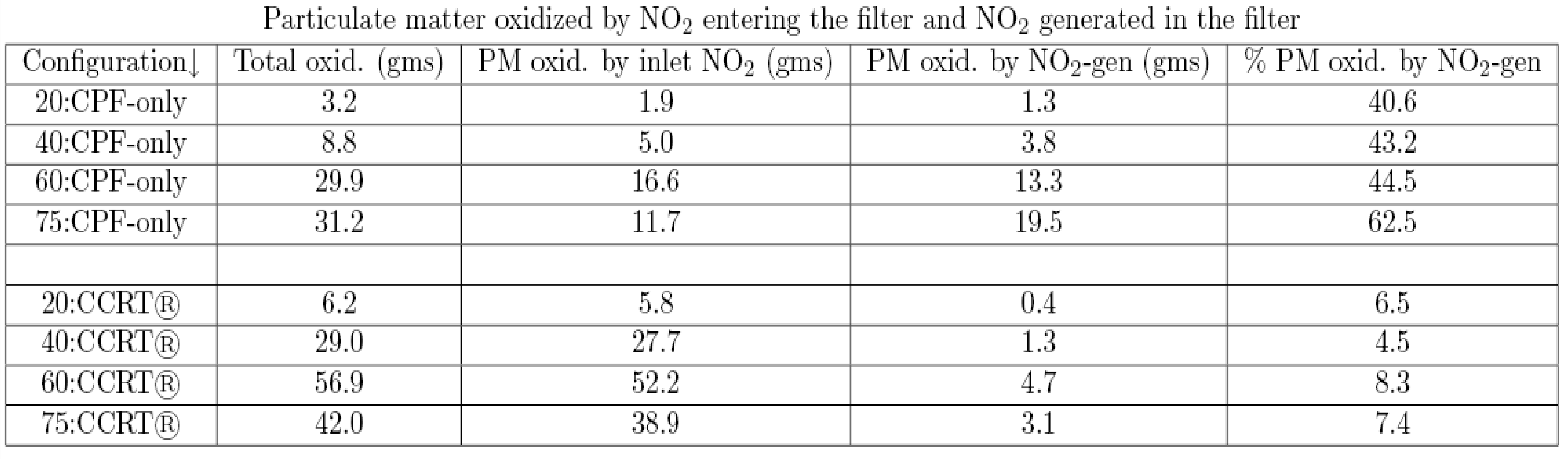
Particulate mass inlet, retained, oxidized and oxidation efficiency in CPF-only and CCRT® configuration

Configuration↓	PM Inlet (g)	PM Retained (g)	PM Oxidized (g)	PM Oxidation Eff. (%)
20: CPF-only	72.9	69.1	3.2	4.4
20: CCRT®	71.8	65.1	6.2	8.6
40: CPF-only	88.5	79.0	8.9	10.0
40: CCRT®	91.2	61.6	29.1	31.9
60: CPF-only	78.6	47.0	31.0	39.5
60: CCRT®	81.3	23.1	57.6	70.1
75: CPF-only	52.2	17.8	33.8	64.8
75: CCRT®	53.0	9.0	43.3	81.7

- The CCRT® configuration is more efficient than CPF-only, in oxidizing particulate, proving the beneficial effect of NO_2 on particulate oxidation.

- Oxidation rates at 20% load (280^{o}C) are only ~9%, NO_2 is more effective at higher temperatures.

Comparison of PM Oxidized by NO_2 Entering the CPF and Being Produced in the CPF After 5 hrs



Particulate matter oxidized by NO_2 entering the filter and NO_2 generated in the filter

Configuration↓	Total oxid. (gms)	PM oxid. by inlet NO_2 (gms)	PM oxid. by NO_2-gen (gms)	% PM oxid. by NO_2-gen
20:CPF-only	3.2	1.9	1.3	40.6
40:CPF-only	8.8	5.0	3.8	43.2
60:CPF-only	29.9	16.6	13.3	44.5
75:CPF-only	31.2	11.7	19.5	62.5
20:CCRT®	6.2	5.8	0.4	6.5
40:CCRT®	29.0	27.7	1.3	4.5
60:CCRT®	56.9	52.2	4.7	8.3
75:CCRT®	42.0	38.9	3.1	7.4

-The catalyst loading in the CPF increases costs and decreases engine performance due to higher backpressures.

-Model results show that the catalyst loading only modestly increases the total particulate oxidized in CCRT® configuration. Its effect is most evident in CPF-only configuration.

Summary and Conclusions

Summary and Conclusions

- No 'catalyst effect' with O_2 in Layer I was required for modeling the CPF particulate oxidation kinetics. All oxidation kinetics were described by thermal and NO_2/Temp. -assisted oxidation of particulate.
- The model showed that NO_2/Temp. is the dominant means of particulate oxidation in the temperature range of 280°C – 460°C. Layer I (20um) was the dominant physical location of particulate oxidation.
- The model shows that oxidation in the pores of the filter wall and particulate cake layer filtration explain the disproportionate decrease in the pressure drop across the filter with respect to particulate mass.

Summary and Conclusions

- The NO_2 production model resulted in the same kinetic factors for all the temperatures and NO_2 concentrations
- The filtration model developed for the particulate cake layer showed that it is a very efficient filter of particles in the exhaust, even more than the filter wall, and overall filtration efficiencies of 98-99% were predicted.
- The catalyst in the CPF significantly increases particulate oxidation rates in the CPF-only configuration. However, it only modestly increases oxidation rates in the CCRT® configuration. Hence, the catalyst loading in the CPF could possibly be reduced without significantly decreasing the passive regeneration performance of the CCRT®.
- The CPF model was an effective tool in developing a physical and chemical understanding of the performance of the CCRT®.

Questions?