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Development of Advanced Diesel Particulate Filtration (DPF) Systems

(ANL/Corning/Caterpillar CRADA)

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PI: **Kyeong Lee**

(Postdoc: Seung Yang)

Argonne National Laboratory

Project ID ace024

DOE Project Managers:

Kenneth Howden & Gurpreet Singh

Office of Vehicle Technologies

U.S. Department of Energy

UChicago Argonne LLC

A U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

Overview

Timeline

- Start: Oct 2006
- Finish: Sept 2009
  (extended to 2011)
- 60% Finished

Budget

- Total Project funding
  - DOE: $1,450K
  - Industry sponsors: $1,450K
- Funding received in FY09
  - $500K
- Funding received in FY10
  - $500K

Barriers

- Increased back pressure and fuel penalty
- Lack of effective regeneration strategies to reduce input energy and deal with low exhaust temperature
- Durability of the system, including filter materials
- Sensor technology

Partners

- Corning and Caterpillar
- University of Illinois – Chicago
- University of Wisconsin – Madison
- Iljin Electric Co.

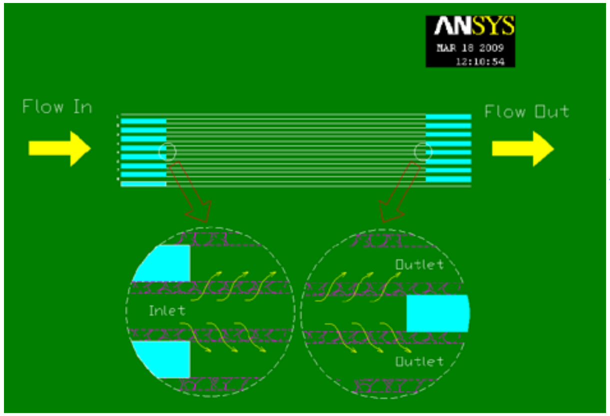
Relevance and Objectives

- Existing DPF systems still need to improve filtration/regeneration efficiencies and pressure drops.
- DPF systems need efficient regeneration strategies, which can control thermal run-away.

  → Accurate measurement of heat release is needed.
- A real-time DPF control/management system is required for developing an advanced DPF system with on-board diagnostics (OBD) capability.
- Predict the transient heat release in DPF regeneration.
  - Derive equations for the oxidation rate of diesel particulates
  - Measure the amount of heat release from the oxidation
- Characterize pressure drops of modified DPF membranes with soot loading.
- Develop a real-time DPF control/management system that can measure the instantaneous mass of soot deposits in a DPF, control DPF regeneration, and provide OBD signals for DPF operation.

Approach – Overall

DPF experiments for filtration, regeneration, μ-imaging



Numerical modeling

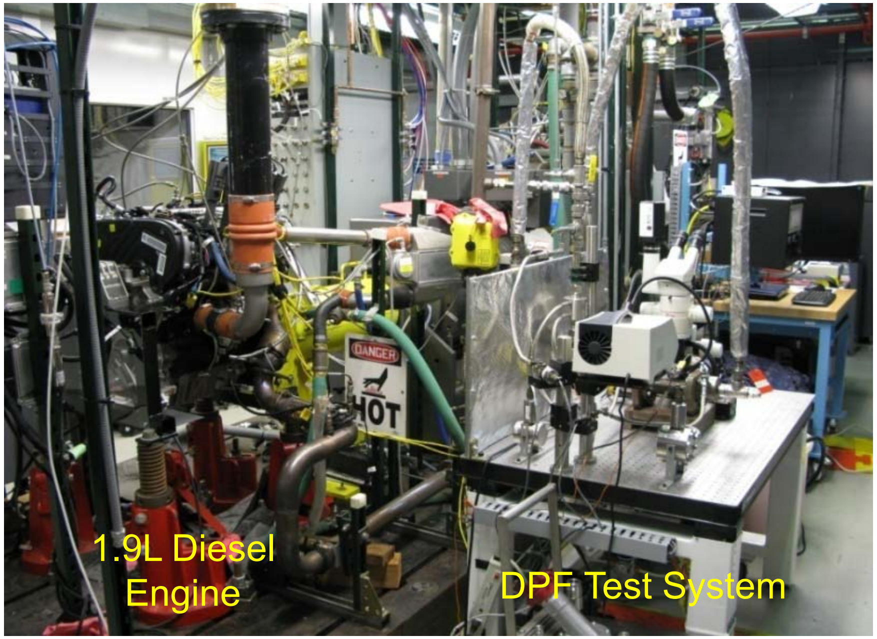
Caterpillar C7 Diesel

Soot oxidation with TGA, DSC

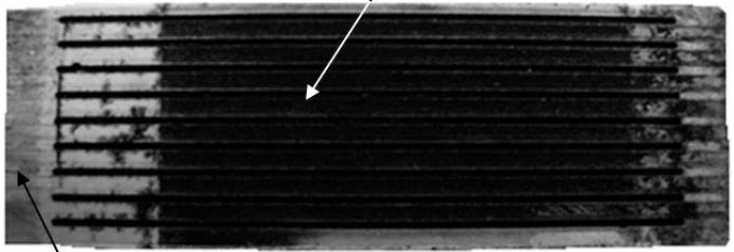
PM mass, filtration efficiency with TEOM

Approach – Year 3

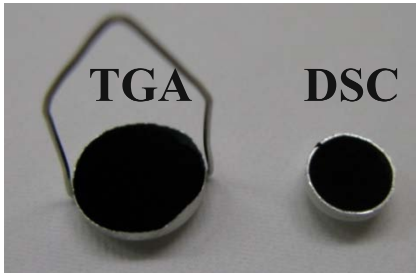
■ Experimental procedure



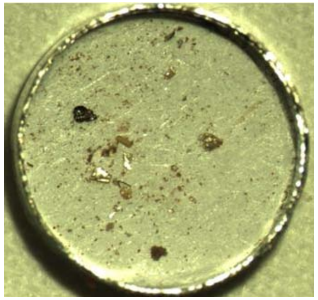
Soot deposit



Bisected non-catalyzed Cordierite membrane



Diesel PM samples



Residues

Technical Accomplishments:
Transient heat release evaluated from oxidation experiment with diesel soot will help DPFs control thermal runaway

- Transient heat release ($\dot{Q}$, *kW*) =

  Oxidation rate of soot ($-dm/dt$, *g/sec*) x

  Specific heat-release from oxidation of soot (q, *kJ/g*)

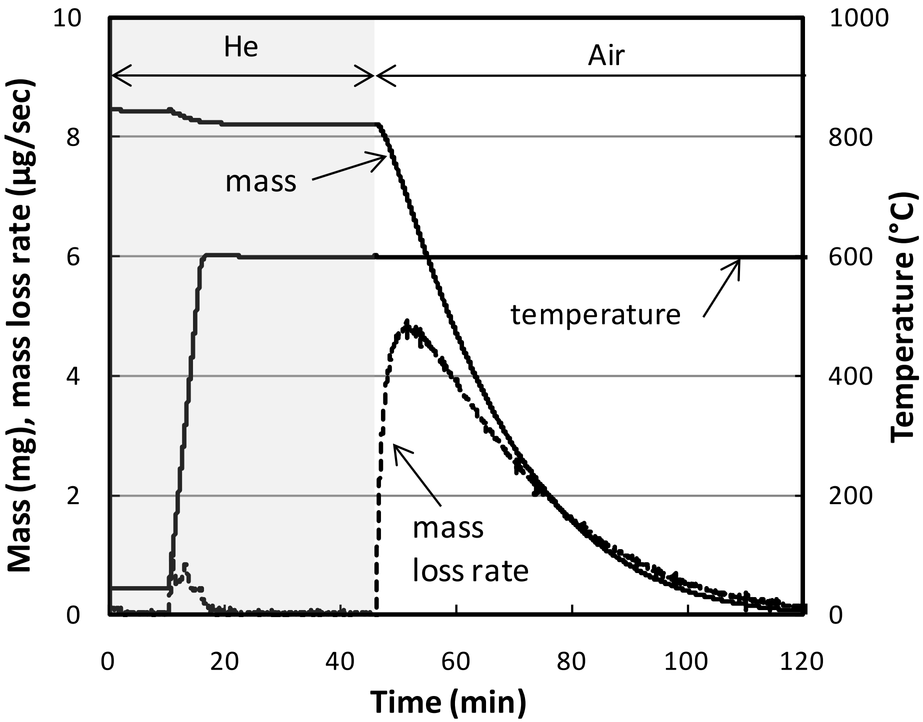
$$\dot{Q} = -\frac{dm}{dt} \cdot q$$

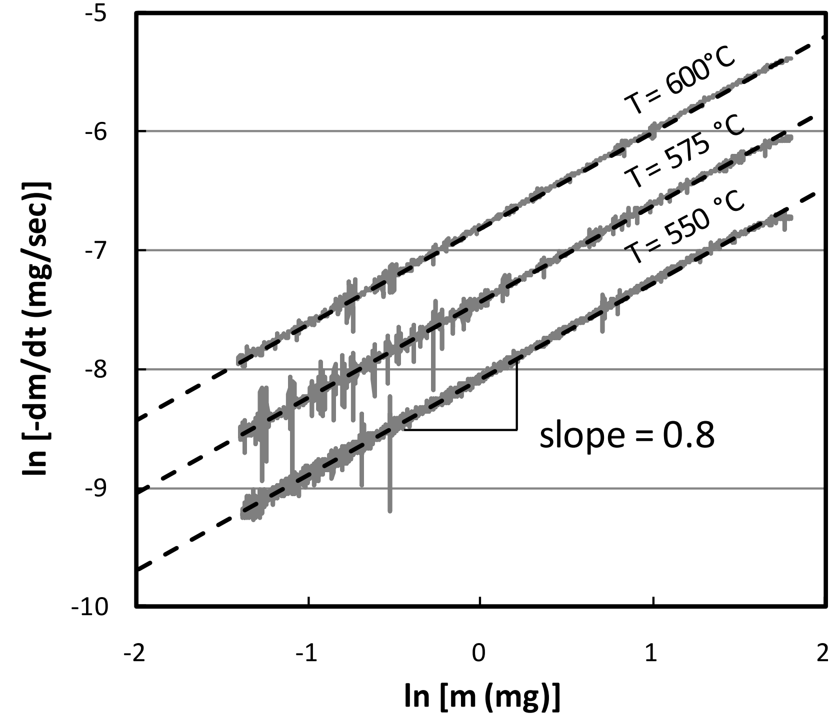
$$-\frac{dm}{dt} = A \cdot exp\left[-\frac{E_a}{RT}\right] \cdot [m]^n \cdot [P_{O_2}]^{n_{O_2}}$$

$$q = \left[\int_{t_1}^{t_2} \frac{dH}{dt} dt\right] \cdot \left[\frac{1}{M}\right]$$

$M=M_0 - M_{soc}$

Oxidation rate of graphite was first evaluated to compare with oxidation behaviors of diesel soot

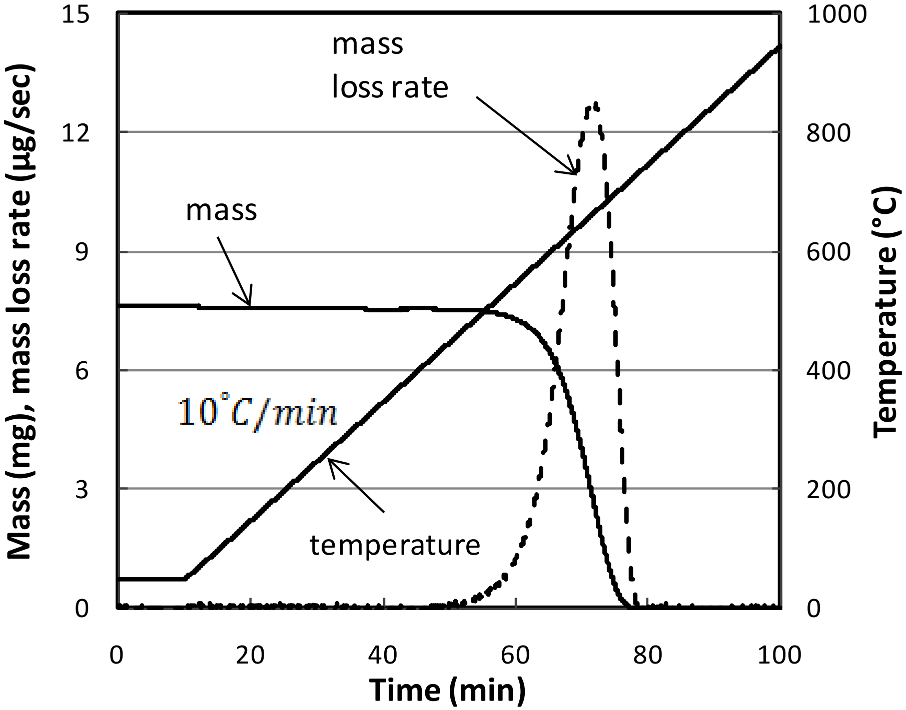


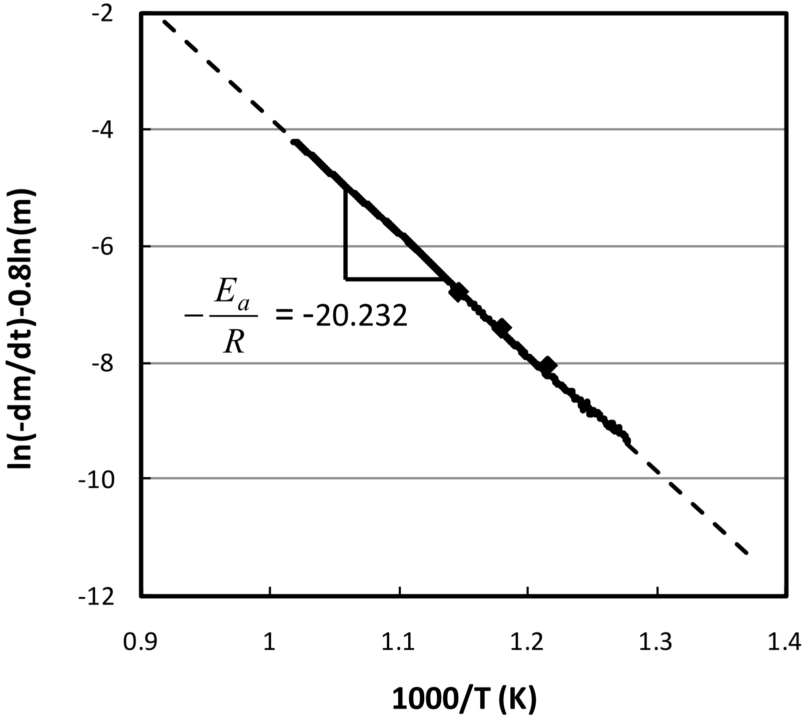


$$ln\left[-\frac{dm}{dt}\right] = n\, ln[m] - \frac{E_a}{R}\cdot\frac{1}{T} + n_{O_2}\, ln[P_{O_2}] + ln[A]$$

$$ln\left[-\frac{dm}{dt}\right] - 0.8\, ln[m] = -\frac{E_a}{R}\cdot\frac{1}{T} + 1.0\, ln[0.21] + ln[A]$$

Progressive heating on samples enabled us to accurately evaluate the activation energy





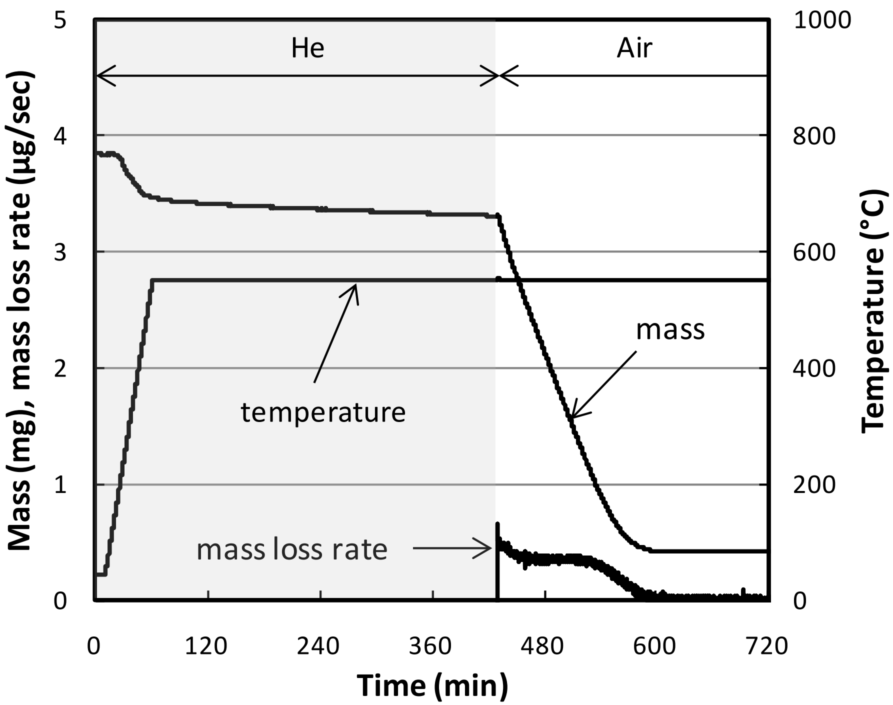
$$ln\left[-\frac{dm}{dt}\right] - 0.8\,ln[m] = -\frac{E_a}{R}\cdot\frac{1}{T} + 1.0\,ln[0.21] + ln[A]$$

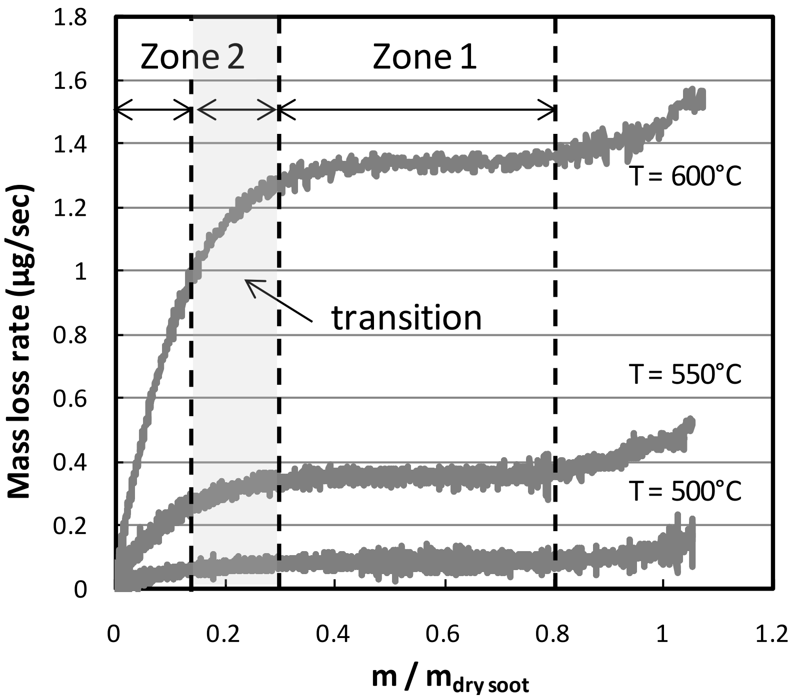
$$-\frac{dm}{dt} = 1.3629\times10^{7} exp\left[-\frac{20230}{T}\right]\cdot[m]^{0.8}$$

E_a=168.2 kJ/mol

A=6.49 x 10^7/sec

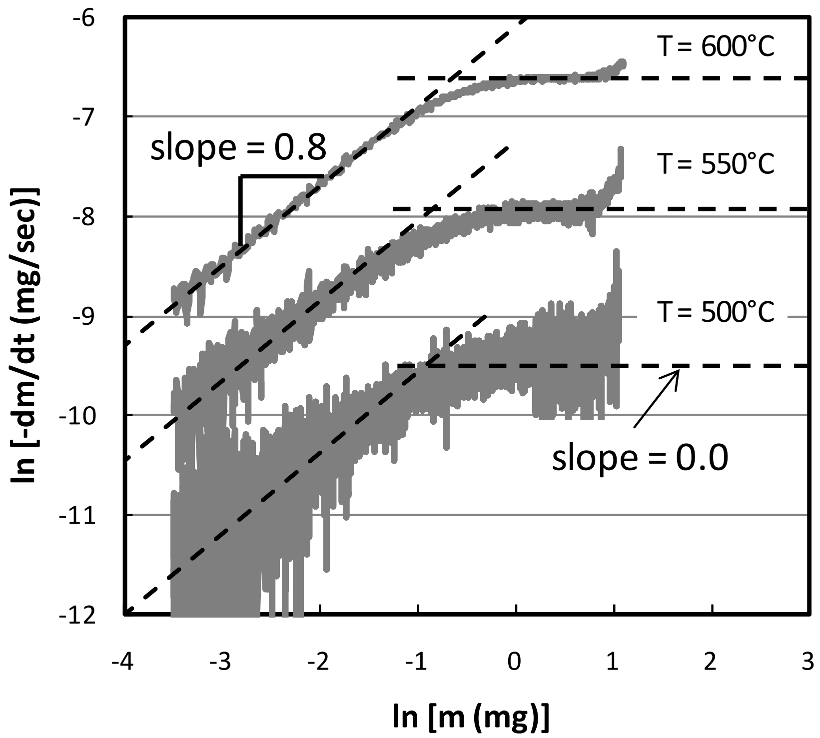
Oxidation of diesel soot shows two different reaction zones





- The content of SOCs in diesel PM turned out to be 20 ± 0.05 wt%.

Oxidation rate equations of diesel soot were derived with accurately evaluating the magnitude of kinetic parameters



$$ln\left[-\frac{dm}{dt}\right] = n\, ln[m] - \frac{E_a}{R}\cdot\frac{1}{T} + n_{O_2}\, ln[P_{O_2}] + ln[A]$$

Reaction Orders

n=0

n=0.8±0.01

Activation Energies (E_a)

155.5 kJ/mol

151.3 kJ/mol

E_a=168.2 kJ/mol for graphite

Pre-exponential Factors (A)

1.26×10^7

1.28×10^7

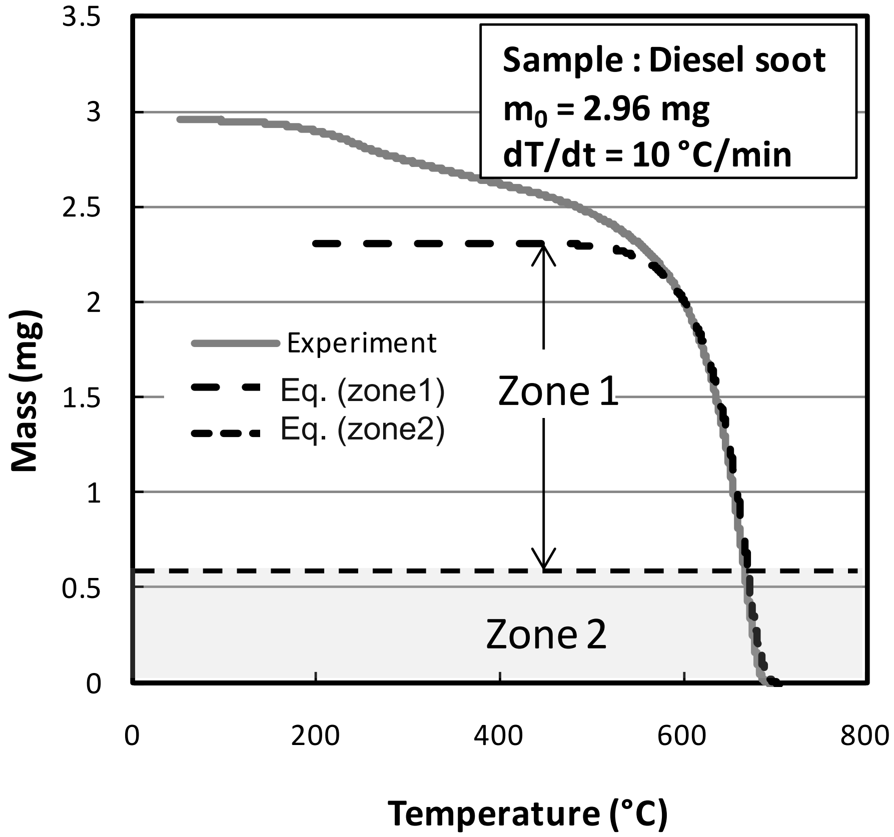
$$-\frac{dm}{dt} = 2.643 \times 10^6 \exp\left[-\frac{18702}{T}\right]$$

(Zone 1)

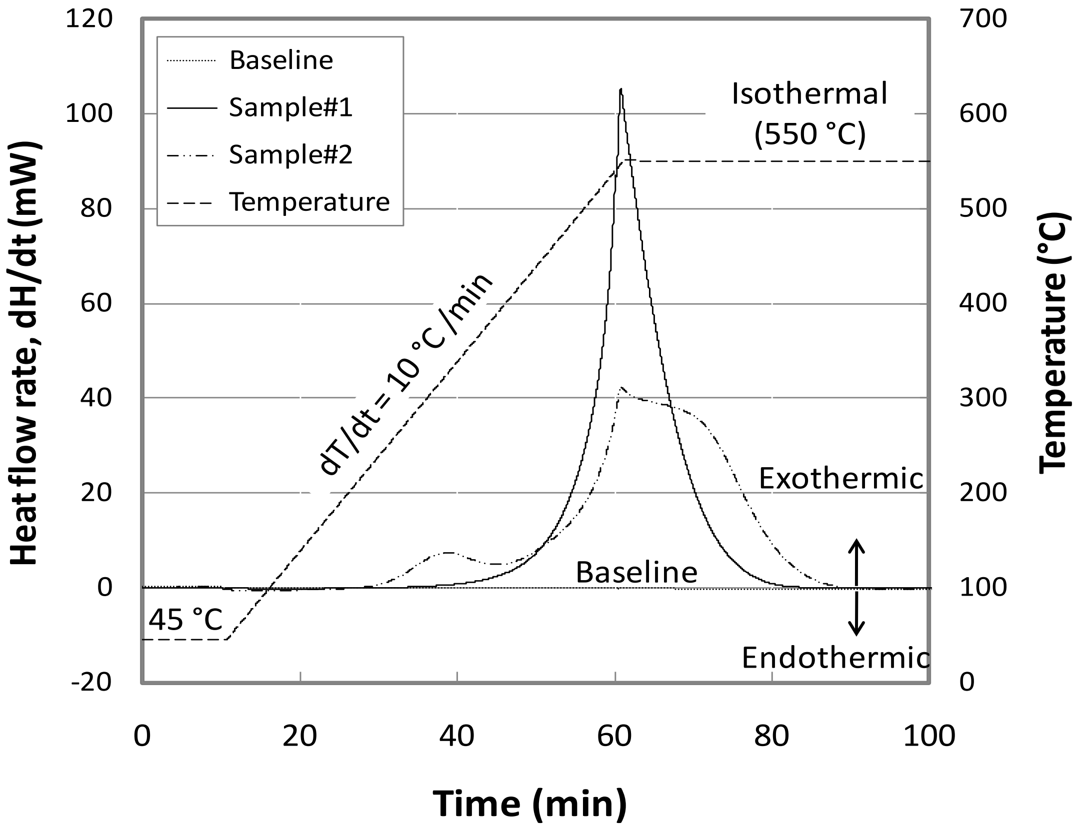
$$-\frac{dm}{dt} = 2.683 \times 10^6 exp\left[-\frac{18197}{T}\right]\cdot[m]^{0.8}$$

(Zone 2)

Mass data calculated by the equations concur with experimental data



Specific heat release from oxidation of diesel soot was evaluated in consideration of soluble organic compounds absorbed in samples



SOC containing soot

Dry soot

Quantity	Sample #1	Sample #2
Initial mass, M_o (mg)	3.725	4.197
Residual mass, M_r (mg)	0.315	0.323
M_o - M_r	3.410	3.874
Heat release (kJ/g)	17.25	14.67
SOC mass, M_{soc} (mg)	0	0.84
Soot mass (M_o - M_r – M_{soc})	3.410	3.034
Heat release by soot (kJ/g)	17.25	17.21
Heat release by SOC (kJ/g)	-	5.50

Evaluation of transient heat release under diesel-like environment is now promising

- Transient heat release during DPF regeneration in air

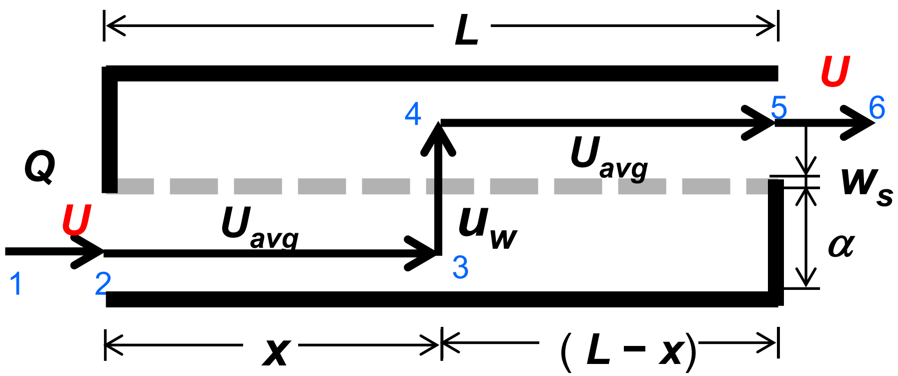
$$\dot{Q} = -\frac{dm}{dt} \cdot q$$

$$-\frac{dm}{dt} = A \cdot exp\left[-\frac{E_a}{RT}\right] \cdot [m]^n \cdot \left[P_{O_2}\right]^{n_{O_2}} \qquad q = \left[\int_{t_1}^{t_2} \frac{dH}{dt} dt\right] \cdot \left[\frac{1}{M}\right]$$

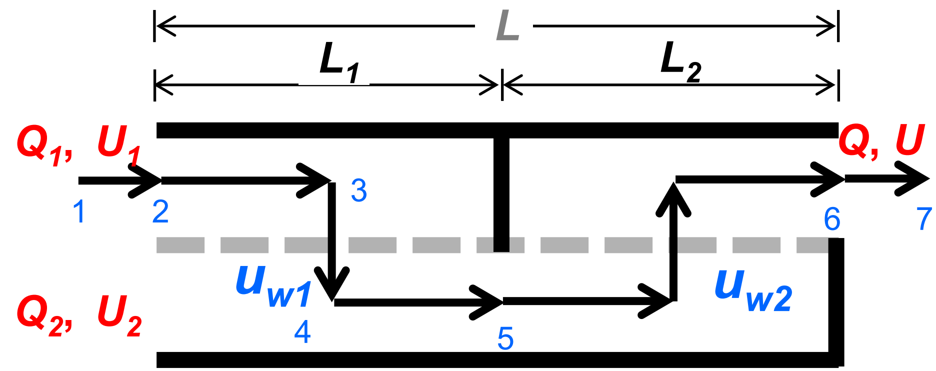
- Diesel soot oxidation experiments will be conducted with various compositions of gaseous emissions in consideration of regeneration conditions in practical DPF systems.
  - NO_x, HC, CO, CO_2, H_2O, etc.

Pressure Drop Model: Total pressure drop has been defined in a quadratic form of flow rate

- ***Conventional*** wall-flow DPF



- ***Modified*** DPF



$$\Delta P = \left(\frac{\mu}{4N} \frac{w_s}{k\alpha} \frac{1}{L} + \frac{2\mu F L}{3\alpha^4 N} \right) Q \quad + \frac{\rho\zeta}{2N^2\alpha^4} Q^2$$

$$\Delta P = \left(\frac{\mu}{4N} \frac{w_s}{\alpha} \frac{1}{k_{app}} \frac{1}{L} + \frac{2\mu F L}{3\alpha^4 N} \right) Q \quad + \frac{\rho\zeta^*}{2N^2\alpha^4} Q^2$$

$$\frac{1}{k_{app}} \frac{Q}{L} \equiv \frac{1}{k} \left(\frac{Q_1}{L_1} + \frac{Q}{L_2} \right)$$

$Q^* = Q_1 / Q$

$L^* = L_1 / L$

$k^* = k_{app} / k$

$$Q^* = \frac{L^*}{k^*} - \frac{L^*}{1 - L^*}$$

N : # of incoming (or outgoing) flow channels

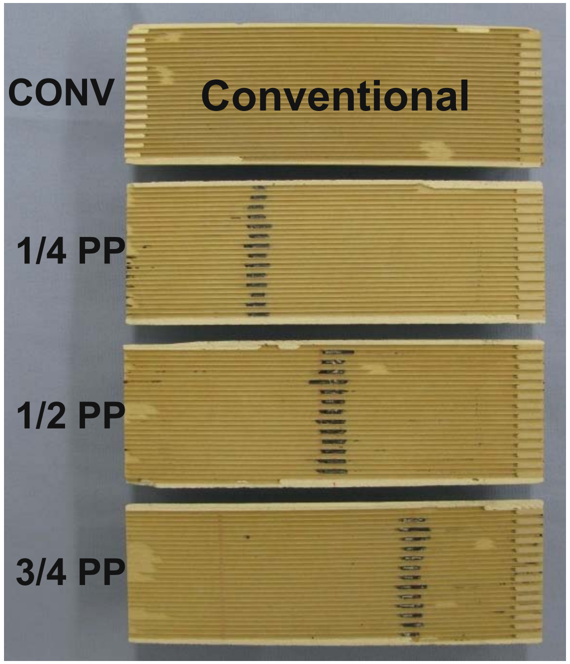
μ: Viscosity, ρ: density, F: Pre-factor

k : permeability, ζ : inertial loss coefficient

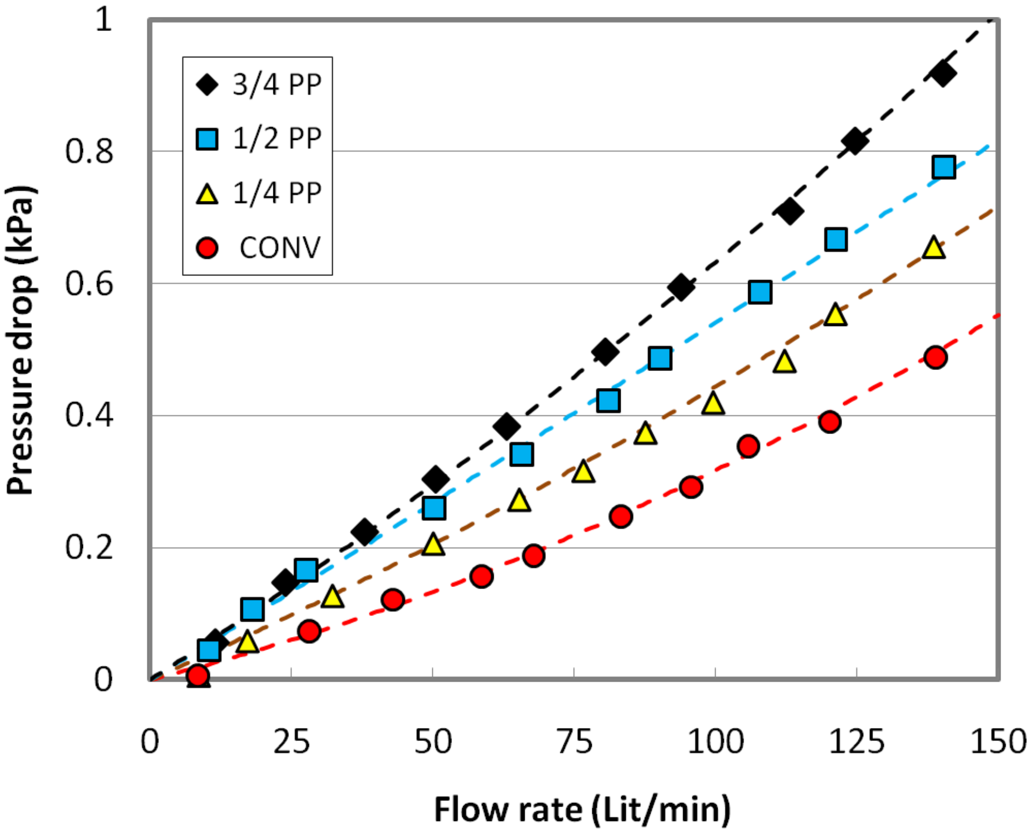
k_{app}: apparent permeability

Permeability (k, k_{app}) and inertial loss coefficients (ζ, ζ^*) can be determined by a flow bench experiment

$$\Delta P = \left(\frac{\mu}{4N} \frac{w_s}{\alpha} \frac{1}{k_{app}} \frac{1}{L} + \frac{2\mu FL}{3\alpha^4 N} \right) Q \quad + \frac{\rho \zeta^*}{2N^2 \alpha^4} Q^2$$

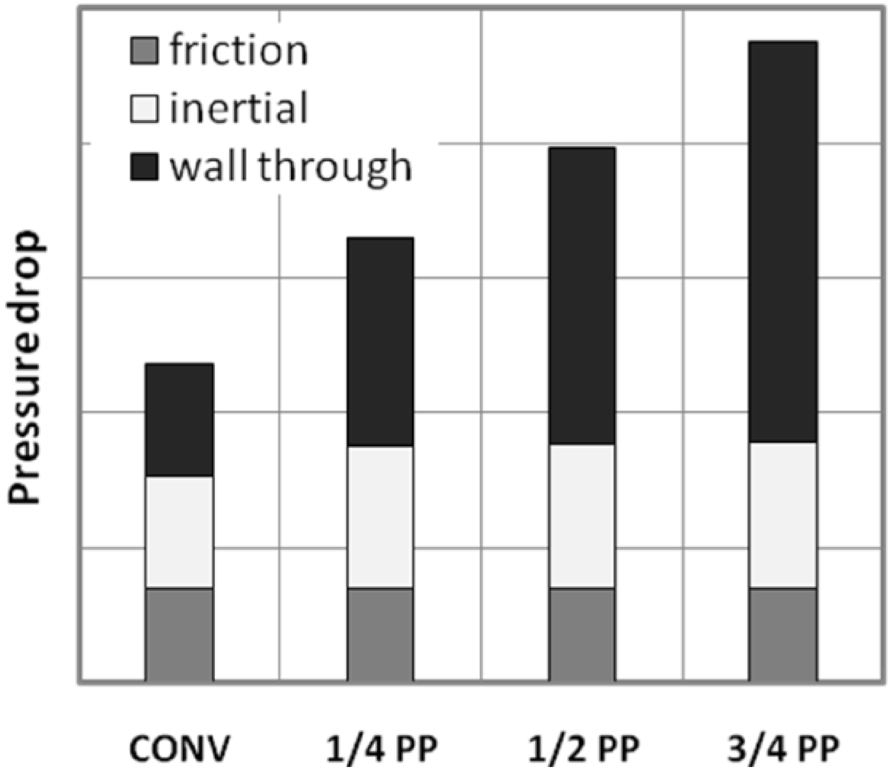


Modified membranes



Pressure drop through the wall is a major contributor to total pressure drop in modified DPFs

$$\Delta P = \left(\frac{\mu}{4N} \frac{w_s}{\alpha} \frac{1}{k_{app}} \frac{1}{L} + \frac{2\mu F L}{3\alpha^4 N} \right) Q \quad + \frac{\rho \zeta^*}{2N^2\alpha^4} Q^2$$



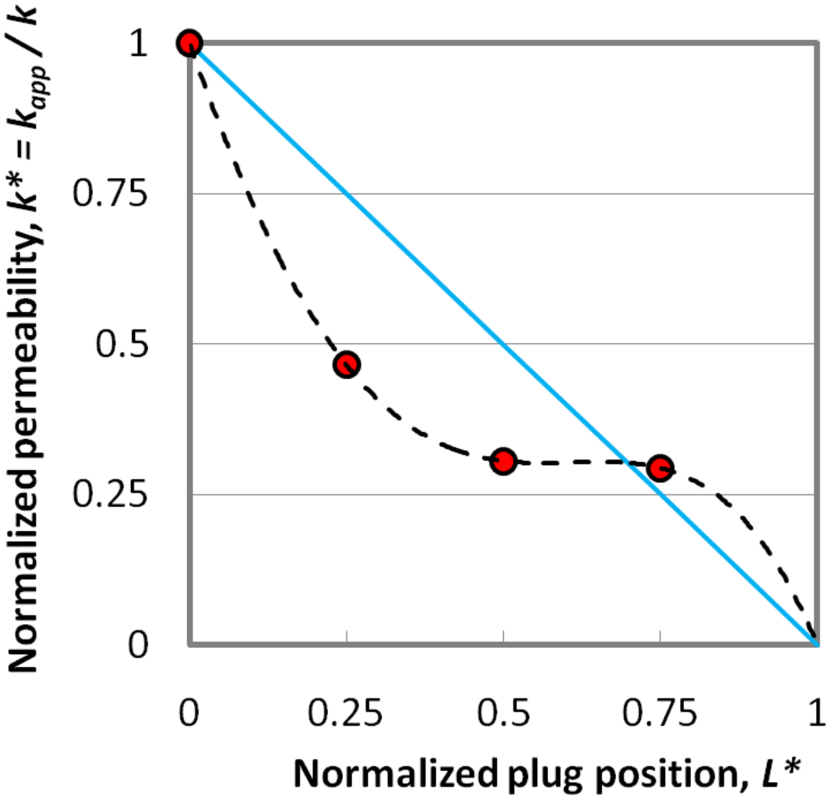
$$\Delta P_{friction} = \frac{2\mu F L}{3\alpha^4 N} Q$$

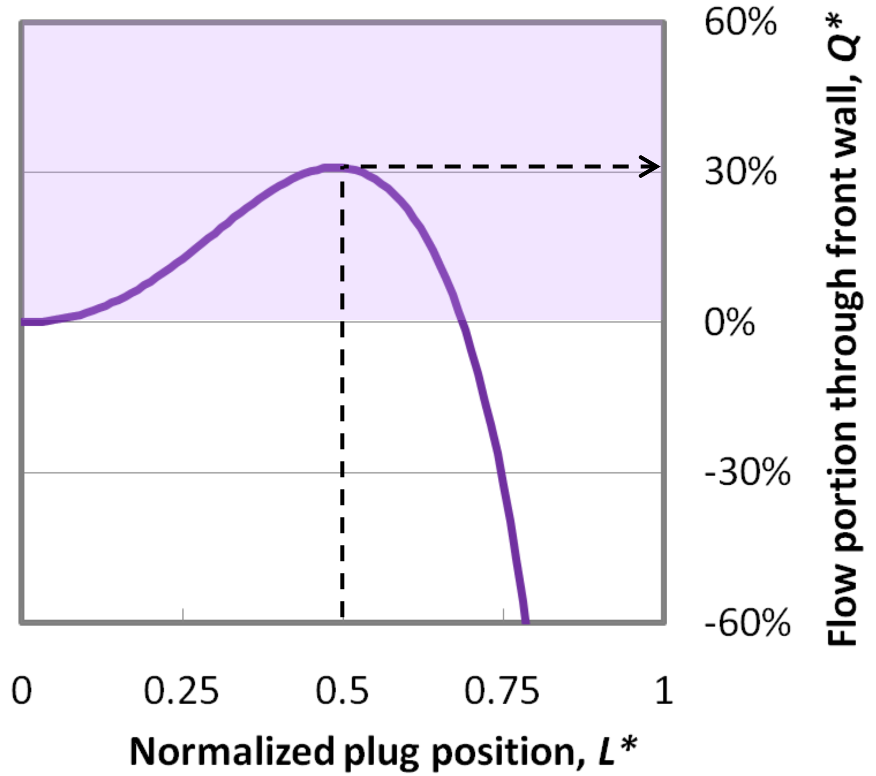
$$\Delta P_{inertial} = \frac{\rho \zeta^*}{2N^2\alpha^4} Q^2$$

$$\Delta P_{wall} = \frac{\mu}{4N} \frac{w_s}{\alpha} \frac{1}{k_{app}} \frac{Q}{L}$$

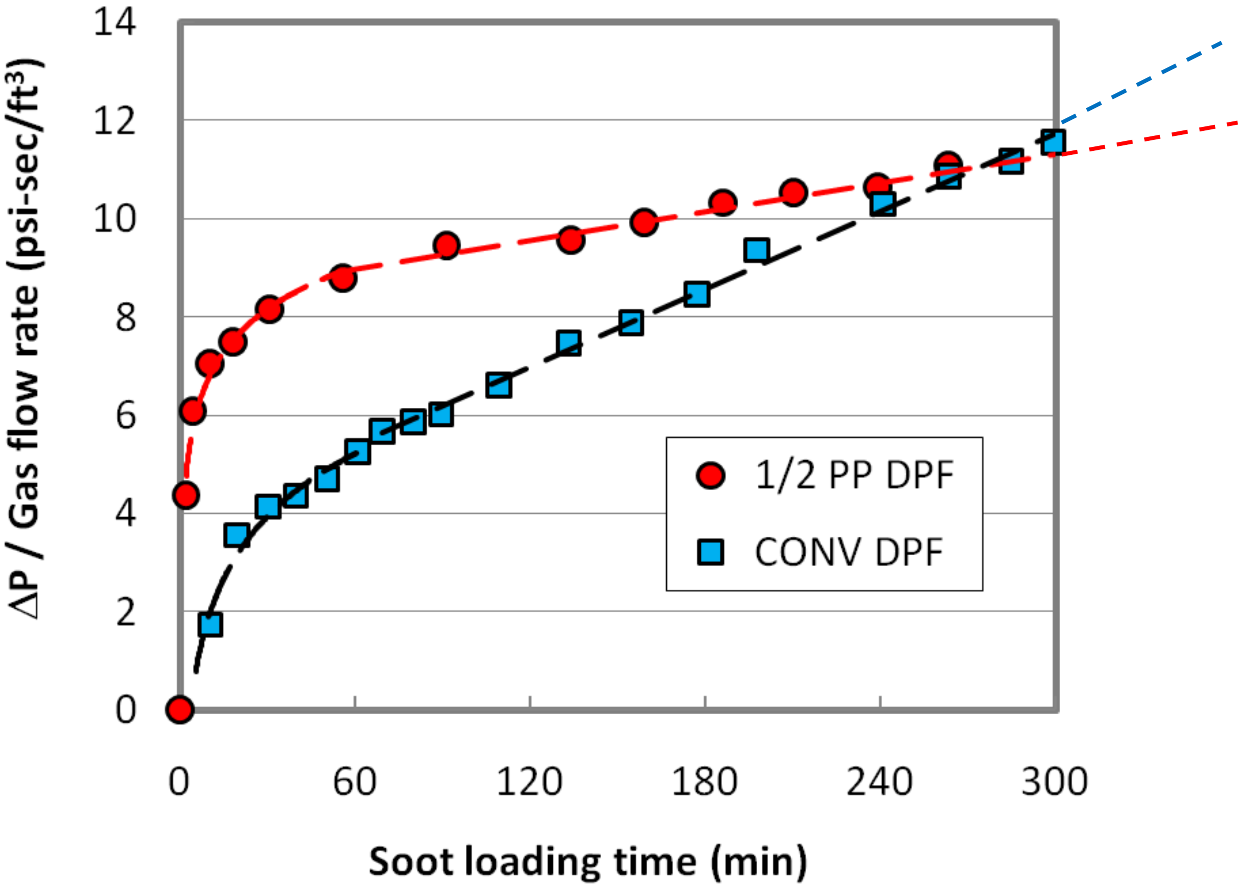
An optimum plug position was determined to be 1/2PP for given membrane physical properties

$$Q^* = \frac{L^*}{k^*} - \frac{L^*}{1 - L^*}$$

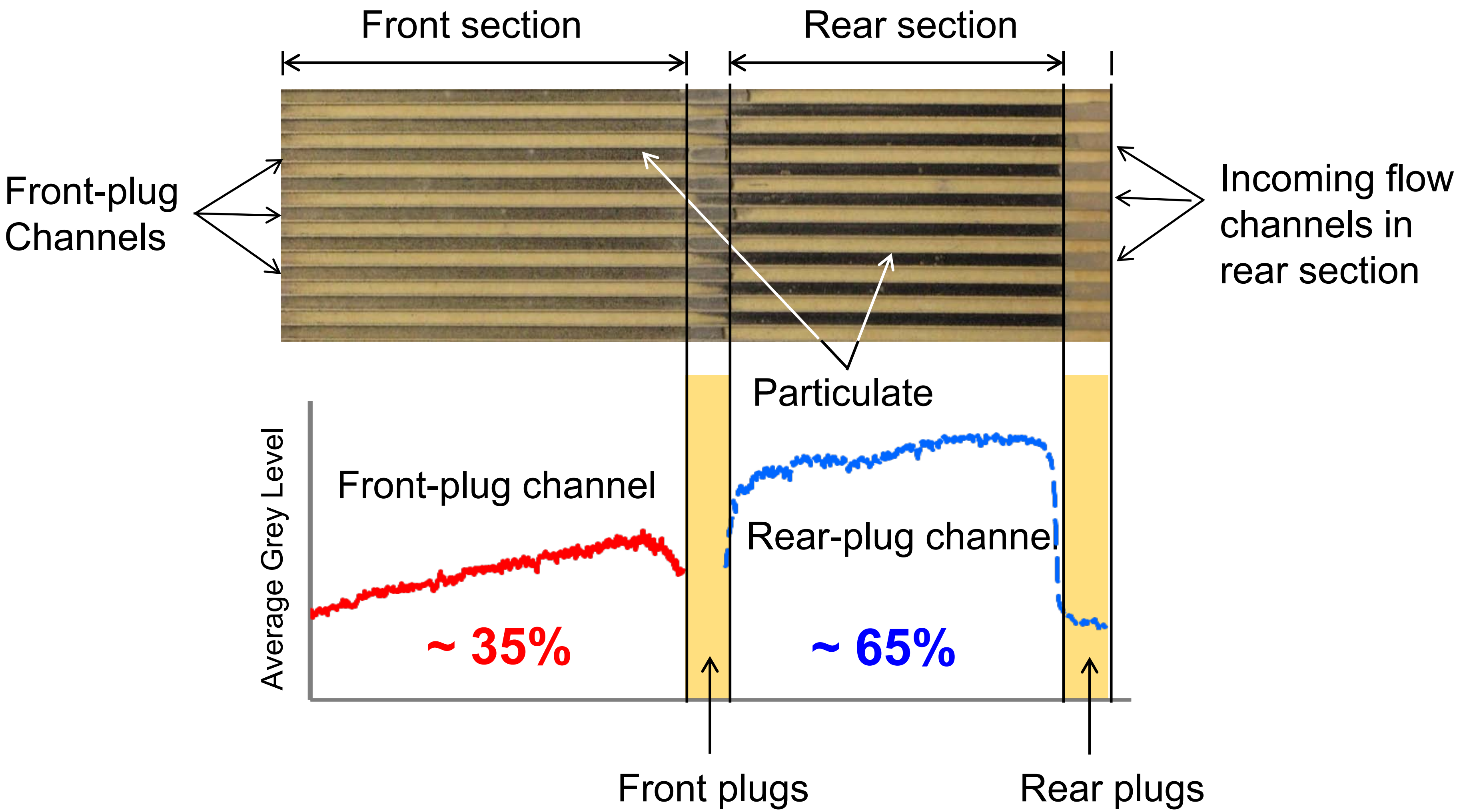




Pressure drops appeared to be higher with the modified DPF membrane for the tested period. However …



The modified DPF membrane allowed a fair amount of soot loading in the front-plug channels



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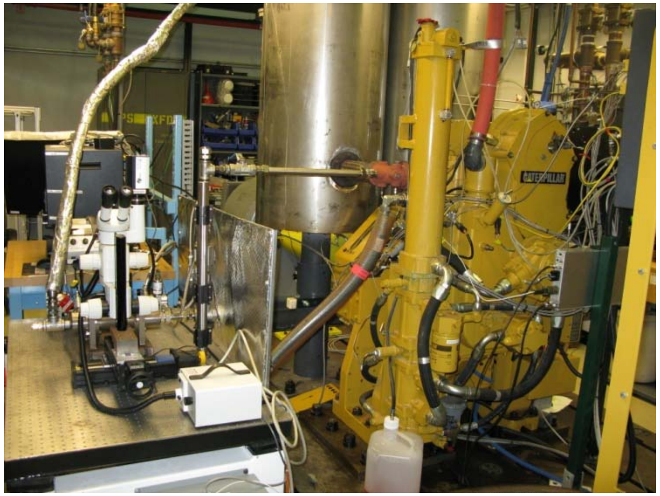
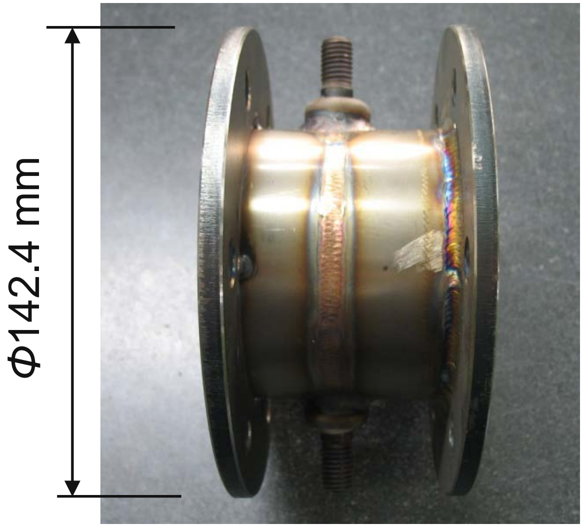
Current status of DPF experiment

- DPF experiments have not been able to be performed due to no extra engine dyno facility for CAT®'s C7 engine (FY09).
- The DPF test bench is being set up with the existing CAT®'s single cylinder diesel engine.
- A DPF regeneration system for experiments has been designed.
- A custom-designed electrical heater unit has been developed for regeneration in collaboration with ILJIN Electric Co.





An invention disclosure has been filed at Argonne under this CRADA

- Industry has developed DPF systems, but their smart control systems are unavailable.
  - Detailed mathematical theories have been derived to define pressure drops in DPF (accurate).
  - Transient mass of soot deposits in DPF can accurately be measured in real time during engine/vehicle operation modes (transient, real-time).
  - No additional exotic hardware, such as soot sensors, is needed (cost effective).
  - DPF monitoring on the OBD system is capable.
  - It works for all engine classes from light-duty to heavy-duty (diverse in application).

Future Work

- Perform soot oxidation experiments with various flue gases (NO_x, HC, CO, CO_2, H_2O) and measure oxidation rates and heat release.
- Continue to characterize the pressure drops in modified membranes with extended soot loading time and evaluate filtration efficiency at various engine operating conditions.
- Conduct filtration experiments with catalyst-coated membranes to measure filtration properties.
- Conduct regeneration experiments.
  - Provide optical images of thermal reaction in regeneration.
- Analyze morphology and nanostructures of soot particles partially oxidized during TGA experiment.
- Continue to validate the invention with CAT® engines and discuss for its patenting with the industry sponsor.

Summary

- Oxidation behaviors of diesel soot and graphite were accurately characterized in air.
  - Oxidation of diesel soot typically revealed two different oxidation zones: a constant oxidation rate zone and an exponentially decreasing zone, whereas
  - Commercial graphite represents an exponentially changing oxidation rate only.
- Transient heat release of diesel soot was evaluated in air.
  - Transient oxidation rates of diesel soot.
  - Specific heat release of both diesel soot and SOCs

    : Dry soot presented an approximately three (3) times higher degree of heat release than SOCs did.
- The plug position of modified DPF membranes was optimized, showing promising results in total pressure drop with soot loading.
- An invention disclosure has been filed.
  - Intelligent DPF Control and Management System.