Systematic Evaluation of PM Loading and Oxidation in Diesel Particulate Filters

Jonas Sjöblom[1]*, Jan Koegler[2], Oskar Sundborg[1] and Alessia Natta[1]

1: Department of Mechanics and Maritime Studies, Chalmers University of Technology, SE 412 96 Gothenburg, Sweden,

2: Volvo Group Trucks Technology, Powertrain Advanced Engineering, Dept. BF61500 Exhaust Aftertreatment, Sven Hultins gata 9B, SE-412 88 Gothenburg, Sweden

**jonas.sjoblom@chalmers.se*

Introduction

Particulate Matter (PM) emissions cause serious health problems

Diesel Particulate Filters (DPF) have high capture efficiencies but with fuel penalty due to pressure drop

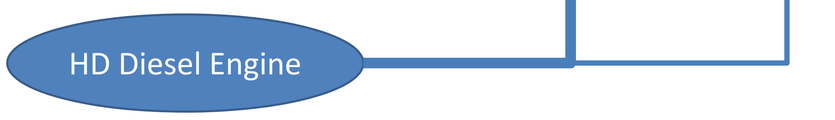
Understanding of DPF is important to ensure low emissions and low fuel penalty

Complex Soot oxidation mechanism include:

- Size distribution depending on engine operation
- PM transformation in upstream Diesel Oxidation Catalyst (DOC) and ageing/oxidation during loading

Objectives

- To bridge between full scale and lab scale experimentation [1]
- To assess PM transformations in full scale [2]
- To evaluate Catalytic effects in DPFs



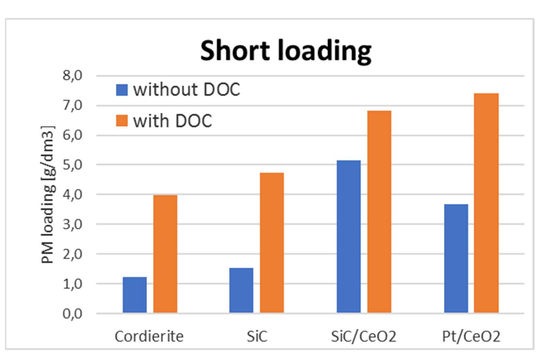
Experiments

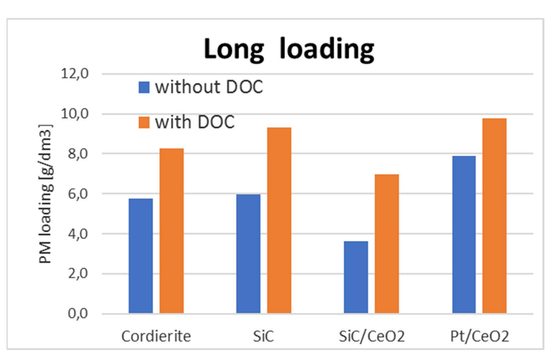
16 different samples

- 4 different mini-DPFs
- With & without upstream DOC
- Long & short loading

Loading using HD diesel engine (Volvo, 11L Eu6 eSCR)

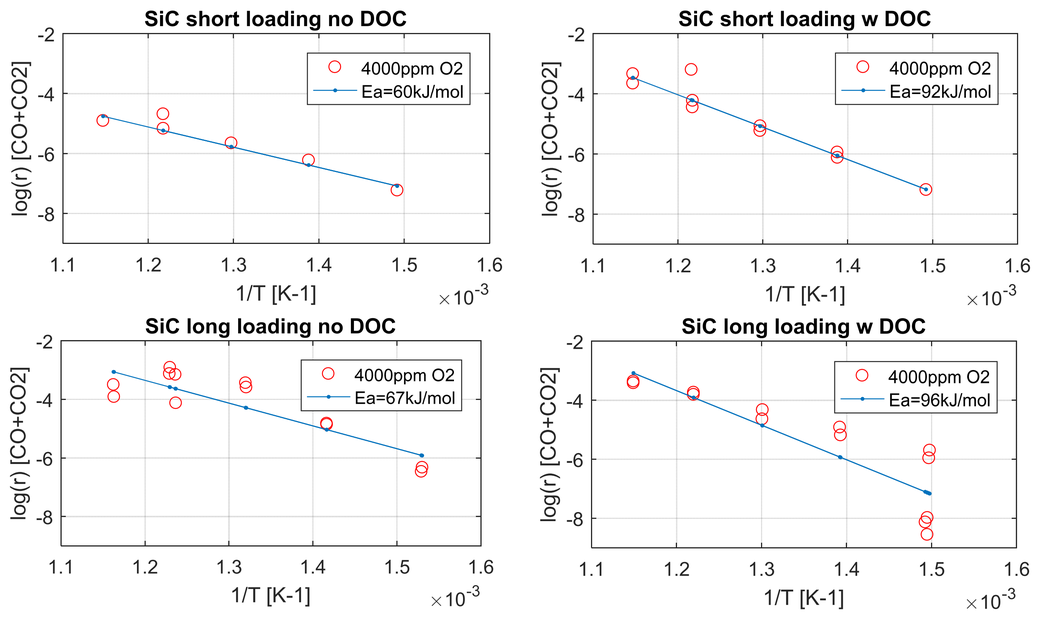
- Oxidation in heated reactor
- Using O_2, NO_2 and O_2+NO_2
- Pulses at constant temperatures





Soot loading results

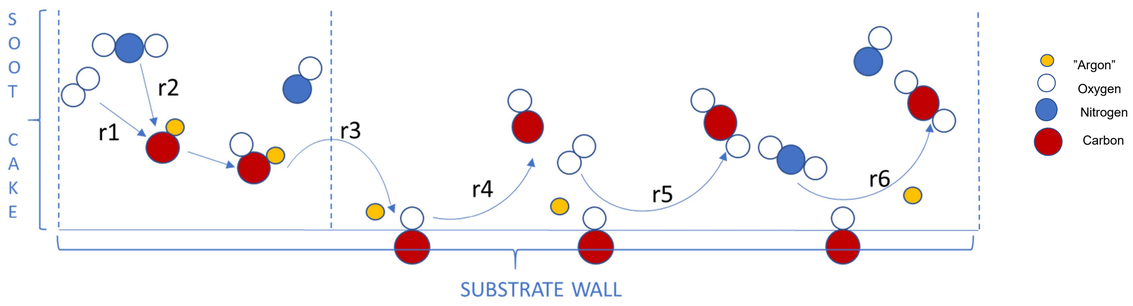
- Higher loading using upstream DOC:
  1. HC stripping in DOC
  2. more uniform Particle Size Distribution (PSD)
  3. More efficient packing of soot cake (less relative pressure drop)
  4. Higher flow through mini-DPF (same "driving force")



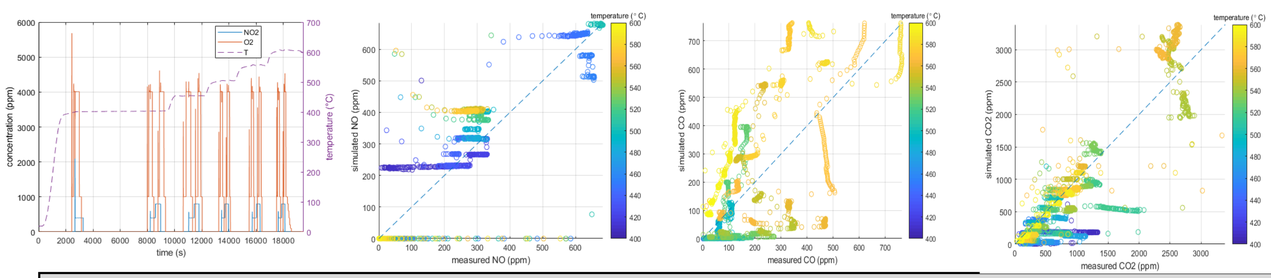
PM reactivity results

- Higher Apparent Activation energies with DOC (stripped HC)
- Better fit for short loading (more homogeneous PM)
- Small Catalytic effect (Except CO/CO_2 for Pt) (not shown)
- Low CO selectivity (CO/CO_X ~ 0.1-0.2), increasing at high conversion (not shown)

Detailed Kinetic Modelling of Soot Oxidation using GT Power



					rate expression	pre-exp	Ea [kJ/mol]
r1)	cake + wall	soot + 0.5 O_2 (g)	→	COAr (g)	$r_1 = A_1 \exp(-Ea_1/RT)\,[O_2]^{0.8}\,[C]^{2/3}$	1.5e9	150
r2)	cake + wall	soot + NO_2 (g)	→	COAr (g) + NO (g)	$r_2 = A_2 \exp(-Ea_2/RT)\,[NO_2][C]^{2/3}$	1.7e5	68
r3)	wall	COAr (g)	→	CO (ads)+ Ar (g)	$r_3 = A_3[COAr]\,\theta_Z$	5.2e9	0
r4)	wall	CO(ads)	→	CO (g)	$r_4 = A_4 \exp(-Ea_4/RT)\,\theta_{CO}$	3.8e7	99
r5)	wall	CO (ads) + 0.5 O_2 (g)	→	CO_2 (g)	$r_5 = A_5 \exp(-Ea_5/RT)\,[O_2]\theta_{CO}$	5.6e8	62
r6)	wall	CO (ads) + NO_2 (g)	→	CO_2 (g) + NO(g)	$r_6 = A_6 \exp(-Ea_6/RT)\,[NO_2]\,\theta_{CO}$	5.6e5	12



Results from detailed kinetic modelling (preliminary results)

- Addition of "pseudo specie" (Ar) to model surface reactions in the soot cake
- Combined mechanism (O_2 & NO_2oxidation)
- Using limited data for calibration (Long loading with DOC, 1st half)
- Can capture mass transfer limitations
- Better fit for CO_2 (than CO & NO)
  - Selectivity not well captured using this mechanism
  - Better DoE suitable for modelling needed

Conclusions

- Upstream DOC transform PM and gives lower pressure drop (higher PM loading) and alters the reactivity (HC, packing)
- Detailed kinetic mechanism proposed using "pseudo specie" capturing co-oxidation of O_2 and NO_2
- Further refinements needed (on-going work)

References

[1] Sjöblom, J. (2013). "Bridging the gap between lab scale and full scale catalysis experimentation." Topics in Catalysis 56(1-8): 287-292.

[2] Sjöblom, J. and H. Ström (2013). "Capture of automotive particulate matter in open substrates." Industrial & Engineering Chemical Research 52(25): 8373–8385.

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