



---

# Flow-Reactor Studies to Support Modeling of the Soot Filters Regeneration Process

*3rd CLEERS Workshop  
October 17-18, Detroit (MI)*

Alex Yezerets, Neal Currier, Sriram Popuri, Arvind Suresh

# Initial Reactor Study of Soot Combustion

---

## Outline:

- Introduction:
  - Soot combustion studies: On-Engine vs. Micro- and Pilot-Reactors
- Experimental
  - Reaction set-up and procedures
- Results
  - Qualitative:
    - Soot combustion by  $O_2$  at different  $H_2O$  concentrations
    - Soot vs. carbon black
  - Quantitative:
    - Kinetic processing of the data
- Conclusions



# Introduction:

## Soot Filters Regeneration Studies

---

### Limitations of the On-Engine Studies

- Soot loading:
  - Uncertainty of soot generation rate and continuous soot combustion rate (especially for CRT and catalyzed traps).
- Soot regeneration:
  - Impossible to vary one parameter at a time (e.g., only temperature)
  - Amount of incoming soot during regen? Other uncertainties (e.g.,  $T_{\text{exhaust}}$  vs.  $T_{\text{filter}}$ )
  - Criteria of success:  $\Delta P = f(\text{soot amount \& distribution, } T, \text{ flow rate, transients})$

### Micro-Reactor Studies

- Fundamental study of the soot oxidation process =  $f(T, O_2, NO, NO_2, H_2O, \text{ etc})$

### Pilot-Reactor Studies

- Oxidation of soot loaded on the soot filter cores:
  - Study of  $\Delta P = f(\text{soot loading, degree of regen})$  at different  $T$  and flow rates
  - How the “engineering” factors (heat & mass transfer) affect the soot combustion?
  - Effect of various catalysts

# Experimental Setup



## Sample

- **Soot:** Real diesel soot sample “A”
- **Carbon black:** Provided by Cabot

## Reactor Loading

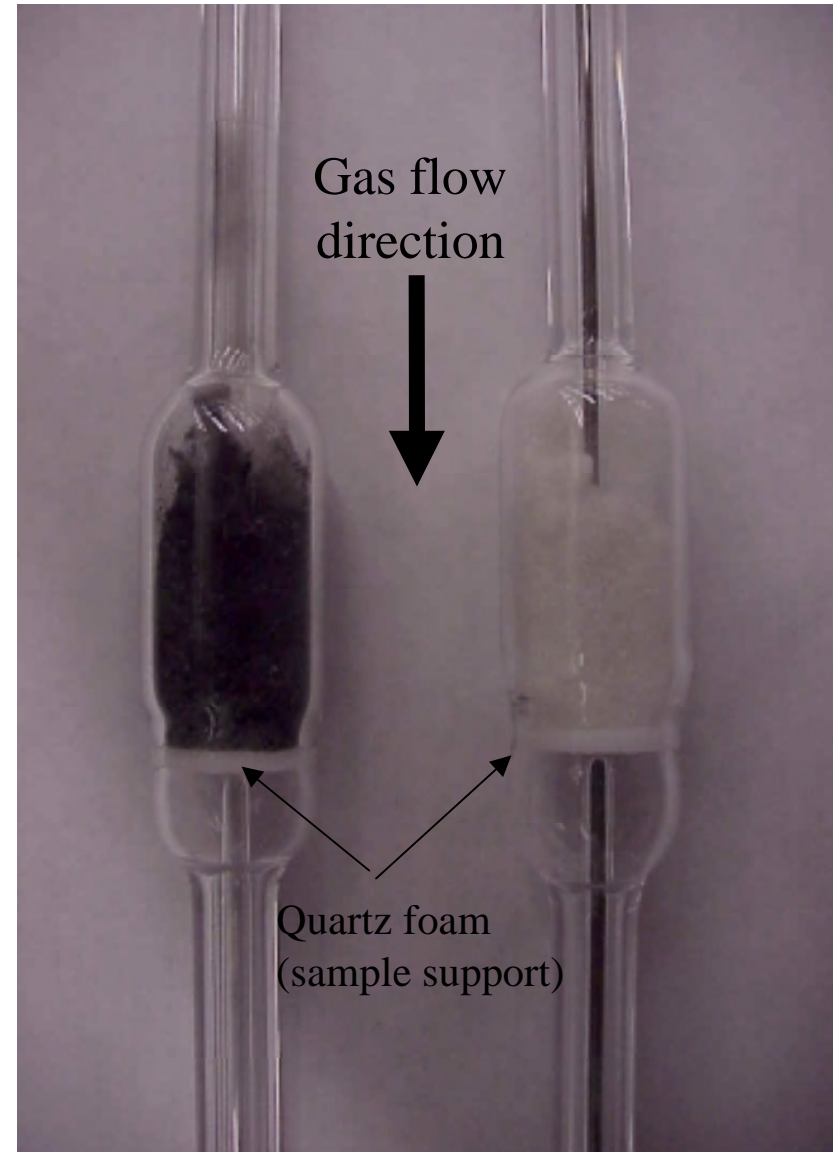
- Soot powder mixed with quartz chips for better heat dissipation

## Gas:

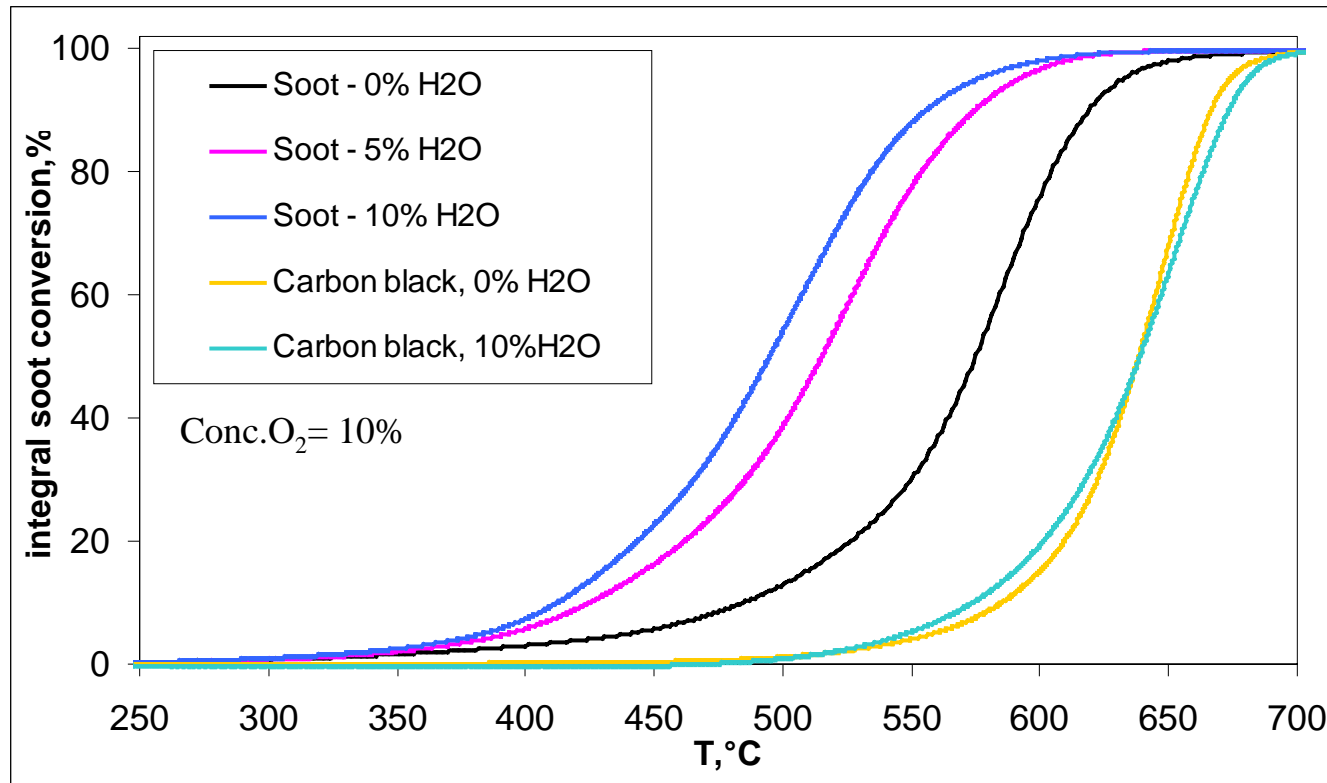
- O<sub>2</sub> -10.0% (vol.), H<sub>2</sub>O 0-10% (vol.) / He

## Analysis:

- “DOC” catalyst downstream (oxidizes CO to CO<sub>2</sub> - to simplify material balancing)
- Mass-spec analyses (broad dynamic range)
- This configuration allowed to perform studies in a broad range of temperatures (conversions)

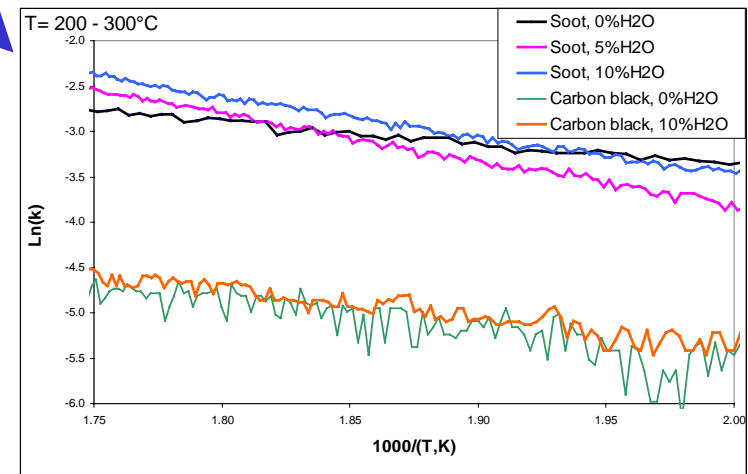
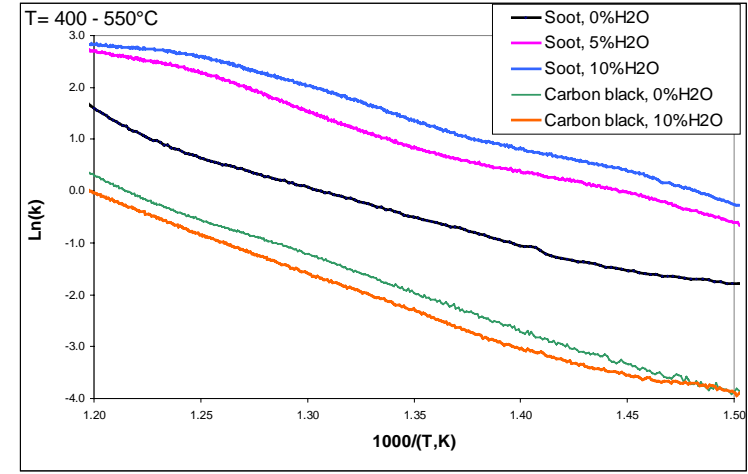
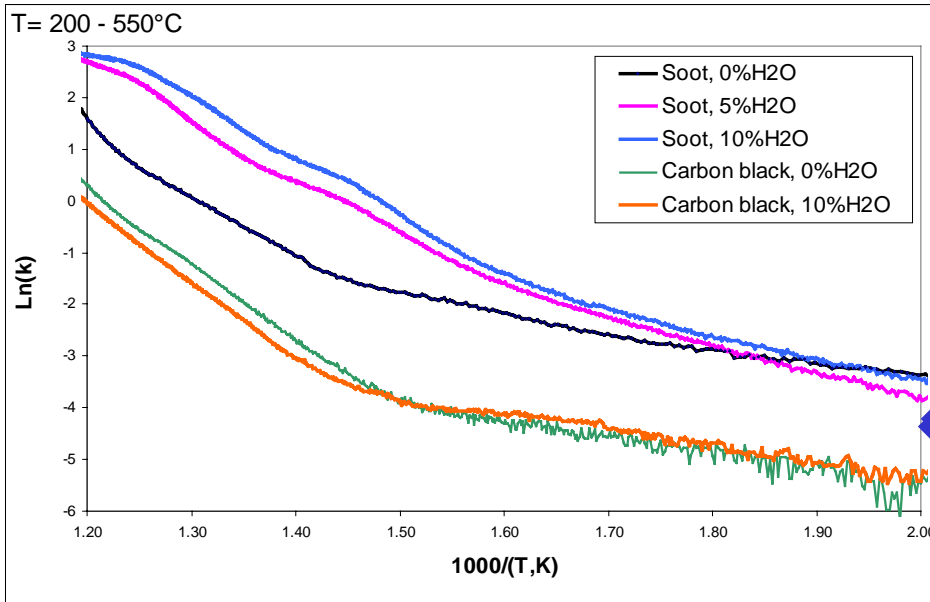


# Effect of H<sub>2</sub>O on soot oxidation by O<sub>2</sub>



- Soot combustion by O<sub>2</sub> was enhanced by the presence of H<sub>2</sub>O up to ~10%.
- Combustion of carbon black was not affected by the presence of 10% H<sub>2</sub>O.
- Origin of soot significantly affects both qualitative and quantitative results (possibly one of the reasons of controversy of the literature data)
- Consistent material recovery was achieved, allowing us to apply quantitative kinetic processing to the data

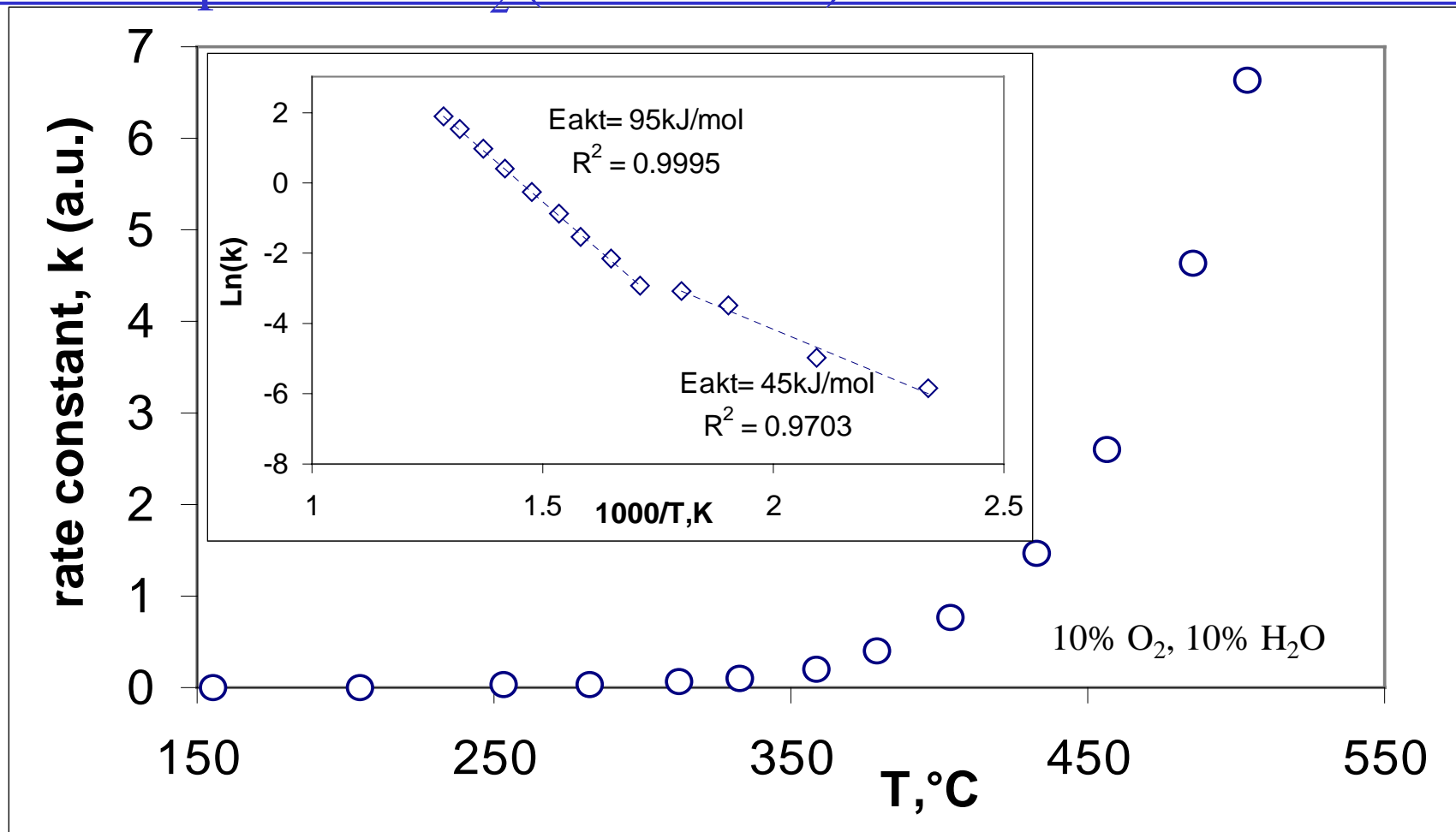
# Arrhenius plot: 200-550°C



H <sub>2</sub> O % vol.	200-300°C		400-550°C	
	E <sub>a</sub> ,kJ/mol	R <sup>2</sup>	E <sub>a</sub> ,kJ/mol	R <sup>2</sup>
<b>Carbon black</b>				
0	<b>32</b>	0.788	<b>117</b>	0.999
10	<b>24</b>	0.914	<b>114</b>	0.993
<b>Soot</b>				
0	<b>21</b>	0.986	<b>92</b>	0.994
5	<b>39</b>	0.986	<b>97</b>	0.986
10	<b>34</b>	0.990	<b>92</b>	0.994

# Advanced experimental technique:

- pulses of O<sub>2</sub> (150-500°C)



Obtained results are **independent** of the experimental technique:

- qualitatively - similar transition from lower to higher  $E_a$
- quantitatively (e.g., for 300-500°C:  $E_a = 92$  vs. 95 kJ/mol)

# Conclusions:

---



- Equipment and methodology for quantitative fundamental studies of soot oxidation were demonstrated.
- Cummins' reactor systems provide unique capabilities for studying soot combustion (sensitivity, time resolution)
- Presence of H<sub>2</sub>O has a different effect on the oxidation of diesel and synthetic soot samples. This emphasizes the dependence of the results on the origin and properties of the soot.
- Unexpected change in the kinetic behavior (reproduced by different techniques) needs to be understood:
  - Does soot undergo some changes during the experiment (“aging”)?
  - Is there initial inhomogeneity of soot samples (“easy”- and “hard”-burning moieties)? Is it related to the soot “age”?