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

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

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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\(_2\)O 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**:  
- $O_2$ -10.0% (vol.), $H_2O$ 0-10% (vol.) / He

**Analysis**:
- “DOC” catalyst downstream (oxidizes CO to $CO_2$ - 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\textsubscript{2}O on soot oxidation by O\textsubscript{2}

- Soot combustion by O\textsubscript{2} was enhanced by the presence of H\textsubscript{2}O up to \(~10\%\).
- Combustion of carbon black was not affected by the presence of 10\% H\textsubscript{2}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

<table>
<thead>
<tr>
<th>H₂O % vol.</th>
<th>200-300°C</th>
<th>400-550°C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Eₐ, kJ/mol</td>
<td>R²</td>
</tr>
<tr>
<td>Carbon black</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>32</td>
<td>0.788</td>
</tr>
<tr>
<td>10</td>
<td>24</td>
<td>0.914</td>
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<tr>
<td>Soot</td>
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</tr>
<tr>
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<td>21</td>
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<tr>
<td>5</td>
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<tr>
<td>10</td>
<td>34</td>
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</tbody>
</table>
Advanced experimental technique:
- pulses of O₂ (150-500°C)

Obtained results are **independent** of the experimental technique:
- qualitatively - similar transition from lower to higher Ea
- 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 H₂O 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”?