Measurements and Predictions of the Aerosol Dynamics of Smoke

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NFPA SUPDET 2022
September 16, 2022
This presentation will include:

1. Motivation for Studying Smoke Dynamics

2. Smoke Distributions and Coagulation Experiments

3. Coagulation Predictions from NIST’s Fire Dynamics Simulator (FDS)

4. Conclusions and Future Work
Motivation: to improve models of smoke dynamics, which affect predictions for egress and life safety

Egress & Life Safety Predictions affected by smoke dynamics: visibility, toxicity, smoke alarm activation

Fire Forensics & Hazardous Material Emissions

[FDS beam detector example case]

[FDS propane flame deposition example case]

[Kerber & Walton, NISTIR 7213, 2005]
Smoldering fires produce mainly spherical particles, and flaming fires produce mainly soot agglomerates.

**Smoldering Fire Smoke**
- mainly condensed liquid spherical particles

**Flaming Fire Smoke**
- mainly soot agglomerates

Soot from propane burner [Brugiere et al. 2014], which had ~ 10 – 1000 primary particles

**Examples of characteristic sizes:**
- aerodynamic diameter,
- volume equivalent diameter,
- light scattering diameter,
- primary particle diameter,
- electric mobility diameter, etc.

Primary particle diameter = 19.7 nm
Fractal dimension = 1.69

[Averill 2010, NIST TN 1661]

[Madrzykowski 2009, NIST TN 1629]
A cascade impactor measured the aerodynamic size distributions, which were converted to the physical size.

MOUDI – micro-orifice low pressure cascade impactor

Measurement

Aerodynamic equivalent sphere

\[ da = 25.3 \, \mu m \]

\[ P_o = 1000 \, \text{kg m}^{-3} \]

Terminal velocity = 0.22 cm s\(^{-1}\)

Density and slip correction

Irregular particle

\[ dp = 18 \, \mu m \]

\[ P_p = 2700 \, \text{kg m}^{-3} \]

\[ x = 1.36 \]

Terminal velocity = 0.22 cm s\(^{-1}\)
The size distributions of both aerosol types were determined using a cascade impactor.

Smoldering Fires - Mineral Oil, \( \rho = 830 \text{ kg/m}^3 \)

Flaming Fires – Soot
\( \rho_{\text{eff}} = 200 \text{ kg/m}^3 \)

Gemini Smoke Detector Analyzer

Mass CDF

<table>
<thead>
<tr>
<th>Diameter, ( \mu m )</th>
<th>Mineral Oil, aerodynamic</th>
<th>Mineral Oil</th>
<th>Soot, aerodynamic</th>
<th>Soot, effective</th>
</tr>
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</table>

**MMD, measured (\( \mu m \))**  
Mineral Oil: 0.392 (± 10 %)  
Soot: 0.760 (± 10 %)

**GSD, measured**  
Mineral Oil: 1.36 (± 10 %)  
Soot: 2.19 (± 10 %)

Certain commercial equipment, instruments, or materials are identified in order to specify the procedures adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.
The decay in number concentration over the observation time is tracked as particles coagulate.

**Fill** with aerosol (mineral oil or soot) with fan on to start experiment well-mixed.

**Smoke Aging Test (7200 s):** CPC tracks number concentration decay from sample tube, with fan off.

**Start and End:**
- Number concentration ($#/m^3$) with CPC
- Mass concentration (kg/m$^3$) with tapered element oscillating microbalance (TEOM)
We modeled the experiments with FDS, which is commonly used to make smoke predictions.

\[ u_{\text{dep}} = u_g + u_{\text{dt}} + u_{\text{th}} \]

Coagulation
\[ \frac{dN}{dt} = f(\Phi, N) \]
To model smoke coagulation in FDS, users specify the aerosol density, bin sizes, and mass distribution.

### Bin Study: generic aerosol inputs

- **Density** = 1000 kg/m³
- **Minimum diameter**, \( m_{\text{min}} \) = 0.08 µm
- **Maximum diameter**, \( m_{\text{max}} \) = 3 µm
- **Number of bins**, \( M \) = 5

\[
s = \left( \frac{m_{\text{max}}}{m_{\text{min}}} \right)^{\frac{1}{M}} = 8.8
\]

\[
m_i = s \ m_{i-1} = 0.08, 0.17, 0.34, 0.7, 1.45, 3 \ \mu m
\]

Total mass concentration = 10 mg/m³

Geometric mean diameter (GMD) = 0.25 µm
Geometric standard deviation = 1.6
The number of bins used to represent the size distribution can affect the accuracy and efficiency of the solutions.

**Size Distributions after 10,000 s of Brownian coagulation only**

- **3 bins**
  - geometric mean diameter (GMD) = 0.25 µm
  - geometric standard deviation = 1.6

- **5 bins**

- **9 bins**

- **15 bins**

**Aerosol Sci. 1999**
Particle number count results for coagulation only using 9 bins and 15 bins were similar to Park et al. calculation.
The quiescent aging experiments modeled the coagulation of mineral oil and soot in FDS.
Two cases were run for each aerosol, with the size distribution represented with 5 bins and with 8 bins.

### Aerosol Parameters Used for FDS Cases

<table>
<thead>
<tr>
<th>Aerosol</th>
<th>Mineral Oil</th>
<th>Soot</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of bins</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td>Minimum bin size (µm)</td>
<td>0.155</td>
<td>0.072</td>
</tr>
<tr>
<td>Maximum bin size (µm)</td>
<td>1</td>
<td>8</td>
</tr>
<tr>
<td>Specified bulk density (kg/m³)</td>
<td>830</td>
<td>200</td>
</tr>
<tr>
<td>Initial mass concentration, measured (mg/m³)</td>
<td>5.8 (± 2 %)</td>
<td>6.312 (± 1 %)</td>
</tr>
<tr>
<td>Initial number concentration, No, measured (/cm³)</td>
<td>6.12 E5 (± 6 %)</td>
<td>6.03 E5 (± 11 %)</td>
</tr>
<tr>
<td>Initial number concentration, No, simulated (/cm³)</td>
<td>3.43 E5</td>
<td>3.36 E5</td>
</tr>
</tbody>
</table>

### Graphs

- **Mineral Oil Size Distribution**
  - 5 bins - initial
  - 8 bins - initial

- **Soot Size Distribution**
  - 5 bins - initial
  - 8 bins - initial
The mineral oil mass concentration decayed by 6% over 2 hrs due to deposition and make-up flow dilution.

Initial mass concentration = 5.8 mg/m³
Final mass concentration = 5.43 mg/m³
FDS predicted shifts in the size distribution for both mineral oil and soot, expected due to coagulation.
FDS predicted a slower decay in N/No for mineral oil because FDS started with a lower initial No.
Agreement between the soot experimental N/No and analytical solution confirmed the effective density used. 

\[ \rho_{\text{eff}} = 200 \text{ kg/m}^3 \]
Conclusions

1. A practical method to model coagulation of smoke, given some information about the structure and size distribution – flaming vs. smoldering smoke

2. Validated FDS predictions for mass concentration (experiments) and number concentration (analytical coagulation solution)

3. FDS results were similar whether 5 bins or 8 bins were used for the size distributions. The computed No had a larger effect on the result.

4. Confirmed the use of a lower effective density for soot, 200 kg/m$^3$ through agreement with the analytical coagulation solution.
   - Could modify FDS to allow a different effective density for each bin size to account for the compactness of smaller agglomerates compared to the sparseness of larger agglomerates.