Aircraft Black Carbon Particle Number Emissions – New Predictive Method & Uncertainty Analysis

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1. Introduction and motivation

2. New method to estimate particle number emissions

3. Results
   1. Validation
   2. Uncertainty analysis
   3. Application to a sample of aircraft activity
   4. Implication for contrail properties

4. Conclusions
Motivation

• Knowledge of soot PSDs and ice nucleation properties is important to accurately predict visible contrail formation

• Higher EI$_n$ leads higher number of ice particles
  • More smaller particles
  • Greater optical depth

• Measurements of ice particles in contrails and lifetimes of contrails suggests EI$_n$ is underpredicted by up to a factor of 3

Q: Is it worth diverting flights to avoid contrail formation?
   • **Quantify BC particle number emissions (and uncertainties)**
   • Contrail model needed to evaluate trade-off with CO$_2$
   • Additional demands on air traffic control and management
Aircraft particle emissions

- Characterised as an **emissions index**: mass/number of particles emitted per kg of fuel burned.

- Mass ($EI_m$) and number ($EI_n$) emissions indices are dependent on the engine thrust setting.

- Size distribution (GMD and GSD) of particles is dependent on the engine thrust setting and characterised by a lognormal distribution.

- Morphology ($D_{fm}$ and $d_{pp}$) of particles is dependent on the engine thrust setting.

Aircraft particle mass (EI_m) estimates

- Smoke number based [1,2]
  - Limited by accuracy of certification smoke numbers

- FOX method [3]
  - Smoke numbers are discarded
  - Semi-empirical model
  - Improved BC mass estimates at ground level and at cruise

- ImFOX [4]
  - ‘Improved FOX’ method
  - Accounts for hydrogen content of fuel (H)
  - Different equations for global air to fuel ratio (AFR) at cruise and ground

- From 2020: ICAO regulation
  - Certification test and limits on non-volatile particulate matter
  - Mass and number

Aircraft particle number ($E_{I_n}$) estimates

- **$E_{I_n}$**
  - $10^{14}$ to $10^{15}$ per kg fuel burned
  - E.g. Kärcher et al. (2016) [1].

- **$E_{I_n}/E_{I_m}$ ratios**
  - $5 \times 10^{15}$ to $1.6 \times 10^{15}$ particles per g(BC)
  - E.g. Döpelheuer (2002) [2].

- **Assumed particle diameter or size distribution**
  - Assume a particle diameter and density
  - E.g. $d = 38$ nm and $\rho = 1000$ kg/m$^3$ (Barrett et al., 2010) [3]

Mobility of fractal aggregates

Free-molecular regime:
\[ \text{Kn} = \frac{\lambda}{d_m} > 1 \] (mean free path >> d)

Diffusion limited cluster aggregation (DLCA):
Aerosols aggregate via random Brownian motion

\[ n_{pp} \approx \left( \frac{d_m}{d_{pp}} \right)^{D_{fm}} \]

Mass of the aggregate is the sum of the mass of primary particles:
\[ m = n_{pp} \rho_0 \left( \frac{\pi}{6} \right) d_{pp}^3 \]

\( D_{fm} \) is the mass-mobility exponent
\( n_{pp} \) is the number of primary particles
\( m \) is the mass of the aggregate
\( \rho_0 \) is the material density of black carbon (1770 ± 8%)
Mass of aggregates

Number of primary particles: \( n_{pp} = \left( \frac{d_m}{d_{pp}} \right)^{D_{fm}} \)

Mass of aggregate: \( m = n_{pp} \rho_0 \left( \frac{\pi}{6} \right) d_{pp}^3 \)

Primary particle diameter: \( d_{pp}[m] = a \ d_m^b \)

\[ \therefore m = \rho_0 \left( \frac{\pi}{6} \right) d_m^\phi a^{3-D_{fm}} \]

where \( \phi = D_{fm} + b(3 - D_{fm}) \)
Number and mass of aggregate population

Mass of a collection of aggregates with size distribution \( n(d_m) \):

\[
M = \int_0^\infty m(d_m) n(d_m) \, d\log d_m
\]

\[
= \rho_0 \left( \frac{\pi}{6} \right) a^{3-D_{fm}} \int_0^\infty d_m^\phi n(d_m) \, d\log d_m
\]

\( n(d_m) \) for non-volatile aircraft PM is typically lognormal (single mode). This then becomes the \( \phi \)-th moment of the lognormal distribution:

\[
M = N \rho_0 \left( \frac{\pi}{6} \right) a^{3-D_{fm}} \text{GMD} \phi \exp \left( \frac{\phi^2 \log(\text{GSD})^2}{2} \right)
\]

Re-arrange for \( N \ldots \)

where \( \phi = D_{fm} + b(3 - D_{fm}) \)

Aircraft PM GMD and GSD

**GMD**

- Ground (CFM56-2-C1, DC-8)
- Ground (Durdina et al. 2014)
- Ground (JT8D-219, MD-88)
- Ground (CF6-80A2, B767-300)
- Ground (CF6-80C2B8F, B767-400ER)
- Ground (PW2037, B757-200)
- Cruise (CFM56-2-C1, DC-8)

Ground GMD:
\[ GMD = 0.2289(F/F_{00} \%) + 14.153 \]
\[ R^2 = 0.7378 \]

Cruise GMD:
\[ GMD = 0.5739(F/F_{00} \%) + 9.9786 \]
\[ R^2 = 0.8926 \]

~ ±25%

**GSD**

- Ground (CFM56-2-C1, DC-8)
- Ground (Durdina et al. 2014)
- Ground (JT8D-219, MD-88)
- Ground (CF6-80A2, B767-300)
- Ground (CF6-80C2B8F, B767-400ER)
- Ground (PW2037, B757-200)
- Cruise (CFM56-2-C1, DC-8)

Ground GSD:
\[ GSD = 0.0039(F/F_{00} \%) + 1.5097 \]
\[ R^2 = 0.7047 \]

Cruise GSD:
Average GSD = 1.72

~ ±14.5%
Mass-mobility exponent - $D_{fm}$

$D_{fm}(SAC) = 2.37$ for $0.03 \ll \frac{F}{F_0} < 0.15$

$D_{fm}(SAC) = 2.50$ for $0.15 \ll \frac{F}{F_0} < 0.30$

$D_{fm}(SAC) = 2.57$ for $0.30 \ll \frac{F}{F_0} < 0.50$

$D_{fm}(SAC) = 2.64$ for $0.50 \ll \frac{F}{F_0} \ll 1.00$

Primary particle diameter - \[ d_{pp}[m] = \alpha d_m^b \]

\[ d_{pp}[m] = 1.62 \times 10^{-5} d_m^{0.39} \]

Dastanpour & Rogak
\[ d_a = d_m \text{ in free-molecular and transition regimes}\]

\[ d_{pp}[m] = 0.0125 d_m^{0.80} \]

Boies et al.

Primary particle diameter - 

\[ d_{pp}[\text{m}] = \alpha \cdot d_m^b \]

\[ d_{pp}[\text{m}] = 1.62 \times 10^{-5} \cdot d_m^{0.39} \]

\[ d_{pp}[\text{m}] = 0.0125 \cdot d_m^{0.80} \]

\[ d_{pp} \] in free-molecular and transition regimes

\[ d_m \] in free-molecular and transition regimes

\[ d_m = d_m \] in free-molecular and transition regimes

\[ E_{\text{I_n}} \] estimates are within ~ ±20%


Results: Validation of \( E_{I_n} \)

\[
E_{I_n} = \frac{E_{I_m}}{\rho_0 \left( \frac{\pi}{6} \right) a^3 - D_{fm} GMD \phi \exp \left( \frac{\phi^2 \log(GSD)^2}{2} \right)}
\]

Ground

\( c.f. \ R^2 = [-0.635, 0.102] \)

Cruise

\( c.f. \ R^2 = [-0.304, 0.156] \)


Application to fleet

- Need to estimate the BC mass emissions ($E_{I_m}$)

$$E_{I_n} = \frac{E_{I_m}}{\rho_0 \left(\frac{\pi}{6}\right) a^{3-D_{fm}} GMD \phi \exp \left(\frac{\phi^2 \log(GSD)^2}{2}\right)}$$

- Sample of Aviation Environmental Design Tool (AEDT) dataset
  - 9th March 2006 23:15:04 to 11th March 2006 08:09:35
  - Flight levels from 15,000 ft to 43,000 ft
  - 3371 flights
    - US Flights $\approx$ 3258
    - Asian Flights $\approx$ 10
    - Transatlantic & EU Flights $\approx$ 103
Results: Estimates of $E_{I_m}$ at cruise

\[ E_{I_n} = \frac{E_{I_m}}{\rho_0 \left(\frac{\pi}{6}\right) \alpha^{3-D_{fm}} GMD \phi \exp\left(\frac{\phi^2 \log(GSD)^2}{2}\right)} \]

![Graph showing comparison between measured and estimated $E_{I_m}$ values with ±50% error range.](image-url)
Results: Uncertainty analysis

\[
\text{EI}_n = \frac{\text{EI}_m}{\rho_0 \left( \frac{\pi}{6} \alpha^3 - D_{fm} \text{GMD} \phi \exp\left( \frac{\phi^2 \log(GSD)^2}{2} \right) \right)}
\]

<table>
<thead>
<tr>
<th>Variable</th>
<th>Fixed F/F\text{00}</th>
<th>Mean (µ)</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>EI\text{m}</td>
<td>0.4</td>
<td>14.2 mg/kg</td>
<td>±50%</td>
</tr>
<tr>
<td>ρ\text{0}</td>
<td>0.4</td>
<td>1770 kg/m\text{3}</td>
<td>±8%</td>
</tr>
<tr>
<td>D\text{fm}</td>
<td>0.4</td>
<td>2.57</td>
<td>±27%</td>
</tr>
<tr>
<td>GMD</td>
<td>0.4</td>
<td>18.52 nm</td>
<td>±25%</td>
</tr>
<tr>
<td>GSD</td>
<td>0.4</td>
<td>1.736</td>
<td>±14.5%</td>
</tr>
</tbody>
</table>

Propagated uncertainty (σ/µ) ~ ±64%
Results: Sensitivity analysis

$E_{I_n} = \frac{E_{I_m}}{\rho_0 \left(\frac{\pi}{6}\right) a^{3-D_{fm}} GMD \phi \exp \left(\frac{\phi^2 \log(GSD)^2}{2}\right)}$

- Uncertainty in inputs propagates to uncertainty in $E_{I_n}$
- GMD, GSD and $E_{I_m}$ are the most critical parameters
- A ±10% change in GMD will result in $E_{I_n}$ varying by approximately -23% to +33%

![Sensitivity index chart](chart.png)
Results: Example flight

- New fractal aggregate approach leads to estimates that are ~2x higher than previous estimates
- There is additional dependence on particle size and morphology
Results: Comparison of fleet average $E_{I_n}$

Upper $\quad \quad 1.9 \times 10^{15} \text{ kg}^{-1}$

Mean $\quad \quad 1.2 \times 10^{15} \text{ kg}^{-1}$

Lower $\quad \quad 4.4 \times 10^{14} \text{ kg}^{-1}$

(a) $\times 10^{14}$

<table>
<thead>
<tr>
<th>Method</th>
<th>Average $BC\ E_{I_n}$ [#/kg-fuel]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FA Approach</td>
<td>$1.04e+15$</td>
</tr>
<tr>
<td>Dopelheuer (2002)</td>
<td>$3.2e+14$</td>
</tr>
<tr>
<td>Barrett et al. (2010)</td>
<td>$9.05e+14$</td>
</tr>
<tr>
<td>Karcher (2016)</td>
<td>$7.82e+14$</td>
</tr>
<tr>
<td>FOX-ASAF Method</td>
<td>$6.5e+14$</td>
</tr>
<tr>
<td>ImFOX Method</td>
<td>$5.50e+14$</td>
</tr>
</tbody>
</table>
## Implications for contrails

Contrail optical depth may be ~20% higher than with previous estimates.

### 220 K [210 K, 225 K]

<table>
<thead>
<tr>
<th>Input Scenario</th>
<th>BC $E I_n$ (kg⁻¹)</th>
<th>Mean Visible Optical Depth ($\tau$)</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>$1.2 \times 10^{15}$</td>
<td>$3 [3.5, 1.3]$</td>
<td>-21% [-23%, -53%]</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>$4.4 \times 10^{14}$</td>
<td>$2.36 [2.68, 0.61]$</td>
<td>-21% [-23%, -53%]</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>$1.9 \times 10^{15}$</td>
<td>$3.20 [3.6, 1.68]$</td>
<td>+7% [+3%, +29%]</td>
</tr>
<tr>
<td>Previous estimates</td>
<td>$\sim 6 \times 10^{14}$</td>
<td>$\sim 2.5$</td>
<td></td>
</tr>
</tbody>
</table>
Conclusions

- New approach based on mobility of fractal aggregates provides more accurate $Ei_n$ estimates than previous methods.

- Large uncertainties remain and sensitivity analysis show that GMD, GSD and $Ei_m$ are most important parameters.

- Fleet average $Ei_n$ of 1.2 $[0.44, 1.9] \times 10^{15}$ per kg of fuel.

- Application to a sample of aircraft activity data suggests average $Ei_n$ are revised upwards by a factor of ~2. Previous estimates are within the lower bound.

- Contrail optical depth may be ~20% higher than previous estimates.
Future work

- Further validation.
- Integrate method into contrail model to quantify any change in contrail properties.
- Are models of ice nucleation in contrails appropriate for fractal aggregates?

- Particle losses when measuring $\text{EI}_n$ through long sample lines:

Acknowledgements

• 2006 AEDT sample dataset used for this study was made available for climate research by FAA within the ACCRI research project.

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Thanks, questions?

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Aircraft particle mass \( (EI_m) \) estimates

- Smoke number based
  - First Order Approximation v3 [1]
  - Aerodyne Research Inc. method [2]
  - Limited by accuracy of certification smoke numbers

- FOX method [3]
  - Smoke numbers are discarded
  - Semi-empirical model fitted to measurements
  - Improved BC mass estimates at ground level and at cruise

\[
C_{BC} \left[ \frac{mg}{m^3} \right] \approx \dot{m}_f \left( A_{form} e \left( -\frac{6390}{T_{fl}} \right) - AFR A_{ox} e \left( -\frac{19778}{T_{fl}} \right) \right)
\]

Formation \quad Oxidation

Aircraft particle mass ($E_{Im}$) estimates

- ImFOX [4]
  - ‘Improved FOX’ method
  - Accounts for hydrogen content of fuel ($H$)
  - Quadratic equation for $A_{form}$ and different equation for $T_4$
  - Different equations for global air to fuel ratio ($AFR$) at cruise and ground

\[ C_{BC} \left(\frac{mg}{m^3}\right) \approx \dot{m}_f e^{13.6-H} \left( A_{form} e^{\left(-\frac{6390}{T_4}\right)} - AFR A_{ox} e^{\left(-\frac{19778}{T_{fl}}\right)} \right) \]

- From 2020: ICAO regulation
  - Certification test and limits on non-volatile particulate matter
  - Mass and number

Results: $E_{I_n}$ versus $E_{I_m}$

SAMPLE III.2
http://doi.org/10.1080/02786826.2015.1078452

Modelled $E_{I_n}$
$R^2 = 0.985$
SAMPLE III.2
$E_{\text{n}}$ dependence on engine thrust and altitude