Item title: SCOPE11 Method for Estimating Aircraft Black Carbon Mass and Particle Number Emissions

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The SCOPE11 method for estimating aircraft black carbon mass and particle number emissions

Akshat Agarwal†, Raymond L. Speth†*, Thibaud M. Fritz†, S. Daniel Jacob‡, Theo Rindlisbacher[§], Ralph Iovinelli‡, Bethan Owen[¥], Richard Miake-Lye[¶], Jayant S. Sabnis†, Steven R. H. Barrett†

†Laboratory for Aviation and the Environment, Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA, United States

‡Federal Aviation Administration, Office of Environment and Energy, Washington DC, United States

[§]Swiss Federal Office of Civil Aviation, CH-3003 Bern, Switzerland

[¥]Manchester Metropolitan University, Manchester, United Kingdom

[¶]Aerodyne Research, Inc., Billerica, MA, United States

*Corresponding author: speth@mit.edu, +1 617 253 1516

This supplemental material is 10 pages long and contains 3 figures, 1 table and 7 equations.

S1. Derivation of volumetric flow rate (Eq 3 in main paper)

The volumetric flow rate, Q, is a parameter required to convert the BC mass concentration to an emissions index. Derivations in the literature have found different coefficients and do not show this derivation as a function of the fuel hydrogen content, H_c. As such, we provide an overview of the method for unmixed engines following Stettler et al (1), but generalize this for a fuel of any Hydrogen content.

We assume the fuel can be written in the form C_nH_m and the resulting combustion reaction is:

$$\mathrm{C}_n\mathrm{H}_m + \left(n + \frac{m}{4}\right)\mathrm{O}_2 \rightarrow n\mathrm{CO}_2 + \frac{m}{2}\mathrm{H}_2\mathrm{O}$$

which assumes 100% combustion efficiency from fuel to products. For H_c = 13.8% and n = 12, we find m = 22.8928 and the resulting moles per emissions product can be calculated.

To estimate the volumetric flow rate, we begin with enforcing conservation of mass. We can convert between our reaction equation and mass by multiply by the molecular masses of each species. As such, 1 kg of fuel would require $\left(n + \frac{m}{4}\right)\frac{M_{O_2}}{M_{C_nH_m}}$ kg of O_2 for complete combustion and similar calculations can be made for the remaining species. Conservation of mass thus results in:

$$\begin{aligned}\dot{m}_{core|exhaust}\left[\frac{\mathrm{kg}}{\mathrm{kg_{fuel}}}\right] &= \dot{m}_{core|in} + \dot{m}_{combustion}\\ &= 0.768\cdot\mathrm{AFR}\cdot\mathrm{N}_2 + 0.232\cdot\mathrm{AFR}\cdot\mathrm{O}_2 + \\ &-\left(n+\frac{m}{4}\right)\frac{M_{O_2}}{M_{C_nH_m}}\mathrm{O}_2 + n\frac{M_{CO_2}}{M_{C_nH_m}}\mathrm{CO}_2 + \frac{m}{2}\frac{M_{O_2}}{M_{C_nH_m}}\mathrm{H}_2\mathrm{O}\end{aligned}$$

where M_i refers to the molecular mass of species i. We use the standard atomic weight values from the International Union of Pure and Applied Chemistry (IUPAC) (2). The volumetric flow rate is then estimated by scaling each term by the appropriate species' density. The densities are calculated at STP using the ideal gas law.

$$\begin{aligned}Q_{core|exhaust}\left[\frac{\mathrm{m}^3}{\mathrm{kg_{fuel}}}\right] &= \left(\frac{0.768}{\rho_{N_2}} + \frac{0.232}{\rho_{O_2}}\right)\cdot\mathrm{AFR}\\ -\left(n+\frac{m}{4}\right)\frac{M_{O_2}}{\rho_{O_2}M_{C_nH_m}}\mathrm{O}_2 &+ n\frac{M_{CO_2}}{\rho_{CO_2}M_{C_nH_m}}\mathrm{CO}_2 + \frac{m}{2}\frac{M_{O_2}}{\rho_{H_2O}M_{C_nH_m}}\mathrm{H}_2\mathrm{O}\end{aligned}$$

For n = 12 and m = 22.8928, the resulting volumetric flow rate is:

$$Q_{core|exhaust}\left[\frac{\mathrm{m}^3}{\mathrm{kg_{fuel}}}\right] = (0.614 + 0.163) \cdot \mathrm{AFR} - 2.376 + 1.609 + 1.534$$
$$= 0.777 \cdot \mathrm{AFR} + 0.767$$

For a mixed turbofan engine, the bypass and core streams are internally mixed, thus the mass concentration is based on the combined flow streams. As such, the volumetric flow rate is adjusted by a factor of (1+BPR), where BPR is the bypass ratio.

$$Q_{mixed|exhaust}\left[\frac{\mathrm{m}^3}{\mathrm{kg_{fuel}}}\right] = 0.777 \cdot \mathrm{AFR} \cdot (1 + \mathrm{BPR}) + 0.767$$

S2. Measurement data and confidence intervals

We include a Microsoft Excel spreadsheet that contains information from dataset-1 and dataset-2 as used to generate the three correlations developed in the main paper. The Excel file contains an “About” tab that details the units and measurement systems used, and 3 additional tabs representing the data points used for the 3 correlations.

Within this Excel file, there are additional tabs that include confidence intervals for the three correlations developed in the main paper (SN-CBC CI, kslm CI and GMD CI). These can be used as look-up tables in order to propagate uncertainties in estimated mass and number emission indices.

S3. Uncertainty in emission index prediction

Figure 5 of the main paper shows the predicted versus measured emission indices (EI) for instrument measured mass (A), exit plane mass (B) and exit plane number (C). While these show the mean results, they do not provide information on the uncertainty. Uncertainties on each of the correlations are available in the form of prediction intervals. Assuming that the prediction intervals are normally distribution around the best fit, we can propagate the uncertainties to an EI using a Monte Carlo sampling approach. The first step involves sampling from three independent Normal distributions. We apply the method to estimate $EI_{m,I}$, $EI_{m,e}$ and $EI_{N,e}$ for each sample that is drawn. Note that since the correlations from SN to $C_{BC,I}$ and $C_{BC,c}$ to GMD were conducted in logspace, the logarithm of the predictions will be normally distributed. We can finally calculate the mean and 95th percentiles over all samples for each EI, where the 95th percentiles represent the uncertainty in our best estimate. We have found that ~2,000 samples is sufficient for the mean and 95th percentiles to converge and for the results presented below we use 10,000 samples.

Figure S1, Figure S2 and Figure S3 show the uncertainty and best estimate for the instrument measured mass, exit plane mass and exit plane number emissions indices. To view the trends more clearly, we only include estimates for the highest thrust variant of each engine.

The uncertainty in $EI_{m,i}$ tends to decrease as its value increases, however the emissions index is also dependent on the mode of operation through the AFR, so this trend is not robust. At low $EI_{m,i}$, the uncertainty spans around 2 orders of magnitudes. This is driven by the prediction intervals in the SN – $C_{BC,i}$ relationship, which spans almost 2 orders of magnitude at SN $\lesssim$ 3. The uncertainties grow further as we move to exit plane mass and finally to exit plane number emissions as well. This is caused by the prediction intervals in the k_{slm} – $C_{BC,i}$ and GMD – $C_{BC,c}$ correlations.

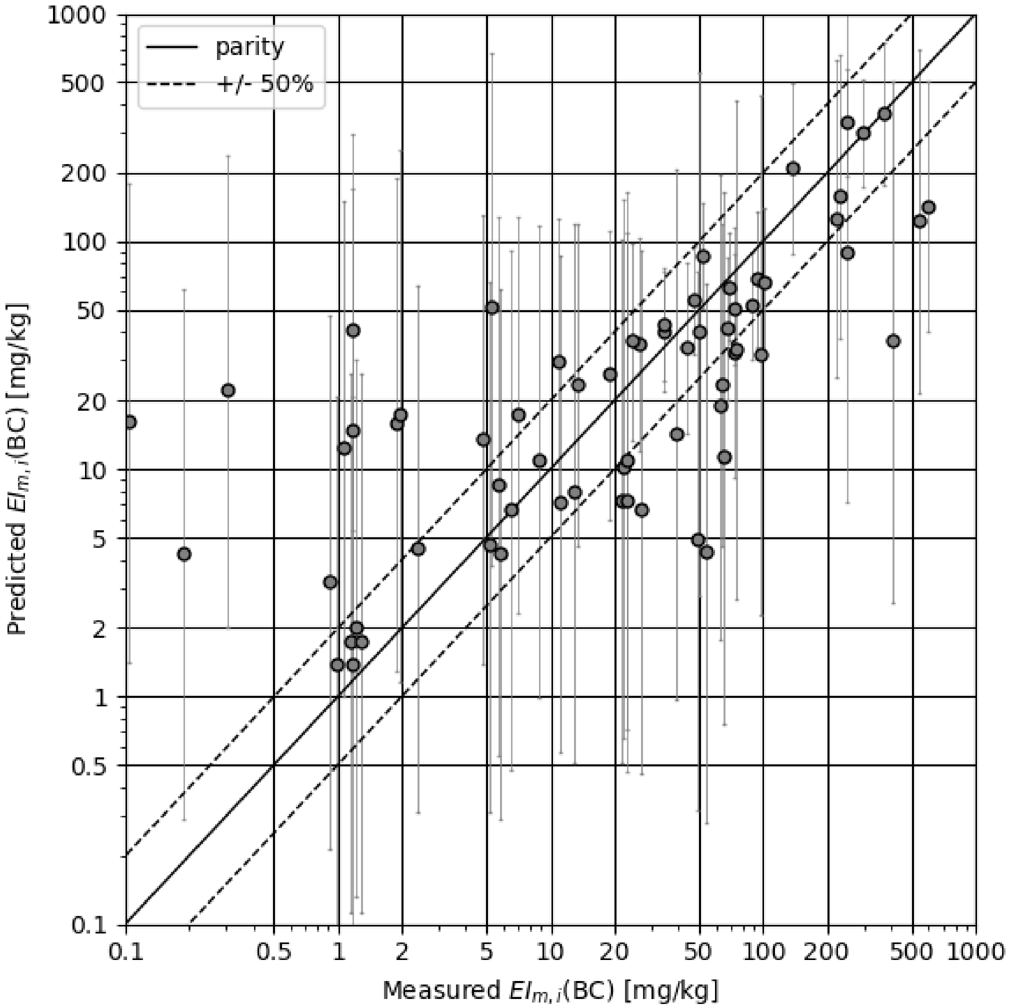

Figure S1: Predicted versus measured instrument measured mass EI with uncertainty

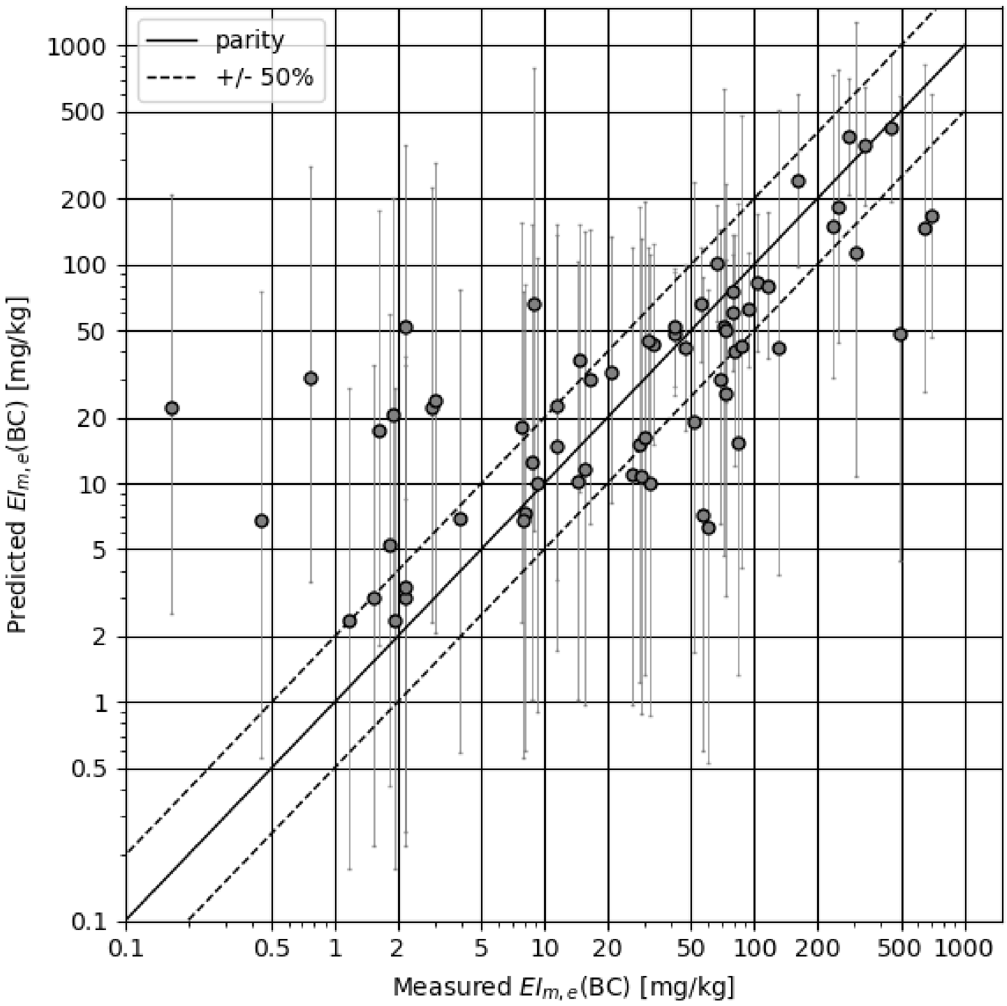

Figure S2: Predicted versus measured exit plane mass EI with uncertainty

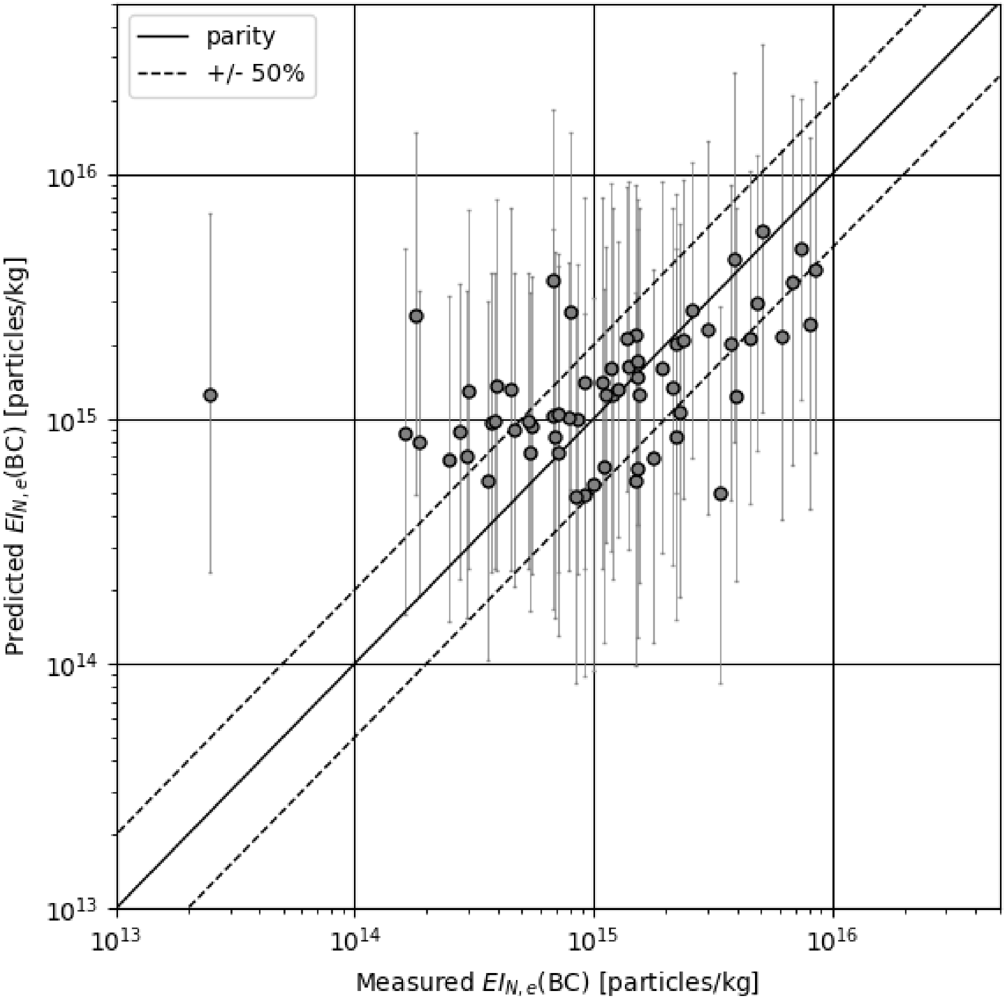

Figure S3: Predicted versus measured exit plane number EI with uncertainty

S4. Distribution of global LTO BC emissions by mode of operation

The Aviation Emissions Inventory Code (AEIC) (3) estimates landing and take-off (LTO) emissions by mode of operation, which include taxi, approach, climb-out and take-off. This allows us to estimate BC mass and number emissions by mode of operation and we can use our upper and lower bound estimates to understand how the uncertainty changes by mode of operation.

Table S1 shows BC mass and number emissions by mode of operation for the SCOPE11, FOA3 (4) and Stettler (5) correlations. As with the total LTO emissions, the SCOPE11 method predicts mass emissions between the FOA3 and Stettler correlations. We also include the uncertainty in the SCOPE11 results for both mass and number emissions. The relative uncertainty (difference between the 95th and 5th percentiles over the mean) increases from between 22% - 27% for approach, climb-out and take-off operations to 45% for taxi operations. This is because taxi operations typically have lower measured SN and this leads to the higher uncertainty from the SN – C_{BC} correlation. The total emissions are driven by the climb-out and take-off modes and thus the relative uncertainty is 28%, following the relative uncertainty in these two modes. For number emissions, the trend is similar with taxi operations having a relative uncertainty of 108%, approach of 94%, climb-out of 67% and take-off of 64%. In this case, however, taxi operations contribute the largest proportion of number emissions and thus lead to a high relative uncertainty in the total number emissions of 92%.

Table S1: Global LTO BC mass and number emissions by mode of operation.

	LTO BC Mass [Gg/yr]				
	Taxi	Approach	Climb-out	Take-off	Total
SCOPE11 (5th – 95th percentile)	0.11 (0.08 – 0.13)	0.08 (0.07 – 0.09)	0.41 (0.37 – 0.46)	0.15 (0.13 – 0.17)	0.76 (0.66 – 0.87)
FOA3 (5)	0.06	0.04	0.30	0.11	0.51
Stettler et al (5)	0.20	0.13	1.65	0.28	2.63
	LTO BC Number [particles/yr]				
	Taxi	Approach	Climb-out	Take-off	Total
SCOPE11	1.30 (0.79 – 2.20)	0.54 (0.35 – 0.86)	0.72 (0.53 – 1.01)	0.25 (0.18 – 0.34)	2.89 (1.89 – 4.55)

S5. SCOPE11 calculation procedure

To aid with implementing the SCOPE11 approach, we include the step-by-step method starting from the Smoke Number (SN) and moving to the mass and number emission indices for a single mode of operation.

Step 1. From the SN, the mass concentration at the instrument ($C_{BC,i}$) can be found using the correlation in Eq 10 of the main paper.

Step 2. The mass emissions index at the instrument ($EI_{m,i}$) is found by multiplying $C_{BC,i}$ with the volumetric flow rate (Q), which is found using Eq 3 in the main paper and the AFR is chosen according to the mode of operation. Note that EI_m at any location can be found by multiplying the C_{BC} at the same location by Q.

Step 3. We can now calculate the mass concentration at the engine exit plane ($C_{BC,e}$)

  a. Use the estimated $C_{BC,i}$ to calculate the system loss correction factor for mass (k_{slm}) from Eq 13 of the main paper.
  b. $C_{BC,e}$ is calculated by multiplying k_{slm} with $C_{BC,i}$.

Step 4. To calculate the particle GMD, we use Eq 15 of the main paper, which first requires us to estimate the mass concentration in the combustor ($C_{BC,c}$).

  a. For static operations, the inlet total temperature (T_t) and pressure (P_t) are identical to the ambient, static temperature (T_a) and pressure (P_a). If the aircraft is moving, we can apply the following equations to estimate total conditions:

$$T_{t2} = T_a + \frac{V^2}{2c_p}$$

$$\frac{P_{t2}}{P_a} = \left(\frac{T_{t2}}{T_2}\right)^{\frac{\gamma}{\gamma-1}}$$

  where c_p is the heat capacity at constant pressure of air, typically ~1,005 kJ/kg/K, $\gamma = 1.4$ is the heat capacity ratio of air, and V is the aircraft velocity.
  b. Knowing the engine's overall pressure ratio (OPR), the combustor inlet temperature (T_{t3}) can be estimated using Eq 9 of the main paper.
  c. The turbine inlet temperature (T_{t4}) and pressure (P_{t4}) are found using Eq 8.
  d. We can thus find the total density (ρ_{t4}) at the turbine inlet using Eq 7.
  e. $C_{BC,c}$ is finally found by applying Eq 6 where the density at STP conditions of 1.2 kg/m^3 is used.
  f. Now we can apply Eq 15 to estimate the GMD at the engine exit plane.

Step 5. The exit plane number emissions index ($EI_{\#,e}$) is found using Eq 4 using a GSD of 1.8, soot density of 1000 kg/m^3. Note that the appropriate exit plane mass emissions index ($EI_{m,e}$) must be used.

References

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