A Methodology to Relate Black Carbon Particle Number and Mass Emissions from Various Combustion Sources

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1. Introduction

- Black Carbon (BC) Particle Number (PN) emissions from the transport sector influences health and climate, yet it's impact remain highly uncertain.
- Health Effects: Ultrafine particles have a higher probability of being deposited into the respiratory system, and translocated towards the circulatory system and internal organs.
- Climate Effects: BC PN emissions from aircraft acts as a condensation nuclei for contrail formation, where the initial contrail properties are strongly correlated to the number of emitted aircraft BC particle per kg of fuel burned (EI_n in kg^{-1}) (*Fig.1*) [1].
- Existing BC EI_n models for aviation emissions assumes that BC particle morphologies remain constant irrespective of engine thrust settings.
- Aims & Objectives:
  1. Develop a new model to estimate BC PN emissions from mass using the theory of fractal aggregates.
  2. Validate the new model using BC measurements from three different emission sources
  3. Perform an uncertainty and sensitivity analysis to understand the accuracy and uncertainty bounds of the outputs of the newly developed model.

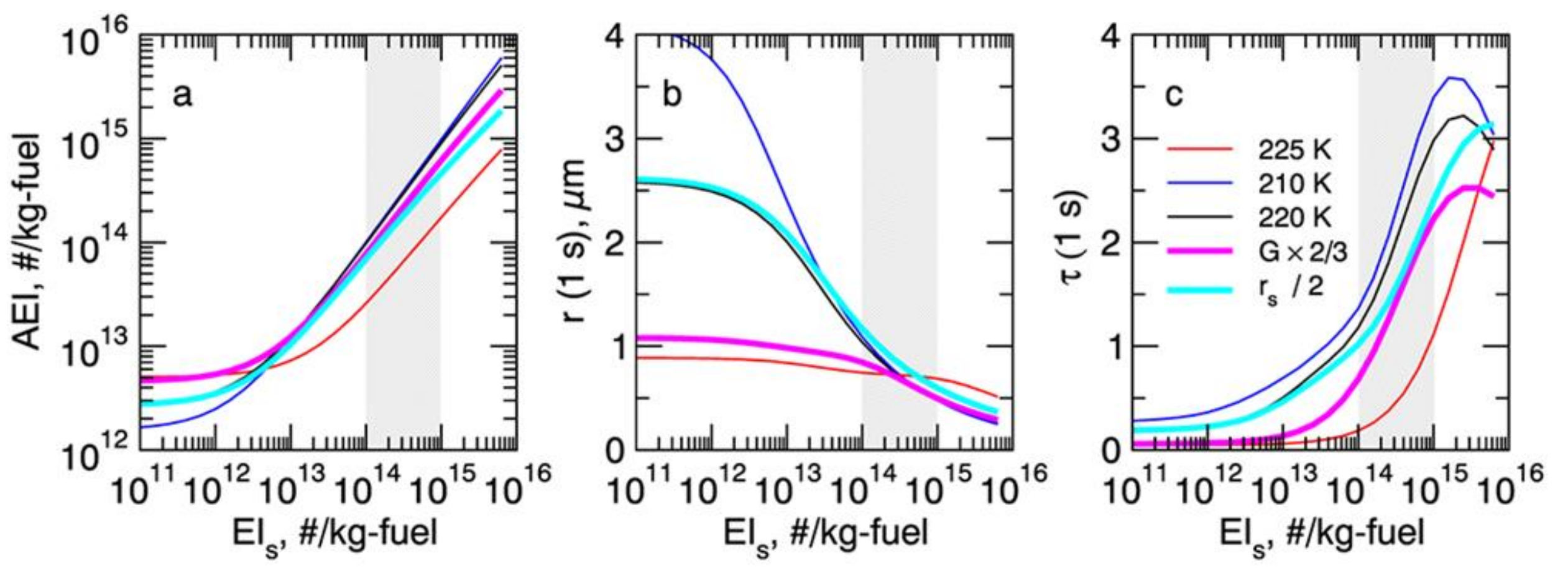


Fig. 1: Changes in contrail properties versus BC EI_n in a young contrail. These contrail properties are reported at a plume age of 1-second. (Source: [1])

2. Theory – Development of a new BC *N* or EI_n Predictive Model

Nomenclature

m	Mass of one BC aggregates	n_{pp}	Number of primary particles in an aggregate
d_m	Aggregate Mobility Diameter	d_{pp}	Primary Particle Diameter
ρ_0	BC Material density	k_a & D_α	Scaling prefactor & projected area exponent
D_{fm}	Aggregate mass-mobility exponent	k_{TEM} & D_{TEM}	TEM prefactor-exponent coefficient pairs
GMD	Geometric Mean Diameter	$n(d_m)$	No. of aggregates for a given mobility diameter range
GSD	Geometric Standard Deviation	M & N	Total mass and number of BC aggregates

- In a free molecular regime, $n_{pp} = k_a(\frac{d_m}{d_{pp}})^{2D_\alpha}$ or $n_{pp} = (\frac{d_m}{d_{pp}})^{D_{fm}}$ [2],
  - where constant values of $k_a = 0.998$ and $D_\alpha = 1.069$ can be used for aggregates formed of polydisperse primary particles, irrespective of the state of sintering [3].
- Total mass of aggregates for a given Particle Size Distribution (PSD):

$$n_{pp} = k_a(\frac{d_m}{d_{pp}})^{2D_\alpha}$$

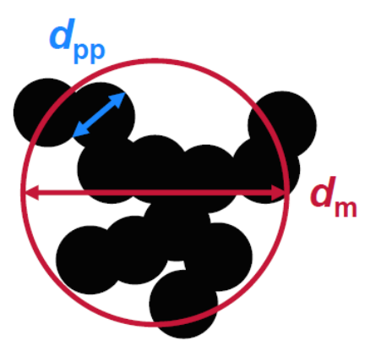
$$d_{pp} = k_{TEM} \times d_m{}^{D_{TEM}} \text{ [4]}$$

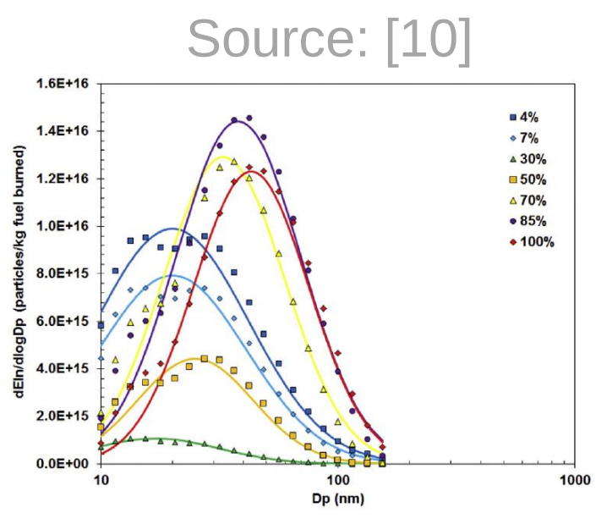
$$m = n_{pp}\rho_0\left(\frac{\pi}{6}\right)d_{pp}{}^3$$

$$n(d_m) = N \times p(d_m)$$

$$M = \int_0^\infty m(d_m)n(d_m)\,dlnd_m \longrightarrow M = Nk_a\rho_0(\frac{\pi}{6})(k_{TEM})^{3-2D_\alpha}\int_0^\infty d_m{}^\varphi\, p(d_m)\,dlnd_m$$

Source: [10]





- Resolve the remaining integral (φ^th moment of a log-normal distribution) & rearrange for *N*:

$$N = \frac{M}{k_a\rho_0(\frac{\pi}{6})(k_{TEM})^{3-2D_\alpha}GMD^\phi \exp(\frac{\phi^2\ln(GSD)^2}{2})}, \text{ where } \phi = 3D_{TEM} + (1 - D_{TEM})2D_\alpha.$$

- BC aggregate morphology and PSD, such as the GMD, GSD and D_{fm} are dependent on engine operating mode & combustion conditions.
- The new Fractal Aggregates (FA) model relates BC mass, number and PSD in one equation.

3. Data & Methodology

- The FA Model is validated with data from (i) An internal combustion engine [5], (ii) An inverted burner [6], and (iii) Two aircraft gas turbine engines at ground and cruise conditions [7], [8].
- An uncertainty analysis for the FA model is performed using the Monte Carlo 1000-member ensembles, while a global sensitivity analysis is accomplished using the Sobol' Method [9].

4. Model Validation

Internal Combustion Engine & Inverted Burner

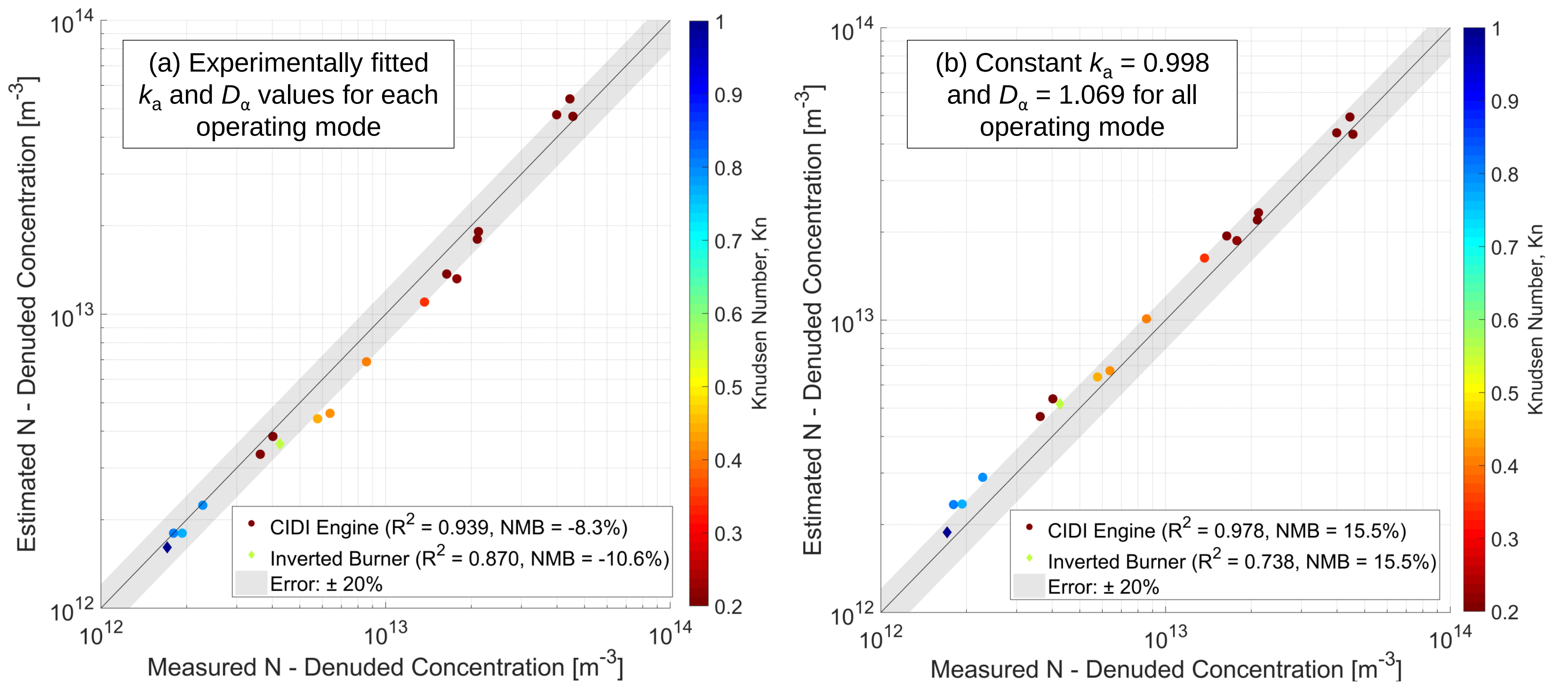


Fig. 2: Validation of the FA Model with data from an internal combustion engine & inverted burner

- For two different sets of k_a and D_α values, the difference in the FA model outputs (estimated *N*) is within ± 20% of the measured *N*. Hence, constant values of k_a = 0.998 and D_α = 1.069 can be used when specific k_a and D_α data for a given operating condition is not available.

Aircraft Gas Turbine Engines at Ground and Cruise Conditions

For aircraft emissions, we assume $k_a = 1$ & $D_\alpha = \frac{1}{2}D_{fm}$ [Recall: $n_{pp} = k_a(\frac{d_m}{d_{pp}})^{2D_\alpha}$ or $n_{pp} = (\frac{d_m}{d_{pp}})^{D_{fm}}$]

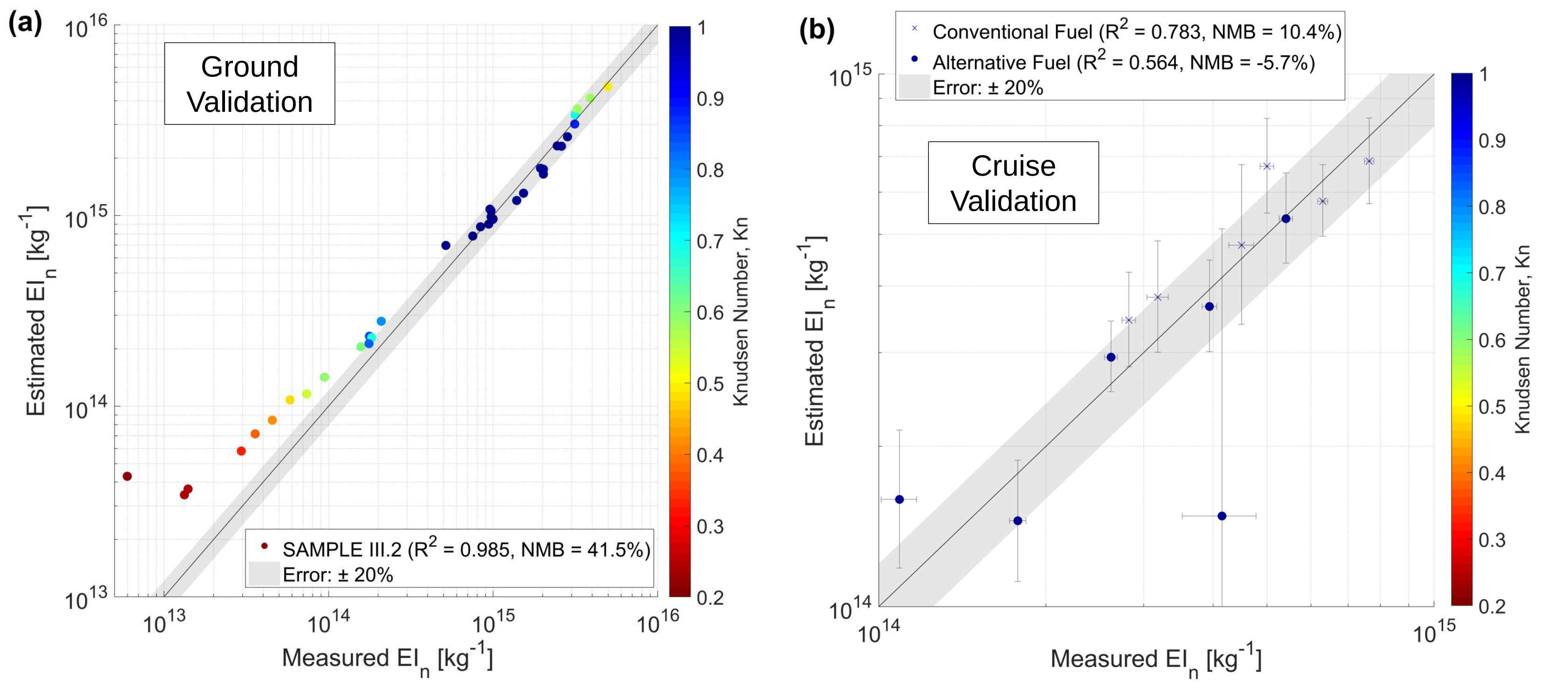


Fig. 3: FA Model validation with aircraft gas turbine engine data at (a) ground and (b) cruise conditions

- For ground validation (Fig. 3a), a systematic overestimation of EI_n is observed at higher thrust settings (data points with lower Kn) as BC aggregates are formed in the continuum regime.

5. Uncertainty & Sensitivity Analysis

- Due to the non-linearity of the FA model, the uncertainty of the estimated *N* or EI_n is asymmetrically distributed (-37%, +55%) at 1.96σ (*Fig. 4a*).
- Sensitivity analysis (*Fig. 4b*) identified that the uncertainties in GSD contribute to the largest sensitivity in the FA model output, followed by inputs of *M*, D_{fm} and GMD.
- A prioritisation can be recommended for future research to measure these critical parameters more accurately to reduce the uncertainty bounds of the FA model outputs.

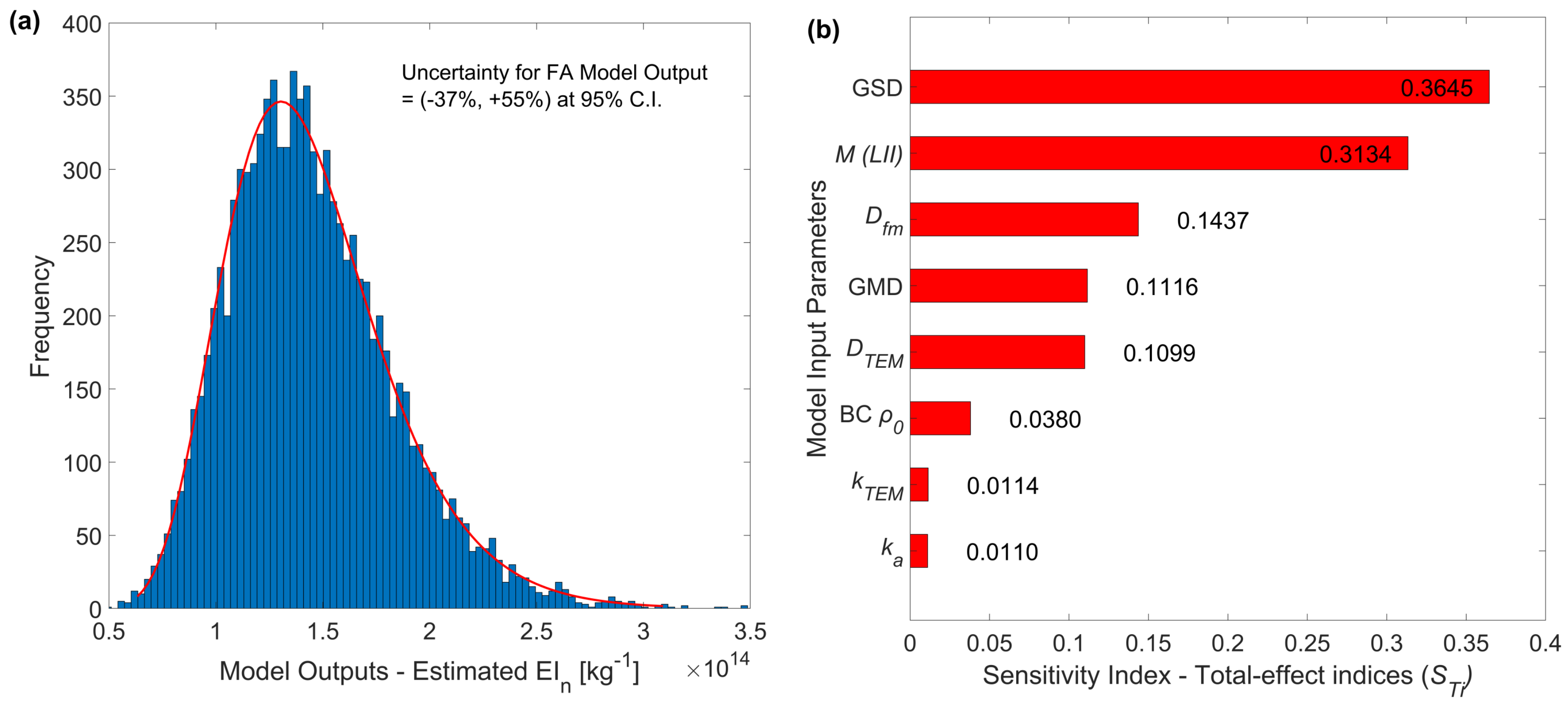
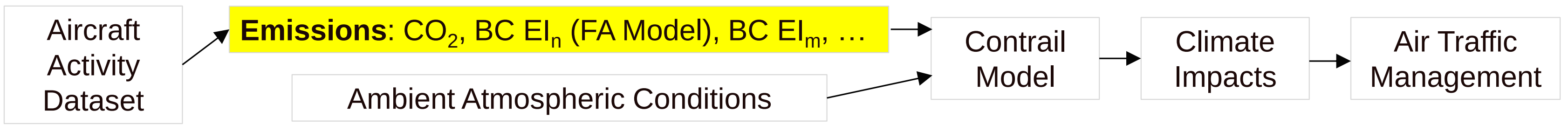


Fig. 4: (a) Uncertainty & (b) Sensitivity Analysis for the FA model outputs (Estimated *N* or EI_n)

Summary & Future Work

- A new methodology to relate BC Particle Number and Mass emissions is developed based on the theory of fractal aggregates, and validated with three different BC emission sources.
- Large uncertainties remain; GMD, GSD, M & D_{fm} inputs are identified as important parameters.
- Future Work: Application of FA Model to estimate BC EI_n for Aviation Emissions



Aircraft Activity Dataset → **Emissions**: CO_2, BC EI_n (FA Model), BC EI_m, … → Contrail Model → Climate Impacts → Air Traffic Management

Ambient Atmospheric Conditions → Contrail Model

References

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