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**DELIVERABLE: D6**

# Refining Methodologies for Estimating Non-Volatile Particulate Matter Emissions from Smoke Number for Regulated and Unregulated Aircraft Turbine Engines

An Agency of the European Union



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## EXECUTIVE SUMMARY

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This report focuses on refining methodologies for estimating non-volatile Particulate Matter (nvPM) emissions from Smoke Number (SN) data for both regulated and unregulated aircraft turbine engines. The study aims to assess and improve the accuracy of existing estimation methods, particularly SCOPE11 and the First-Order Approximation version 4 (FOA4), by evaluating their performance across a wide range of engine types and operational conditions.

The study conducted extensive engine emission tests on 12 turbofan engine types, including three unregulated engines, using both conventional Jet A-1 fuel and blends with Sustainable Aviation Fuel (SAF) components. Data was collected using standardized Swiss (CH) and European (EUR) nvPM reference systems, and the data was analyzed to refine the correlations between SN and nvPM mass and number emissions.

Key findings demonstrate that while the SCOPE11 methodology accurately predicts nvPM mass emissions for engines with unmixed exhaust nozzles, it tends to overestimate emissions for mixed-flow turbofan (MTF) engines, particularly those with high bypass ratios. This overestimation is especially critical for unregulated engines with rated thrusts of less than 26.7 kN, which continue to rely on SN as a primary metric for nvPM emissions.

The report proposes several improvements to the SCOPE11 model, including engine-specific adjustments for MTF engines with high bypass ratios, which would improve the accuracy of nvPM emission estimates for unregulated engines. Additionally, the study explores alternative approaches, such as direct correlations between SN and Emission Indices (EIs) and updated particle size distribution parameters.

In conclusion, the report emphasizes the need for further refinement of existing models to ensure their applicability across different engine configurations, particularly for unregulated engines that continue to use SN as a key measure of nvPM emissions. These refinements are essential for providing more accurate and reliable emissions data, which is crucial for regulatory compliance, environmental impact assessments, and ongoing efforts to reduce aviation's environmental footprint.

## CONTRIBUTIONS

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Dr. Lukas Durdina (ZHAW / GreenLet Research): conceived and designed the analysis; collected data using the Swiss nvPM system; performed the analysis; wrote the paper

Dr. Jacinta Edebeli (ZHAW): collected data using the Swiss nvPM system; developed data processing tools and contributed to data analysis

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Mr. Curdin Spirig, Mr. Tobias Frischknecht, Mr. Manuel Roth (ZHAW): collected data using the Swiss nvPM system

Dr. Andrew Crayford (CU): collected data using the European nvPM system; reviewed the paper; coordinated the technical work

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## LIST OF ABBREVIATIONS

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- **AFR:** Air-Fuel Ratio
- **APC:** Advanced Particle Counter (AVL)
- **ARP:** Aerospace Recommended Practice
- **BPR:** Bypass Ratio
- **CAEP:** Committee on Aviation Environmental Protection
- **CH:** Swiss (related to the Swiss nvPM reference system)
- **CSM:** Chell Smoke Meter
- **DF:** Dilution Factor
- **EASA:** European Union Aviation Safety Agency
- **EI:** Emission Index
- **EEP:** Engine Exit Plane
- **EUR:** European (related to the European nvPM reference system)
- **FOA:** First-Order Approximation
- **GMD:** Geometric Mean Diameter
- **GSD:** Geometric Standard Deviation
- **HEFA-SPK:** Hydrotreated Esters and Fatty Acids-Synthetic Paraffinic Kerosene
- **ICAO:** International Civil Aviation Organization
- **LPC:** Low-Pressure Compressor
- **LTO:** Landing and Take-Off
- **MSS:** Micro Soot Sensor
- **MTF:** Mixed-Flow Turbofan
- **N/M:** Number-to-Mass Ratio
- **nvPM:** Non-Volatile Particulate Matter
- **OEM:** Original Equipment Manufacturer
- **PSD:** Particle Size Distribution
- **RMSE:** Root Mean Square Error
- **SAE:** Society of Automotive Engineers
- **SAF:** Sustainable Aviation Fuel
- **SN:** Smoke Number
- **STP:** Standard Temperature and Pressure (273.15 K, 101.325 kPa)
- **VBV:** Variable Bleed Valve

Moreover, the next abbreviations will be used for each SAMPLEIV Consortium Partner:

*Table 1: SAMPLEIV Consortium Partners Abbreviations*

<b>SAMPLEIV Consortium Partner</b>	<b>Abbreviation</b>
INSTITUTO NACIONAL DE TÉCNICA AEROSPAIAL “ESTEBAN TERRADAS”	INTA
ROLLS-ROYCE PLC	RR
THE UNIVERSITY OF MANCHESTER	UoM
CARDIFF UNIVERSITY	CU
ZHAW ZURICH UNIVERSITY OF APPLIED SCIENCES	ZHAW
UNIVERSIDAD POLITÉCNICA DE MADRID	UPM

# 1. BACKGROUND AND OBJECTIVES

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Following 40 years since its introduction, Smoke Number (SN), which afforded a measure of visible smoke in engine exhaust plumes, was phased out and replaced by the introduction of the ICAO CAEP/11 nvPM LTO mass and number standard on 1 January 2023 for turbofan and turbojet engines with rated thrust >26.7 kN. However, for the foreseeable future, the SN standard will continue to be used for small engines <26.7 kN that are excluded from the nvPM and gaseous emissions standards. Thus, SN remains the only (indirect) measure of nvPM and anchor for estimating nvPM emissions of unregulated engines. It is also essential for estimating nvPM emissions of large engines that were out of production before the introduction of the nvPM standard but will continue to operate for decades.

The state-of-the-art methods for estimating nvPM mass and number emissions from SN are SCOPE11 and the first-order approximation version 4 (FOA4) ((Agarwal et al., 2019; ICAO, 2020). In both methods, nvPM mass concentration at the engine exit plane is determined from an empirical correlation between SN and nvPM mass. The next step calculates EI nvPM mass using assumed air-fuel ratios (AFR) for each LTO mode. The FOA4 method is derived from SCOPE11, and the EI nvPM mass calculations are identical. EI nvPM number is calculated from mass by assuming a lognormal particle size distribution (PSD) with a geometric standard deviation (GSD) of 1.8, average particle density of 1 g/cm<sup>3</sup> and a given geometric mean diameter (GMD). FOA4 assumes GMD of 20 nm for taxi and approach and 40 nm for climb and take-off. The SCOPE11 method determines exit plane GMD from an empirical correlation with combustor exit nvPM mass concentration.

This report addresses the following tasks:

- Review the current methodology for estimating nvPM mass and number EIs using nvPM and SN data collected using standardized sampling and measurement systems
- Evaluate the applicability of the SN-nvPM methodology for unregulated turbofan engines <26.7 kN rated thrust
- Propose improvements to the standardized SN-nvPM methodology
- Explore direct correlations between SN and emission indices of nvPM mass and number

## 2. DATA COLLECTION AND PROCESSING

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### 2.1. Engine emission tests

Emission tests of 12 turbofan engine types with rated thrust from 15 to 350 kN were conducted in test cells and on-wing tests. Three engines were rated <26.7 kN (6000 lbf) and thus are excluded from the current gaseous and nvPM emissions certification scheme. All engines featured various rich-burn combustion systems; thus, this study does not include staged lean-burn combustors. Four of the 12 engine types had a mixed exhaust nozzle, and exhaust measurements were performed in the mixed-flow configuration. The engines burned Jet A-1 fuel, either conventional petroleum-derived fuel or blends with a synthetic blending component – namely, synthetic paraffinic kerosene derived from hydrotreated esters and fatty acids (HEFA-SPK). The blend ratios were up to ~50%. The fuel hydrogen content across all tests ranged from 13.7 to 14.5% by mass.

The emission tests were conducted independently using either the Swiss (CH) nvPM reference system SMARTEMIS or the European (EUR) nvPM reference system. Exhaust samples were extracted within 0.1 – 1.7 m downstream of the engine exit plane, following the SAE Aerospace Recommended Practice (ARP) 6320. and the ICAO Annex 16 standard (ICAO, 2017; SAE International, 2021). Detailed descriptions of the EUR and CH systems are available in the existing literature (Durand et al., 2021; Durdina et al., 2021, 2023; Lobo et al., 2015).

### 2.1. nvPM mass and number emissions

The CH and EUR standardized systems reported nvPM mass and number concentrations using nominally identical nvPM instruments: the AVL Micro Soot Sensor (MSS) for the nvPM mass and the AVL Advanced Particle Counter (APC) for the nvPM number concentration. The EUR and CH systems were compared in parallel on large turbofan engines during the nvPM standard development (Lobo et al., 2020) and recently using a combustor rig (Crayford et al., 2022)

### 2.2. Smoke number

In parallel with the nvPM system, the SN was measured according to the SAE ARP 1179D (SAE, 2011). In the CH system, SN samples were collected using a Chell CSM2000 smoke meter. The smoke meter sampled in the gas line in parallel with the gas analyzers. The instrument was programmed to collect 16.2 kg exhaust gas per m<sup>2</sup> of filter paper (Whatman Grade 4) with a nominal flow rate of 14 l/min. The reflectance of clean and stained filters was measured using a compliant reflectometer Photovolt 577PC.

In the EUR system, SN was sampled using an updated version of the Chell smoke meter, the CSM2001, where the flows were controlled using a mass flow controller instead of a volume displacement meter. The reflectance was measured using a Photovolt 577(5G) reflectometer.

### 2.1. Data cleaning and analysis

The real-time nvPM and gaseous data were averaged for 60 seconds and matched with the SN sampling periods. Data points were excluded when the nvPM mass concentration measured was affected by the shedding of large particles re-entrained from the nvPM system cyclone separator (i.e., the nvPM mass measured included excess nvPM not originating from the engine), as described by Durdina et al. (2024). The final dataset included 380 SN-nvPM pairs.

### 3. CALCULATION STEPS FROM SN TO EI MASS AND NUMBER

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In the currently used methodology for estimating nvPM mass and number EIs, the following steps are undertaken:

- Step 1 – determine nvPM mass concentration at the engine exit plane from an empirical correlation with SN
- Step 2 – calculate the EI of nvPM mass
- Step 3 – parametrize the PSD
- Step 4 – calculate the EI of nvPM number from nvPM mass

Below, these steps are reviewed using the empirical data obtained from the CH and EUR nvPM reference systems.

## 4. STEP 1 - SN-NVPM MASS CORRELATION

### 4.1. History

Before introducing the nvPM certification standard, SN was the only measure of certified turbofan and turbojet engine particle emissions, previously commonly referred to as smoke or soot. ICAO's Committee on Aviation Environmental Protection (CAEP) recognized this gap and looked for an interim solution to estimate nvPM mass emissions from SN. Researchers developed various correlations between PM mass concentration (gravimetric measurements) and SN in the 1970s and 1980s (Lefebvre, 1985; Wayson et al., 2009). In the early 2000s, a literature review of the various methodologies provided a basis for the initial first-order approximation. In 2007, CAEP accepted the FOA3.0 methodology for internal use, which was later implemented in the first version of the ICAO Airport Air Quality Manual (ICAO, 2020). The downside of this methodology was that it was not based on a correlation with nvPM mass, as defined and measured in the newly developed standard (ICAO, 2017).

### 4.2. SCOPE11 and FOA4

The development and validation of the CAEP/10 and CAEP/11 nvPM standards provided an opportunity to update the SN – nvPM methodology. The CAEP/10 mass concentration standard establishes an equivalency between SN and nvPM mass such that the exhaust non-visibility criterion is carried forward in the new standard. OEMs submitted datasets of SN with nvPM mass and number emissions measured in parallel. The new method for estimating nvPM mass and number from SN was named SCOPE11 (Agarwal et al., 2019). SCOPE11, with some simplified assumptions (discussed below), was accepted as FOA4 and implemented in the 2<sup>nd</sup> edition of the ICAO Doc 9889 Airport Air Quality Manual (ICAO, 2020).

SCOPE11 establishes a fit function between SN and the nvPM mass at the instrument corrected for dilution (DF1) and thermophoretic losses in the sampling system's collection section. The function is a product of an exponential function and a logistic function:

$$\text{nvPM}_{\text{mass,inst.}} \times \text{DF1} \times k_{\text{thermo}} = \frac{k_1 e^{k_2 \text{SN}}}{1 + e^{k_3(\text{SN} + k_4)}} \quad (1)$$

Table 2 summarizes the parameters for the best fit and the lower and upper bounds of a 90% prediction band. This correlation does not distinguish between mixed and unmixed exhaust nozzles.

Table 2 SCOPE11 fit parameters in the SN-nvPM mass correlation

Parameter	Best fit	Lower bound (90% prediction interval)	Upper bound (90% prediction interval)
k <sub>1</sub>	648.4	378.5	1146.2
k <sub>2</sub>	0.0766	0.0776	0.0776
k <sub>3</sub>	-1.098	-1.098	-1.098
k <sub>4</sub>	-3.064	-5.066	-1.480

The SCOPE11 best fit, the prediction interval, and the empirical data from this study are shown in Figure 1. The empirical data are differentiated by engine size and type of exhaust nozzle. The unmixed nozzle means that the core and bypass flows are not internally mixed, and exhaust measurements were taken in the hot exhaust downstream of the engine core nozzle. In a mixed-flow turbofan (MTF) engine, the bypass and core flows are internally mixed using a lobed mixer. The exhaust samples were taken downstream of the common nozzle, where the exhaust was diluted with the bypass air.

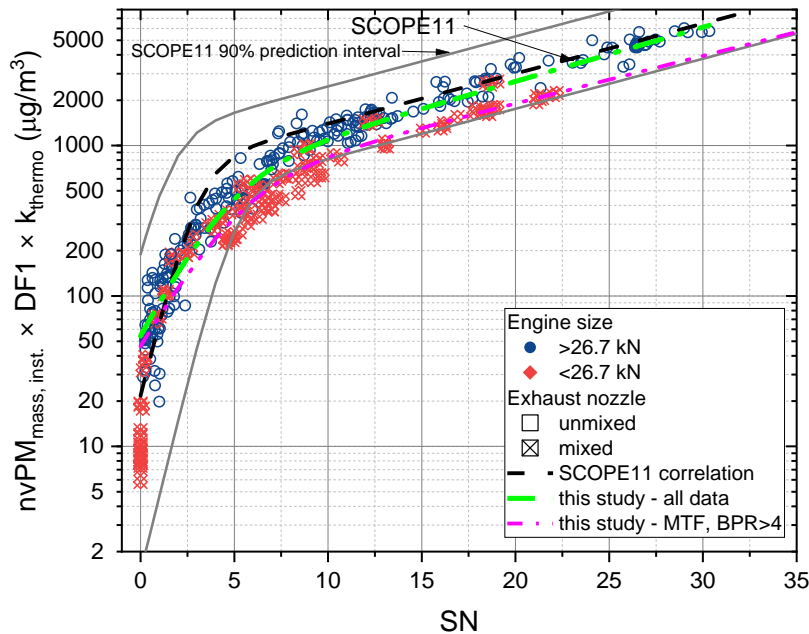


Figure 1 Comparison of the empirical results with the established SCOPE11 correlation between nvPM mass and SN.

All samples obtained from unmixed nozzles were within the 90% prediction band of the SCOPE11 correlation. The correlation predicts our results well for  $SN < 3$  and  $SN > 10$ , while it overpredicted our results outside of this interval. This can be seen by comparing the dashed black and green lines. The green line represents the fit of eq. (1) to all data in this study ( $R^2=0.95$ ).

The MTFs with high bypass ratio (BPR) in this study showed lower nvPM mass for a given SN than the samples obtained from unmixed nozzles. Our dataset includes one large mixed-flow turbofan with a BPR 6 at the design point (take-off). All the unregulated engines are MTFs with a design BPR range from 1.9 to 4.5. The engine with 1.9 BPR agreed well with the SCOPE11 correlation, whereas all the other high BPR engines were significantly lower. While the dataset is limited, it can be hypothesized that this effect could be explained by the changing GMD of the size distribution with thrust and the penetration efficiency of the smoke number filter paper. For all engines studied here, the GMD increased with thrust (Durdina et al., 2024). The filtration efficiency of the SN filter is the highest at the largest GMD (Stettler et al., 2013). Thus, for a given nvPM mass, the SN is the highest for the largest GMD. Due to the dilution with bypass air, the MTF engines may have larger GMD at lower nvPM mass concentration at the instrument compared to core flow samples. A fit of eq. (1) to the MTF engines with  $BPR > 4$  is visualized with the dashed magenta line ( $R^2=0.985$ ). For  $SN > 5$ , this line follows well the lower prediction bound of the SCOPE11 correlation. The fit parameters determined for the data in this study are summarized in Table 3.



Table 3 SCOPE11 fit parameters for data in this study

Parameter	All data	MTF with BPR>4
$k_1$	508.37	441.98
$k_2$	0.083	0.073
$k_3$	-0.498	-0.316
$k_4$	-4.377	-4.85

Figure 2 shows the data from this study color-coded with fuel type. The blue symbols represent samples taken with regular petroleum-based Jet A-1 fuel. The green symbols represent samples taken using blends with HEFA-SPK. The blend ratios were up to ~50%. The samples with SAF blends followed the same nvPM-SN relationship as the Jet A-1 samples for a given engine type.

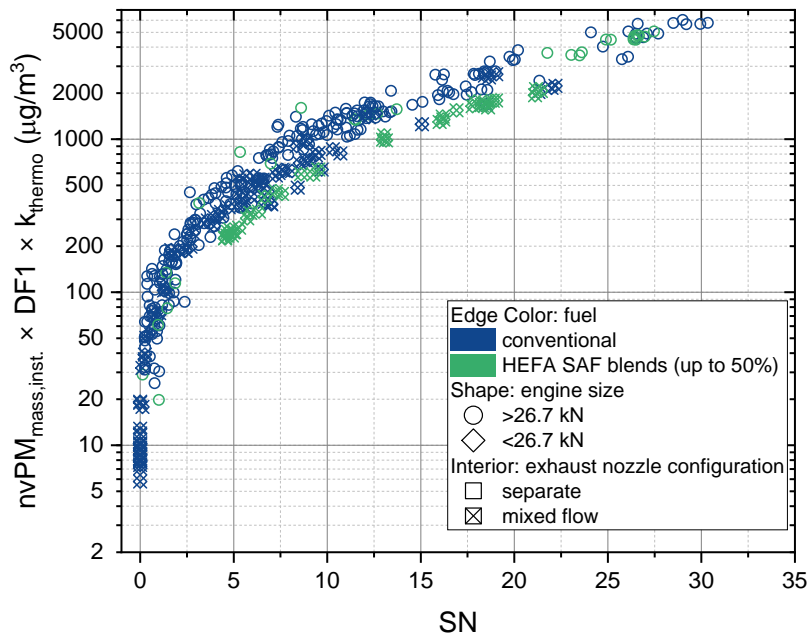


Figure 2 nvPM mass concentration vs smoke number color-coded with fuel type.

### 4.3. System loss correction

In addition to the thermophoretic loss correction factor accounted for in the SCOPE11 correlation, the nvPM mass concentration must be corrected for sampling system losses. The dominant loss mechanism is diffusion. SCOPE11 estimates the loss correction factor  $k_{SL\text{mass}}$  from a correlation with  $\text{nvPM mass} \times \text{DF1} \times k_{\text{thermo}} \times (1 + \text{BPR}_{\text{mix}})$ .  $\text{BPR}_{\text{mix}}$  is the design bypass ratio of MTF engines. This parameter is set to 0 for unmixed exhaust samples. The mass-based loss is dominated by larger particles, and thus, the loss correction factor is significantly lower than for the nvPM number. The  $k_{SL\text{mass}}$  parametrization in SCOPE11 has a lower bound of ~1.17 and an upper bound of ~2.0.

Figure 3 compares  $k_{SL\text{mass}}$  calculated using the SAE ARP6481 method (SAE International, 2019) without measured PSD (squares),  $k_{SL\text{mass}}$  determined using measured PSD in size bins from ~6 to ~240 nm without any assumption about the PSD shape (circles), and the SCOPE11

parametrization (triangles). Durand et al. (2023) compared and discussed the first two system loss correction methods in detail. The SCOPE11 parametrization is a fit to the  $k_{SL_{mass}}$  determined using SAE ARP6481. The SCOPE11 data have a distinct offset of  $\sim 10\%$  (higher) compared to the ARP6481 and PSD-based  $k_{SL_{mass}}$ . Additionally, it can be seen that SCOPE11 overpredicted the PSD-based loss correction factor in the thrust range of 20-45%. In this range, some engines produced their minimum nvPM mass concentration. However, the GMD, which drives the size-dependent losses, was the smallest at idle (3-8% thrust) for all engines tested. The ARP6481 data also tended to overpredict the PSD-based loss correction factors, likely due to the high measurement uncertainty of nvPM mass at or below the limit of detection.

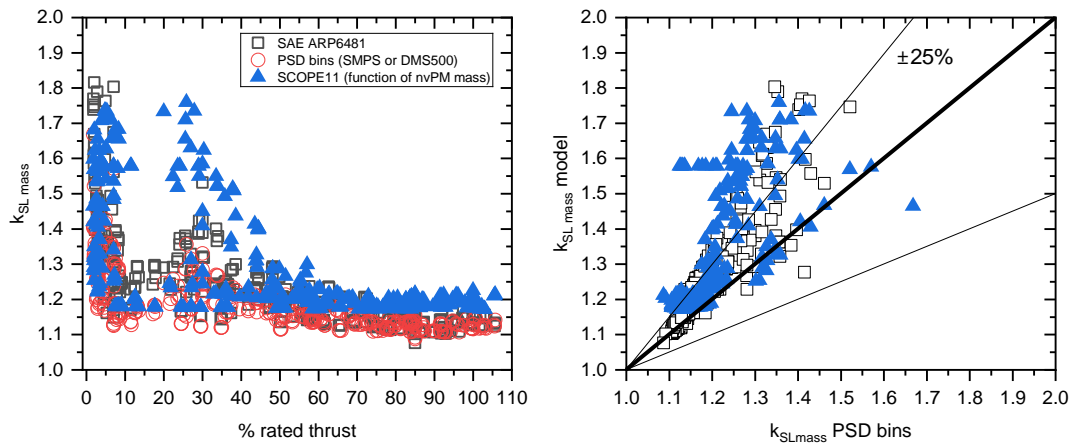


Figure 3 mass-based system loss correction factors as a function of thrust (left) and a parity plot between the model-based  $k_{SL}$  and  $k_{SL}$  determined using measured PSD (right).

#### 4.4. Potential improvements

The SCOPE11 correlation was found representative of the data collected in this study, especially for engines with separate exhaust and bypass nozzles. However, the SCOPE11 model may overpredict the nvPM mass—SN relationship for MTF engines, especially those with high bypass ratios. The analysis presented here, suggests that the lower bound of the SCOPE11 90% prediction interval may be more appropriate for MTF engines with high BPR.

The additional uncertainty of MTF engines is that BPR is not a constant. BPR as a function of static thrust may vary by up to a factor of 2 (decreasing with increasing thrust), and the information is proprietary. However, for regulated engines, the BPR at take-off can be found in the ICAO emissions databank (ICAO, 2023). Another practical issue with sampling mixed exhaust is the mixer efficiency, which is  $\ll 100\%$ . Thus, the core and bypass flows are not perfectly mixed, and the sample is diluted by an unknown fraction of the bypass flow.

The system loss correction factor in SCOPE11 is parametrized as a function of nvPM mass and was found to overpredict the losses at engine conditions that produced low nvPM mass, but not the smallest GMD. Durdina et al. (2024) recently developed a correlation between GMD and % rated thrust for 19 turbofan engine types, including the engines in this study. Thus, a parametrization of  $k_{SL_{mass}}$  as a function of thrust could be explored. Such a parametrization will not be applicable for engines with staged lean-burn combustion systems, which is not an issue in the context of this work since all modern in-service lean-burn engines have been certified for nvPM emissions and no SN-nvPM correlation is needed.

## 5. STEP 2 – EI MASS

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### 5.1. Air-fuel ratio

The EI of nvPM (mg/kg fuel burned) can be estimated by multiplying the nvPM mass concentration by the engine core flow per kg of fuel burned,  $Q$  ( $\text{m}^3/\text{kg}$  fuel). The SCOPE11 method updated the  $Q$  parametrization of Wayson et al. (2009) for fuel with a hydrogen mass content of 13.8% (reference value for the ICAO Annex 16 vol. II correction of nvPM emissions for fuel composition effects) (ICAO, 2017):

$$Q = 0.776\text{AFR}(1 + \text{BPR}_{\text{mix}}) + 0.767 \quad (2)$$

where  $\text{BPR}_{\text{mix}}$  is the bypass ratio for MTF engines, and where the SN was measured in the mixed-flow configuration. For samples from the engine core, this parameter is set to 0. The air-fuel ratio is the mass-based ratio of engine core air and fuel flows. It is not specified at which thermodynamic station the AFR is determined. However, since AFR is used in SCOPE11 to estimate the turbine inlet temperature (thermodynamic station 4), we can assume the AFR concerns this station. Due to the extraction of air from the compressor for high-pressure turbine nozzle and blade cooling (~8-12% of the high-pressure compressor inlet flow (Kurzke & Halliwell, 2018)), the AFR at station 4 is lower than at the turbine exit (station 5). Here, it is assumed that the AFR is reported for station 5, which is equal to the AFR at the exit of an unmixed exhaust nozzle (station 8), but it is not representative of an AFR at the exit of a mixed flow nozzle.

Figure 4 compares AFR5 modeled for five large turbofan engines and three small unregulated engines and the representative ICAO LTO values. The AFR5 values were obtained using either a 0D thermodynamic model calibrated to engine performance data or directly from engine performance data.

At low thrust, the AFR is affected by the handling bleed between the low-pressure compressor (LPC) exit and high-pressure compressor (HPC) inlet, which offloads the first HPC stages at low load to prevent compressor surge. The variable bleed valve (VBV) scheduling and amount of bleed air (% of HPC inlet flow) vary with engine conditions and engine types. The VBV is fully open at idle and closed from medium to maximum thrust. The VBV scheduling may cause a distinct step change in the AFR characteristic. Due to a lack of accurate data, all models shown here, except for one, do not consider handling bleed.

The stars illustrate the representative AFR for the LTO modes approved by engine OEMs. The values were then interpolated to calculate EIs for non-LTO test points. The interpolated reference AFRs compare well to our data of AFR5 for both regulated and unregulated engines, especially >30% thrust. The variability increases with decreasing thrust. Following consideration of the LTO AFR values representative of unregulated engines a polynomial fit is applied in the analysis below.

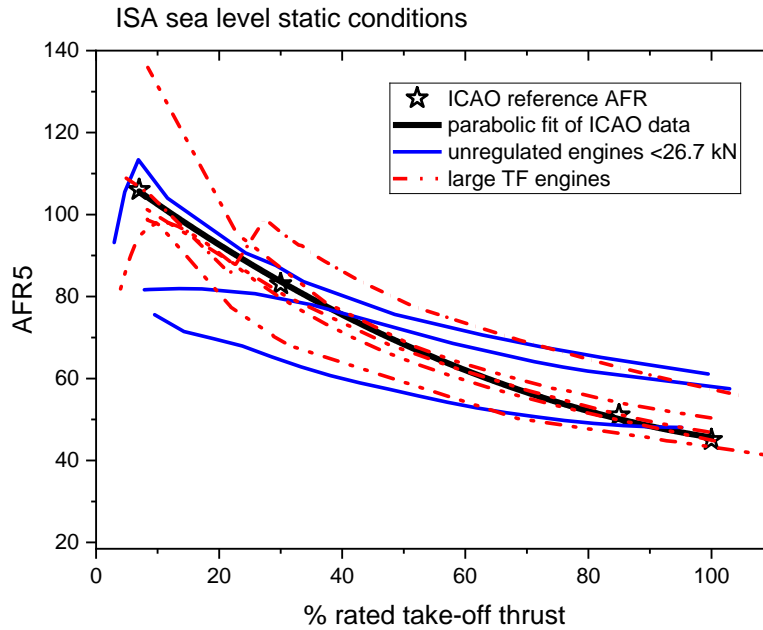


Figure 4 Comparison of modelled AFR at the thermodynamic station 5 for various engines in this study and the assumed ICAO AFR for the LTO modes.

## 5.1. EI mass comparison

Figure 5 compares the nvPM mass EIs calculated using the SCOPE11 method with the measured EIs corrected for sampling system loss using measured PSD (black circles). The predicted EIs strongly correlated with the observations ( $R^2=0.8$ ,  $RMSE=124$  mg/kg). However, it can be seen that the default SCOPE11 correlation overpredicted the EIs for the MTF engines. However, it is noted that excluding the MTF engines with  $BPR>4$  from the comparison led to a significantly better correlation and overall agreement ( $R^2=0.96$ ,  $RMSE=22$  mg/kg). Applying eq. (1) using the updated parameters from Table 3 for MTF engines significantly improved the agreement between observed and predicted values (magenta-coloured circles) with  $R^2=0.94$  and  $RMSE=49$  mg/kg.

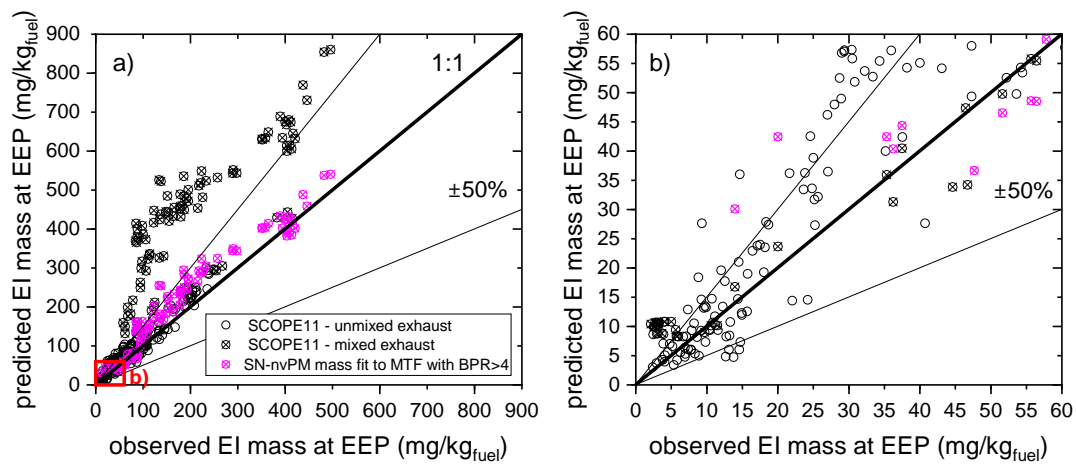


Figure 5 Comparison of nvPM mass emission indices modeled using SCOPE11 and those measured and loss-corrected to engine exit plane using measured PSD. Panel (b) shows the data highlighted by the rectangle in panel (a).

## 5.2. Potential improvements

There are two main sources of uncertainty in the predicted EIs:

- Correlation between SN and nvPM mass
- AFR

It is seen that the SCOPE11 correlation agreed well with the measurements of engines reported here, inclusive of an unmixed exhaust nozzle and a low bypass ratio engine with a mixed nozzle. Most unregulated engines feature a mixed exhaust nozzle, and therefore, the accuracy of the EIs predicted using the default SCOPE11 correlation may be low. Therefore, a new correlation is proposed using measurement data for MTF engines with BRP > 4.

The AFR is a proprietary value, but it is shown that the interpolated ICAO reference values are reasonable for a wide range of engines, including small turbofans <26.7 kN. This data suggests that some small turbofan engines may have lower AFR at low thrust than large ones. However, a larger dataset would be needed to provide updated reference AFR values.

## 6. STEP 3 – PARTICLE SIZE DISTRIBUTION

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nvPM in aircraft gas turbine engine exhaust can generally be well approximated by a monomodal lognormal distribution. However, to characterize the distribution and convert it from mass to number space, GMD, GSD, and effective density,  $\rho$  is required.

Durdina et al. (2024) characterized the nvPM PSD of 19 turbofan engine types and found GMD ranging from  $\sim 7$  nm to  $\sim 50$  nm. The GMD typically increases with thrust for engines with a rich burning primary zone. The GSD also varies with thrust and engine type and ranges from 1.7 to 2.5. The effective density of nvPM varies with particle size, thrust, and engine type. Durdina et al., (2014) determined thrust and size-dependent density for a CFM56-7B engine, reporting mean effective densities in the range from  $\sim 0.8$  to  $\sim 1.1$  g/cm<sup>3</sup> which can be used for estimating mass concentration from number-based integrated PSD and size-dependent density.

Durdina et al. (2024) investigated the average nvPM density as a ratio of nvPM mass measured using the MSS to the integrated PSD volume at STP. The average effective nvPM density ranged from 0.3 g/cm<sup>3</sup> to 1.3 g/cm<sup>3</sup>, with a mean value of 0.74 g/cm<sup>3</sup>.

In SCOPE11, the GMD is estimated from a correlation with nvPM mass concentration at the combustor exit. The combustor exit concentration is obtained by multiplying the exit plane concentration by the ratio of gas densities at station 4 and station 0 (ambient). The total pressure and temperature at station 4 are estimated from a simple energy balance across the combustor, where overall pressure ratio, % thrust, and the AFR are required as input terms (Agarwal et al., 2019). In FOA4, the GMD input is simplified by assuming a fixed GMD for a given LTO mode: 20 nm at 7% and 30% and 40 nm at 85% and 100% thrust.

In both SCOPE11 and FOA4, the GSD is assumed to be 1.8, and the constant effective density is assumed to be 1 g/cm<sup>3</sup>, which is a limitation given both terms, as stated above, are impacted by engine type and thrust level.

## 7. STEP 4 – EI NUMBER

With the assumptions made about the size distribution, the EI nvPM number can be estimated from EI nvPM mass using eq. (3):

$$EI_{\text{number}} = \frac{6EI_{\text{mass}}}{\pi \cdot \rho \cdot GMD^3 e^{4.5(\ln GSD)^2}} \quad (3)$$

### 7.1. FOA4

Figure 6 compares the nvPM number EIs calculated using the FOA4 method with the measured EIs corrected for sampling system loss using measured PSD (black circles). Unsurprisingly, the correlation between the predicted and observed data is much worse than for EI mass with low  $R^2$  and high RMSE (Table 4). The large spread on the y-axis is likely due to the assumed constant GMD for the LTO modes. Since FOA4 prescribes GMD for the LTO modes only, we excluded data that could not be considered representative of an LTO point for any thrust rating of a given engine type.

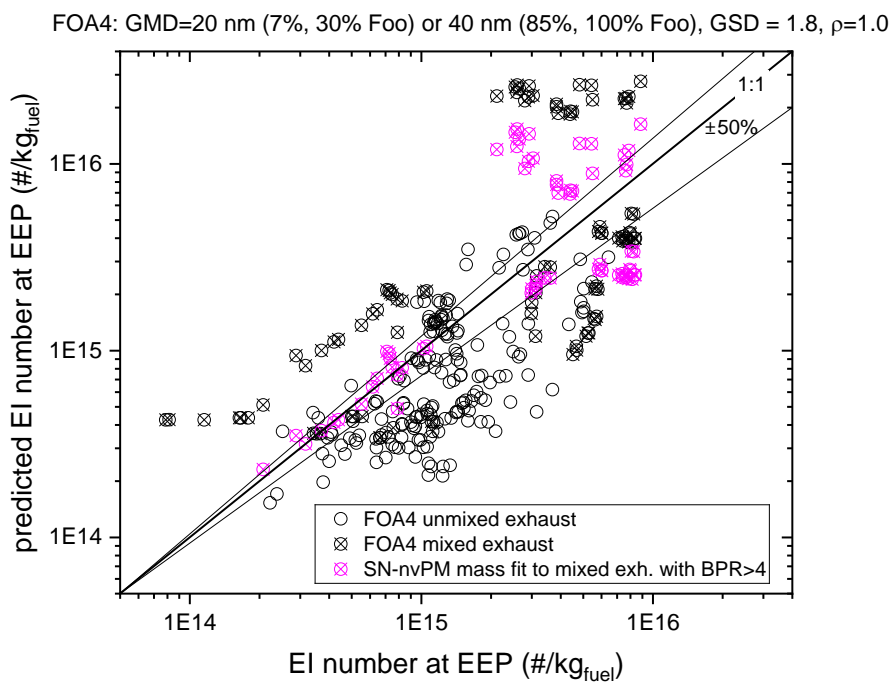


Figure 6 Comparison of nvPM number emission indices modeled using FOA4 and those measured and loss-corrected to engine exit plane using measured PSD.

Table 4 statistics of FOA4 for EI number

Method and data	R <sup>2</sup> of linear interpolation	RMSE (#/kg fuel)
FOA4 all data	0.15	5.65e15
FOA4 core flow only	0.28	1.35e15
FOA4 MTF with adjusted SN-nvPM mass correlation	0.03	5e15

## 7.2. SCOPE11

Compared to FOA4, SCOPE 11 has the advantage that the GMD is parametrized as a function of nvPM mass and is, therefore, not limited to the four GMD values prescribed for the LTO modes. However, the predicted GMDs were as small as 4.5 nm, which is unrealistically low (smaller than observed primary particle sizes in aircraft engine soot (Liati et al., 2014)) and may lead to overestimating the EI number at conditions with low measured nvPM mass concentration (high measurement uncertainty).

Applying SCOPE11 to all data led to a much better correlation and lower RMSE than FOA4 (Table 5). SCOPE11 had a much lower spread on the y-axis, with good agreement for observed EIs >~8e14.

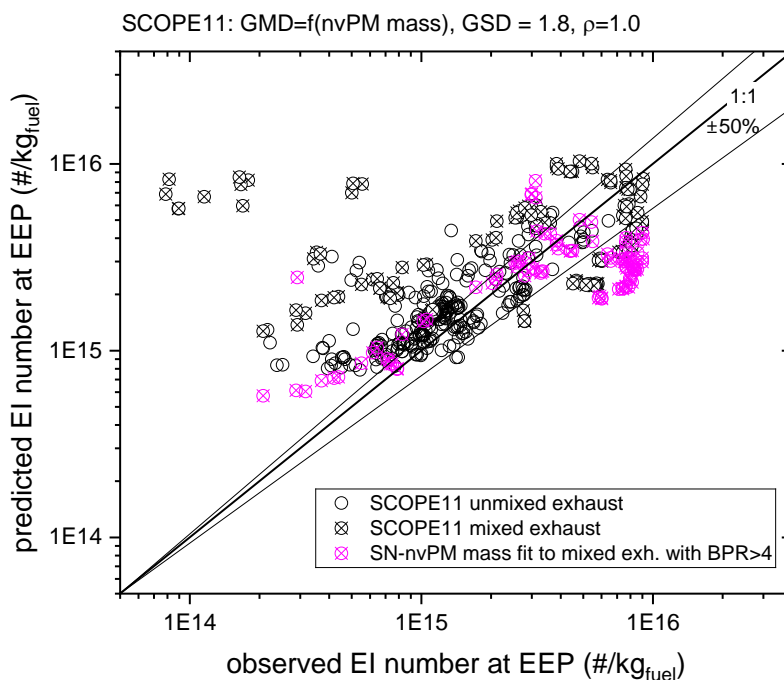


Figure 7 Comparison of nvPM number emission indices modeled using SCOPE11 and those measured and loss-corrected to engine exit plane using measured PSD.



Table 5 statistics of SCOPE11 for EI number

Method and data	R <sup>2</sup> of linear interpolation	RMSE (#/kg fuel)
SCOPE11 all data	0.3	2.13e15
SCOPE11 core flow only	0.04	1.77e15
SCOPE11 MTF with adjusted SN-nvPM mass correlation	0.1	3.5e15

## 7.3. Parametrizations using recent research results

### 7.3.1. Updated lognormal distribution properties

In Figure 8, the SCOPE11 SN-nvPM mass correlation with nominal parameters is used (black symbols) along with the updated fit functions for MTF engines (magenta symbols). The PSD was parametrized using results from Durdina et al. (2024) where GMD was parametrized as a function of thrust (eq. (4)).

$$GMD = 12.91 + 0.264 \left( \frac{F}{F_{00}} \right) \cdot 100 \quad (4)$$

The GSD was assumed constant and equal to 2.05; similarly, density was assumed constant and equal to 0.74 g/cm<sup>3</sup>.

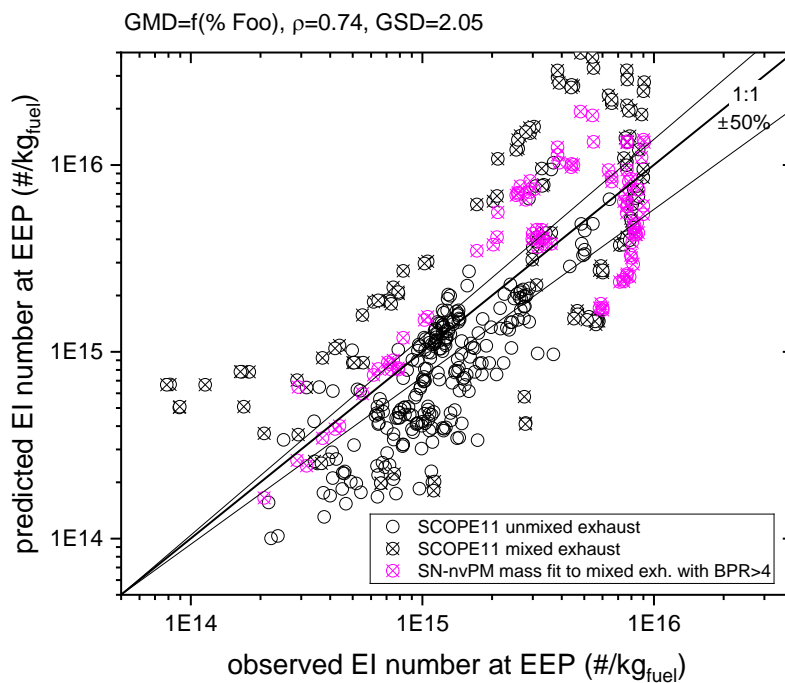


Figure 8 Comparison of nvPM number emission indices modeled using SCOPE11 SN-nvPM mass correlation with updated PSD parameters and those measured and loss-corrected to engine exit plane using measured PSD.

Using eq. (4) for GMD improved the correlation and overall agreement with observations compared to FOA4 (Table 6). Thus, this new parametrization could be used to update FOA4. The overall agreement with the observed EI number did not improve compared to SCOPE11. However, SCOPE11 is challenging to implement for airport emission inventories due to the lack of nvPM mass concentrations in the ICAO engine emissions databank, which are needed as input for the GMD.

Table 6 statistics of SCOPE11 for EI number with updated PSD parametrization

Method and data	R <sup>2</sup> of linear interpolation	RMSE (#/kg fuel)
SCOPE11 all data	0.34	5.57e15
SCOPE11 core flow only	0.36	1.2e15
SCOPE11 MTF with adjusted SN-nvPM mass correlation	0.16	4e15

### 7.3.2. Calculation using N/M as a function of GMD

An alternative to the updated PSD parametrization is the use of a correlation between nvPM number to mass ratio (N/M) with GMD. Durdina et al. (2024) showed a strong correlation between these two parameters. The relationship can be parametrized using eq. (5) with the parameters in Table 7.

$$\frac{N}{M} = t_0 \left( -\ln \left( \frac{GMD - y_0}{A} \right) \right)^{\frac{1}{b}} \quad (5)$$

After determining the GMD using eq. (3), the EI number is calculated by multiplying EI mass is by the N/M obtained for the calculated GMD.

Table 7 parameters in the N/M - GMD correlation

Parameter	Value
t <sub>0</sub>	2.86e13
y <sub>0</sub>	10.52
A	37.5
b	0.724

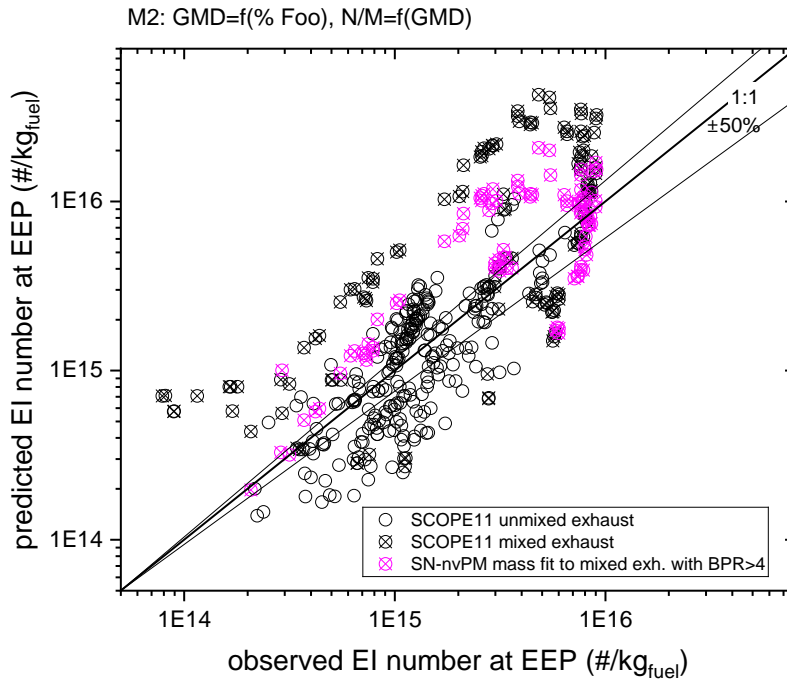


Figure 9 Comparison of nvPM number emission indices modeled using SCOPE11 SN-nvPM mass correlation and  $N/M$  as a function of GMD with those measured and loss-corrected to engine exit plane using measured PSD.

This parameterization did not significantly improve the updated lognormal distribution (Table 8, Figure 9). A slight improvement can be seen for the core flow data.

Table 8 statistics of SCOPE11 for EI number using  $N/M$  as a function of GMD

Method and data	$R^2$ of linear interpolation	RMSE ( $\#/kg \text{ fuel}$ )
SCOPE11 all data	0.31	6.82e15
SCOPE11 core flow only	0.37	1.15e15
SCOPE11 MTF with adjusted SN-nvPM mass correlation	0.25	4.7e15

## 8. DIRECT CORRELATIONS BETWEEN SN AND EI MASS AND NUMBER

The established methodology follows the steps detailed above, demonstrating a strong correlation between nvPM mass and SN. Due to the assumptions made in the conversion from nvPM mass to EI mass and EI number, the agreement of the predicted EI number with observations is rather poor. The question remains – could a correlation linking EIs directly with SN be determined with better accuracy? Figure 10 provides a hint. The EI mass correlated well with SN with two distinct curves for the unmixed and mixed-flow engines.

$$EI_{\text{mass}} = 3 + 7.07SN \quad (6)$$

$$EI_{\text{mass,MTF}} = 3 + 21.41SN \quad (7)$$

These correlations could be used as rough estimates. The same cannot be said about the EI number, which did not correlate with SN. However, a potential variation of the methods above could include estimating EI mass using eq. (6) and (7), and converting EI mass to number using lognormal distribution assumptions; however, further validation across a range of engines and power conditions would be required.

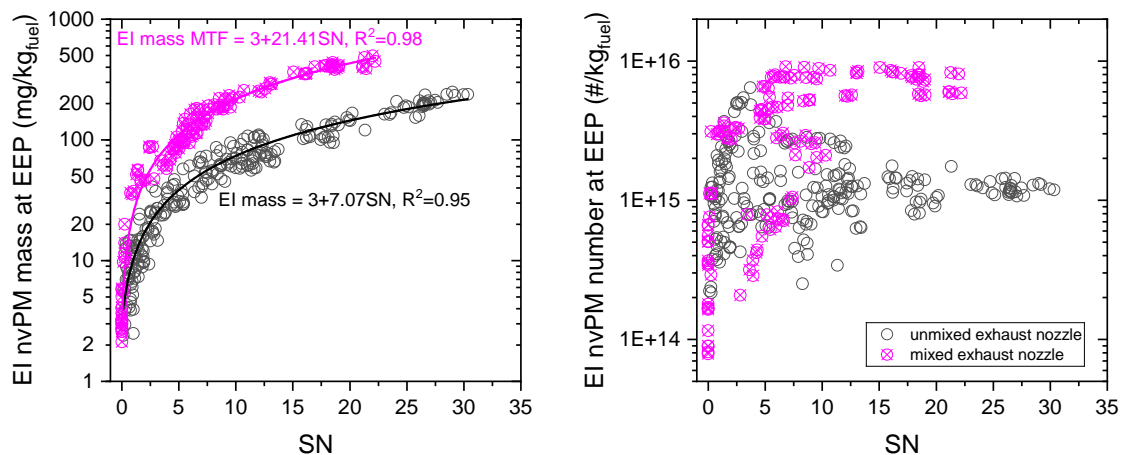


Figure 10 Correlations between EI nvPM mass and SN (left) and EI nvPM number and SN (right).

## 9. SUMMARY AND CONCLUSIONS

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- SN-nvPM mass correlation

The correlation between SN and nvPM mass concentration used in the SCOPE11 and FOA4 methods is appropriate, especially for engines without a mixed exhaust nozzle. All samples obtained from unmixed nozzles with conventional fuels and HEFA-SPK blends were within the 90% prediction band. This study's MTF engines with a high bypass ratio with exhaust sampled in mixed-flow configuration showed lower nvPM mass for a given SN than the samples obtained from unmixed nozzles. It is hypothesized that this observation could be explained by the effects of GMD on the filtration efficiency of the smoke number filter papers (increasing with increasing GMD). MTF engines exhibit larger GMD at lower nvPM mass concentration due to the dilution with bypass and, therefore, may have higher SN at lower nvPM mass due to higher filtration efficiency on the prescribed Whatman 4 filter paper than unmixed engines. Therefore, an alternative correlation is proposed by fitting the (limited) data for MTF engines with BPR>4, which aligned well with the lower band of the 90% prediction interval of the SCOPE11 correlation.

It is noted that the measurements here were obtained predominantly with one nvPM sampling and measurement system and one smoke analysis system. Therefore, it was not possible to assess the reproducibility of the observations.

- EI nvPM mass

The assumed reference AFRs for the LTO points and their interpolation are reasonable for regulated and unregulated engines. This data suggests that some small turbofan engines may have lower AFR at low thrust than large ones (i.e., burning richer). Overall, the predicted EI mass for unmixed engines agreed well with observations, with most points within 50% of the 1:1 line and  $R^2=0.96$ . The nominal SCOPE11 correlation SN-nvPM mass correlation overpredicted the EIs for the MTF engines. Using the adjusted model with our fit parameters improved the agreement significantly.

- EI nvPM number

The uncertainty of the EI number is expected to be much higher than for mass due to the assumptions made in the mass-to-number conversion and the measurement uncertainty of nvPM mass at low concentrations. Between the two standard options, FOA4 with fixed GMD for LTO modes and SCOPE11 with GMD correlated with combustor-exit nvPM mass concentration, SCOPE11 provided significantly better agreement with observations (~60% lower RMSE when applied to all data in this study). The practical application of SCOPE11 is limited because the ICAO emission databank does not include nvPM mass concentrations at the engine exit plane, which is the necessary input parameter. Also, it was observed that GMDs predicted by SCOPE11 were as low as 4.5 nm, which is below any nvPM GMD observed at the EEP with reasonable certainty.

Two alternative methods to FOA4 were therefore proposed. Firstly, the lognormal distribution parameters were adjusted using the latest research findings, with GMD parametrized as a linear function of % thrust and adjusted GSD and density. The second approach correlated the nvPM number to mass ratio (N/M) with GMD, again parametrized as a linear function of thrust. Both these methods provided better correlation between predicted and observed values and better agreement (lower RMSE) for unmixed engines than FOA4. The first approach utilizing updated lognormal PSD parameters is more robust and could be considered an update of the FOA4 used in the ICAO Airport Air Quality Manual (Doc 9889).

- Direct correlations between SN and EI nvPM mass and number

EI nvPM mass correlated strongly with SN ( $R^2=0.95-0.98$ ), with two distinct functions for unmixed and mixed flow nozzles. However, such a correlation was not found feasible for nvPM number.

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