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## Predicting aviation non-volatile particulate matter emissions at cruise via convolutional neural network

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1	Predicting Aviation Non-Volatile Particulate Matter Emissions at Cruise via
2	Convolutional Neural Network
3	
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13	ABSTRACT
14	Aviation emissions are the only direct source of anthropogenic particulate
15	pollution at high altitudes, which can form contrails and contrail-induced clouds, with
16	consequent effects upon global radiative forcing. In this study, we develop a predictive
17	model, called APMEP-CNN, for aviation non-volatile particulate matter (nvPM)

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18	emissions using a convolutional neural network (CNN) technique. The model is
19	established with data sets from the newly published aviation emission databank and
20	measurement results from several field studies on the ground and during cruise
21	operation. The model also takes the influence of sustainable aviation fuels (SAFs) on
22	nvPM emissions into account by considering fuel properties. This study demonstrates
23	that the APMEP-CNN can predict nvPM emission index in mass ( $EI_m$ ) and number ( $EI_n$ )
24	for a number of high-bypass turbofan engines. The accuracy of predicting $\mathrm{EI}_m$ and $\mathrm{EI}_n$
25	at ground level is significantly improved ( $R^2 = 0.96$ and 0.96) compared to the published
26	models. We verify the suitability and the applicability of the APMEP-CNN model for
27	estimating nvPM emissions at cruise and burning SAFs and blend fuels, and find that
28	our predictions for $EI_m$ are within $\pm 36.4\%$ of the measurements at cruise and within
29	$\pm33.0\%$ of the measurements burning SAFs in average. In the worst case, the APMEP-
30	CNN prediction is different by -69.2% from the measurements at cruise for the JT3D-
31	3B engine. Thus, the APMEP-CNN model can provide new data for establishing
32	accurate emission inventories of global aviation and help assess the impact of aviation
33	emissions on human health, environment and climate.

## 35 HIGHLIGHTS

36	• Application of convolutional neural network for aviation emission predictions.
37	• Good agreement on nvPM emissions at cruise between measurements and
38	calculation.
39	• Capability of predicting nvPM emissions for aircrafts burning SAFs.
40	
41	KEYWORDS
42	Aircraft engine, Aviation emission, Non-volatile particulate matter, Sustainable
43	aviation fuel, Cruise, Convolutional neural network
44	
45	SYNOPSIS
46	The results of this paper provide accurate predictions of nvPM emissions from in-use
47	aircraft engines, which impact airport local air quality and global radiative forcing.
48	
49	GRAPHICAL ABSTRACT



#### 51 **1. INTRODUCTION**

52 In the past twenty years, impacts from aviation emissions on human health, airport 53 local air quality, and climate change have attracted increasing interest (Stettler et al., 54 2011; Yim et al., 2013; Yim et al., 2015). Non-volatile particulate matter (nvPM) as one 55 of the major pollutants from aviation has been widely studied (Liati et al., 2014; Lobo 56 et al., 2015; Lobo et al., 2016) and currently regulated in engine certification process 57 by the International Civil Aviation Organization (ICAO) (ICAO, 2021). At present, 58 aviation is the only anthropogenic source that emits nvPM at cruise altitude (~ 10,000 59 m) in the upper troposphere or lower stratosphere (Jensen and Toon, 1997; Peck et al., 60 2013). In fact, more than 90% of global aviation fuel is consumed at cruise altitude 61 (Zhang et al., 2019). 62 Aviation nvPM, often assumed to be predominantly composed of black carbon 63 (BC) or soot, has been widely considered as one of the major contributors to climate 64 change (Lee et al., 2009; Lee et al., 2021). The nvPM emissions from aviation at cruise 65 altitude can influence the global radiation balance via two mechanisms: (i) the direct absorption of solar radiation. The nvPM strongly absorbs solar light in the spectral 66 range from ultraviolet to infrared (Lee et al., 2021). Additionally, compared to the nvPM 67

68 emissions from other anthropogenic sources, nvPM from aviation emission has a long

69	lifetime cycle, which thus leads to an appreciable positive radiative forcing (RF) (Bond
70	et al., 2013); (ii) an indirect effect by forming contrails and contrail cirrus, which could
71	be more significant than the direct effect (Bond et al., 2013). A recent study on the
72	V2527-A5 engine of a research A320 airplane by Voigt et al. (Voigt et al., 2021)
73	demonstrated that contrail ice particles (IP) are closely correlated to nvPM emissions
74	and 80-90% of the IP have nvPM cores, indicating that such particles, although small
75	in particle size (~ 20-30 nm), can serve as ice nucleus (IN) at the cruise condition (e.g.
76	at T = 230 K and P = 25 kPa). From a recent study by Lee et al., the net effective RF
77	induced by aviation activities is $\pm 100.9 \text{ mW/m}^2$ in 2018 mostly attributed to contrail
78	cirrus (+57.4 mW/m <sup>2</sup> ) (Lee et al., 2021). It is generally agreed that the RF of contrail
79	cirrus will increase in the coming years. This increase was estimated to occur by a factor
80	of 3 from 2006 to 2050, reaching to 160 or even 180 mW/m <sup>2</sup> by then, attributed to both
81	a large increase in air traffic and a slight shift in the air traffic towards high altitudes
82	(Wilkerson et al., 2010; Bock and Burkhardt, 2019). According to the report by the
83	Intergovernmental Panel on Climate Change (IPCC), RF from aviation could have a 7%
84	contribution to anthropogenic RF by 2050 (Sabogal, 2011). A recent study provided
85	experimental evidence that burning sustainable aviation fuels (SAF) can result in a 50
86	to 70% reduction of ice number concentration and a slight increase in ice crystal size

87	(Voigt et al., 2021). Although the formation and the evolution of contrails and contrail
88	cirrus is one of the main undetermined factors that influence the prediction of future
89	global radiation balance (Solomon et al., 2007), the microphysical interaction between
90	aircraft nvPM emissions and the formation of contrails is still not fully understood.
91	Precise prediction of aviation nvPM emissions, especially those at cruise altitude,
92	becomes critical in assessing the complex influences of aviation on climate. At present,
93	there are several approaches being used to estimate the emission index for mass and
94	number of nvPM (EI <sub>m</sub> and EI <sub>n</sub> ), including the first order approximation version $3.0$
95	(FOA3) (Wayson et al., 2009), the formation and oxidation (FOX) (Stettler et al.,
96	2013a), the improved formation and oxidation (ImFOX) (Abrahamson et al., 2016), the
97	approximation for soot from alternative fuels (ASAF) (Speth et al., 2015), and the
98	smoke correlation for particle emission-CAEP11 (SCOPE11) (Agarwal et al., 2019).
99	The FOA3 converts the results of smoke measurements, smoke numbers (SN), into
100	nvPM mass concentrations. It was approved by ICAO (ICAO, 2011) in 2007 to evaluate
101	nvPM emissions around airports worldwide. However, the SN instrument measures the
102	light opacity of the particles collected on filter papers (ICAO, 2008). Its application to
103	aviation emissions has been limited by two factors: insensitivity to ultrafine particles
104	and insufficient resolution (Jones, 2002; Rye et al., 2012; Stettler et al., 2013b). Modern

105	high-bypass turbofan aircraft engines such as the CFM56 and IAE-V2500 generate
106	nvPM emissions in the range of 20-100 nm (Saffaripour et al., 2020; ICAO, 2021). For
107	these engines, correlations between the nvPM mass concentrations and the SN are
108	usually poor (Abrahamson et al., 2016). The FOX does not depend on SN measurement,
109	but uses engine conditions as the input variables, thus avoiding the intrinsic
110	uncertainties of SN measurement. However, the fuel parameters are not incorporated in
111	the FOX model, so it may not be readily used to predict $EI_m$ from SAFs, yet a study by
112	Christie et al. showed that the FOA3 could still be valid for blends of SAFs with the
113	conventional jet fuels (Christie et al., 2017). It has also been found that the predicted
114	EIm by FOX were about 4 times higher than the measurements (Abrahamson et al.,
115	2016; Durdina et al., 2016; Durdina et al., 2017). In addition, Agarwal et al. developed
116	a method for estimating $EI_m$ and $EI_n$ from aircraft engines, called SCOPE11 (Agarwal
117	et al., 2019). This method predicts $EI_n$ by assuming a log-normal size distribution and
118	correlating geometric mean diameter (GMD) and geometric standard deviation (GSD)
119	with a function of measured nvPM mass concentration. Similarly, because it is difficult
120	to accurately measure the low SN produced by modern high bypass engines, the
121	SCOPE11 is unreliable to predict nvPM emissions for low-emission engines.
122	SAF is one of the major and attractive solutions adopted by the global aviation

123	community to mitigate aviation impact on climate (Undavalli and Khandelwal, 2021).
124	A number of dedicated measurement programs have been carried out to evaluate the
125	reduction of aviation emissions by using SAFs (Anderson et al., 2011; Beyersdorf et al.,
126	2014; Moore et al., 2017; Durdina et al., 2021). For the purpose of estimating the effects
127	of a variety of SAFs on nvPM emission mitigation, a new method called ASAF has
128	been developed (Speth et al., 2015). The ASAF models the total rate of polycyclic
129	aromatic hydrocarbons (soot precursor) formation as the sum of a component
130	independent of fuel aromatic content and a component proportional to fuel aromatic
131	content, and establishes the relationship between the total amount of nvPM generation
132	and engine thrust setting, aromatic content of SAF and conventional aviation fuel.
133	Through some assumptions and mathematical processing as well as combining with
134	other estimation models suitable for conventional aviation fuel, the nvPM emissions
135	burning SAFs can be predicted by the ASAF approach.
136	Most of the current predicting methods aim to estimate nvPM emissions around
137	airports, which are important to local air quality and human health. However, in
138	evaluating the influence of aviation on global radiative balance, emissions at cruise

139 altitude contribute the most because the majority of the aviation fuel is consumed during

140 cruise operation. A common approach to predict emissions at cruise altitude is to

141	extrapolate the ground measurement values using dynamic ratios based on the
142	Döpelheuer and Lecht correlation (Döpelheuer and Lecht, 1998). Abrahamson et al.
143	developed the ImFOX, which can be directly used to predict nvPM emissions at cruise
144	and burning SAFs (Abrahamson et al., 2016). However, the ImFOX only considers the
145	hydrogen content of fuels and ignores the influence of other components, such as
146	naphthalene and aromatics (Abrahamson et al., 2016), making the emission estimation
147	values of the mode accurate for some specific data, but much less for other data, so the
148	estimation values are still not satisfactory (Durdina et al., 2017). Previous studies
149	showed that the content of naphthalene and aromatics in fuel can greatly affect aviation
150	nvPM emissions (Moore et al., 2015; Durdina et al., 2017).
151	In recent years, artificial intelligent technologies such as machine learning
152	methods have been applied broadly and successfully in various research areas (Ma et
153	al., 2018; Nielsen and Voigt, 2018). As a representative of machine learning methods,
154	neural network can obtain better fitting accuracy than the conventional linear statistical
155	models by introducing nonlinear functions (Ukrainec et al., 1989). Until now, in the
156	field of aviation emission estimation, there has been no attempt of using neural
157	networks. Given that the prediction of aviation nvPM emissions is in fact a multiple
158	regression problem, we believe that applying the convolutional neural network (CNN)

159 approach in this field could provide a reasonable solution.

160	In this study, we develop a new approach based on CNN to estimate nvPM
161	emissions from aircraft engines, by using a large variety of parameters about engine
162	parameters, fuel properties, and ambient conditions as inputs. In particular, the newly
163	published ICAO emission databank from ground tests and a series of open data from
164	cruise experiments are utilized to develop the CNN model, which is capable of handling
165	multi-dimensional data sets unlike the conventional empirical models. This study aims
166	to address the following unsolved issues: (i) how to accurately predict emissions at
167	cruise altitude based on emission measurements on the ground; (ii) how to estimate the
168	impact of SAF under a wide range of engine conditions because there is limited
169	experimental data using the SAF currently available. This approach can be used to
170	improve nvPM inventory prediction from the current fleet and will be beneficial to
171	evaluate the impact of aviation nvPM emissions on environment and climate change.

172

## 173 2. MATERIALS AND METHODS

In this study, we categorize five measurement data groups from four of previous
aircraft field measurements either on the ground or at cruise altitude (Petzold et al.,
Schumann et al., 2002; Anderson et al., 2011; Moore et al., 2017; Voigt et al.,

1//	2021), and the ICAO 2021 Aircraft Engine Emissions Databank (EEDB) (ICAO, 2021).
178	The comprehensive variables representing engine specific parameters (ESP), engine
179	operational parameters (EOP), fuel properties (FP), and ambient conditions (AC) and
180	nvPM emission data are used for the development of the predictive model of aviation
181	nvPM emissions. We consider the influencing factors of nvPM emissions as the results
182	of ESP, EOP, FP and AC, no matter whether the aircraft is on the ground or at cruise,
183	burning conventional aviation fuels or SAFs. The input variables for the APMEP-CNN
184	model in predicting $EI_m$ and $EI_n$ are the same and listed in the Table 1.

185

1 77

## Table 1. Input Variables for the APMEP-CNN Model

	Input	Variables	
ESP	EOP	AC	FP
pressure ratio bypass ratio	fuel flow rate	ambient temperature	aromatics content
maximum rated thrust	thrust ratio	ambient pressure	

#### 186 **2.1. Measurement Data Sources**

1.1

## 187 **2.1.1. Emission Data for Aircrafts on the Ground**

188 The EEDB provides the average values of nvPM emission measurement data for

189 each engine with maximum rated thrust of more than 26.7 kN during the landing and

190	take-off (LTO) cycle, which contains four specified thrust settings (ICAO, 2021). The
191	EEDB includes the following information: (i) engine certification data, including
192	bypass ratio, overall pressure ratio, and the maximum rated thrust under international
193	standard atmospheric sea level static conditions ( $T = 288$ K, $P = 101325$ Pa); (ii) fuel
194	and combustion data, including the average heat of combustion of the fuel, hydrogen
195	content, aromatics content, naphthalene content, sulfur content, and fuel flow rate; (iii)
196	ambient data, including pressure, temperature, and relative humidity. In the EEDB,
197	there are a total of 784 sets of measurement data for 196 engines from ten aircraft engine
198	manufacturers. As shown is the EEDB, some of the reported $EI_m$ and $EI_n$ are corrected
199	for system losses in accordance with the ICAO Appendix 8 of Annex 16 Vol II, but
200	others are not.

## 201 **2.1.2. Emission Data for Aircrafts at Cruise**

Three of the five data groups used in the CNN modeling are the emission data of aircrafts at cruise from three field studies by Moore et al. (Moore et al., 2017), Voigt et al. (Voigt et al., 2021), and Schumann et al. (Petzold et al., 1999; Schumann et al., 2002), respectively. Moore et al. measured the emissions of the CFM56-2C1 engine equipped with the NASA DC-8 research aircraft from the NASA HU-25 Falcon aircraft using the NASA Langley Aerosol Research Group (LARGE) suite of in situ instruments, which

208	were not corrected for diffusional, inertial and sedimentation losses given uncertainties
209	associated with the condensation particle counter (CPC) detection efficiency curves
210	(Moore et al., 2017). The uncertainty associated with neglecting these corrections was
211	estimated to be 7%-9% on $EI_n$ and around 3% on $EI_m$ (Moore et al., 2017). They
212	examined the influence of three different fuels, a low-sulfur-content Jet-A fuel, a
213	medium-sulfur-content Jet-A fuel and a 50/50 (by volume) blend of the low-sulfur-
214	content Jet-A fuel with an hydrotreated esters and fatty acids (HEFA) biojet fuel, on
215	nvPM emissions at cruise (Moore et al., 2017). In the process of studying the influence
216	of clean aviation fuels on the formation of contrail-induced clouds, Voigt et al.
217	measured the emissions of the IAE-V2527-A5 engine equipped with an Airbus A320-
218	232 aircraft with CPCs based on TSI, Model 3010 counters (TSI, Inc, USA), and
219	provided the measured values of nvPM emissions under different fuel components, in
220	which CPC data have been corrected for reduced detection efficiencies in low pressure
221	environments and particle losses in the thermodenuder, with an overall uncertainty in
222	nonvolatile particle number concentrations of $\pm 15\%$ (Voigt et al., 2021). Schumann
223	et al. compiled the cruise data of aircraft nvPM emissions during the experiment of
224	SULFUR 1-7, including the CF6-80C2A2, CFM56-3B1, CFM56-5C4 and PW JT3D-
225	3B engines, and studied the influence of different sulfur contents on the composition of

227 data, the loss correction was not mentioned in the paper.

## 228 2.1.3. Emission Data for Aircrafts burning Sustainable Aviation Fuels

229	The last data group is the compiled aircraft emission data based on the Alternative
230	Aviation Fuel EXperiment I (AAFEX-I) field measurement campaign (Anderson et al.,
231	2011), where five different fuels were tested: a standard JP-8 (or baseline) fuel and
232	several commercially available SAFs, such as a Fischer-Tropsch (FT) fuel synthesized
233	from natural gas (FT-1), a FT fuel prepared from coal (FT-2), and 50:50 blends of FT-
234	1 and FT-2 with JP-8. The influence on the gaseous and PM emissions burning different
235	fuels for CFM56-2C1 engines was systematically investigated by National Aeronautics
236	and Space Administration (NASA) and collaborators. The CFM56 engine series are the
237	most widely used engine type on commercial aircraft at present (almost all B737 use
238	one version of this engine type). It should be noted that the AAFEX data sets are not
239	corrected for the system line losses or background aerosol interference, different from
240	the ICAO EEDB in the sampling, measurements and reporting practices since the ICAO
241	EEDB complies with the Annex 16 requirements on nvPM emissions.
242	2.2. Modeling Procedure – the Convolutional Neural Network Method

243 The existing nvPM emission prediction models of aircraft engines are different in

244	mechanism, characteristics and details, from the FOA3 which depends on SN and
245	converts SN into nvPM mass concentrations, to the semi-empirical FOX and ImFOX
246	which predict nvPM mass emissions based on the proprietary engine cycle data. In this
247	study, we develop a new modeling method to predict nvPM emission indices for
248	individual aircraft engine, based on the CNN technology. CNN is an end-to-end feature
249	extraction method, of which two-dimensional (2D) convolution is suitable for image
250	processing and one-dimensional (1D) convolution is usually used to deal with multiple
251	regression problems. The detailed modelling procedure of the CNN approach used in
252	this study is shown in Fig. 1.
253	There are four major steps during the CNN modeling procedure: data processing,
254	model selection, model training and model prediction. In the first step, a process of
255	feature selection is performed on the data relevant to nvPM emission. During the
256	process, the Pearson correlation coefficient (PCC) and the maximum information
257	coefficient (MIC) (Reshef et al., 2011) are used to select the attributing features that
258	have a greater correlation with emission indices, to reduce modelling complexity, to
259	improve the model capability and robustness, and to ensure the model accuracy. The
260	selected features are the input variables for the APMEP-CNN model, which are listed
261	in Table 1. After the feature selection, the EEDB data group with high-correlation

262	characteristics are divided into three sets to train, validate and test the model. The
263	training set, which uses approximately 60% of all the data, is to process the training
264	error with the gradient descent method and learn the common parameters (such as
265	weight coefficients, deviations, etc.) of the constructed regressor; the validation set,
266	using 20% of all the data, is to adjust the hyperparameters of the regressor (such as the
267	epochs, the number of network layers, the number of neurons in each layer, etc.) and
268	preliminarily evaluate the capability of the model; and the test set, using the other 20%
269	of all the data, is to measure the performance of the regressor and evaluate the
270	generalization ability of the final model. About 60% of the other four data groups are
271	used for testing as well, 20% and 20% are used for training and validation in order to
272	make a correction to the data-driven model burning SAFs or at cruise.



274 Figure 1. Establishment procedure of the proposed APMEP-CNN modelling approach. **a.** Data processing; **b.** Model selection; **c.** Model training; **d.** Model prediction.  $X_1$ ,  $X_2$ , 275 276  $X_3$  represent the normalized model training set, validation set and test set inputs.  $X'_1$ ,  $X'_2$ ,  $X'_3$  represent the input of model training set, validation set and test set after 277 principal component analysis.  $Y_1$ ,  $Y_2$ ,  $Y_3$  represent the experimental values of model 278 training set, validation set and test set processed by 'A' scaler.  $Y'_1$ ,  $Y'_2$ ,  $Y'_3$  represent 279 the output of model training set, validation set and test set in the iterative process.  $Y_3''$ 280 281 represent the output of model test set after inverse processing by 'A' scaler. 'A' scaler:

282 logarithm the data before standardization.

283	All data are converted to be dimensionless by scaling to eliminate the problem of
284	excessive differences among the used data, caused by the dimensional differences. The
285	scaling process is beneficial to accelerate the convergence speed of model training and
286	to improve the accuracy of the model. Among the data sets, the independent variables
287	are normalized. To obtain better results in testing, $\mathrm{EI}_m$ and $\mathrm{EI}_n$ are converted to
288	logarithms, and then the logarithm of $\mathrm{EI}_n$ is standardized. The goal of principal
289	component analysis (PCA) is to map a high-dimensional data set into a low-
290	dimensional space through certain linear projections, then to maximize the amount of
291	data information (maximum variance) in the projected dimensions, leading to a
292	reduction of data dimensions and still retaining original data characteristics. The
293	dimensions after PCA for $EI_m$ and $EI_n$ are seven and eight, then the $EI_m$ and $EI_n$ are
294	modeled as seven-dimensional and eight-dimensional structural models, respectively.
295	In the step of model selection, a hyperparametric data set is established by setting
296	different numbers of hidden layers (1, 2), numbers of neurons (16, 32, 64, 128, 256,
297	512, 1024), epochs (500-5000 with a step of 50), and batch sizes (16, 32, 64, 128, 256,
298	512). A grid search experiment is then carried out on hyperparameters using K-fold
299	cross-validation. Models with different hyperparameters are trained in the step of model
300	training.

301 In this study, 1D convolution and max pooling operations are used to transform 302 the high-dimensional data of the input layer to the hidden layer, extracting its features to reduce the dimensionality of the original data set effectively. The 1D convolution 303 kernel and the pooling kernel slide along different experiment data to obtain features of 304 ESP, EOP, FP and AC. As shown in Fig. 2 for EIn, the experiment data have dimension 305 N (N = 8). Blue boxes represent the convolution kernel with window length M (M = 3) 306 307 and step length 1, and the feature dimension obtained by convolution is N - M + 1. Yellow boxes represent the pooling kernel with window length P(P=2), and the feature 308 dimension obtained by pooling is (N - M + 1) / P. Then, we have established a 309 310 convolution-pooling module, and the feature mapping by convolution and pooling are 311 shown in Eqs. 1 and 2 respectively.

$$v_j^l = f\left[\sum_{i \in N} v_j^{l-1} k_{ij}^l + b_j^i\right] \tag{1}$$

where  $v_j^l$  is the convolution feature mapping of the *j*-th output of the neuron in layer  $l, v_j^{l-1}$  is the output of layer l-1, which is the input of layer  $l, k_{ij}^l$  is the coefficient in a convolution kernel from the *i*-th neuron in layer l-1 to the *j*-th neuron in layer  $l, b_j^l$  is the deviation of the *j*-th neuron in layer l, f is the Relu activation function (Glorot et al., 2011).

$$\nu_j^l = \max_{i^{l-1} \in \mathbb{N}} \nu_j^{l-1} \tag{2}$$

317 where  $v_j^l$  is the pooling feature mapping of the *j*-th output of the neuron in layer l, 318  $v_j^{l-1}$  is the output of layer l-1, which is the input of layer l,  $i^{l-1} \in N$  represents N





320

Figure 2. Operating principle of convolution kernel and pooling kernel. The blue and yellow boxes represent a convolution kernel with window length 3 and a pooling kernel with window length 2. The feature maps are obtained by sliding over the data related to engine emissions.

As shown in Fig. 3, the CNN constructed in this study for predicting  $EI_m$  is composed of two convolution layers with the window lengths of three and two, two max pooling layers with the window lengths of two and one, one flatten layer, one dropout layer and one fully connected layer. For  $EI_n$ , there are also two convolution

329	layers with the window lengths of three and two, two max pooling layers with the
330	window lengths of two and one. The pre-processed data is first extracted and
331	dimensioned through the convolution layer and pooling layer, and then input to the
332	flatten layer, which is used for the transition from the convolution layer to the fully
333	connected layer to make the multi-dimensional data one-dimensional. The function of
334	dropout layer is to randomly delete the neurons in the fully connected neural network
335	with specified probability, to reduce the over-fitting effect and to enhance the robustness
336	of the model. The last fully connected layer is used to synthesize the extracted features,
337	which is described by the weight matrix of each neuron connection obtained by using





Figure 3. Network structure of the proposed APMEP-CNN model.

340

341 In the step of model training, the loss is calculated by taking the absolute value of

512	the difference between the actual experimental value and the predicted value of the
343	model, then put into the model to adjust the weights of all connections in the network,
344	where, an adaptive optimization algorithm, called Adam, is used to be the optimizer
345	(Kingma and Ba, 2014), with mean square error (MSE) as the loss function. This
346	process continued until the set conditions are reached.
347	Finally, as the result of model selection, it is determined that the number of hidden
348	layers is one and one; the number of neurons is 256 and 256; the epoch is 2840 and
349	3925; and the batch size is 128 and 256 for $EI_m$ and $EI_n$ respectively.
350	
351	3. RESULTS AND DISCUSSION
352	3.1. Training/Validation and Test Results of the Convolutional Neural Network
352 353	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method
352 353 354	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method In this study, the EEDB data group at ground level, namely take-off condition,
<ul><li>352</li><li>353</li><li>354</li><li>355</li></ul>	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method In this study, the EEDB data group at ground level, namely take-off condition, climb-out condition, approach condition, idle condition, are divided into three sets, in
<ul> <li>352</li> <li>353</li> <li>354</li> <li>355</li> <li>356</li> </ul>	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method In this study, the EEDB data group at ground level, namely take-off condition, climb-out condition, approach condition, idle condition, are divided into three sets, in which approximately 60% for training, 20% for validation, 20% for testing, while the
<ul> <li>352</li> <li>353</li> <li>354</li> <li>355</li> <li>356</li> <li>357</li> </ul>	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method In this study, the EEDB data group at ground level, namely take-off condition, climb-out condition, approach condition, idle condition, are divided into three sets, in which approximately 60% for training, 20% for validation, 20% for testing, while the other field measurement results are also divided into three sets, 20% for training, 20%
<ul> <li>352</li> <li>353</li> <li>354</li> <li>355</li> <li>356</li> <li>357</li> <li>358</li> </ul>	3.1. Training/Validation and Test Results of the Convolutional Neural Network Method In this study, the EEDB data group at ground level, namely take-off condition, climb-out condition, approach condition, idle condition, are divided into three sets, in which approximately 60% for training, 20% for validation, 20% for testing, while the other field measurement results are also divided into three sets, 20% for training, 20% for validation, and 60% for testing. The training/validation and the test results of EIm

360	are shown in Fig. 4. There are 789 sets of data corrected and 51 sets of data uncorrected,
361	thus the APMEP-CNN is a mixed model. To investigate the influence from the
362	corrections for system losses, we establish three CNN models, labelled as model A, B,
363	C, by using the fully corrected data, or the completely uncorrected data, or the mixed
364	data, respectively. All the three models are used to calculate the nvPM emissions of five
365	designated engines to evaluate the system error caused by the use of uncorrected data.
366	The results (take RRMSE as the error index) are as follows: the $EI_m$ calculated with
367	model A differs from the experimental value by 0.161, the $EI_n$ differs by 0.067; the $EI_m$
368	calculated with model B differs by 0.237, the $EI_n$ differs by 1.131; the $EI_m$ calculated
369	with model C differs by 0.300, and the $EI_n$ differs by 0.098. Therefore, the $EI_m$ system
370	error caused by the use of the uncorrected data is 0.237, and the $EI_n$ system error is
371	1.131.
372	The predicted training/validation and test values of $EI_m$ and $EI_n$ are in great
373	agreement with the experimental data. As shown in Fig. 4b, 98.10% of the predicted
374	$\mathrm{EI}_{\mathrm{m}}$ are within a factor of two from the measured $\mathrm{EI}_{\mathrm{m}}$ , compared to 48.3% for FOA3,

375 14.6% for FOX and 24.7% for ImFOX. Similarly, 99.37% of the predicted  $EI_n$  are 376 within a factor of two from the measured  $EI_n$  in Fig. 4d. From a consequent correlation

377 analysis, the test results are satisfactory with the relative root mean square error





Figure 4. Comparison between the predicted and measured emission indices using the APMEP-CNN for the training/validation and test data sets. **a.** Results of  $EI_m$  from the training (60%) and validation (20%) data set; **b.** Results of  $EI_m$  from the test (20%) data set; **c.** Results of  $EI_n$  from the training (60%) and validation (20%) data set; **d.** Results of  $EI_n$  from the test (20%) data set. Shaded gray areas with different transparency

389 represent error bounds with different sizes.



In order to evaluate the predictive accuracy of the APMEP-CNN compared with other existing models, measurement data in the EEDB related to 76 aircraft engines for APMEP-CNN, FOX and ImFOX, and 74 for FOA3, are utilized to predict nvPM emissions during the LTO cycle (These measurement data haven't been used in the training or validation step, but only for testing. The data in Section 3.3 and 3.4 is the same). In Fig. 5, a comparison between predicted and measured values of EI<sub>m</sub> at the ICAO certification test points (i.e., 7, 30, 85, 100% thrust) using four models is shown



in a log-log scale.

399

Figure 5. Comparison between predicted EI<sub>m</sub> using different models with measured
 EI<sub>m</sub> in the ICAO EEDB. Shaded gray areas with different transparency represent error

402 bounds with different sizes.

403 The prediction of the APMEP-CNN correlates better with the measurements than

404	those of FOA3, FOX and ImFOX, with RRMSE = 0.22, $R^2 = 0.98$ for APMEP-CNN;
405	RRMSE = 0.92, $R^2 = 0.67$ for FOA3; $R^2 < 0$ for FOX and ImFOX. When using the
406	FOX to estimate $EI_m$ , about 17.1% of the total results are negative. For the current
407	version of FOX and ImFOX, the predicted $\mathrm{EI}_{\mathrm{m}}$ are overestimated especially at take-off
408	and climb-out, as displayed in Fig. 5. The negative $R^2$ values indicates that FOX and
409	ImFOX perform worse than a mean EI <sub>m</sub> value, suggesting that these two methods might
410	be unsuitable for newer high-bypass gas turbine engines in the EEDB. However, the
411	FOX and the ImFOX are promising in describing the clear trend between $\mathrm{EI}_{\mathrm{m}}$ and thrust,
412	also they are suitable for predicting nvPM emissions from older engines (Stettler et al.,
413	2013a; Abrahamson et al., 2016). As shown in Fig. 5, the majority of $EI_m$ predicted by
414	FOA3 are lower than the measured values. There may be three reasons for the
415	underestimation from FOA3: (i) the insufficient resolution in measuring SN at low
416	emissions, since the prediction of the FOA3 is based on the SN measurements of aircraft
417	engines, which tend to underestimate when the emissions are low (Stettler et al., 2013b);
418	(ii) the insensitivity in detecting small particles as nvPM from turbofan aircraft engines
419	is normally in the range of 20-100 nm (Saffaripour et al., 2020); and (iii) the difference
420	in the SN measurements by engine manufacturers. However, the FOA3 is still highly
421	valuable because it can be applied universally across all combustor technologies as long

422 as SN can be accurately measured (Abrahamson et al., 2016). For four thrust settings,

423 97.4% of the APMEP-CNN predictions agree to within a factor of two from the424 measurements, representing an improvement compared with other methods.

425 **3.3. Predictions of nvPM Emissions at Cruise** 

426 Because the training and validation processes have used the measurement results 427 at both the ground level and cruise, the APMEP-CNN can also be used to predict nvPM 428 emissions during cruise operations. Our prediction are compared with previous 429 measurement studies on six commercial aircraft engines, including CF6-80C2A2, CFM56-3B1, CFM56-5C4, JT3D-3B, CFM56-2C1, and V2527-A5 during the 430 431 SULFUR 1-7 experiments, the ACCESS experiments and the ECLIF projects (Petzold et al., 1999; Schumann et al., 2002; Moore et al., 2017; Voigt et al., 2021). The predicted 432 values and the measurement values are listed in Table 2, in which the predicted EI<sub>m</sub> of 433 434 the CF6-80C2A2, CFM56-3B1, CFM56-5C4, JT3D-3B, CFM56-2C1 and V2527-A5 435 engines are different from the measurements (Petzold et al., 1999; Schumann et al., 2002; Moore et al., 2017; Voigt et al., 2021) by 21.1%, 27.3%, 60.0%, -69.2%, 4.5% 436 and \* respectively (\* means there is no measurement data), while for the predicted EI<sub>n</sub>, 437 the differences are 38.8%, 44.3%, 53.3%, -24.8%, 36.5% and 46.6%, respectively. 438 Conventionally, both the FOA3 and the FOX predict engine emissions during 439

440	cruise operation by using the dynamic ratio relationship proposed by Döpelheuer and
441	Lecht to scale the ground values to the cruise values (Döpelheuer and Lecht, 1998;
442	Stettler et al., 2013a). When the ICAO-certified SN results are used to estimate nvPM
443	emissions at cruise, the predicted values of $\mathrm{EI}_{\mathrm{m}}$ are usually smaller than the
444	measurement results. Some previous studies have shown that the updated FOA3 could
445	also lead to an underestimation(Stettler et al., 2013a; Abrahamson et al., 2016) The
446	ImFOX uses a direct cruise prediction method (Abrahamson et al., 2016), which only
447	needs the information for fuel flow rate and fuel hydrogen content as the inputs to
448	calculate the $EI_m$ at cruise. However, we find that the ImFOX predictions of $EI_m$ are
449	quite different from the measurement results. In terms of parameter selection, the
450	APMEP-CNN model is quite different from the conventional models, capable of
451	considering more relevant parameters as the input parameters, thus can provide better
452	predictions than the conventional models.

•						
Aircraft	A310-300	B737-300	A340	B707	DC-8	A320
Engine	CF6-80C2A2	CFM56-3B1	CFM56-5C4	JT3D-3B	CFM56-2C1	V2527-A5
Power (%)	18.9	22.5	19.9	40.0	24.8	29.9
EI <sub>m</sub> _measured <sup>a</sup>	$19\pm10$	11 ± 5	$10\pm3$	$500\pm100$	22 °	١

453	Table 2. Com	narison between	Measured ar	nd Predicted	Emission	Indices at	Cruise
тЈЈ	Table 2. Com	parison between	micasurcu ai	iu i i cuicicu	L'importon	mulces at	Ciuise

EI <sub>n</sub> _measured <sup>b</sup>	$6\pm1.2$	$3.5\pm 0.7$	$1.8\pm0.5$	$17\pm3$	4.99 °	27
EI <sub>m_</sub> APMEP-CNN <sup>a</sup>	23 <sup>d</sup>	14 <sup>d</sup>	16 <sup>d</sup>	154 <sup>d</sup>	23 °	48
EI <sub>n</sub> _APMEP-CNN <sup>b</sup>	8.33 <sup>d</sup>	5.05 <sup>d</sup>	2.76 <sup>d</sup>	12.78 <sup>d</sup>	6.81 °	39.58

<sup>a</sup> In the unit of mg/kg-fuel; <sup>b</sup> In the unit of 10<sup>14</sup> #/kg-fuel; <sup>c</sup> Not corrected for system losses; <sup>d</sup> There are no data for the aromatics content in these measurements, thus we establish a model using hydrogen content as one of the CNN input variables, instead of aromatic content; \ No measurement data.

## 454 **3.4.** Predictions of nvPM Emissions burning Sustainable Aviation Fuels

455	Because the training and validation processes have used the measurement results
456	from aircraft engines burning both conventional aviation fuels or SAFs, the APMEP-
457	CNN can also be used to predict nvPM emissions burning different fuels. The predicted
458	$EI_m$ of the CFM56-2C1 engine burning JP-8, FT-1, FT-2, the mixed fuel Blend-1 and
459	Blend-2 under different engine thrusts are shown in Fig. 6, in comparison with the
460	measured results. The APMEP-CNN can predict the values of $EI_m$ with RRMSE = 0.48,
461	$R^2 = 0.89$ , and $EI_n$ with RRMSE = 0.27, $R^2 = 0.91$ .



463 Figure 6. Comparison between the predicted emission indices of nvPM using the 464 APMEP-CNN model with the measured results for the CFM56-2C1 engine while burning JP-8, FT-1, FT-2, Blend-1 and Blend-2 during the AAFEX-I campaign. a) The 465 EI<sub>m</sub> burning JP-8 vs engine power; **b**) The EI<sub>m</sub> burning FT-1 and FT-2 vs engine power; 466 c) The EI<sub>m</sub> burning Blend-1 and Blend-2 vs engine power; d) The EI<sub>n</sub> burning JP-8 vs 467 engine power; e) The EI<sub>n</sub> burning FT-1 and FT-2 vs engine power; f) The EI<sub>n</sub> burning 468 Blend-1 and Blend-2 vs engine power. 469 As displayed in six subgraphs of Fig. 6, the APMEP-CNN is able to capture the 470

- 471 relationship between the nvPM emissions and the variation in fuel composition, in
- 472 which the increase of aromatic and naphthalene content or the decrease of hydrogen
- 473 content results in the increase of EI<sub>m</sub> and EI<sub>n</sub>, as observed by previous studies (Marx

474	and Namer, 1988; Corporan et al., 2004; Corporan et al., 2007; DeWitt et al., 2008;
475	Timko et al., 2010; Corporan et al., 2011; Cain et al., 2013; Beyersdorf et al., 2014;
476	Brem et al., 2015; Durand et al., 2021). The reason for the predictive accuracy of the
477	APMEP-CNN model maybe twofold: (i) the APMEP-CNN considers both fuel
478	components and engine optional parameters,; (ii) the APMEP-CNN uses the most
479	recent emission measurements of $EI_m$ and $EI_n$ from the ICAO EEDB (ICAO, 2021).
480	This also confirms the important influence of fuel properties on aviation nvPM
481	formation (Moore et al., 2015).

### 483 **4. CONCLUSIONS**

In conclusion, with the newly published ICAO emission databank and extra open 484 485 measurement results from several field campaigns including cruise tests and SAF tests, 486 we develop the APMEP-CNN, a new aviation nvPM emission predictive model via 487 convolutional neural network, which can predict nvPM emissions on the ground and at 488 cruise for a large number of high-bypass commercial aircraft turbofan engines burning either conventional aviation fuels or SAFs. The developed APMEP-CNN model has 489 been demonstrated to be able to provide relatively accurate estimates of nvPM 490 emissions. Further measurements of aviation emissions during cruise operation will be 491

492 helpful to further verify the APMEP-CNN and eventually enable establishment of a493 more accurate global inventory of aviation nvPM emissions.

494 In despite of the success in predicting aviation nvPM emissions, the APMEP-CNN still has two intrinsic limitations: (i) the complexity of such brain-inspired neural 495 496 networks makes them remarkably capable, yet it also renders them opaque to human 497 understanding, turning them into 'black-box' systems, which means that researchers 498 cannot trace the course of the neural network calculations. However, we demonstrated 499 that the satisfactory estimation of nvPM emissions can be achieved with a certain 500 degree of accuracy; (ii) compared with traditional aviation nvPM emission prediction 501 methods, the APMEP-CNN usually needs a large quantity of measurement data. Although this approach makes a reasonable prediction of nvPM emissions, the amount 502 of training data could be still insufficient, and the acquisition of a large number of 503 504 relevant data is a major challenge in the field of aviation emission, especially at cruise. 505 Alternatively, a flight simulation ground test facility, which can simulate flight conditions by providing airflow at pressures and temperatures experienced at cruise, 506 may be used to alleviate the scarcity of cruise data by conducting cruise-like 507 experiments with dramatically lower costs and higher accuracy. In the future, with the 508 509 continuous progress of relevant measurements both on the ground and at cruise (or

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510	cruise simulation ground tests) burning both conventional aviation fuels and SAFs, the
511	APMEP-CNN may achieve even more accurate prediction results. To address the
512	opaqueness issue of mainstream neural networks, some new and promising transparent
513	machine learning techniques could be utilized, which could offer system transparency
514	to enable us to form coherent explanations of the system's decisions and actions without
515	sacrificing prediction accuracy.

## 517 NOMENCLATURE

Abbreviation	Full Name
AAFEX-I	Alternative Aviation Fuel EXperiment I
AC	Ambient Condition
ACCESS	Alternative Fuel Effects on Contrails and Cruise Emissions Study
APMEP-	Aviation nvPM Emission Prediction Based on the Convolutional
CNN	Neural Network
ASAF	Approximation for Soot from Alternative Fuels
BC	Black Carbon
BP	Back Propagation

CNN	Convolutional Neural Network
CPC	Condensation Particle Counter
EEDB	Engine Emissions Database
EIm	Mass Emission Index
EIn	Number Emission Index
ЕОР	Engine Operational Parameter
ESP	Engine Specific Parameter
FOA3	First Order Approximation Version 3.0
FOX	Formation and Oxidation
FP	Fuel Property
FT	Fischer-Tropsch
GMD	Geometric Mean Diameter
GSD	Geometric Standard Deviation
HEFA	Hydrotreated Esters and Fatty Acids
ICAO	International Civil Aviation Organization
ImFOX	Improved Formation and Oxidation
IN	Ice Nucleus
IP	Ice Particle

IPCC	Intergovernmental Panel on Climate Change
LARGE	Langley Aerosol Research Group
LTO	Landing and Take-off
MIC	Maximum Information Coefficient
MSE	Mean Square Error
NASA	National Aeronautics and Space Administration
nvPM	Non-volatile Particulate Matter
PCA	Principal Component Analysis
PCC	Pearson Correlation Coefficient
R <sup>2</sup>	the Coefficient of Determination
RF	Radiative Forcing
RRMSE	Relative Root Mean Square Error
SAF	Sustainable Aviation Fuel
SCOPE11	Smoke Correlation for Particle Emission–CAEP11
SN	Smoke Number
1D	One-Dimensional
2D	Two-Dimensional

#### 519 DECLARATION OF COMPETING INTEREST

520 The authors declare that they have no known competing financial interests or personal 521 relationships that could have appeared to influence the work reported in this paper. 522 523 ACKNOWLEDGMENTS 524 This work was mainly supported by the National Natural Science Foundation of China 525 (51922019 & 51920105009). This work was also partially supported by National 526 Engineering Laboratory for Mobile Source Emission Control Technology (NELMS2018A02), Open Foundation of Beijing Key Laboratory of Occupational 527 Safety and Health (2019) and the Reform and Development Project of Beijing 528 529 Municipal Institute of Labour Protection (2020).

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