

1 **Full-coverage 1 km daily ambient PM_{2.5} and O₃ concentrations of China in**
2 **2005-2017 based on multi-variable random forest model**

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23 **Abstract**

24 The health risks of fine particulate matter (PM_{2.5}) and ambient ozone (O₃) have been
25 widely recognized in recent years. An accurate estimate of PM_{2.5} and O₃ exposures is
26 important for supporting health risk analysis and environmental policy-making. The
27 aim of our study was to construct random forest models with high-performance, and
28 estimate daily average PM_{2.5} concentration and O₃ daily maximum of 8h-average
29 concentration (O₃-8hmax) of China in 2005-2017 at a spatial resolution of 1km×1km.
30 The model variables included meteorological variables, satellite data, chemical
31 transport model output, geographic variables and socioeconomic variables. Random
32 forest model based on ten-fold cross validation was established, and spatial and
33 temporal validations were performed to evaluate the model performance. According
34 to our sample-based division method, the daily, monthly and yearly estimations of
35 PM_{2.5} from test datasets gave average model fitting R² values of 0.85, 0.88 and 0.90,
36 respectively; these R² values were 0.77, 0.77, and 0.69 for O₃-8hmax, respectively.
37 The meteorological variables and their lagged values can significantly affect both
38 PM_{2.5} and O₃-8hmax estimations. During 2005-2017, PM_{2.5} exhibited an overall
39 downward trend, while ambient O₃ experienced an upward trend. Whilst the spatial
40 patterns of PM_{2.5} and O₃-8hmax barely changed between 2005 and 2017, the temporal
41 trend had spatial characteristic. The dataset is accessible to the public at
42 <https://doi.org/10.5281/zenodo.4009308> (Ma et al., 2021), and the shared data set of
43 Chinese Environmental Public Health Tracking: CEPHT
44 (<https://cepht.niehs.cn:8282/developSDS3.html>).

45 **1 Introduction**

46 Air pollution is becoming a main concern of modern society due to various health
47 risks. According to the latest Global Burden of Disease (GBD) report, air pollution
48 has caused approximately 6.67 million deaths (95% UI: 5.90-7.49 million), and
49 ranked fourth on the global list of death-related risk factors in 2019 (Health Effects
50 Institute, 2020; Murray et al., 2020). Ambient fine particulate matter (PM_{2.5}) and
51 ambient ozone (O₃) have been identified and proven to be related to many health
52 outcomes. China is known to be one of the countries with the most serious air
53 pollution in the world. Strict pollution control measures (including *the Air Pollution*
54 *Prevention and Control Action Plan* and *three-year action plan to fight air pollution*)
55 were enacted by the Chinese government to control and reduce air pollution since
56 2013. The implementation of these measures has resulted in a markable drop of
57 emissions and PM_{2.5} concentration. However, the occasional pollution events, as well
58 as the short development history of air quality monitoring network, have brought
59 many difficulties to accurately capture the temporal and spatial patterns of PM_{2.5} and
60 O₃ concentrations. Therefore, it is difficult to develop a complete decision-making
61 basis for handling air pollution. In addition, there are gaps in epidemiological studies
62 linking air pollutants to health outcomes, due to the lack of accurate measurements of
63 PM_{2.5} and ambient O₃ concentrations. To this end, an accurate estimate of PM_{2.5} and
64 O₃ exposures is essential to support health risk analysis and environmental
65 policy-making.

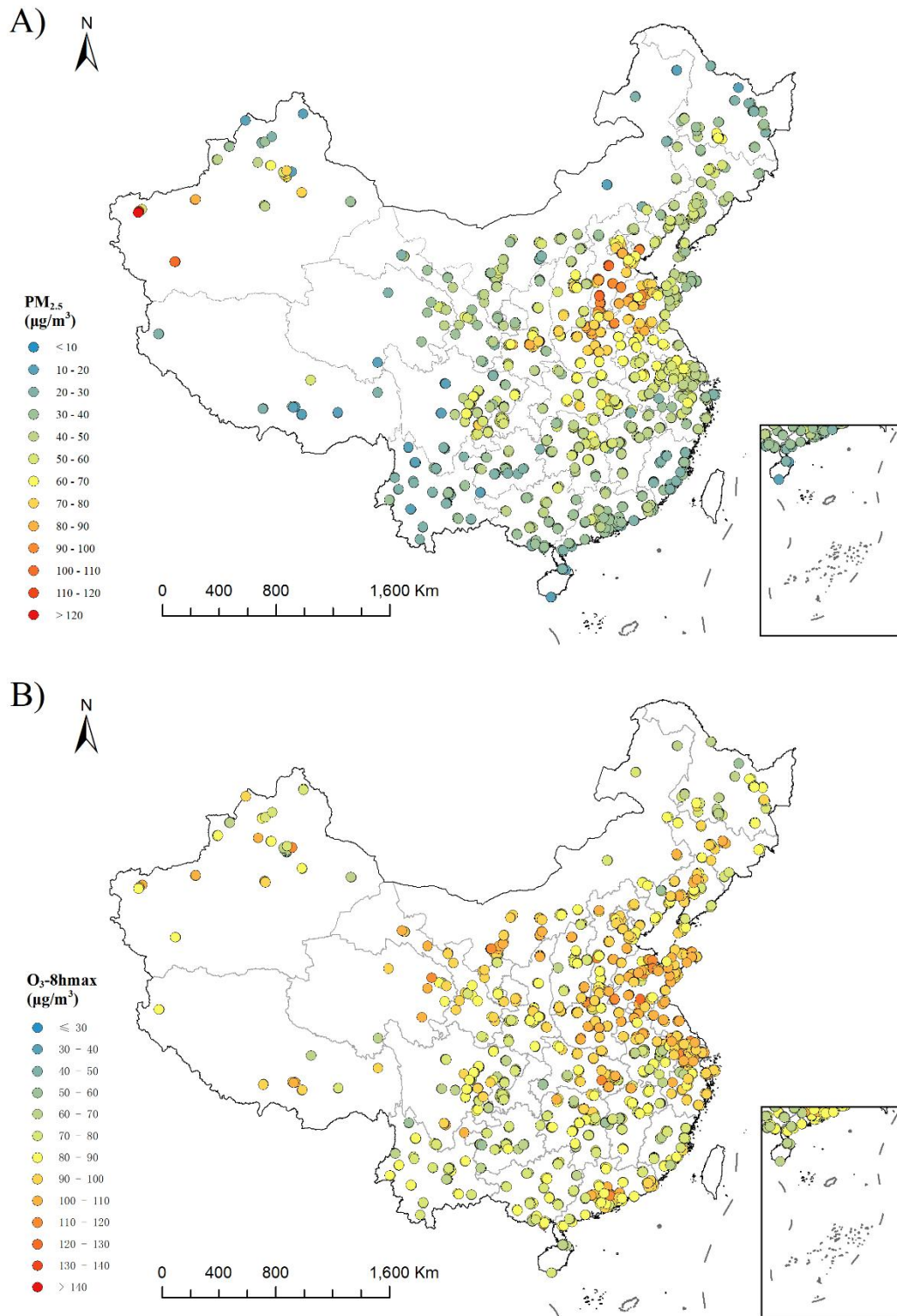
66

67 Suitable model variables and advanced estimation method are important to achieve
68 accurate modeling. Basically, PM_{2.5} is jointly affected by both natural conditions and
69 human activities over space and time, e.g., Aerosol Optical Depth (AOD),
70 meteorological conditions, geographic factors and human-related features (Wei et al.,
71 2021). While O₃ is a secondary pollutant, which is produced by a series of complex
72 photochemical reactions on the basis of precursor including nitrogen oxides (NO_x)
73 and volatile organic compounds (VOCs) under the action of high temperature and
74 strong radiation. These complex characteristic puts forward higher requirements on
75 the ability of the modeling method to handle multi-variable, and capture the
76 non-linear relationships between variables and air pollutants. Many models have been
77 developed to estimate the spatiotemporal distribution of PM_{2.5} and O₃ concentrations
78 in China. Machine-learning approaches (e.g., random forest (RF), extreme gradient
79 boosting and deep belief network models) can mine useful information from a large
80 amount of input data and explore the nonlinear relationship, bring a better
81 performance in modeling work (Chen et al., 2018, 2019; Di et al., 2017; Li et al.,
82 2017; Wei et al., 2019; Zhan et al., 2018). However, most of these estimation datasets
83 cannot balance long time series and high spatiotemporal resolution. Besides, there is
84 no long-term estimation dataset for both PM_{2.5} and O₃ concentrations with high
85 temporal and spatial resolution for supporting epidemiological research. Therefore, by
86 incorporating multi-source data into random forest models, this study makes an
87 attempt to estimate the high-resolution (1km×1km) ambient PM_{2.5} and O₃
88 concentrations of China in 2005-2017.

89

90 **2. Method**

91 The model variables of this study include meteorological variables, geographical
92 variables, socio-economic variables, satellite data and chemical transport model
93 output in 2013-2017. Daily average $PM_{2.5}$ and O_3 daily maximum of 8h-average
94 concentration (O_3 -8hmax) monitoring data of 1479 sites in 2013-2017 was obtained
95 (Fig. 1; Fig. S1 and Fig. S2). A $1km \times 1km$ standard grid is created across the country
96 ($35.55^\circ N$ to $43.12^\circ N$, and $112.95^\circ E$ to $120.35^\circ E$) with a total of 9495025 grid cells.
97 The coordinate system of the grid is WGS-84; and the projection of the grid is the
98 Albers Conical Equal Area Projection. We construct high-performance random forest
99 (RF) models (temporal resolution: daily; spatial resolution: $1km \times 1km$), and estimate
100 the grid daily average $PM_{2.5}$ concentration and O_3 -8hmax concentration of China in
101 2005-2017.



102

103 **Fig.1 Station distribution in China and average ground monitoring concentration based on**
 104 **the available data of PM_{2.5} (A) and O₃-8hmax (B) from 2013 to 2017**

105

106 **2.1 Data set**

107 The model variables used in this study mainly include Aqua AOD for PM_{2.5} modeling,
108 GEOS-Chem chemical transport model output for O₃ modeling, and some variables
109 shared by PM_{2.5} and O₃: 13 meteorological variables (includes boundary layer height,
110 surface pressure, 2 meter dew point temperature, evaporation, albedo, low cloud cover,
111 medium cloud cover, high cloud cover, total precipitation, 10 meter U wind
112 component, 10 meter V wind component, 2 meter surface temperature and surface
113 solar radiation downwards) and its lag 1 and lag 2, geographic and socio-economic
114 variables, such as Digital Elevation Model (DEM), Normalized Difference Vegetation
115 Index (NDVI), population, Gross Domestic Product (GDP), road network and dummy
116 variables (includes season, month, and spatial dummy variables, province). A more
117 detailed description of the model variables is given in Table S1. The processing
118 method has been described in detail in our earlier studies (Ma et al., 2021; Zhao et al.,
119 2019). Briefly, most of the model variables are processed into 1km×1km resolution
120 based on the standard grid using interpolation methods (such as inverse distance
121 weighted and bilinear algorithm) in ArcGIS 10.2 and Python 2.7. For example, AOD
122 is processed by ENVI 5.3+IDL and extracted into standard grid using ArcPy, then the
123 inverse distance weighted interpolation is carried out to obtain the 1km×1km
124 resolution data. For the long-term variables, the corresponding monthly and annual
125 level value is assigned to each day. Subsequent modeling work was carried out based
126 on the data set that covering monitoring data and all variables.

127

128 **2.2 Random forest model**

129 Random forest is an ensemble machine learning method consisting of many
 130 individual decision trees growing from bagged data and its prediction is a vote result
 131 of those trees (Breiman, 2001). The RF algorithm primarily integrates learning
 132 principles, trains several individual learners, and finally forms a strong learner
 133 through a certain combination strategy; through multiple rounds of training, multiple
 134 prediction results are obtained, and the final results are obtained after average
 135 aggregation.

136

137 The random forest models are established using the 10-fold cross validation method.
 138 First, this method randomly divides the modeling data set into 10 parts; then 9 of them
 139 are used for modeling, the remaining one is used for estimation and be compared with
 140 observations. The verification is repeated until every part is predicted. In this way, the
 141 modeling and verification of estimation are repeated 10 times in total, and the average
 142 values of the 10 runs is took as the final result, i.e., the CV-R². The formulae of the
 143 models are as follows:

144

$$145 \quad PM_{2.5ij} = f(METE_{ij}, lag1METE_{ij}, lag2METE_{ij}, AOD_{ij}, LD_j, ROAD_j, NDVI_j, ELE_j, GDP_j, \\ 146 \quad POP_j, SEASON_i, MON_i, PRO_j) \quad (1)$$

$$147 \quad O_{3-8hmaxij} = f(METE_{ij}, lag1METE_{ij}, lag2METE_{ij}, GEOS_{ij}, LD_j, ROAD_j, NDVI_j, ELE_j, \\ 148 \quad GDP_j, POP_j, SEASON_i, MON_i, PRO_j) \quad (2)$$

149

150 where $PM_{2.5ij}$ and $O_{3-8hmaxij}$ are the $PM_{2.5}$ and $O_{3-8hmax}$ concentrations on day i in

151 grid cell j ; $METE_{i,j}$ is 13 meteorological variables on day i in grid cell j , and lag 1
152 $METE_{i,j}$ and lag2 $METE_{i,j}$ represent corresponding one-day lag and two-day lag
153 values, respectively; $GEOS_{i,j}$ and $AOD_{i,j}$ are the GEOS-Chem model output and AOD
154 value on day i in grid cell j ; LD_j , $ROAD_j$, $NDVI_j$, ELE_j , GDP_j and POP_j are the land
155 use coverage, length of a variety of roads, NDVI, elevation, GDP and population in
156 grid cell j , respectively; $SEASON_i$, MON_i and PRO_j are the season and month of day i ,
157 and province of grid cell j , respectively.

158

159 In general, the random forest parameters that need to be adjusted include $n_estimators$
160 (number of decision trees) and the max_depth (maximum depth of the trees). Unlike
161 the previous methods of manually adjusting parameters, the parameters of random
162 forest were optimized using GridSearchCV, which can realize cross-validated
163 grid-search over a parameter grid. After GridSearchCV, we set max_depth as 36 and
164 $n_estimators$ as 200 for $PM_{2.5}$ modeling. For O_3 -8hmax modeling, we set max_depth
165 as 54 and $n_estimators$ as 200.

166

167 **2.3 Validation method**

168 To comprehensively verify the model performance, we construct the main models
169 using sample-based division method. Models using spatial-based and temporal-based
170 division method are further construct to test the model performance in spatial and
171 temporal scale.

172

173 The data set was randomly divided into training set (90% of the records) and test set
174 (10% of the records) by using the sample-based division method. We construct the
175 main model using the training set with a 10-fold cross-validation. Since the data in the
176 test set is not used in the main model, "true model performance" can be verified. The
177 coefficient of determination (R^2) of main model on test set (test- R^2), and the
178 verification indicators of model uncertainty, the root mean square error (RMSE) and
179 mean absolute error (MAE) are calculated for the $PM_{2.5}$ and O_3 -8hmax model,
180 respectively. The monthly and yearly test- R^2 are also calculated.

181

182 For the spatial verification, 90% of the monitoring stations are randomly selected. The
183 monitoring data of these stations is used as the training set, and the monitoring data of
184 remaining stations is used as the testing set. For the temporal verification, all date in
185 2013-2017 is randomly divided into nine and one, and the data in these dates is used
186 as training and test sets, respectively. After that, the test- R^2 , RMSE and MAE are
187 calculated.

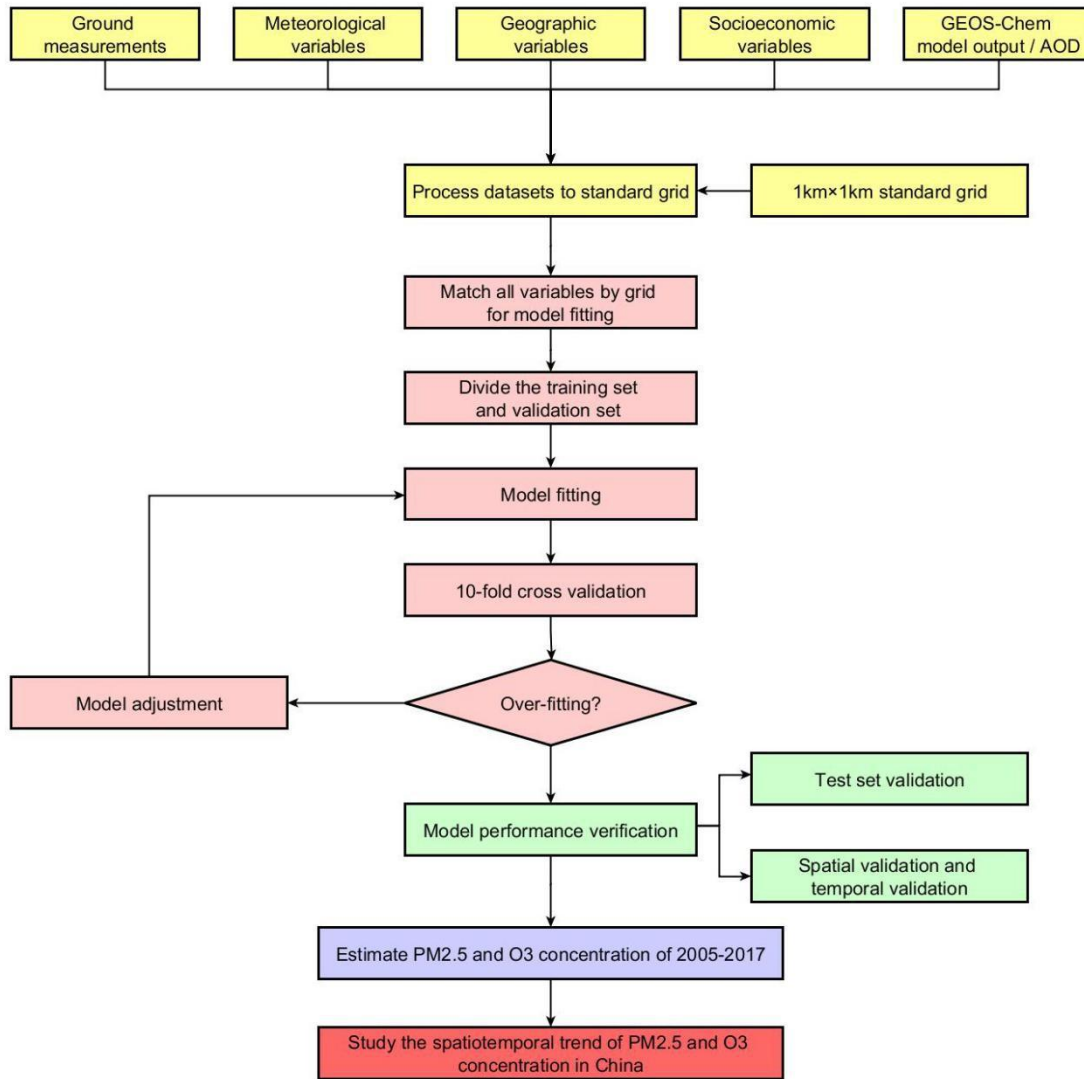
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189 **2.4 Estimation of daily $PM_{2.5}$ and ambient O_3 of China from 2005 to 2017**

190 Based on the final models of $PM_{2.5}$ and O_3 -8hmax, we estimate the gridded daily
191 average $PM_{2.5}$ concentration and O_3 -8hmax concentration of China in 2005-2017. The
192 spatial pattern and temporal trend of $PM_{2.5}$ and O_3 -8hmax concentrations are analyzed,
193 and compared with other modeling products.

194

195 The modeling and estimations are performed in Python 2.7.13 using the
 196 scikit-learn-0.20.3 and GridSearchCV packages. The workflow of this study is
 197 displayed in Fig. 2.



198
 199 **Fig. 2 The workflow of modeling process in the study**

200
 201 **3 Results and Discussion**

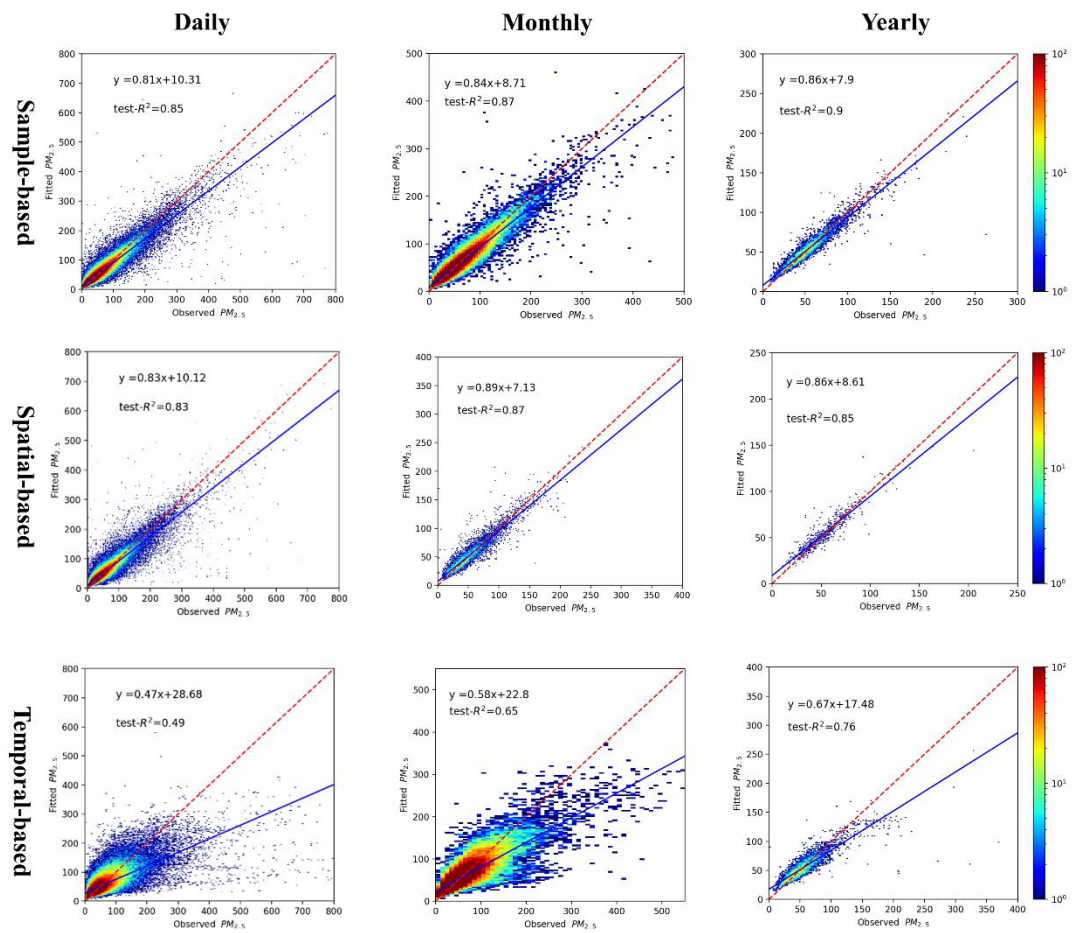
202 A total of 981744 monitoring data records were used in the final model-fitting data set.
 203 The mean \pm standard deviation of $PM_{2.5}$ and ambient O_3 concentrations in 2013-2017
 204 were $59.60 \pm 45.85 \mu g/m^3$ and $86.72 \pm 47.73 \mu g/m^3$, respectively. The results of

205 descriptive analysis for variables included in PM_{2.5} and O₃-8hmax model is shown in
206 Table S2.

207

208 **3.1 Model fitting and validation**

209 The cross-validation results indicate that the estimated PM_{2.5} and O₃-8hmax
210 concentrations matched reasonably with the observed PM_{2.5} and O₃-8hmax
211 concentrations, with high fitted test-R² values. According to our sample-based
212 division method, the test-R² values of the estimated daily, monthly and yearly PM_{2.5}
213 concentrations were 0.85, 0.88 and 0.90, respectively (Fig. 3). Likewise, the test-R²
214 values of the estimated daily, monthly and yearly O₃-8hmax concentrations were 0.77,
215 0.77 and 0.69, respectively (Fig. 4). The RMSE and MAE for PM_{2.5} in daily level
216 were 17.72 and 9.37 µg/m³; for O₃-8hmax, the values were 23.10 and 15.43 µg/m³.
217 The model performance is comparable to previous studies (Di et al., 2017; Li and
218 Cheng, 2021; Liu et al., 2020; Wei et al., 2021, 2020, 2019). At provincial/city level,
219 The model performance of PM_{2.5} estimations of Shanghai, Beijing, Hubei, Hebei and
220 Sichuan ranked the top 5 with relatively high test-R² (≥0.90), while those of Tibet,
221 Qinghai, Gansu, Anhui and Yunnan were less accurate with relatively low test-R²
222 values (<0.70). The model performance of O₃-8hmax estimations of Beijing,
223 Chongqing, Shanghai, Tianjin and Henan ranked the top 5 with relatively high test-R²
224 values (≥0.83), while those of Gansu, Anhui, Heilongjiang, Guizhou and Tibet were
225 poorer with relatively low test-R² values (<0.62) (Table S3).

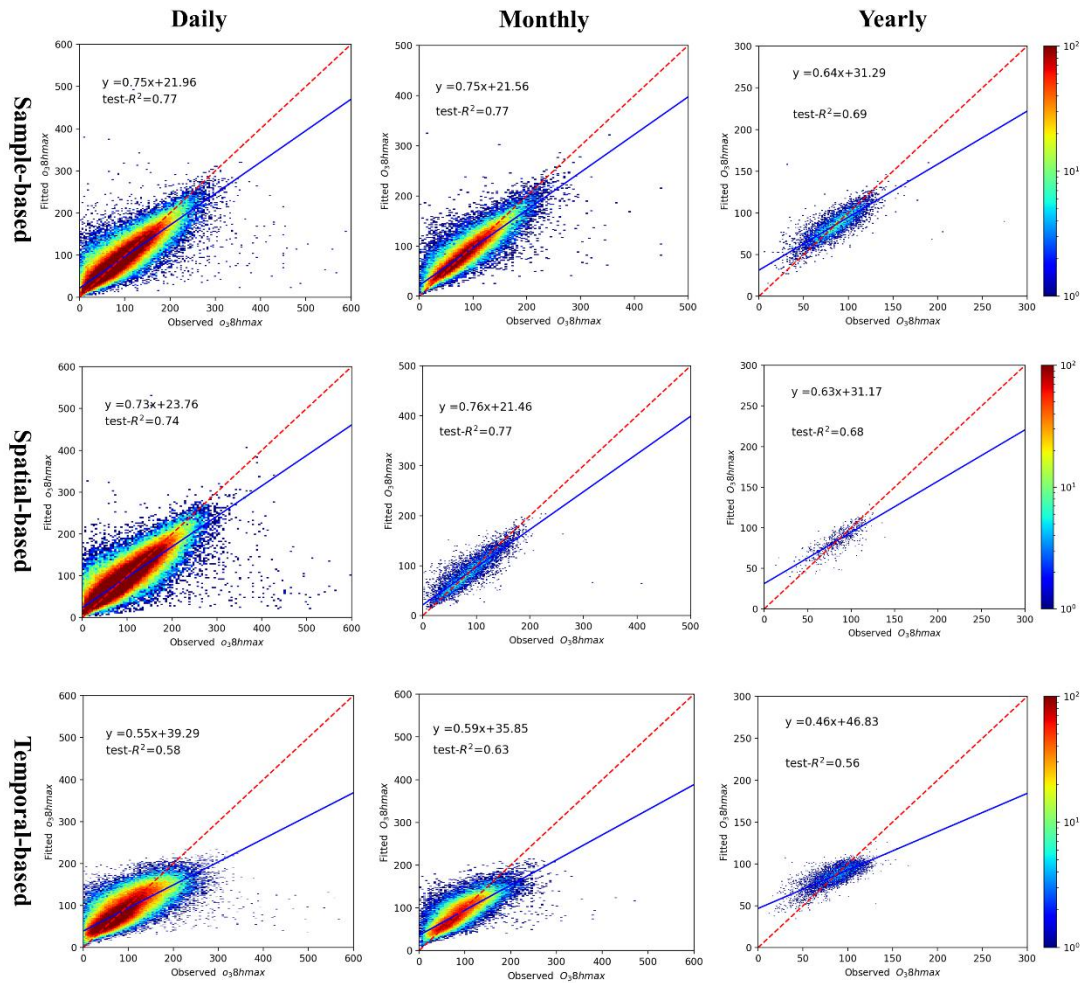


226

227 **Fig. 3 The density plot of PM_{2.5} model**

228 From left to right is different temporal scale: daily, monthly and yearly; From top to bottom is

229 different validation method: sample-based, spatial-based and temporal-based.



230

231 **Fig. 4 The density plot of O₃-8hmax model**

232 From left to right is different temporal scale: daily, monthly and yearly; From top to bottom is
 233 different validation method: sample-based, spatial-based and temporal-based.

234

235 The spatial and temporal test-R² of our models explained the uncertainty to some
 236 content (Fig. 3 and Fig. 4). The spatial test-R² values for daily, monthly and yearly
 237 PM_{2.5} estimation were 0.83, 0.87 and 0.85, respectively; while those of daily, monthly
 238 and yearly O₃-8hmax estimations were 0.74, 0.77 and 0.68, respectively. The
 239 relatively high spatial test-R² demonstrates the reasonable performance of our models
 240 in areas without monitoring stations. The temporal test-R² values of daily, monthly
 241 and yearly PM_{2.5} estimations were 0.49, 0.65 and 0.76, respectively; while those of

242 daily, monthly and yearly O₃-8hmax estimations were 0.58, 0.63 and 0.56,
243 respectively. These results indicate the uncertainty of our models when modeling data
244 in historical period, although the performance is among the best compared with
245 previous studies. The simulation accuracy is a universal issue in the present studies of
246 air pollutant concentrations in historical period without monitoring data. Further
247 efforts are need to improve the model performance of historical estimations.

248

249 **3.2 Feature importance**

250 The feature importance of the variables in our random forest models is presented in
251 Table S4-1 and S4-2. Similar to previous studies (Chen et al., 2018; Zhan et al., 2018),
252 the meteorological factors and their lagged values can significantly affect both PM_{2.5}
253 and O₃-8hmax modeling. Moreover, the specific features for PM_{2.5} and O₃, AOD and
254 GEOS-Chem output, also demonstrated high importance in modeling work.

255

256 For PM_{2.5} modeling work (Table S4-1), the meteorological variables (boundary layer
257 height, evaporation, 2 meter dew point temperature) and its lagged effect were among
258 the top ten important factors, totaling 33.6% in modeling work. The lagged effects
259 greatly contributed to PM_{2.5} modeling. For example, the lag1 boundary layer height
260 ranked first (17.2%) in our study, which is similar to previous studies (Zhao et al.,
261 2019). The interpolated AOD (5.6%), DEM (4.9%) and season (3.7%) also
262 demonstrated high importance, which showed crucial effects of satellite data, terrain
263 distribution characteristics in the study area, and study period on PM_{2.5} modeling. The

264 relative contribution of land-use, NDVI, population density, road length and GDP are
265 negligible (the importance scores less than 1%). Unlike DEM, these factors are
266 subjected to the influence of socioeconomic status in study area. In the future study,
267 the integration of these factors with a higher temporal resolution might change its
268 contribution to the estimation.

269

270 The feature importance of ambient O₃ is consistent with its formation and dissipation
271 mechanism: surface solar radiation downwards and its lagged effect according for
272 39.2% in modeling work (Table S4-2). Other meteorological factors (2 meter
273 temperature, boundary layer height, 10 meter V wind component, and low cloud cover)
274 according for totaling 9.54% importance scores. Our analysis also suggests the high
275 importance of GEOS-Chem model (7.2%), altitude (1.9%), and dummy factors
276 including year (2.2%) and province (1.6%) in O₃ modeling. By contrast, the relative
277 contribution of land-use, NDVI and road length are negligible (the importance scores
278 less than 1%). The high importance rank of population and GDP might be attributed
279 to the relatively high sensitivity of O₃ to anthropogenic emission sources (compared
280 to PM_{2.5}).

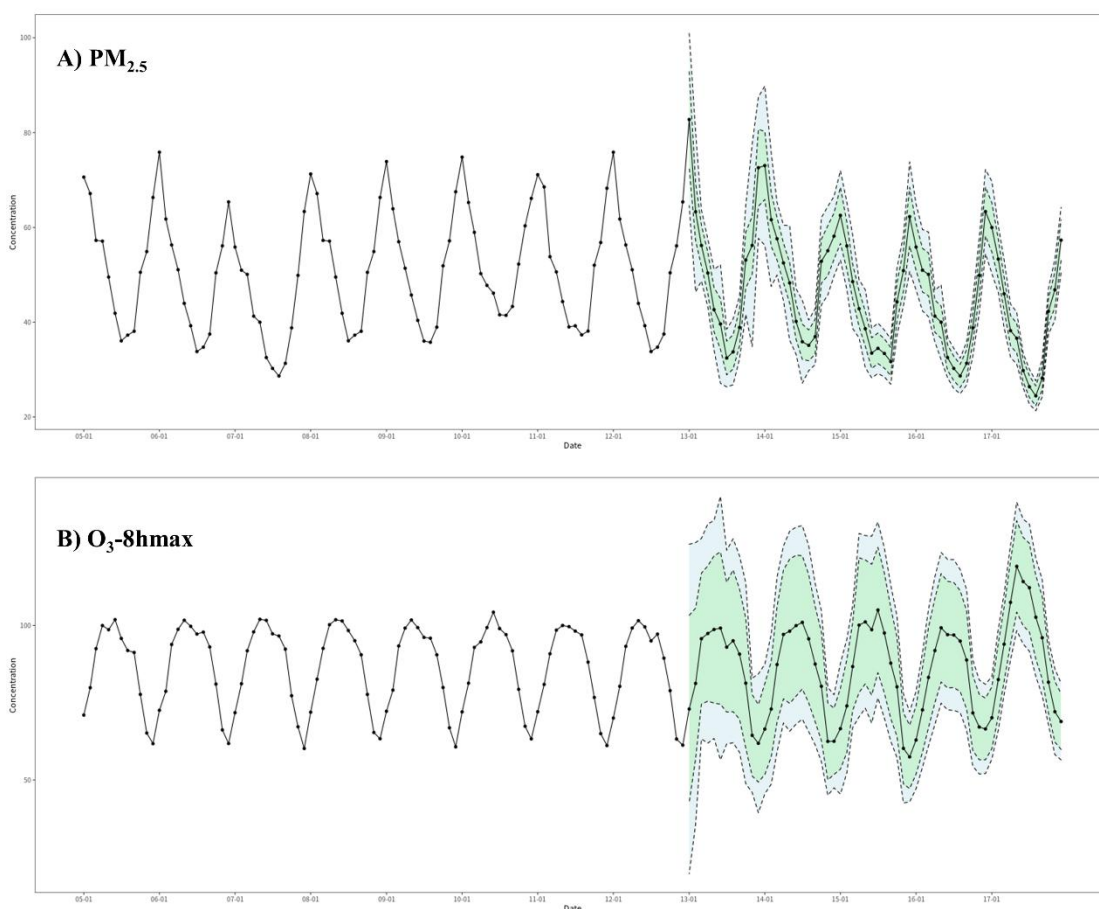
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282 **3.3 The spatial characteristics and temporal trend of PM_{2.5} and ambient O₃ of**

283 **China from 2005 to 2017**

284 During 2005-2017, PM_{2.5} showed an overall downward trend, while ambient O₃
285 showed an upward trend in recent years (Fig. 5, Fig. S3-S6). Relative to 2005, PM_{2.5}

286 concentration has increased by $2.60 \mu\text{g}/\text{m}^3$ in 2013. Nevertheless, after the
287 implementation of the *Air Pollution Prevention and Control Action Plan*, a strict
288 pollution control measure, $\text{PM}_{2.5}$ concentration has declined by $11.041 \mu\text{g}/\text{m}^3$ in 2017
289 (relative to 2013). This has resulted in a downward trend of $\text{PM}_{2.5}$ concentration in
290 2005-2017: $\text{PM}_{2.5}$ concentration in 2017 has decreased by $8.44 \mu\text{g}/\text{m}^3$ relative to 2005
291 (Fig. 5 and Fig. S3). In key pollution areas, with the implementation of various air
292 pollution prevention and control policies, $\text{PM}_{2.5}$ levels in the Beijing-Tianjin-Hebei
293 region have dropped the most, but the overall concentration levels are still higher than
294 those in the Yangtze River Delta and Pearl River Delta (Fig. S4). For O_3 -8hmax,
295 upward barely changed. Relative to 2005, O_3 -8hmax concentrations in 2013 and 2017
296 have increased by $0.39 \mu\text{g}/\text{m}^3$ and $7.83 \mu\text{g}/\text{m}^3$, respectively. The upward trend during
297 2005-2017 was mostly due to the significant changes between 2013 and 2017: relative
298 to 2013, the O_3 -8hmax concentration has increased by $7.44 \mu\text{g}/\text{m}^3$ in 2017 (Fig. 5 and
299 Fig. S5). The Beijing-Tianjin-Hebei region has shown an obvious upward trend since
300 2013; while the Pearl River Delta region change trend is not obvious (Fig. S6). During
301 the strict pollution control period, VOC emissions were not effectively controlled
302 could be one of the main reasons. Therefore, integrated management of VOCs and
303 NO_x in key industries and areas is important.



304

305 **Fig.5 The temporal trend of PM_{2.5} and O₃-8hmax concentration in China from 2005-2017**

306 The black dots represent the monthly average PM_{2.5} and O₃-8hmax concentration from 2005 to

307 2017, the blue color band represents the range of the monthly average PM_{2.5} and O₃-8hmax

308 concentration plus or minus the RMSE value from 2013-2017 (period with monitoring data), and

309 the green color band represents the range of the monthly average PM_{2.5} and O₃-8hmax

310 concentration plus or minus the MAE value from 2013-2017 years.

311

312 The seasonal distributions of PM_{2.5} and O₃-8hmax concentrations were obvious

313 during 2005-2017 (Fig. S7 and Fig. S8). The lowest seasonal PM_{2.5} concentration

314 occurred in summer, with an average concentration of $33.6 \pm 11.39 \mu\text{g}/\text{m}^3$; and the

315 highest seasonal PM_{2.5} concentration occurred in winter, with an average

316 concentration of $57.4 \pm 21.76 \mu\text{g}/\text{m}^3$. In winter, temperature inversion occurs frequently,

317 and the thickness of the mixed layer is low, which is not conducive to the diffusion of

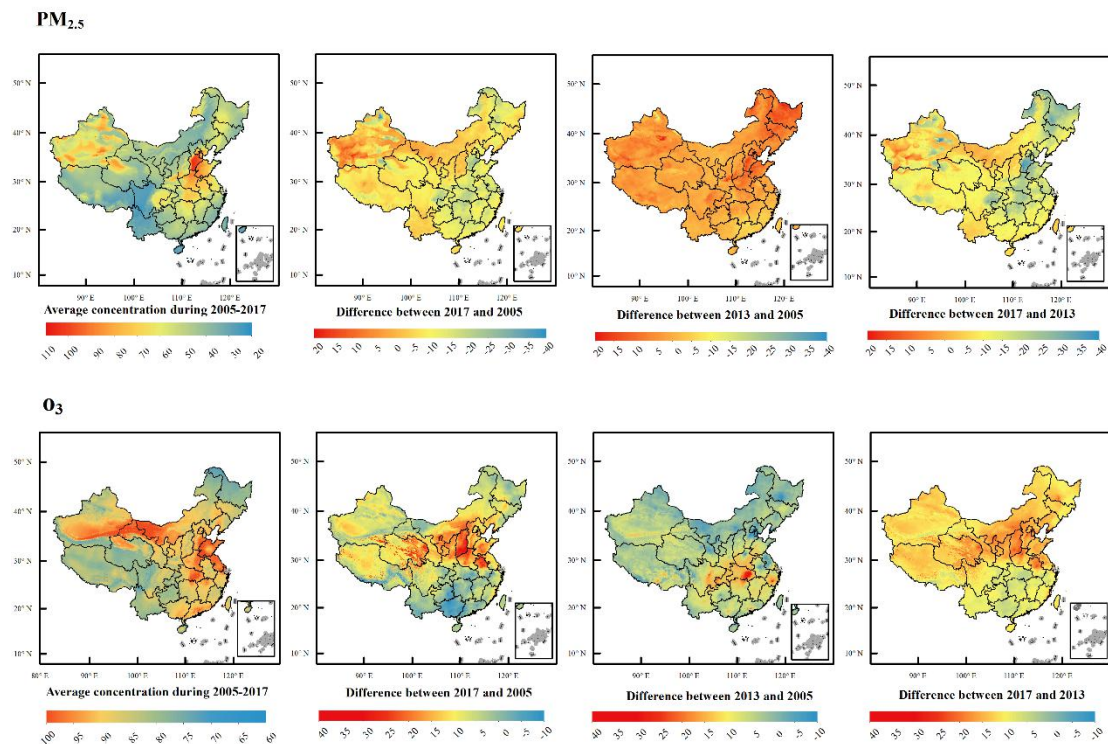
318 pollutants, which leads to the accumulation of PM_{2.5} near the ground (Sun et al, 2014).

319 In opposite, the lowest seasonal O₃-8hmax concentration was in winter, with an
320 average concentration of 72.65±6.28μg/m³; The highest seasonal O₃-8hmax
321 concentration was in summer, with an average concentration of 97.44±13.58μg/m³.
322 Temperatures and solar radiation conditions in summer increase the incidence of
323 severe O₃ pollution events, which is consistent with its formation and dissipation
324 mechanism.

325

326 The PM_{2.5} concentrations in Beijing-Tianjin-Hebei, Chengdu-Chongqing and Xinjiang
327 regions are higher than other regions, followed by the central China. The PM_{2.5}
328 concentrations in the southwestern regions (Yunnan and Tibet) and western part of
329 Sichuan Province, are the lowest, followed by the inner-north regions and the south
330 and southeastern regions (Fig. 6, Fig. S3 and Fig. S4; Table S5). The O₃-8hmax
331 concentrations in the Bohai Rim, Yangtze River Delta, Pearl River Delta and other
332 economically developed regions, southern Xinjiang, Inner Mongolia, and northeastern
333 Gansu are relatively high (Fig. 6, Fig. S5 and Fig.6; Table S5). This spatial pattern
334 barely changed during 2005-2017 (Fig. S3 and Fig. S5), but the temporal trend
335 showed spatial characteristic (Fig. 6; Fig. S4 and S6). For PM_{2.5} concentration, the
336 key pollution areas were severely polluted during 2005-2013. The air pollution
337 control measures of these regions were strict during 2013-2017, thus the decline was
338 obvious, especially for the Beijing-Tianjin-Hebei region. For O₃-8hmax concentration,
339 the growth rate was not obvious (except for the eastern part of Hubei Province) during
340 2005-2013. However, after 2013, there was a clear upward trend across the country,

341 especially in the northern China.



342
343 **Fig. 6 Estimated annual mean and difference of PM_{2.5} and O₃-8hmax concentration in China**
344 **during 2005 to 2017**

345 The first row is maps of PM_{2.5} related indicators, and the second row is maps of O₃-8hmax related
346 indicators. From left to right are average concentration during 2005-2017, the difference between
347 2017 and 2005, the difference between 2013 and 2005, and the difference between 2017 and 2013.

348

349 **3.4 Evaluation of the PM_{2.5} and O₃ concentration products with comparison with** 350 **other products**

351 Our estimation datasets include the PM_{2.5} and O₃-8hmax concentration data of China
352 in 2005-2017 with a spatial resolution of 1km×1km resolution. With high spatial and
353 temporal resolutions, our validation results are comparable with other modeling work
354 (see Table S6). Considering the future application in epidemiological research, our
355 estimation datasets would be useful: for acute effects studies, the high spatial
356 resolution would effectively reduce exposure errors; for chronic effects studies,

357 long-term exposure data is essential for the development of cohort studies.
358
359 Nevertheless, our estimation datasets also contain some limitations. First, we did not
360 use emission data in our model limited by coarse resolution. However the newly
361 published high-resolution emission inventory of China (<http://meicmodel.org/>) may
362 be utilized in future estimation studies to improve accuracy. Second, our modeling
363 still has spatial and temporal uncertainties. In areas where monitoring sites are
364 sparsely distributed, such as western China, it may be difficult to accurately capture
365 the association between air pollution concentrations and variables. The model
366 validation of historical period is also limited. Third, the interpolation process of model
367 features inevitably introduces systematic errors. Therefore, more high-quality and
368 high-resolution basic data would be needed in the future.

369

370 **4 Data availability**

371 The estimated PM_{2.5} and O₃ data are freely accessible at
372 <https://doi.org/10.5281/zenodo.4009308> (Ma et al., 2021), and the shared data set of
373 Chinese Environmental Public Health Tracking: CEPHT
374 (<https://cepht.niehs.cn:8282/developSDS3.html>).

375

376 **5 Conclusions**

377 We constructed random forest models for simulating of daily average PM_{2.5} and
378 O₃-8hmax concentrations of China during 2005-2017, with referential feature list and

379 comparable model performance. The estimation dataset would be useful for
380 supporting both long-term and short-term epidemiological studies. The model can be
381 further used for simulating daily concentrations of longer time period. The key
382 findings are summarized as follows. First, RF model proved its superiority in our
383 study and can be further used in the future estimation of air pollutant concentration.
384 Second, meteorological data is the most sensitive to PM_{2.5} and O₃ modeling. For
385 PM_{2.5} modeling work, boundary layer height, evaporation, 2 meter dew point
386 temperature and its lagged effects showed the highest sensitivity. For O₃ modeling
387 work, surface solar radiation downwards and its lagged effect were the most sensitive.
388 Third, PM_{2.5} concentration has trended downward in China, and the key polluted areas
389 during 2005-2013 were effectively controlled during 2013-2017. O₃ concentration has
390 trended upward in China, especially in the northern China during 2013-2017.

391

392 **Author Contribution**

393 Runmei Ma, Jie Ban and Qing Wang: Software, Investigation, Validation, Formal
394 analysis, Data curation, Writing - original draft. Yayi Zhang: Formal analysis,
395 Visualization. Yang Yang, Shenshen Li and Wenjiao Shi: Methodology, Writing -
396 Review & Editing. Tiantian Li: Conceptualization, Methodology, Writing - Review &
397 Editing.

398

399 **Competing Interests**

400 The authors declare that they have no conflict of interest.

401

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