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Supplement of

FastCTM (v1.0): Atmospheric chemical transport modelling with a principle-informed neural network for air quality simulations

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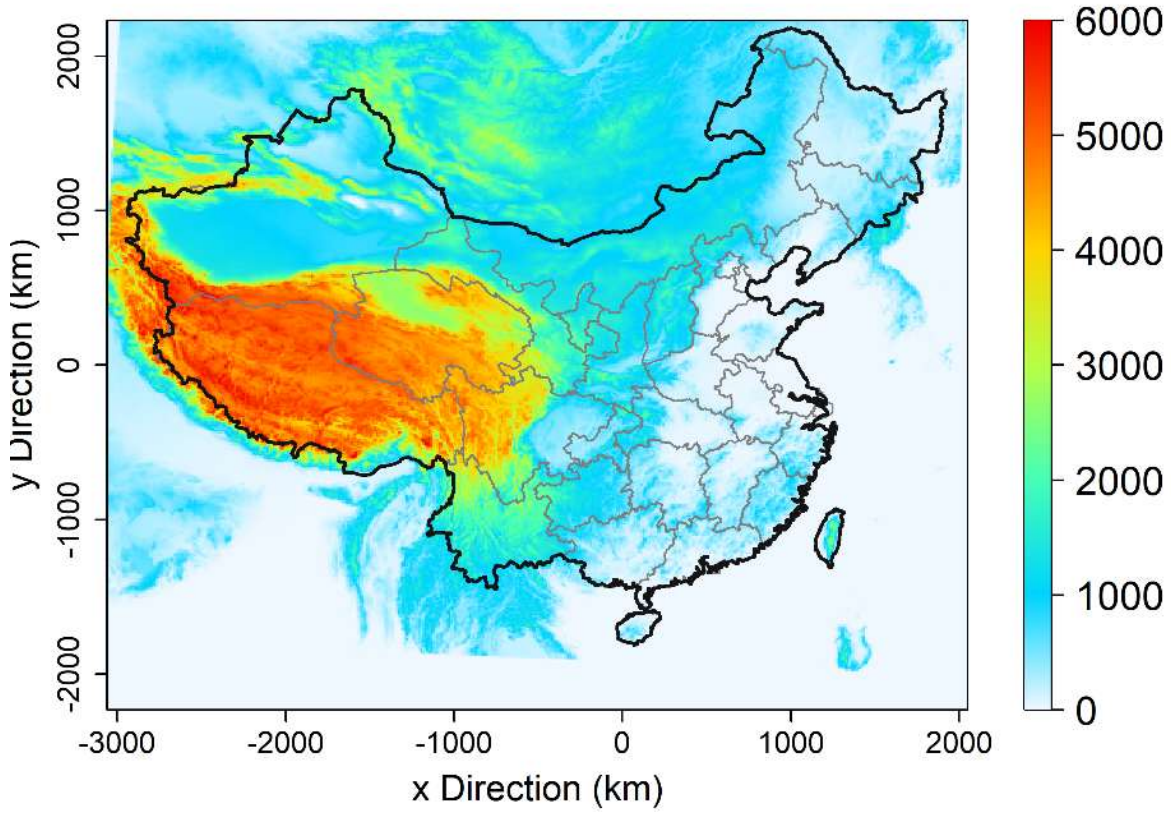


Figure S1: The spatial coverage for CMAQ simulation in 12-km resolution. The colour in this figure represent elevations above sea level.

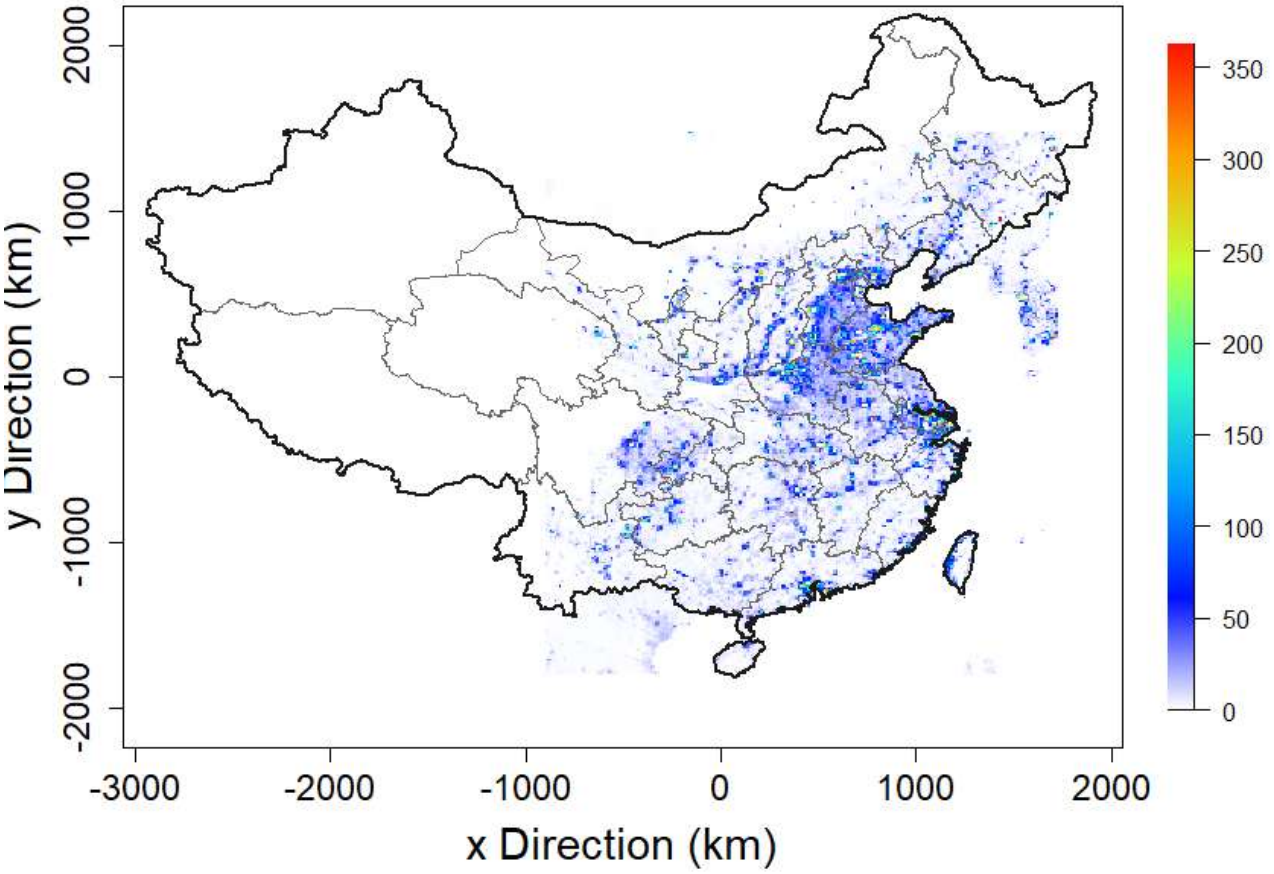


Figure S2: Annual average emissions (g/s) of NOx used in this study.

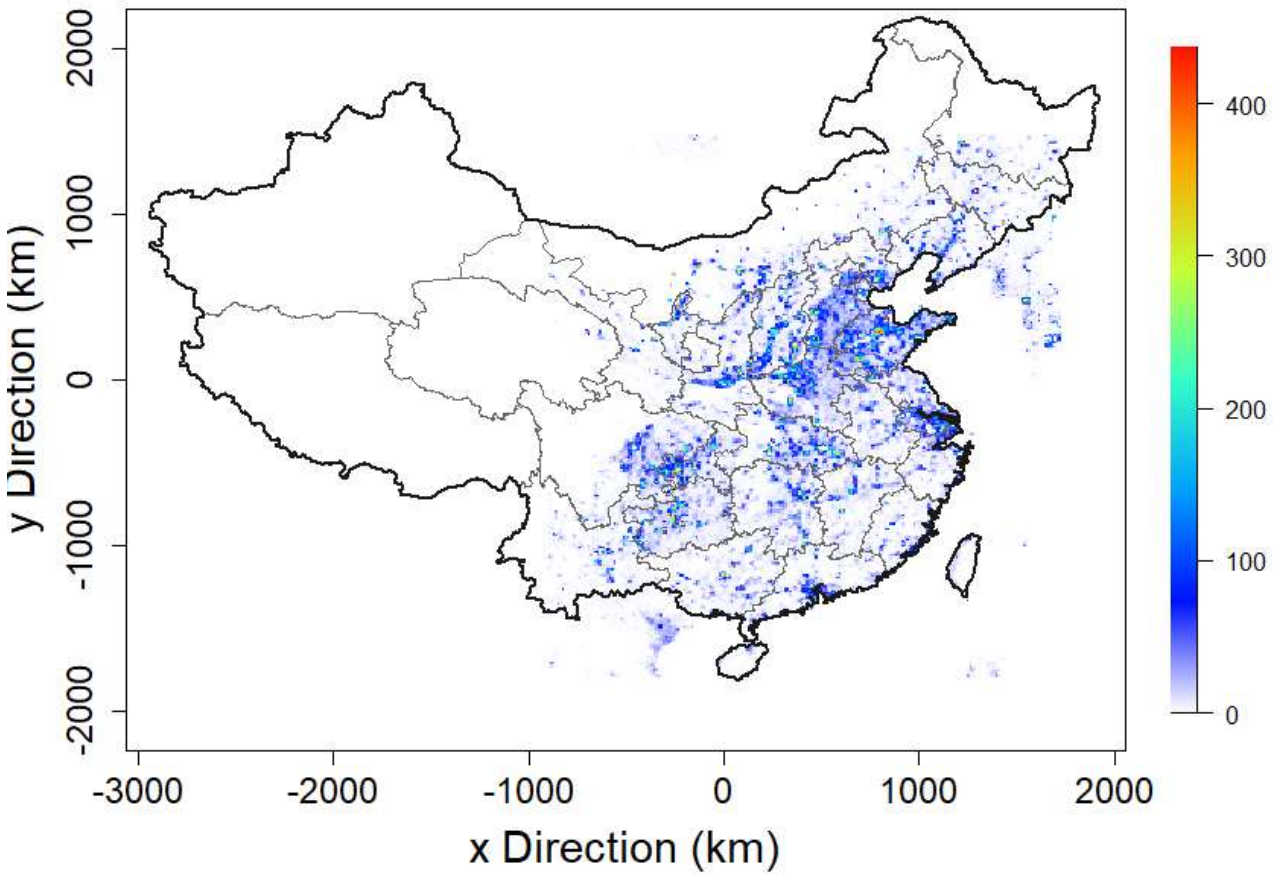


Figure S3: Annual average emissions (g/s) of SO_2 used in this study.

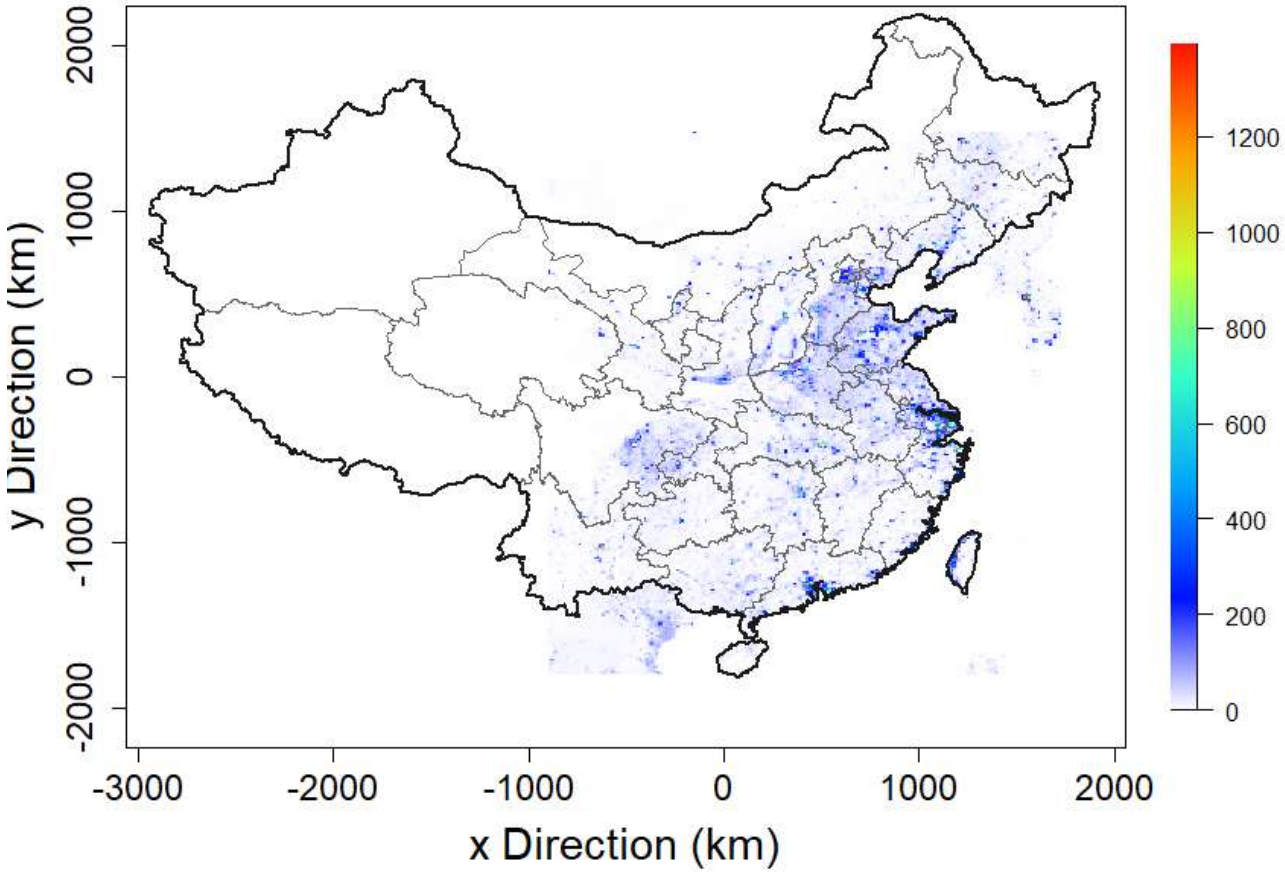


Figure S4: Annual average emissions (g/s) of VOC used in this study.

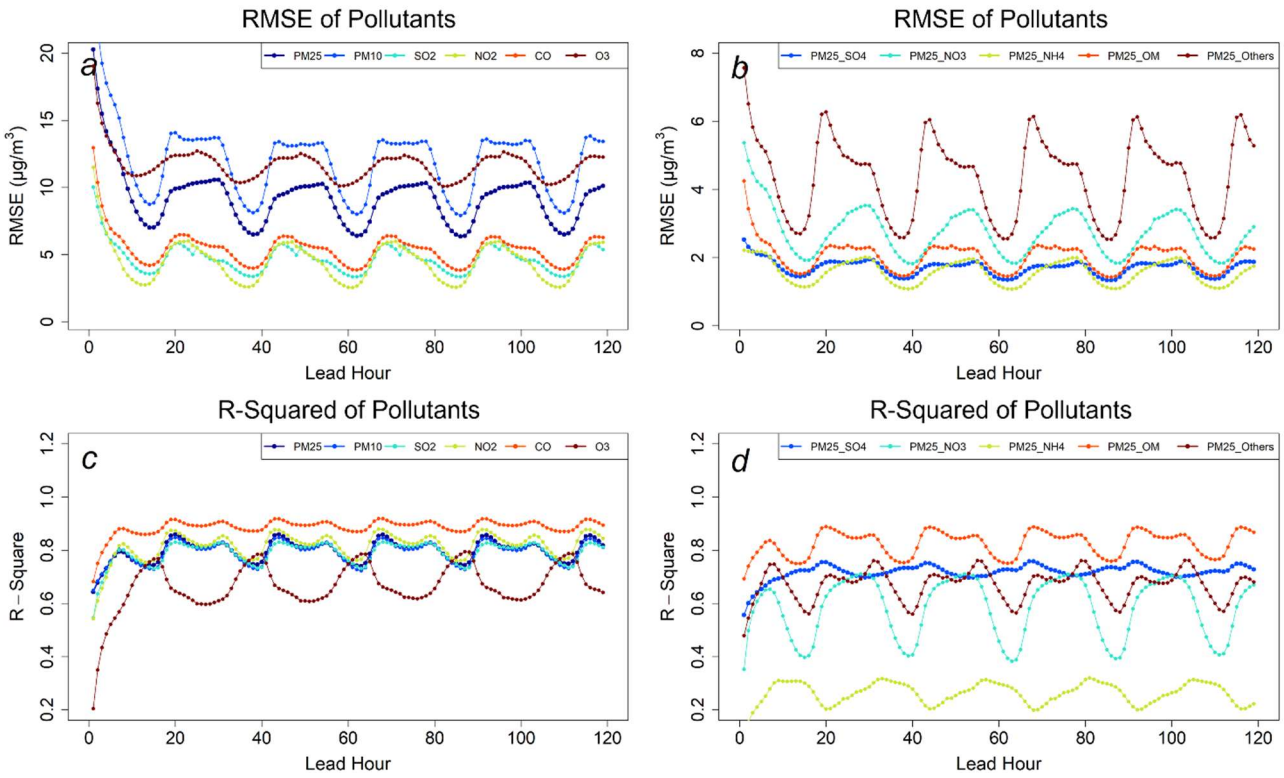


Figure S5: The evaluation metrics of RMSE and R^2 for air pollutants' concentration forecasts with the FASTCTM model initialized with fields in zero values.

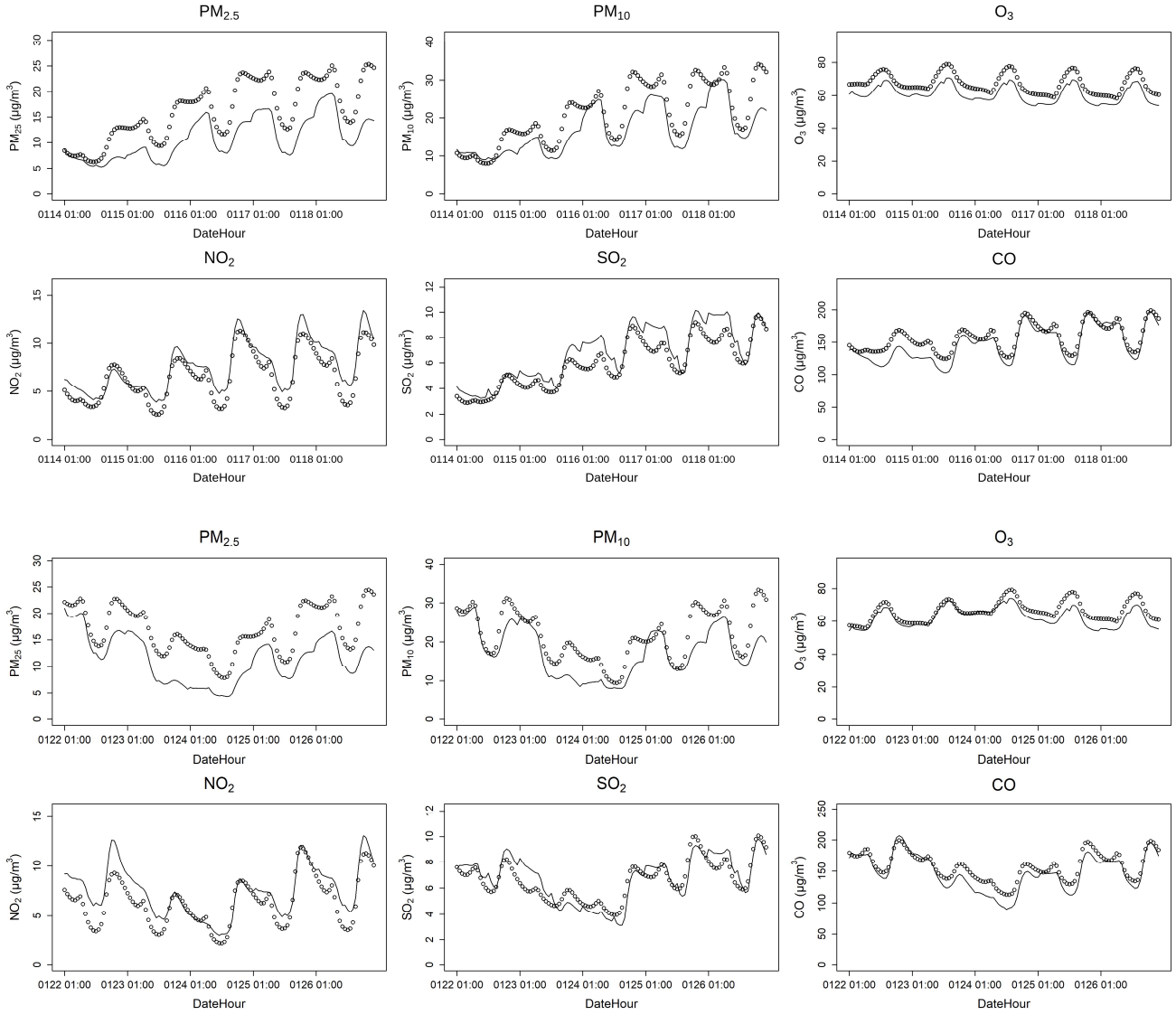
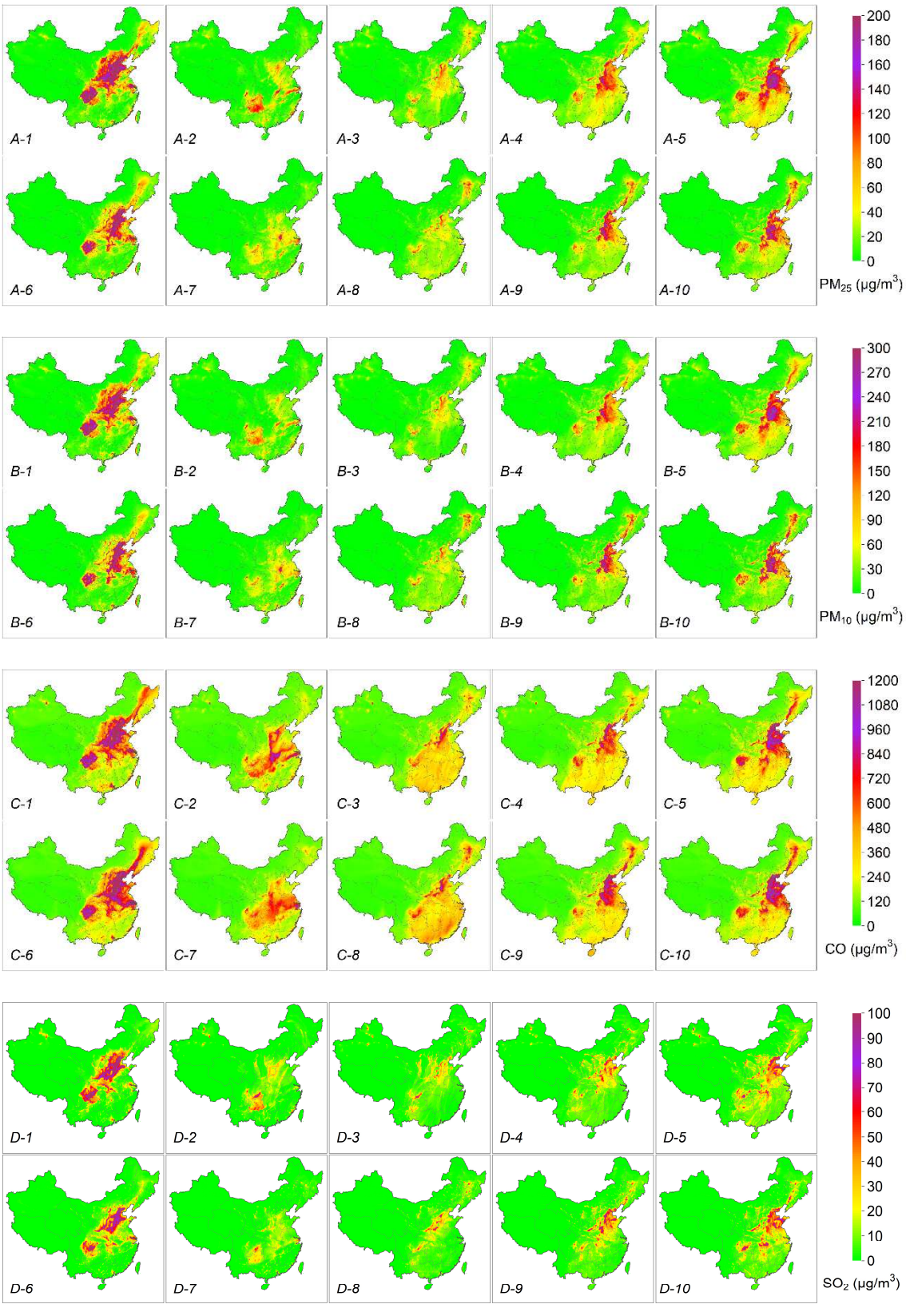


Figure S6: Time series of hourly air pollutant concentrations averaged for all China with the circles represent CMAQ forecasts and the solid black lines represent FastCTM forecasts: prediction cycle starting on January 14, 2023 (top) versus prediction cycle starting on January 22, 2023 (bottom).


A-1
A-2
A-3
A-4
A-5
A-6
A-7
A-8
A-9
A-10
200
180
160
140
120
100
80
60
40
20
0
PM25 (μg/m3)
B-1
B-2
B-3
B-4
B-5
B-6
B-7
B-8
B-9
B-10
300
270
240
210
180
150
120
90
60
30
0
PM10 (μg/m3)
C-1
C-2
C-3
C-4
C-5
C-6
C-7
C-8
C-9
C-10
1200
1080
960
840
720
600
480
360
240
120
0
CO (μg/m3)
D-1
D-2
D-3
D-4
D-5
D-6
D-7
D-8
D-9
D-10
100
90
80
70
60
50
40
30
20
10
0
SO2 (μg/m3)

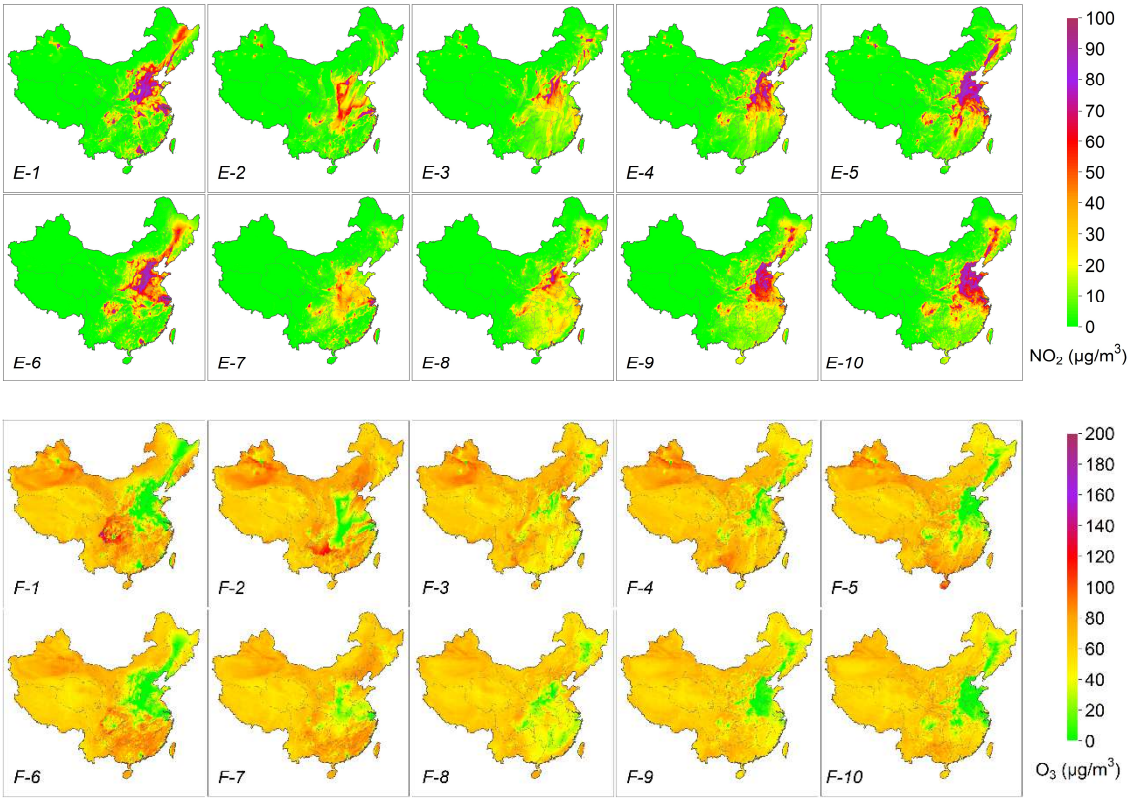


Figure S7: Air quality forecast examples of CMAQ and FastCTM at leading time of 24, 48, 72, 94 and 120 hours starting from 0:00 on March 4th, 2023. Panel A-F respectively refers to $PM_{2.5}$, PM_{10}, CO, SO_2, NO_2 and O_3. The 1-5 sub-panels in the first row (1-5) in each panel are the CMAQ forecasts, while the 6-10 sub-panels in the second row are FastCTM forecasts.

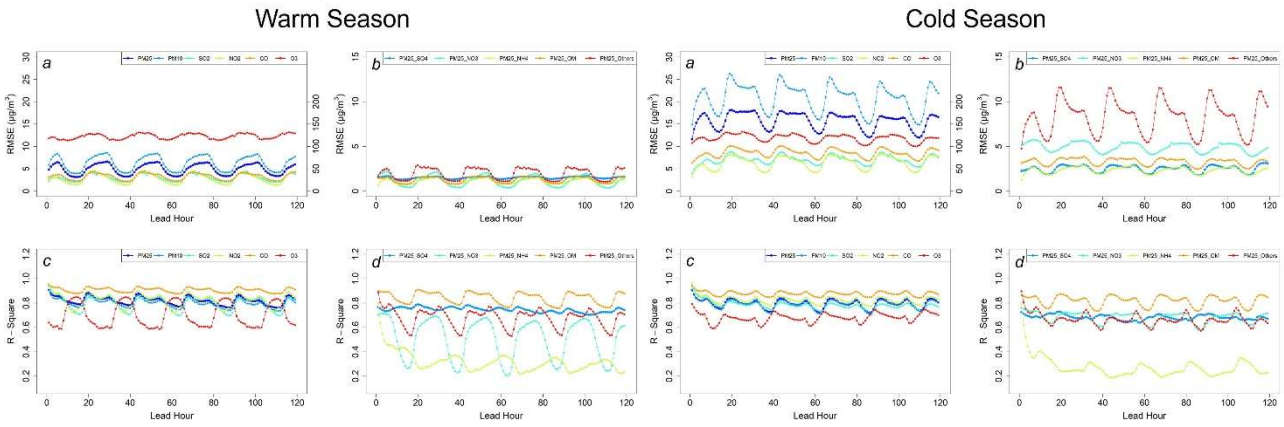


Figure S8: The evaluation performances of random forest forecasts against CMAQ forecasts in warm season of 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a).

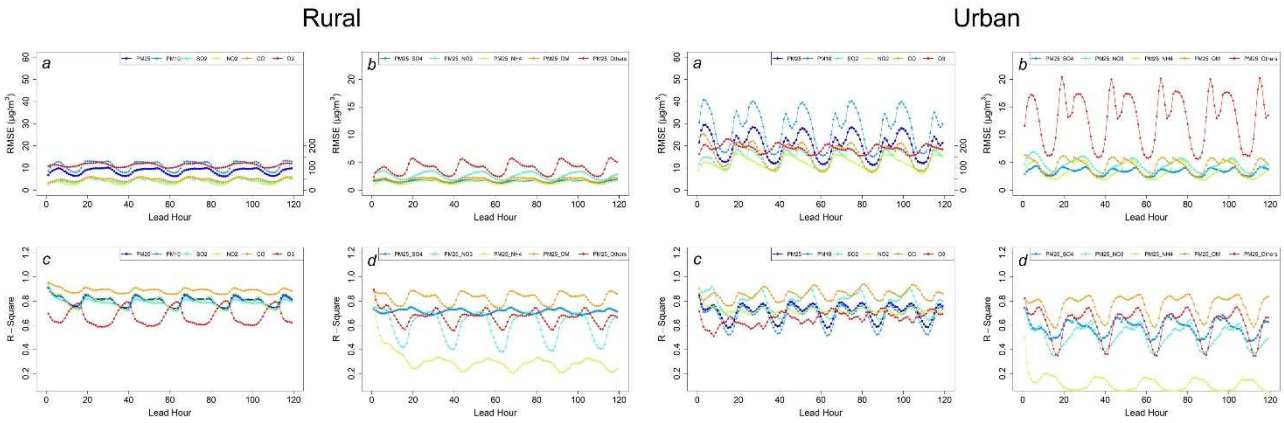


Figure S9: The evaluation performances of FastCTM forecasts against CMAQ forecasts in rural and urban areas in 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a).

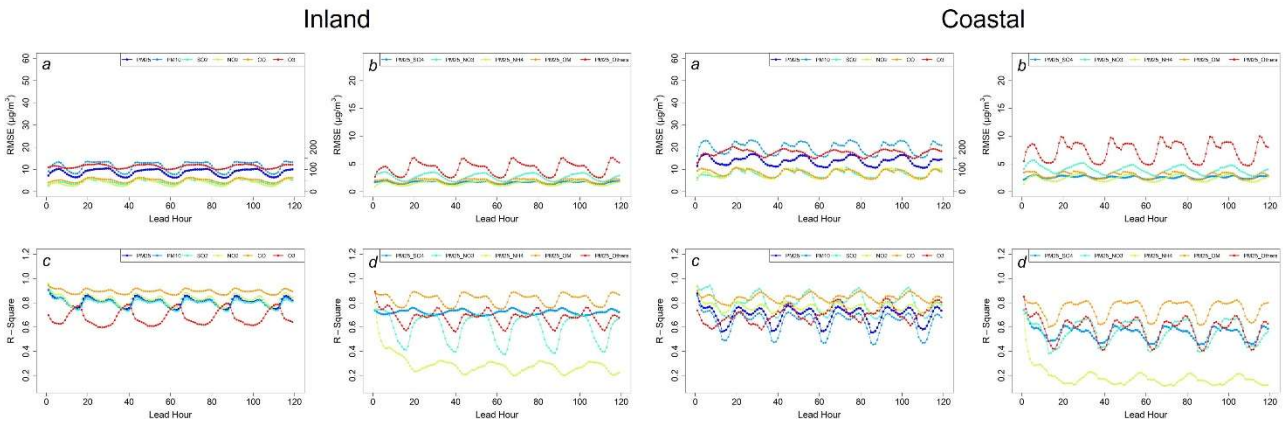


Figure S10: The evaluation performances of FastCTM forecasts against CMAQ forecasts in inland and coastal areas in 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a)

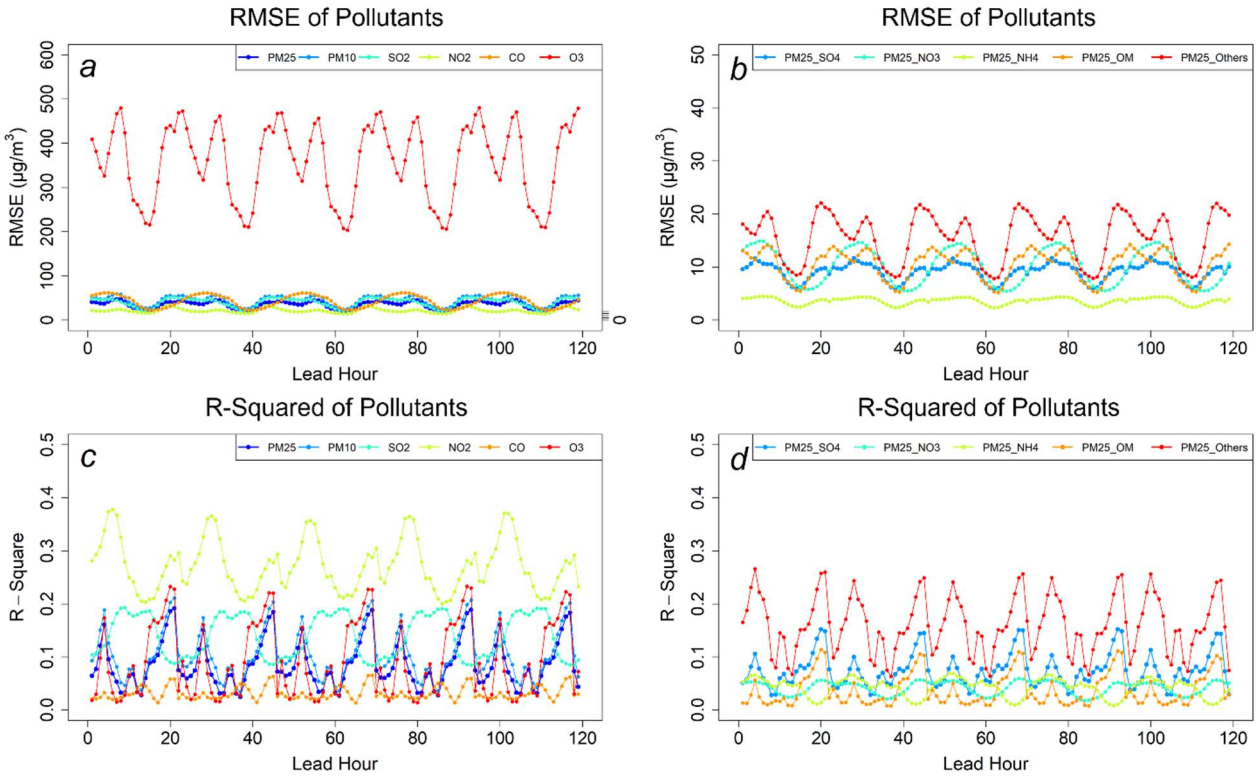


Figure S11: The evaluation performances of linear regression forecasts against CMAQ forecasts in 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a).

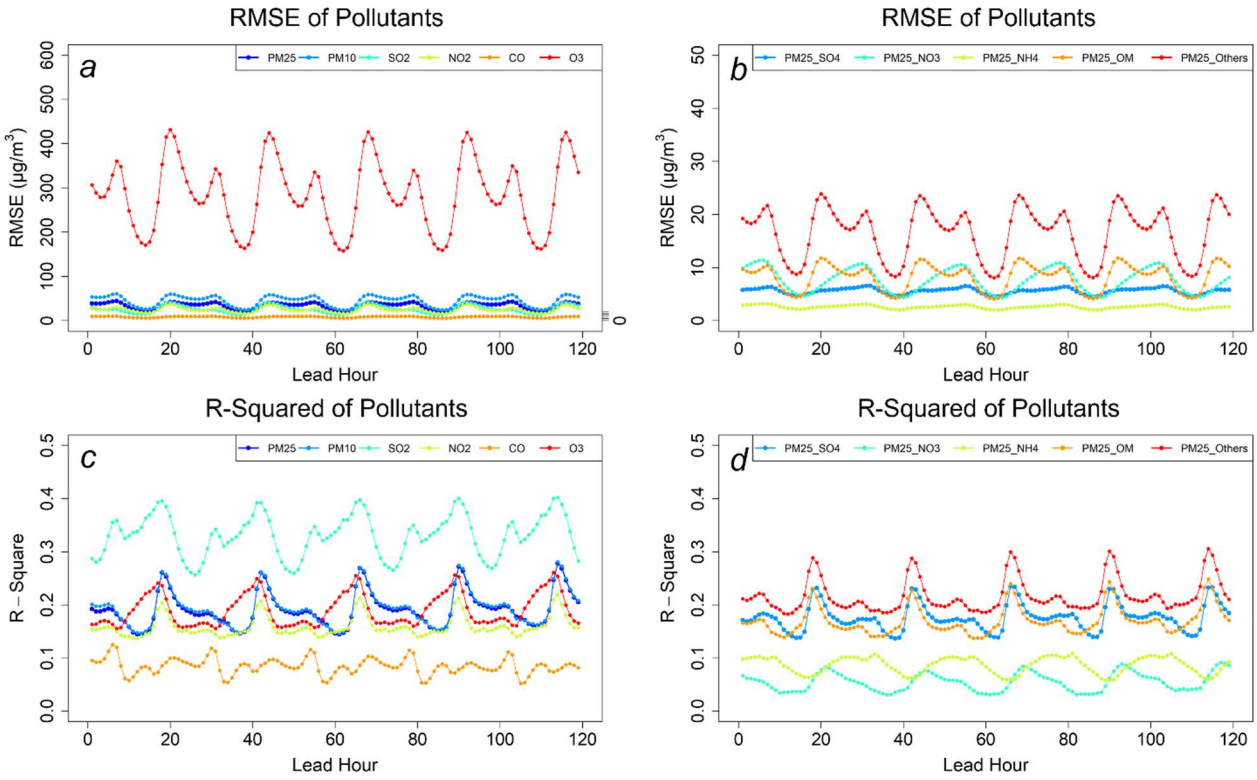


Figure S12: The evaluation performances of random forest forecasts against CMAQ forecasts in 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a).

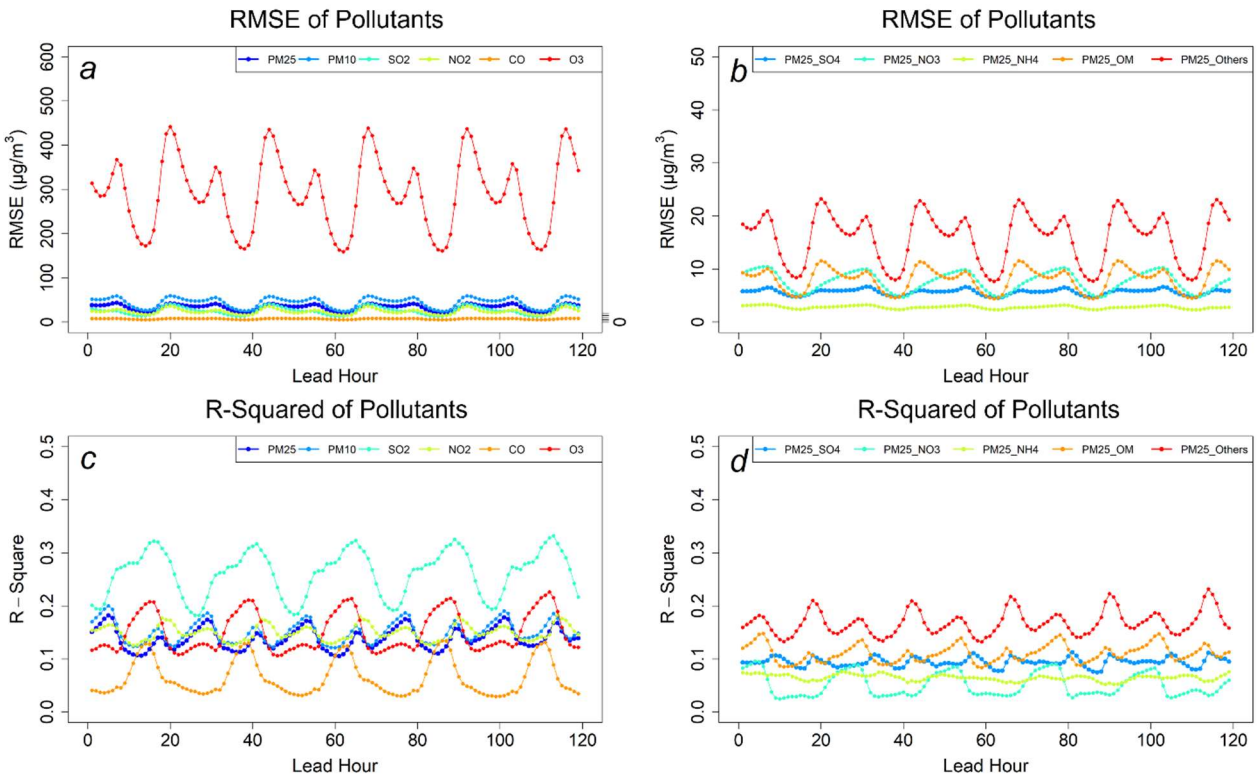


Figure S13: The evaluation performances of XGBoost forecasts against CMAQ forecasts in 2023. Panel (a) and (b) respectively show RMSE values of criteria pollutants and the $PM_{2.5}$ components of. Panel (c) and (d) respectively show R^2 values. It should be noted that RMSE value of CO corresponds to the right axis in panel (a).

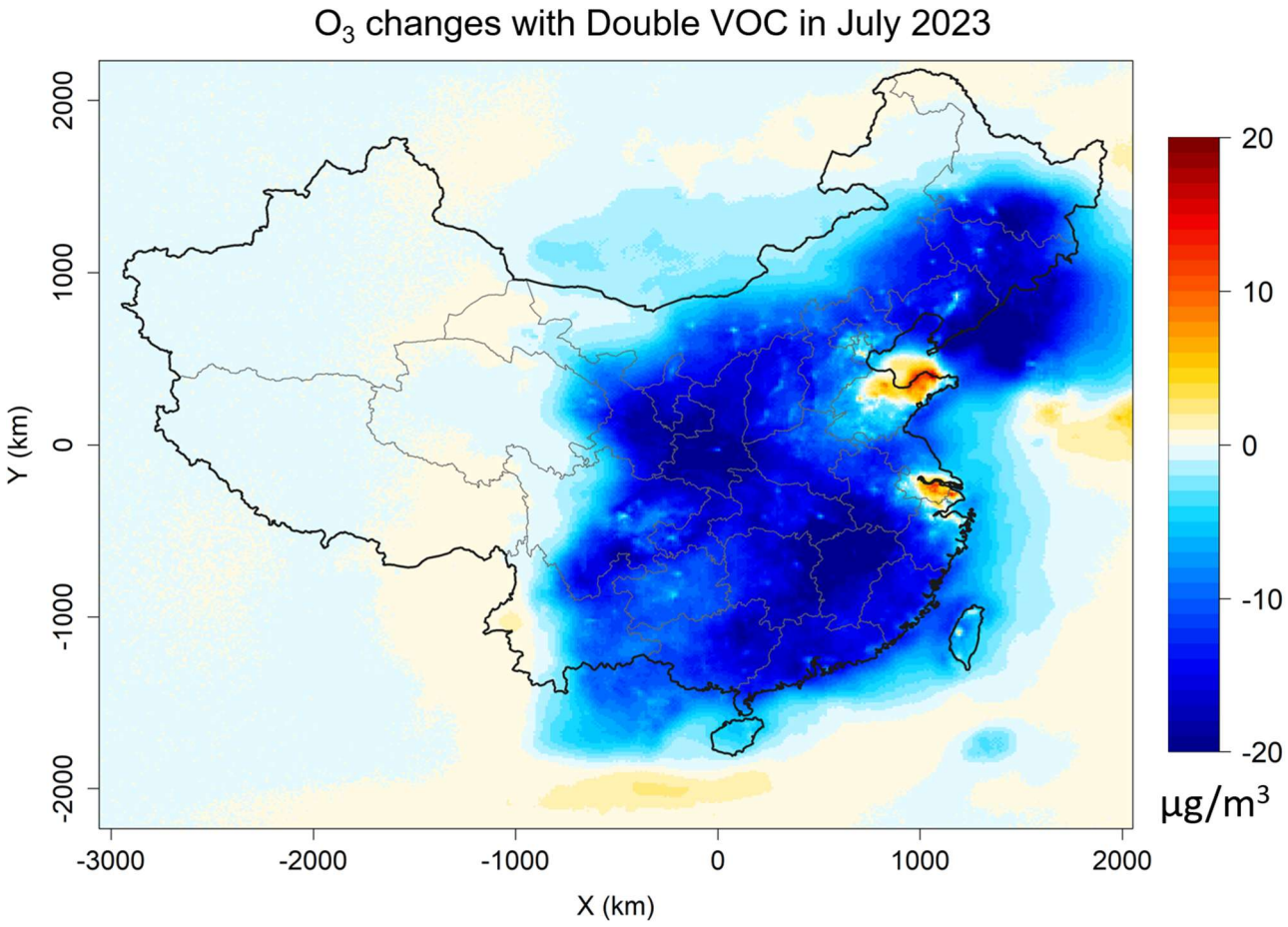


Figure S14: Predicted average changes of hourly O_3 concentrations in 5 lead-days with doubled VOC emissions in July 2023.

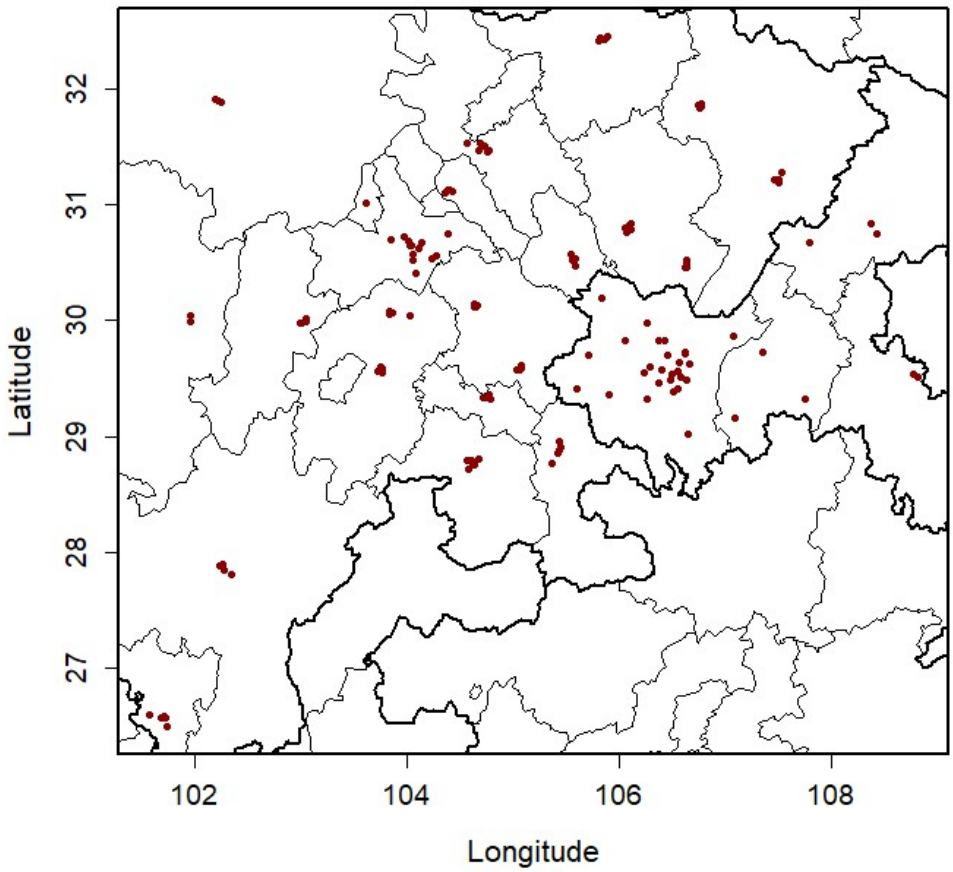


Figure S15: The locations of national air quality monitors used for evaluation FastCTM responses to emission changes.

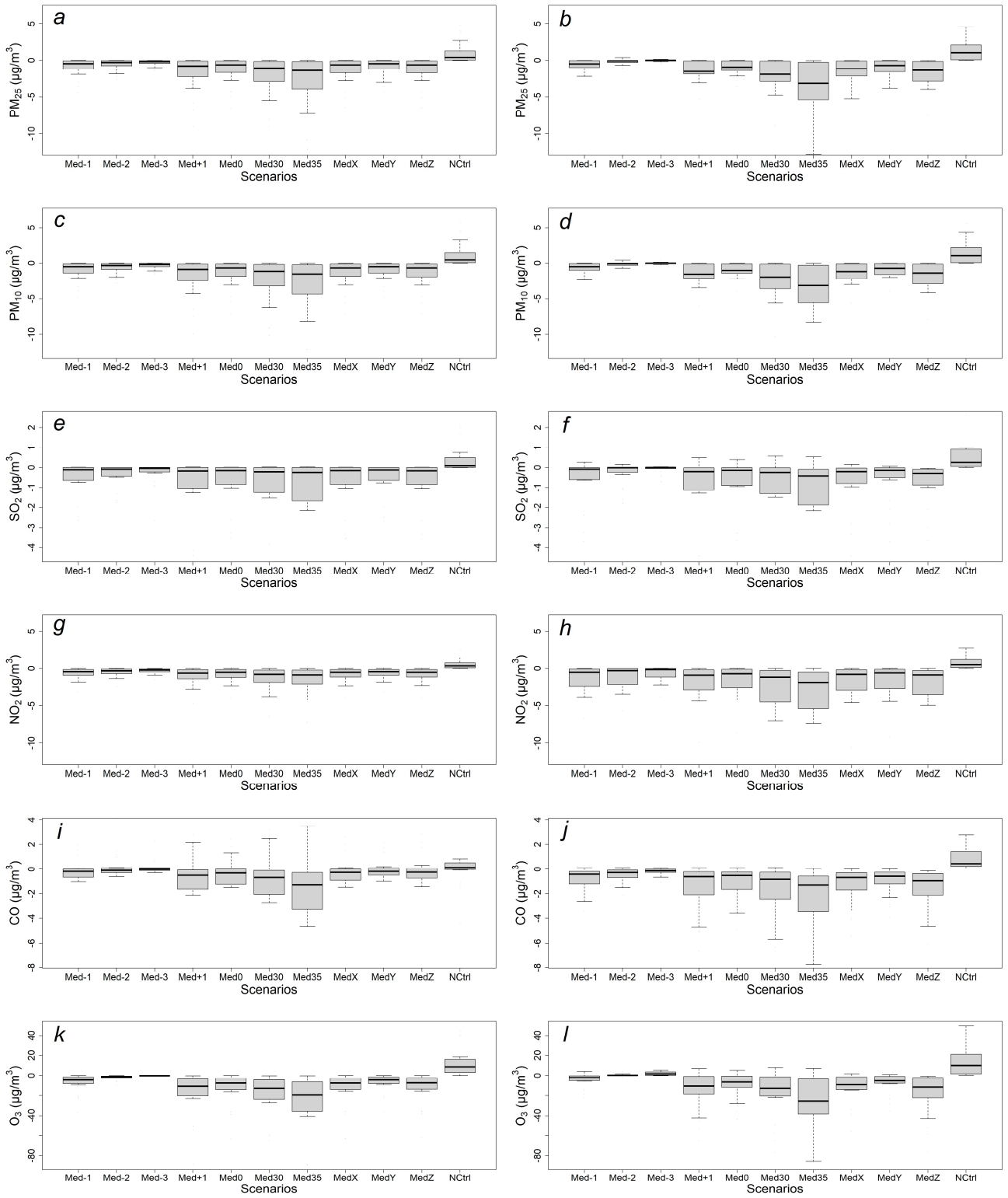


Figure S16: Air pollutant concentration changes in terms of base case simulated by CMAQ (subplots of a, c, e, g, i and k in first column) and by FastCTM (subplots of b, d, f, h, j and l in second column) in January 2019.

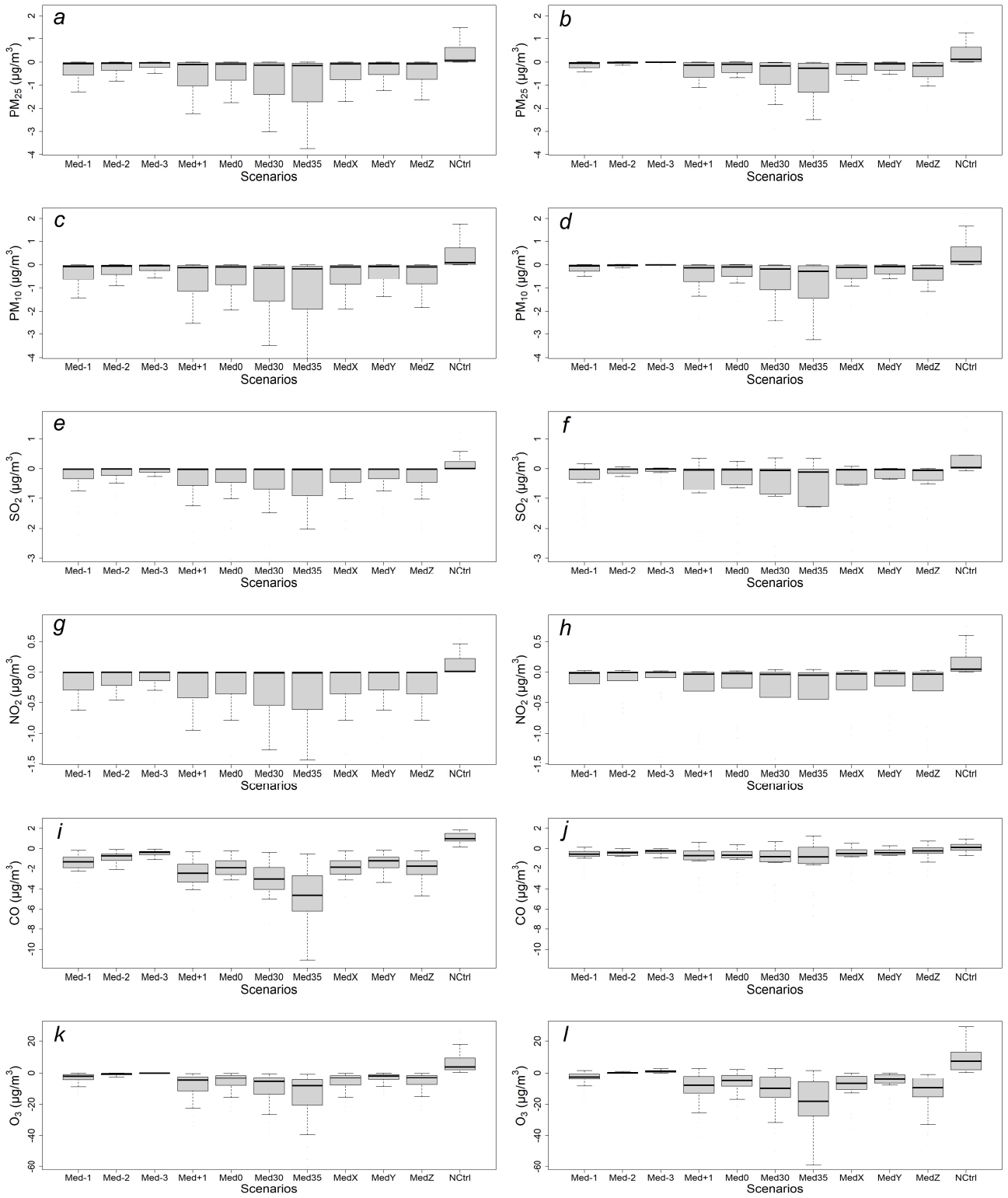


Figure S17: Air pollutant concentration changes in terms of base case simulated by CMAQ (subplots of a, c, e, g, i, and k in the first column) and by FastCTM (subplots of b, d, f, h, j, and l in the second column) in July 2019.