

1 *Supplement of*

2 **Elucidating the pollution characteristics of nitrate, sulfate and ammonium in**
3 **PM_{2.5} in Chengdu, southwest China based on long-term observations**

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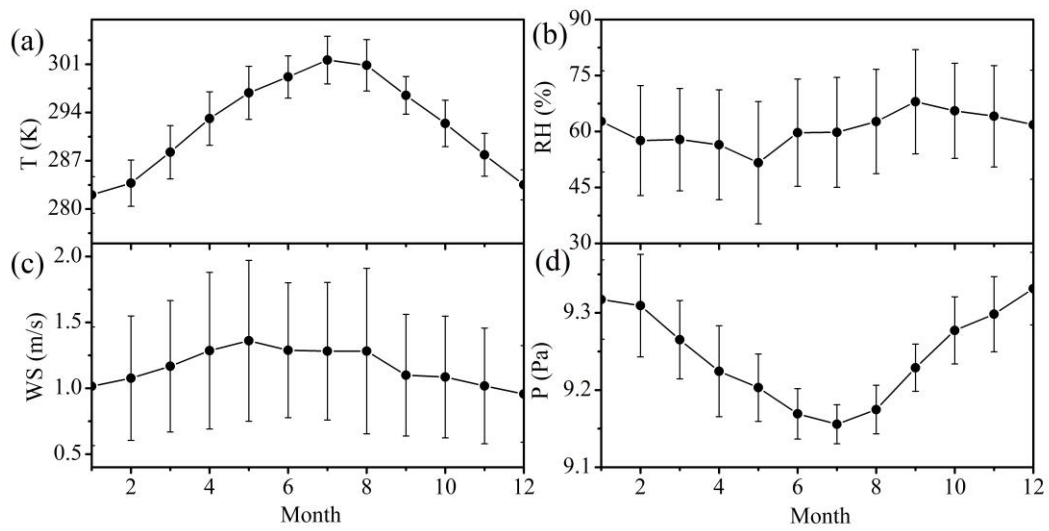
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17 (Qinwen Tan)

18 Table S1. Comparison of PM_{2.5}, NO₂ and SO₂ (μg/m³) mass concentrations from 2013
19 to 2017.

	2013	2014	2015	2016	2017
PM _{2.5}	97	77	64	63	56
NO ₂	63	59	53	54	53
SO ₂	31	19	14	14	11

Data from Chengdu Municipal Ecology and Environment Bureau: Ambient air quality report, last access: 12
February 2020

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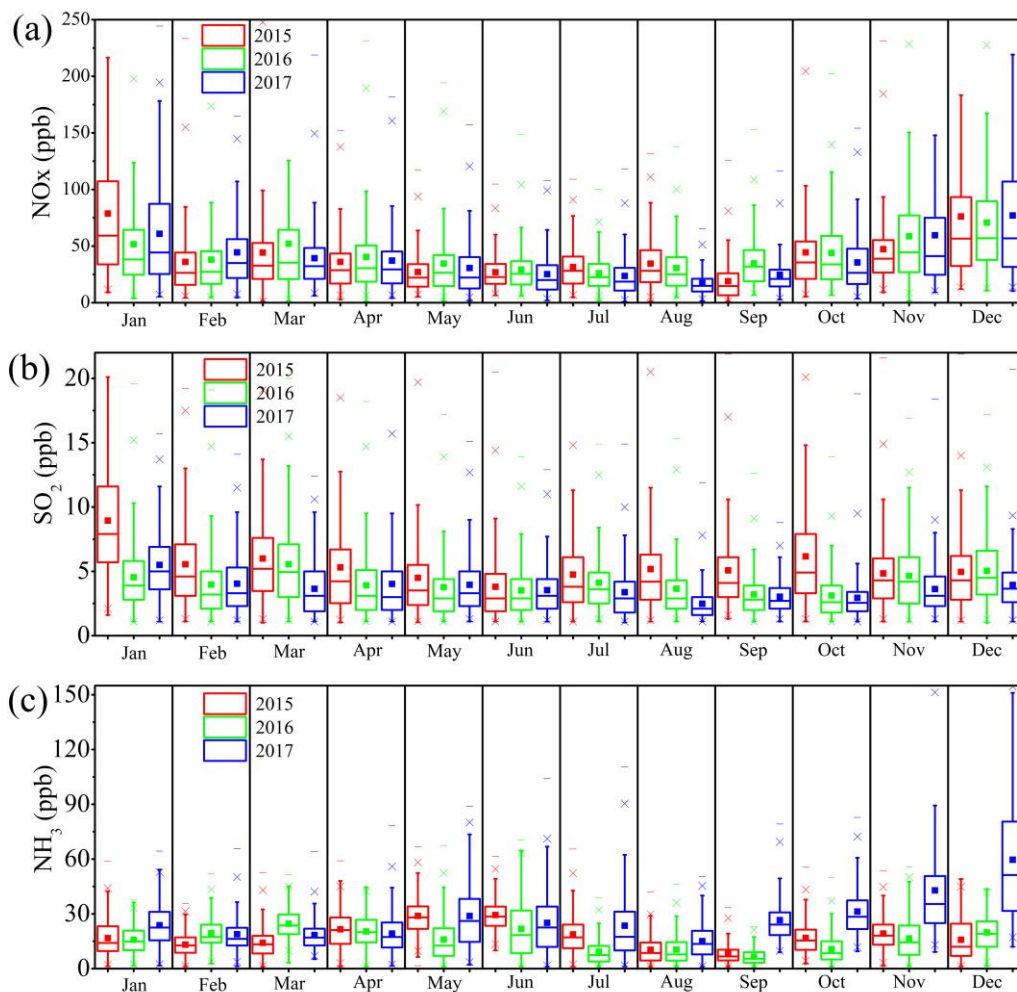
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22 Fig. S1. Monthly variations in meteorological conditions during the observations

23 (2015-2017).

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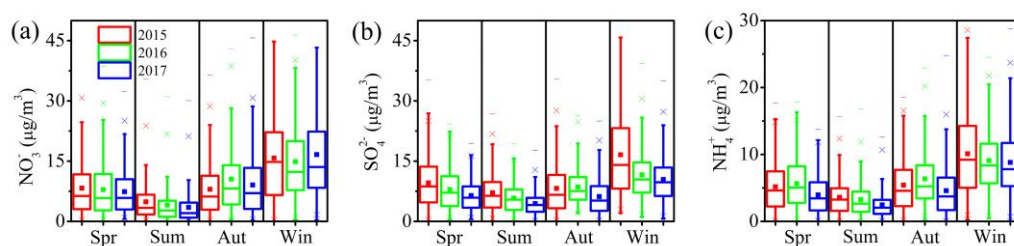
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27 Fig. S2. Monthly variations in NO₂, SO₂ and NH₃ concentrations from 2015 to 2017.

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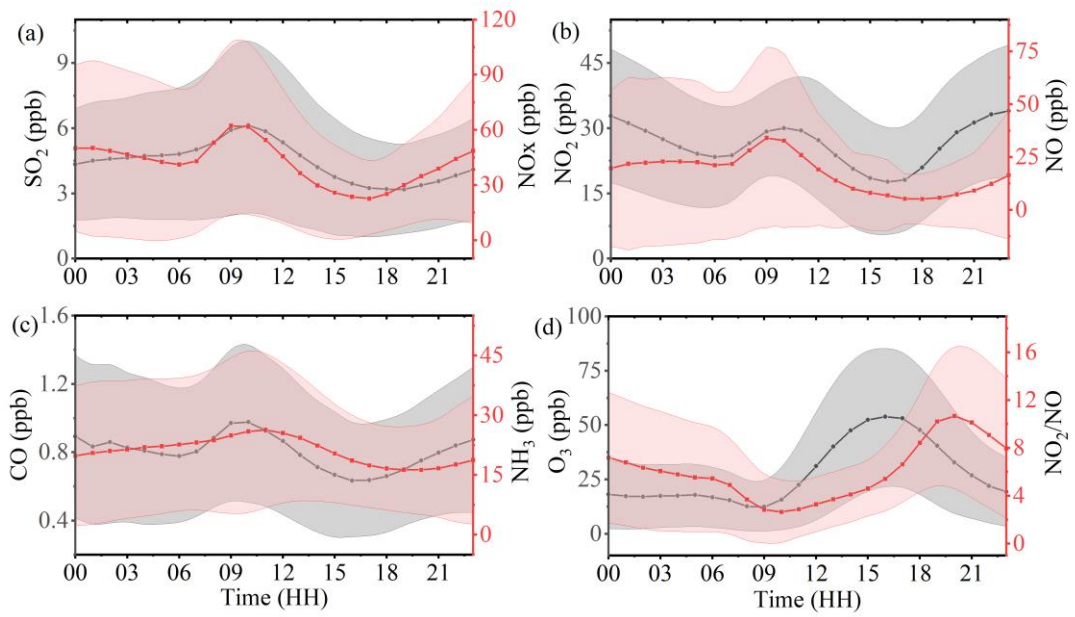


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30 Fig. S3. Seasonal variations in NO₃⁻, SO₄²⁻ and NH₄⁺ mass concentrations from 2015

31 to 2017.

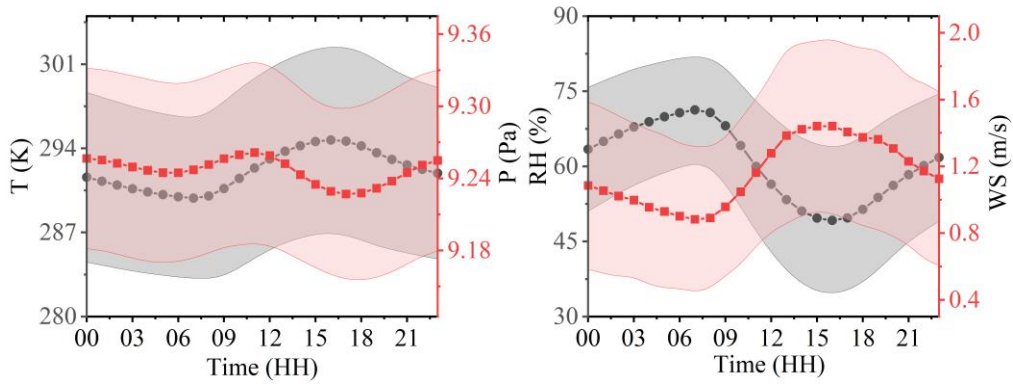
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34 Fig. S4. Diurnal variations in gaseous pollutants from 2015 to 2017.

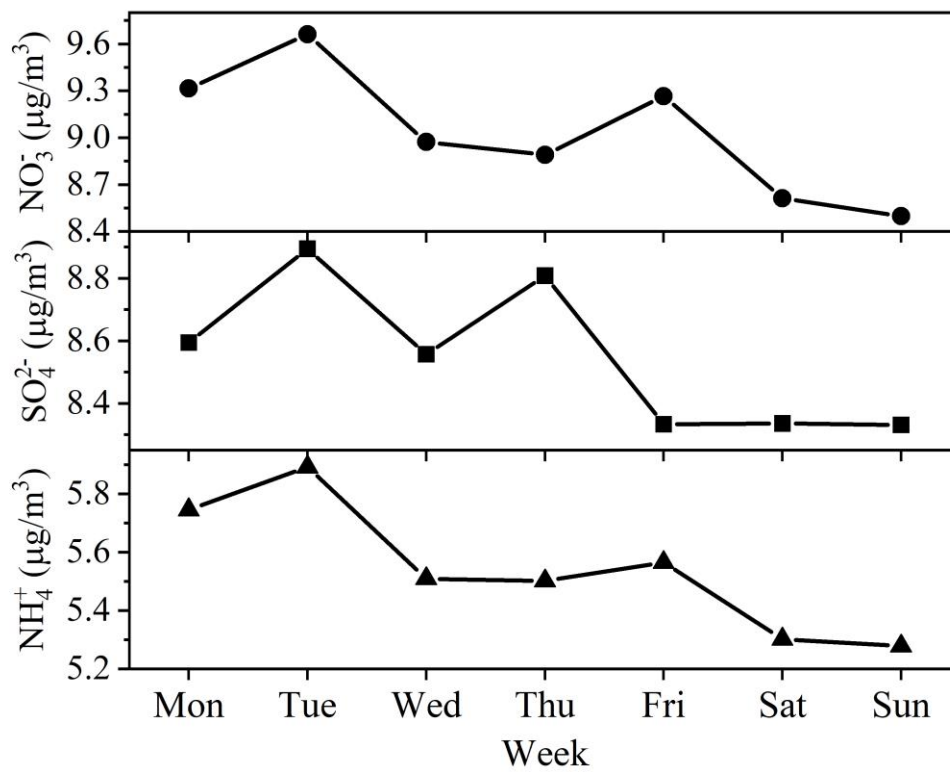
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37 Fig. S5. Diurnal variations in metrological conditions from 2015 to 2017.

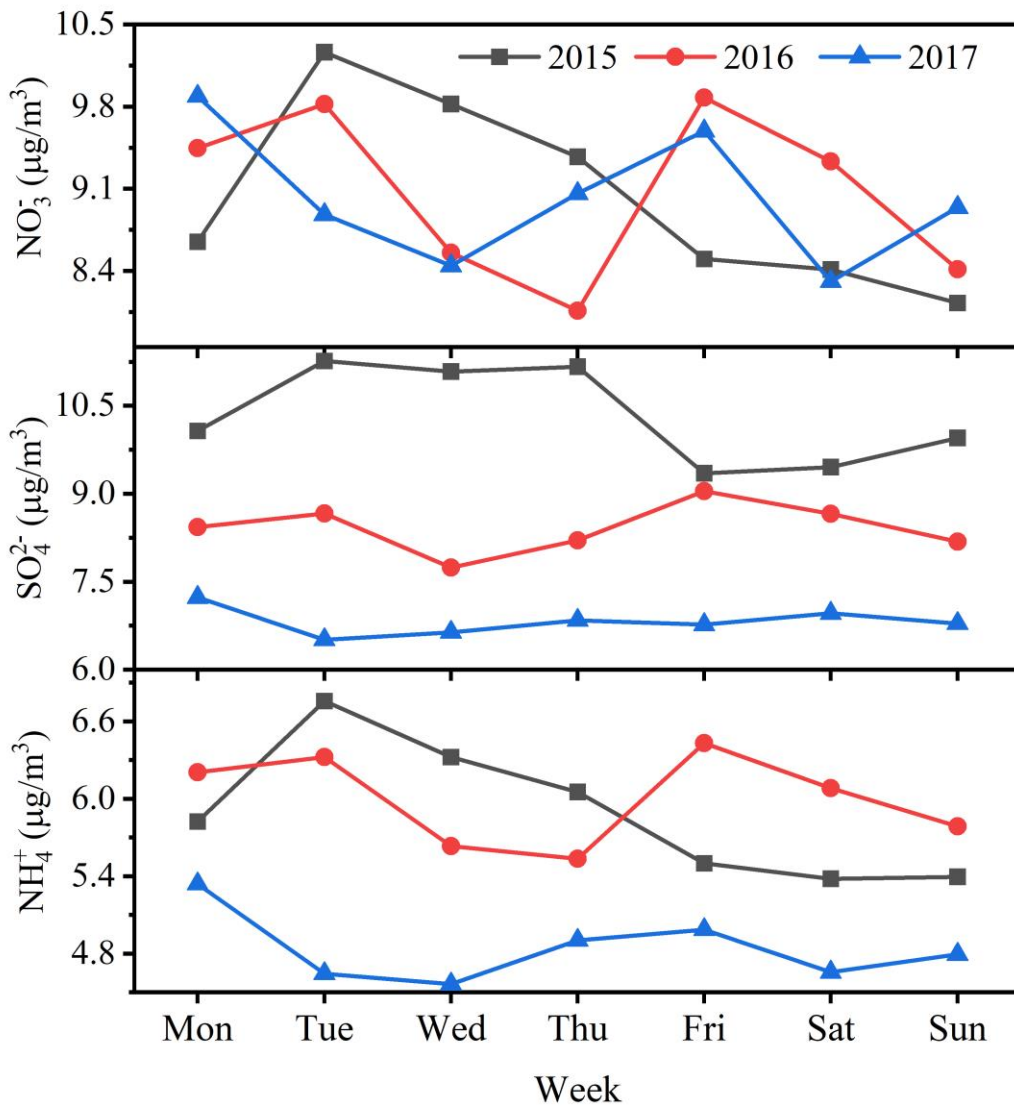
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40 Fig. S6. Weekly variations in NSA during the overall observation period.

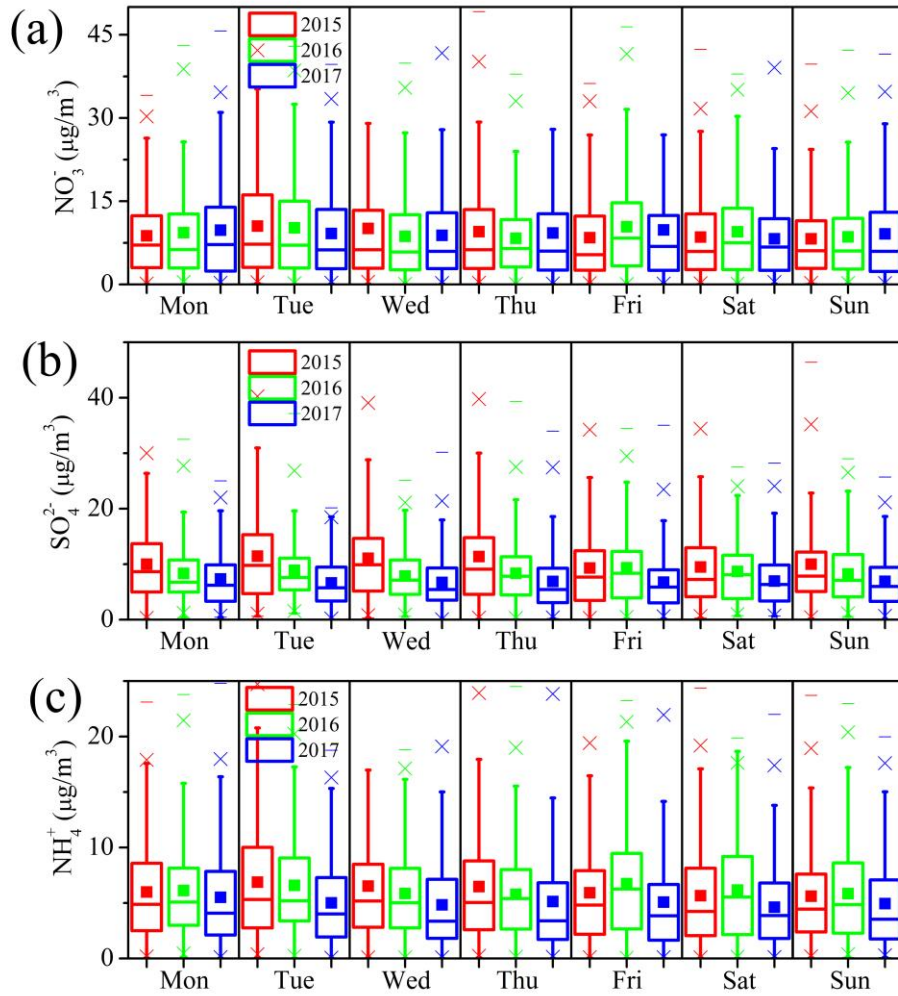
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43 Fig. S7. Weekly variations in NSA from 2015 to 2017 (Broken line diagram).

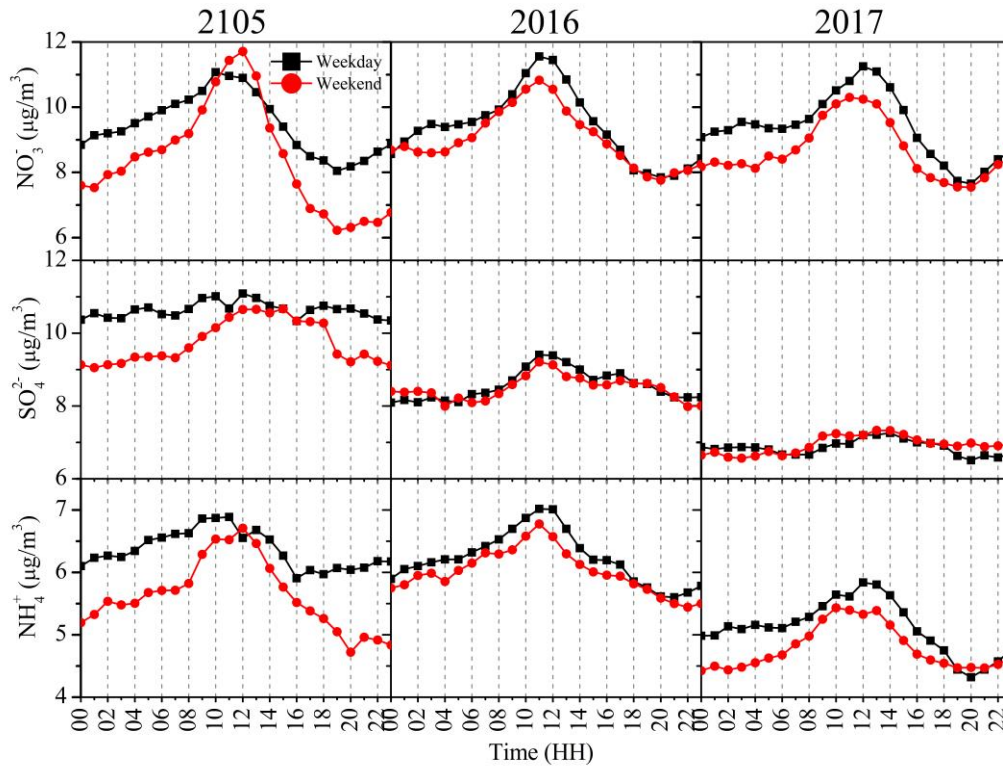
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46 Fig. S8. Weekly variations in NSA from 2015 to 2017 (Box diagram).

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49 Fig. S9. Diurnal variations in NSA during weekdays and weekends from 2015 to 2017.

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51 Table S2. Correlation analysis of Fe and Mn concentrations with SOR and NOR under
 52 different PM_{2.5} concentrations.

		(Fe+Mn) under different PM _{2.5} concentrations					
		0-50	50-100	100-150	150-200	200-250	>250
SOR	R ²	0.0061	0.0989	0.1118	0.0245	-0.0010	-0.0007
	r	-0.0789**	-0.3149**	-0.3352**	-0.1593**	0.0264	0.0416
	k	-0.0412	-0.0968	-0.0898	-0.0386	0.0062	0.0086
NOR	R ²	0.0014	0.0418	0.0036	0.0258	0.1132	0.1544
	r	0.0392**	-0.2050**	-0.0645**	0.1632**	0.3384**	0.3952**
	k	0.0083	-0.0285	-0.0081	0.0203	0.0408	0.0423

R²: Coefficient of determination of the regression analysis; r: Pearson's correlation coefficient;

k: Slope of regression analysis; **: Level of significance: p < 0.01.

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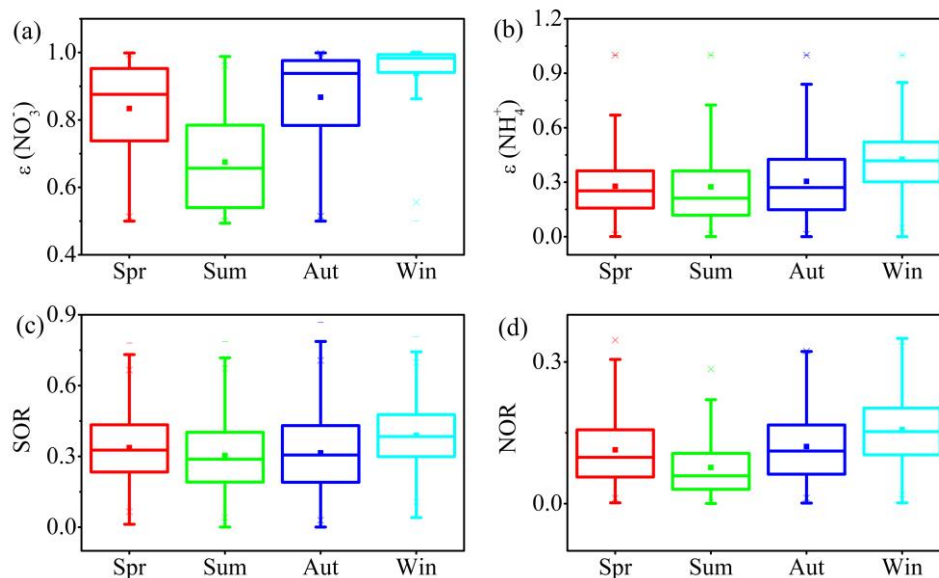
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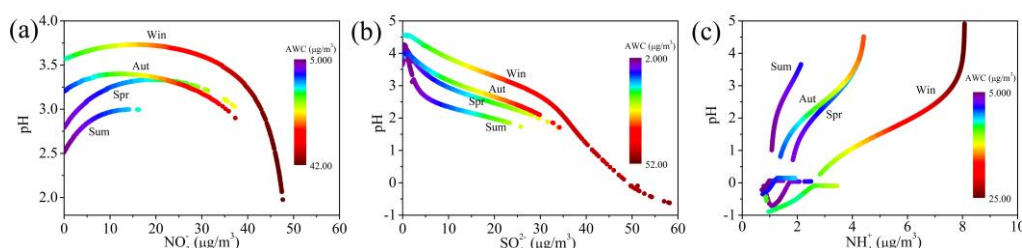
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58 ISORROPIA-II thermodynamic model sensitivity analysis

59 The sensitivity analysis of NSA was simulated by changing the pollutant concentration
 60 input into the ISORROPIA-II thermodynamic model by controlling the variable method.
 61 Variables: SO_4^{2-} , NO_3^- and NH_3 (measurement data during observation periods);
 62 Invariants: temperature (T), RH, Na^+ , Cl^- , Ca^{2+} , K^+ and Mg^{2+} (mean values of
 63 measurement data during observation periods). For example, to study the response of
 64 ammonium and nitrate to changes in sulfate concentration, the Variable is SO_4^{2-} and
 65 Invariants include temperature (T), RH, Na^+ , Cl^- , Ca^{2+} , K^+ , Mg^{2+} , NO_3^- and NH_3 . The
 66 degree of response is expressed by the coefficient of variation: standard deviation/mean
 67 value*100.



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 69 Fig. S10. (a) Gas-particle phase partitioning of NO_3^- . (b) Gas-particle phase partitioning
 70 of NH_4^+ . (c) SOR. (d) NOR.



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 72 Fig. S11. The effect of changes in NO_3^- , SO_4^{2-} , NH_4^+ and aerosol water content (AWC)
 73 on pH.

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76 Table S3. Simulation of NSA emission reduction control effect (%) and its influence on pH based on the ISORROPIA-II thermodynamic model.

Reduction	Only Reduction NO ₃ ⁻				Only Reduction SO ₄ ²⁻				Only Reduction NH ₃				Synergistic			
	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺	PH	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺	PH	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺	PH	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺	PH
5%	14.48	5.31	18.46	3.56	9.81	9.95	18.84	3.60	11.69	5.44	17.59	3.49	15.06	10.26	21.63	3.57
10%	18.62	5.30	20.35	3.57	9.25	14.97	21.11	3.67	13.18	5.86	18.72	3.43	19.70	15.14	26.67	3.61
15%	22.81	5.29	22.26	3.63	8.77	19.99	23.35	3.73	14.93	6.33	20.01	3.37	24.37	20.04	31.65	3.63
20%	27.05	5.28	24.20	3.60	8.30	25.01	25.63	3.82	16.99	6.96	21.52	3.29	29.01	25.04	36.63	3.69

Synergistic: simultaneous emissions reductions of NO₃⁻, SO₄²⁻ and NH₃

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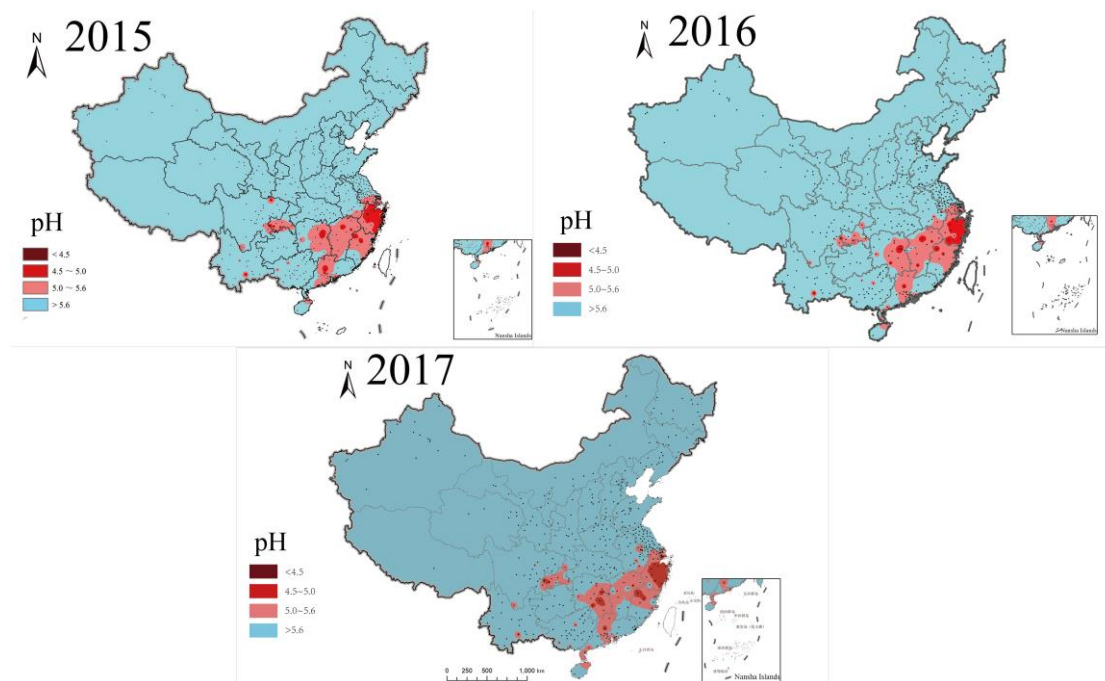
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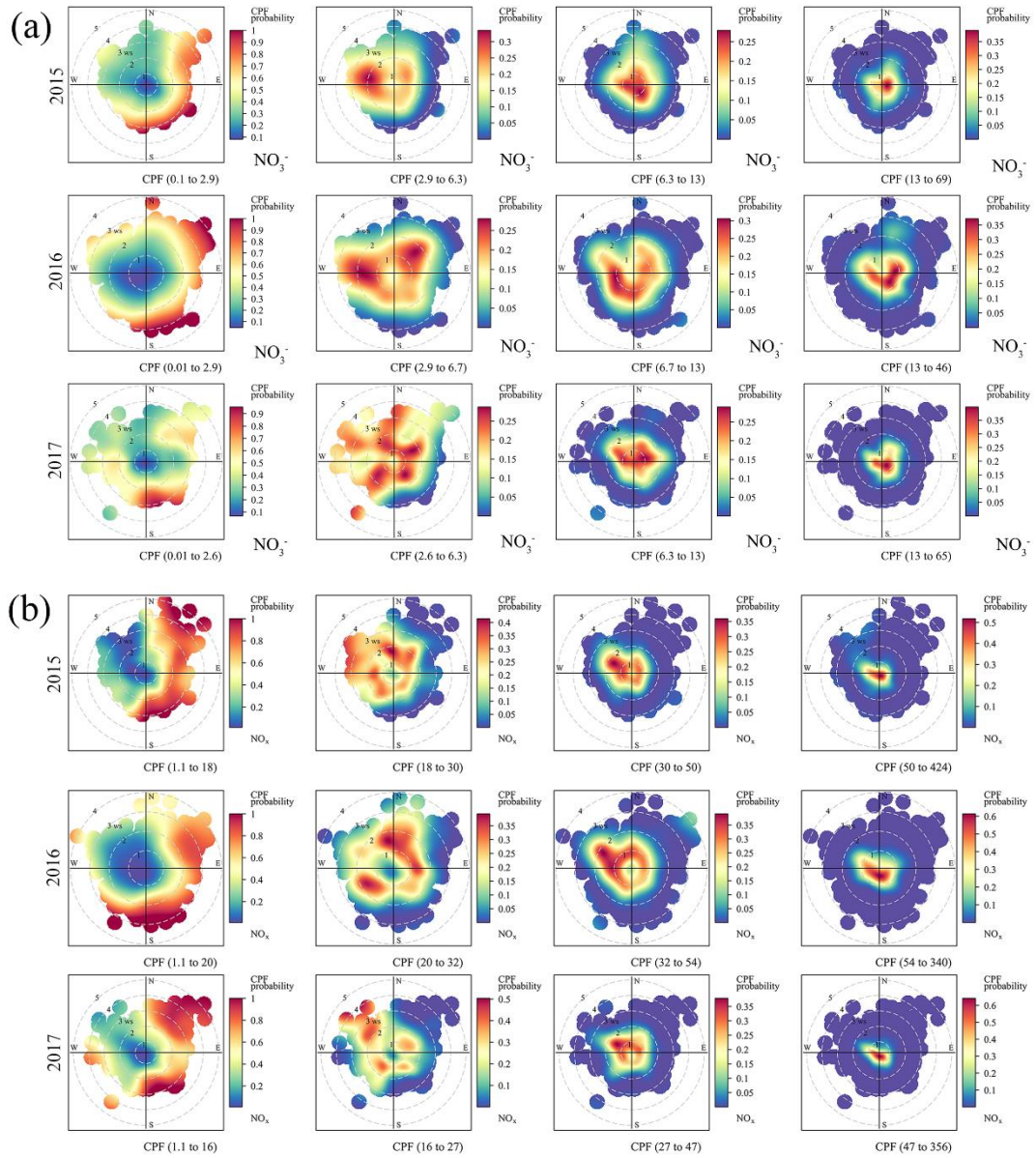


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85 Fig. S12. Acid rain distribution in China

86 (<http://www.mee.gov.cn/hjzl/zghjzkqb/lnzghjzkqb/>, last access: 12 February 2020).

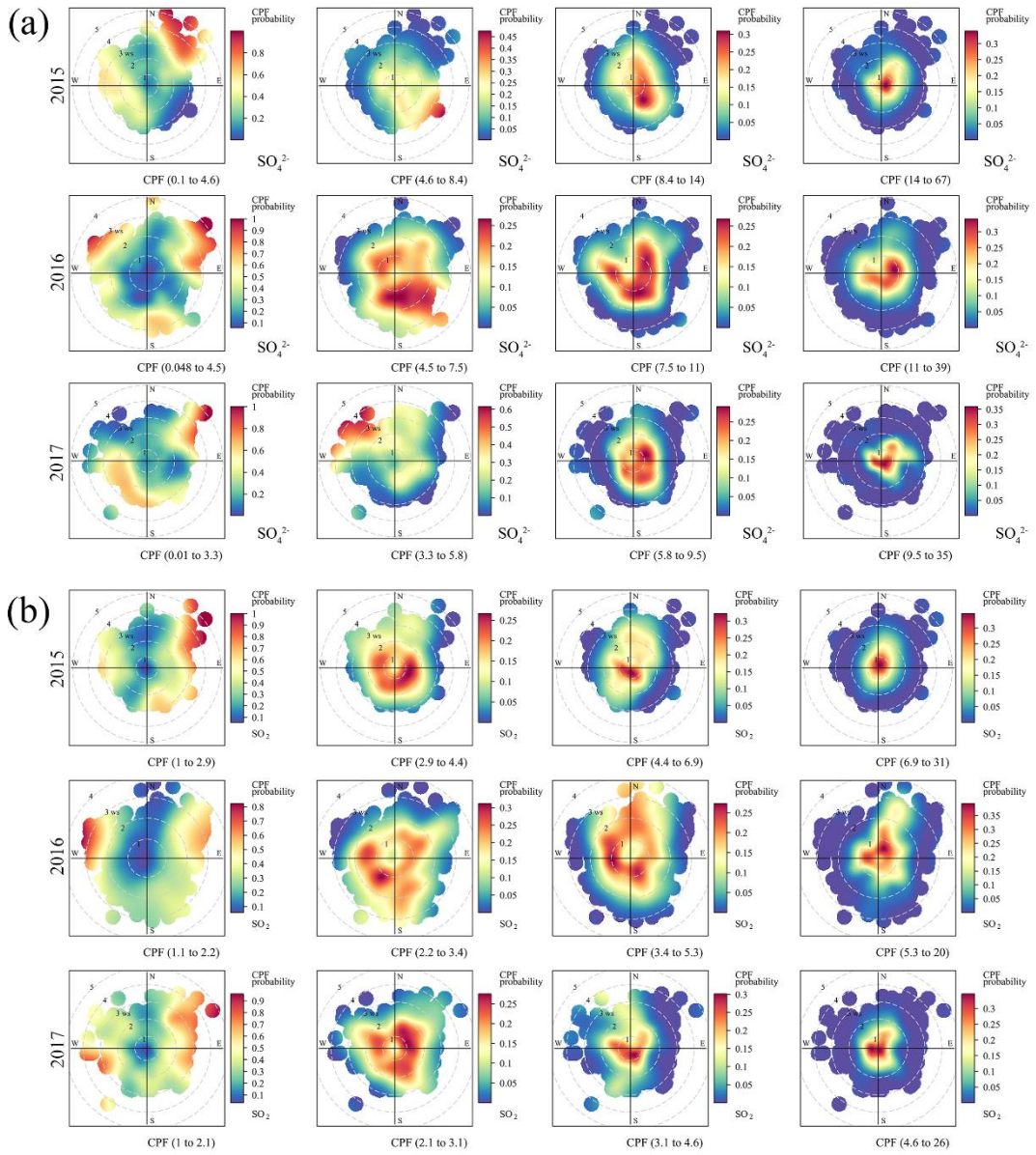
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89 Fig. S13. PolarPlot of the NO_3^- ($\mu\text{g}/\text{m}^3$) and NO_x (ppb) concentrations from 2015 to
 90 2107 in Chengdu based on the conditional probability functions (CPF) for the following
 91 ranges of percentile intervals: 0-25%, 25-50%, 50-75%, and 75-100%. (a) NO_3^- . (b)
 92 NO_x .

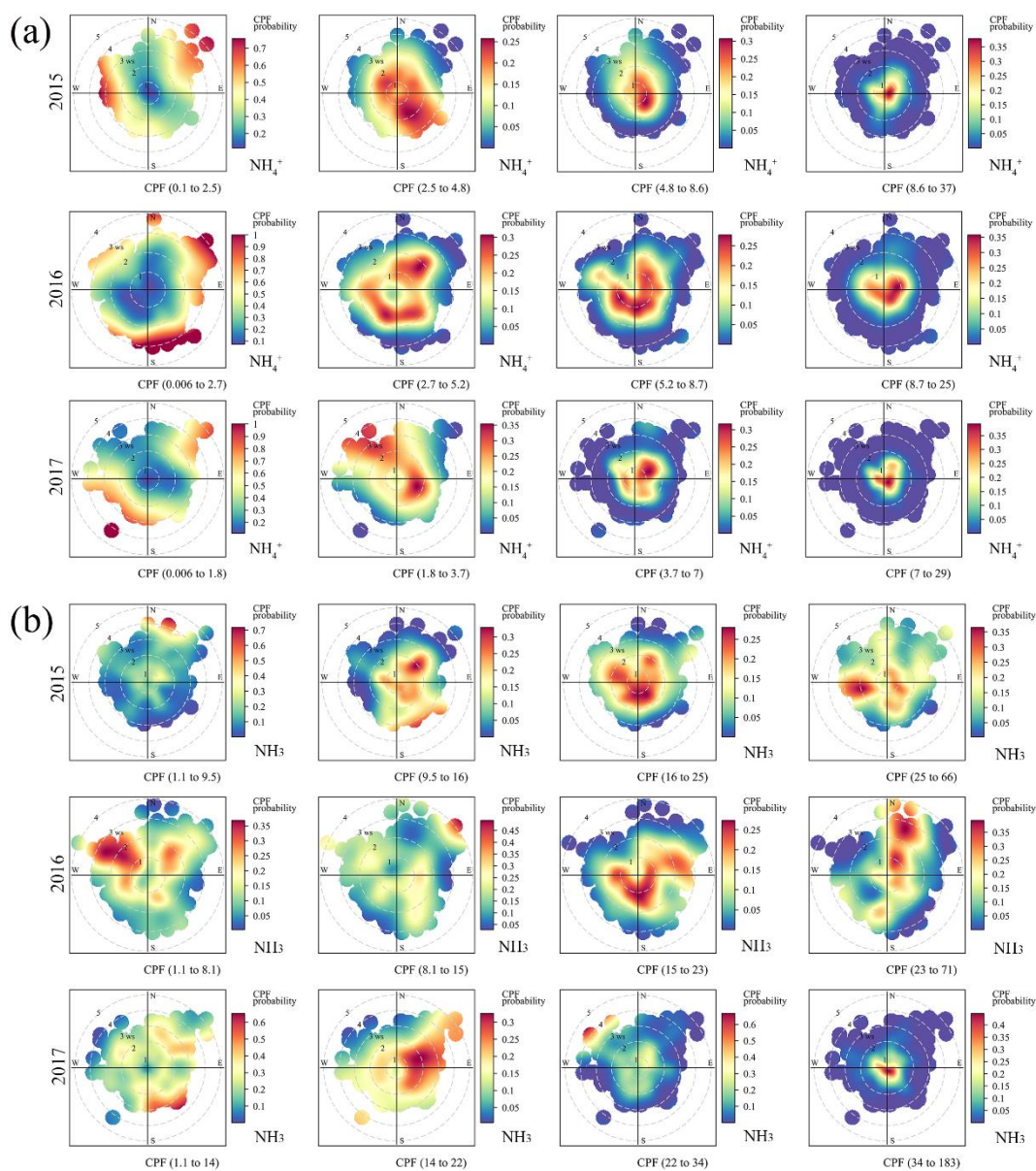
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95 Fig. S14. PolarPlot of the SO₄²⁻ (μg/m³) and SO₂ (ppb) concentrations from 2015 to
 96 2107 in Chengdu based on the CPF for the following ranges of percentile intervals: 0-
 97 25%, 25-50%, 50-75%, and 75-100%. (a) SO₄²⁻. (b) SO₂.

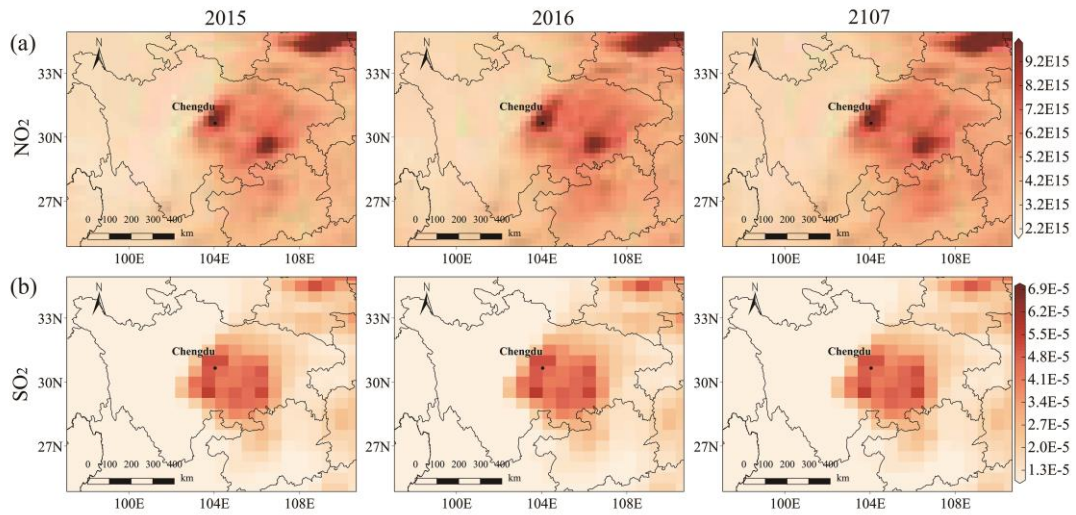
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100 Fig. S15. PolarPlot of the NH_4^+ ($\mu\text{g}/\text{m}^3$) and NH_3 (ppb) concentrations from 2015 to
 101 2017 in Chengdu based on the CPF for the following ranges of percentile intervals: 0-
 102 25%, 25-50%, 50-75%, and 75-100%. (a) NH_4^+ . (b) NH_3 .

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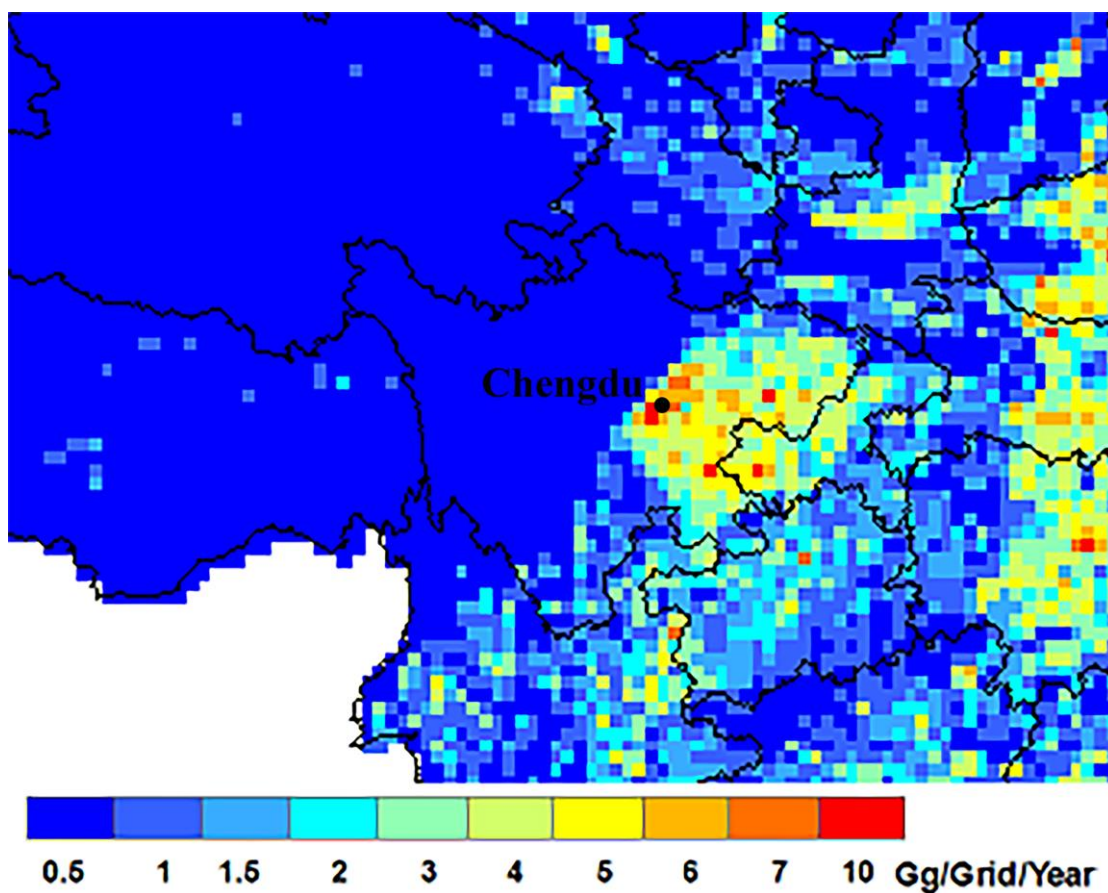


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105 Fig. S16. Spatial distribution characteristics of NO₂ and SO₂ in the Sichuan Basin in
 106 Southwest China from 2015 to 2017. (Data are from
 107 <https://giovanni.gsfc.nasa.gov/giovanni/>, last access: 12 February 2020). (a) Nitrogen
 108 dioxide (NO₂) total column (30% cloud screened) (1/cm²), data source: OMI. (b) Sulfur
 109 dioxide (SO₂) column mass density (kg/m²), data source: MERRA-2 Model.

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113 Fig. S17. Gridded NH₃ emissions in southwest China in 2016 from the Multiresolution
114 Emission Inventory for China (MEIC, website: www.meicmodel.org, last access: 12
115 February 2020).