

Table S1 Seasonal aerosol pH in response to changing NHR (training data).

	Observed NHR	Deviation +20% NHR	Deviation -20% NHR	Estimated NHR	Remove p < 0.05 factors Estimated NHR
pH-Winter	4.87 ± 0.48	4.70 ± 0.49	5.03 ± 0.48	4.99 ± 0.49	4.95 ± 0.49
pH-Spring	4.26 ± 0.59	4.16 ± 0.60	4.39 ± 0.57	4.12 ± 0.61	4.09 ± 0.61
pH-Summer	3.93 ± 0.70	3.83 ± 0.71	4.03 ± 0.69	4.00 ± 0.73	4.05 ± 0.75
pH-Autumn	4.80 ± 0.64	4.69 ± 0.64	4.93 ± 0.63	4.55 ± 0.64	4.57 ± 0.64

*The observed NHR denotes the measured ammonium conversion ratio. Deviation +20% NHR represents 1.2 times the observed NHR, and deviation -20% NHR represents 0.8 times the observed NHR. The estimated NHR was derived through multiple linear regression analysis, and the estimated NHR after removing factors with $p < 0.05$ was obtained through multiple linear regression analysis.

Table S2 Seasonal Δ pH-total and the independent contribution of each factor.

	Δ pH -total	Δ pH -T	Δ pH- RH	Δ pH- SO ₄ ²⁻	Δ pH- NH _x	Δ pH- NO ₃ ⁻	Δ pH- Cl ⁻	Δ pH- NVCs	Δ pH- others
Win-Spr	-1.17	-0.62	0.05	0.19	-0.89	-0.01	-0.06	0.02	0.14
Spr-Sumr	-0.98	-0.49	0.02	0.00	0.21	0.05	-0.02	-0.38	-0.38
Sum-Aut	0.63	0.65	0.34	-0.21	-0.22	0.28	0.01	-0.06	-0.16
Aut-Win	1.52	0.54	0.04	-0.21	0.70	-0.18	0.04	-0.06	0.64

(The Δ pH-others represents the residual change of pH not captured by these single-factor replacements)

Table. S3 The numbers of PM_{2.5}, PM₁₀ and O₃ pollution days in different seasons

	Winter	Spring	Summer	Autumn
PM _{2.5} ($\mu\text{g m}^{-3}$)	67	17	2	10
PM ₁₀ ($\mu\text{g m}^{-3}$)	44	7	0	9
O ₃ ($\mu\text{g m}^{-3}$)	0	7	33	3

The daily averaged concentrations value exceeding national air quality standards of China

Table S4 Results of T-test and F-test

Winter Model	T-test			F-test		Model Summary		
	Non-standardized coefficient	T	Sig.	F	Sig.	R	R ²	Estimated standard error
Constant	1.204	3.029	0.003					
SO ₄ ²⁻	-0.003	-5.531	0.000					
NO ₃ ⁻	0.006	15.476	0.000					
K ⁺	0.023	4.297	0.000	295.93	P < 0.01	0.88	0.77	0.082
Mg ²⁺	0.328	3.134	0.002					
Ca ²⁺	-0.017	-1.578	0.115					
T	-0.004	-2.581	0.010					
RH	0.001	0.060	0.952					
Spring Model	T-test			F-test		Model Summary		
Constant	0.533	2.835	0.005					
SO ₄ ²⁻	0.006	12.774	0.000					
NO ₃ ⁻	0.005	15.513	0.000					
K ⁺	-0.018	-2.745	0.006	219.02	P < 0.01	0.83	0.69	0.044
Mg ²⁺	-0.065	-0.898	0.370					
Ca ²⁺	-0.017	-3.375	0.001					
T	-0.001	-2.018	0.044					
RH	-0.009	-0.581	0.562					
Summer Model	T-test			F-test		Model Summary		
Constant	-1.389	-9.369	0.000					
SO ₄ ²⁻	0.007	18.481	0.000					
NO ₃ ⁻	0.006	14.972	0.000					
K ⁺	0.010	0.864	0.388	339.18	P < 0.01	0.82	0.67	0.045
Mg ²⁺	0.021	1.794	0.073					
Ca ²⁺	-0.003	-1.281	0.200					
T	0.005	9.903	0.000					
RH	0.066	5.279	0.000					
Autumn Model	T-test			F-test		Model Summary		
Constant	0.656	4.944	0.000					
SO ₄ ²⁻	0.006	16.318	0.000					
NO ₃ ⁻	0.003	15.854	0.000					
K ⁺	-0.003	-0.637	0.524	537.31	P < 0.01	0.86	0.74	0.057
Mg ²⁺	-0.064	-4.426	0.000					
Ca ²⁺	-0.040	-12.934	0.000					
T	-0.001	-3.197	0.001					
RH	0.012	1.435	0.152					

Table S5 Pearson correlation among factors in each season

Winter	NHR	SO₄²⁻	NO₃⁻	K⁺	Mg²⁺	Ca²⁺	T	RH
NHR	1							
SO ₄ ²⁻	0.803**	1						
NO ₃ ⁻	0.862**	0.959**	1					
K ⁺	0.754**	0.849**	0.822**	1				
Mg ²⁺	0.412**	0.316**	0.361**	0.477**	1			
Ca ²⁺	0.229**	0.147**	0.189**	0.360**	0.689**	1		
T	-0.142**	-0.097*	-0.099*	-0.090*	-0.047	0.046	1	
RH	0.339**	0.390**	0.367**	0.479**	0.018	-0.024	-0.224**	1
Spring	NHR	SO₄²⁻	NO₃⁻	K⁺	Mg²⁺	Ca²⁺	T	RH
NHR	1							
SO ₄ ²⁻	0.701**	1						
NO ₃ ⁻	0.743**	0.674**	1					
K ⁺	0.261**	0.397**	0.489**	1				
Mg ²⁺	-0.273**	-0.032	-0.072	0.376**	1			
Ca ²⁺	-0.327**	-0.104**	-0.116**	0.306**	0.898**	1		
T	-0.041	0.129**	-0.051	-0.149**	0.076*	0.051	1	
RH	0.151**	0.024	0.101**	0.117**	-0.248**	-0.242**	-0.845**	1
Summer	NHR	SO₄²⁻	NO₃⁻	K⁺	Mg²⁺	Ca²⁺	T	RH
NHR	1							
SO ₄ ²⁻	0.751**	1						
NO ₃ ⁻	0.677**	0.664**	1					
K ⁺	0.385**	0.544**	0.383**	1				
Mg ²⁺	0.245**	0.125**	0.174**	-0.053	1			
Ca ²⁺	-0.016	0.013	-0.093**	0.473**	0.006	1		
T	0.072*	-0.037	-0.294**	-0.112**	0.215**	0.170**	1	
RH	0.057	0.064*	0.352**	0.05	0.044	-0.167**	-0.840**	1
Autumn	NHR	SO₄²⁻	NO₃⁻	K⁺	Mg²⁺	Ca²⁺	T	RH
NHR	1							
SO ₄ ²⁻	0.786**	1						
NO ₃ ⁻	0.779**	0.801**	1					
K ⁺	0.274**	0.329**	0.501**	1				
Mg ²⁺	-0.067*	0.084**	-0.159**	-0.399**	1			
Ca ²⁺	-0.236**	-0.084**	0.043	0.556**	-0.236**	1		
T	0.135**	0.290**	0.071**	-0.485**	0.420**	-0.300**	1	
RH	0.229**	0.211**	0.130**	-0.129**	0.300**	-0.283**	-0.103**	1

** . At the 0.01 level (two-tailed), the correlation is significant

* . At the 0.05 level (two-tailed), the correlation is significant

Table S6 Aerosol acidity in various parts of China

Sampling Site	Year	Season	pH	Reference
Qinglin	2021 - 2022	Winter	4.6 ± 1.2	Liu et al. (2025)
Xi'an	2017	Winter	5.0 ± 0.6	Wu et al. (2018)
		Summer	4.1 ± 1.2	
Beijing	2016 - 2017	Winter	4.5 ± 0.7	Ding et al. (2019)
		Spring	4.4 ± 1.2	
		Summer	3.8 ± 1.2	
		Autumn	4.3 ± 0.8	
	2015 - 2016	Winter	4.3 ± 0.3	Liu et al. (2017)
	2014	Winter	4.1 ± 1.4	Tan et al. (2018)
Spring		2.1 ± 0.7		
Summer		1.8 ± 0.5		
Autumn		3.1 ± 1.2		
Tianjin	2015	Winter	4.9 ± 0.8	Shi et al. (2019)
Xiamen	2018	Winter	3.5 ± 0.4	Xu et al. (2025)
		Spring	3.0 ± 0.5	
		Summer	2.7 ± 0.5	
		Autumn	2.5 ± 0.5	
Guangzhou	2012 - 2013	All	2.5 ± 0.7	Jia et al. (2020)
Shanghai	2019 - 2020	Winter	3.5 ± 0.4	Fu et al. (2022)
		Spring	3.1 ± 0.5	
		Summer	2.6 ± 0.5	
		Autumn	2.7 ± 0.6	
This Study	2022	Winter	4.9 ± 0.4	
		Spring	3.4 ± 0.7	
		Summer	2.8 ± 0.7	
		Autumn	3.2 ± 0.7	

Table S7 Average mass concentrations of NO₃, SO₄²⁻, NH₄⁺, PM_{2.5}, ALWC, H_{air}⁺ and pH under clean and polluted conditions by season. The last column shows the pvalue from independent T-tests comparing pH between clean and polluted days for each season

Winter	PM_{2.5} (µg m ⁻³)	SO₄²⁻ (µg m ⁻³)	NO₃⁻ (µg m ⁻³)	NH₄⁺ (µg m ⁻³)	RH (%)	T (K)	pH	ALWC (µg m ⁻³)	H_{air}⁺ (µg m ⁻³)	T-test
Average	93.5 ± 40.2	7.3 ± 4.7	16.3 ± 11.9	7.3 ± 5.7	65 ± 21	278.2 ± 4.2	4.8 ± 0.5	80.4 ± 112.9	1.0E-06	
Clean	56.4 ± 10.5	5.9 ± 2.8	11.7 ± 4.9	5.6 ± 2.4	75 ± 16	278.2 ± 3.8	4.8 ± 0.4	63.3 ± 78.1	5.2E-07	p < 0.01
Polluted	114.9 ± 34.7	9.4 ± 5.4	23.8 ± 12.4	10.6 ± 6.1	71 ± 18	277.3 ± 4.1	5.0 ± 0.3	94.3 ± 130.6	1.0E-06	
Spring	PM_{2.5}	SO₄²⁻	NO₃⁻	NH₄⁺	RH	T	pH	ALWC	H_{air}⁺	T-test
Average	61.4 ± 40.8	4.3 ± 1.7	6.4 ± 7.1	2.5 ± 2.6	62 ± 18	291.2 ± 5.8	3.6 ± 0.5	55.7 ± 132.2	6.4E-06	
Clean	42.2 ± 14.0	4.4 ± 1.6	6.8 ± 7.4	3.0 ± 2.7	70 ± 18	291.0 ± 5.8	3.3 ± 0.7	58.9 ± 140.5	6.8E-06	p < 0.01
Polluted	111.9 ± 35.1	7.0 ± 1.7	16.8 ± 8.1	6.0 ± 3.1	67 ± 21	288.1 ± 5.5	4.0 ± 0.3	32.5 ± 34.0	3.1E-06	
Summer	PM_{2.5}	SO₄²⁻	NO₃⁻	NH₄⁺	RH	T	pH	ALWC	H_{air}⁺	T-test
Average	33.3 ± 13.7	3.5 ± 2.2	1.0 ± 1.2	1.1 ± 0.9	61 ± 16	302.0 ± 4.1	2.7 ± 0.7	10.0 ± 25.1	9.9E-06	
Clean	30.7 ± 8.3	4.2 ± 2.2	1.2 ± 1.4	1.5 ± 0.9	66 ± 16	302.2 ± 4.1	2.8 ± 0.7	10.2 ± 25.4	1.0E-05	p > 0.01
Polluted	92.2	4.0	1.1	1.3	57	302.2	2.7	3.8	8.9E-06	
Autumn	PM_{2.5}	SO₄²⁻	NO₃⁻	NH₄⁺	RH	T	pH	ALWC	H_{air}⁺	T-test
Average	43.1 ± 25.1	4.4 ± 3.1	8.7 ± 10.8	3.8 ± 4.1	80 ± 13	290.3 ± 5.1	3.3 ± 0.7	76.2 ± 121.0	1.8E-05	
Clean	36.8 ± 15.3	4.4 ± 2.9	6.1 ± 6.3	3.1 ± 2.5	82 ± 13	290.6 ± 5.2	3.1 ± 0.7	61.9 ± 111.5	1.8E-05	p < 0.01
Polluted	90.9 ± 8.6	7.7 ± 1.0	29.7 ± 3.1	14 ± 1.3	86 ± 9	286.5 ± 1.3	3.9 ± 0.1	171.6 ± 149.5	1.7E-05	

*Only two polluted days in summer; so no SD calculated.

Table S8 Sensitivity of PM_{2.5} pH to SO₄²⁻, NH_x, NO₃⁻, Cl⁻, Ca²⁺, RH and T. The greater the relative standard deviation (RSD), the greater the impact of the variable change.

Impact factor	SO ₄ ²⁻	NH _x	NO ₃ ⁻	Cl ⁻	RH	T	Ca ²⁺
Winter RSD (%)	5.83	4.66	0.85	0.96	4.48	4.38	3.25
Spring RSD (%)	5.58	28.34	4.11	0.23	10.85	9.22	8.75
Summer RSD (%)	21.79	9.06	1.76	0.06	12.11	7.13	6.16
Autumn RSD (%)	6.09	39.77	9.39	0.50	4.39	6.19	1.41

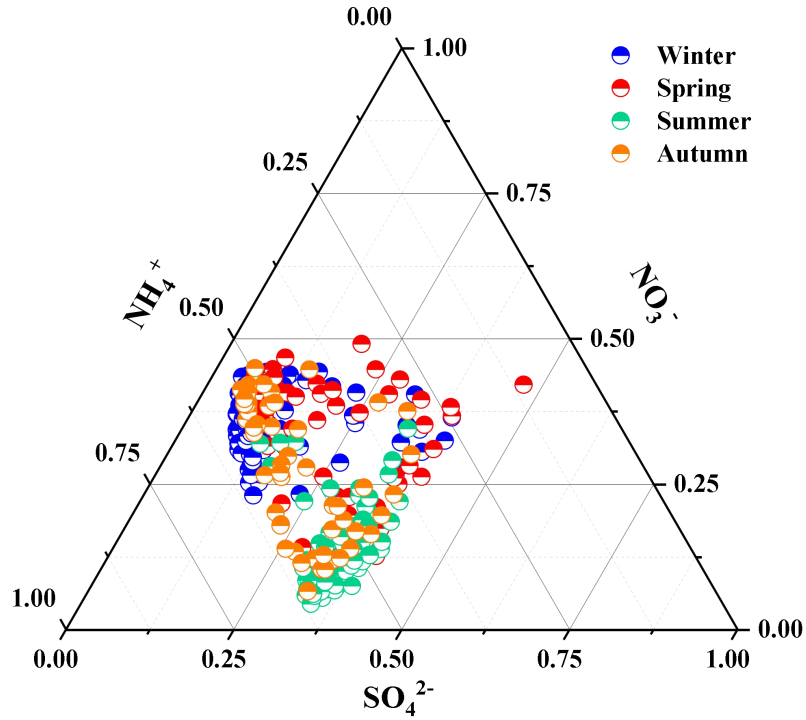


Fig. S1 Ternary diagram of molar concentration ratio of SO_4^{2-} , NO_3^- and NH_4^+ in each season

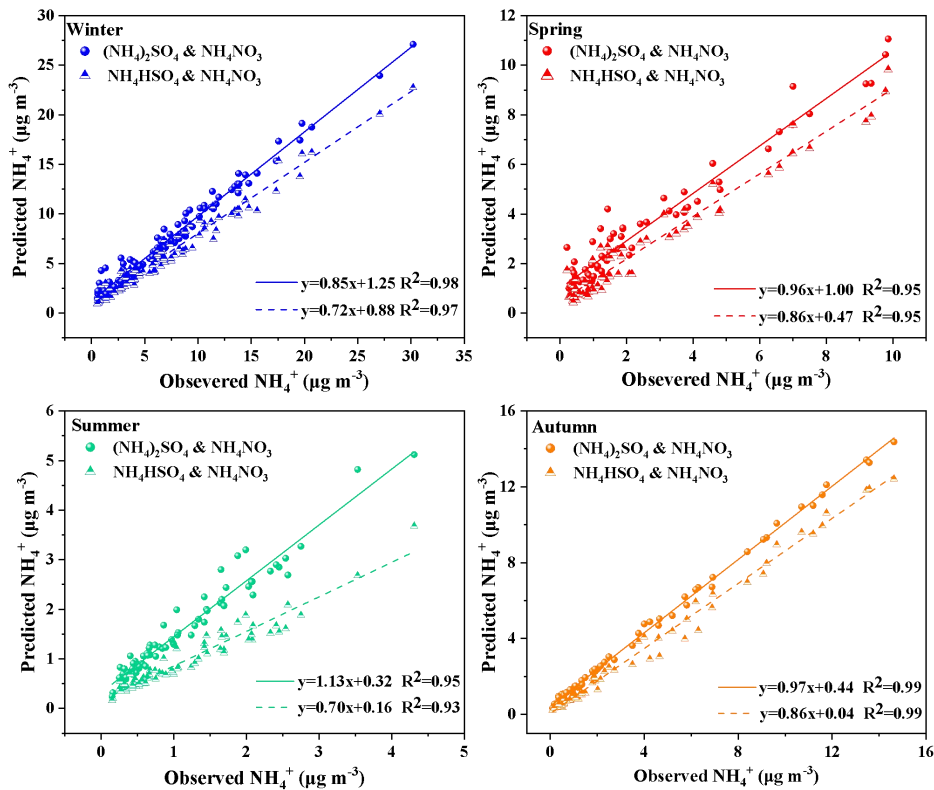


Fig. S2 Linear relationship between observed and predicted values of NH_4^+

(When NH_4^+ , SO_4^{2-} , and NO_3^- exist in the atmosphere as $(\text{NH}_4)_2\text{SO}_4$ and NH_4NO_3 , the predicted NH_4^+ concentration is calculated as: $[\text{NH}_4^+] = [\text{NO}_3^-] \times 18/62 + [\text{SO}_4^{2-}] \times 36/96$; When exist as NH_4HSO_4 and NH_4NO_3 , it is calculated as: $[\text{NH}_4^+] = [\text{NO}_3^-] \times 18/62 + [\text{SO}_4^{2-}] \times 18/96$, $\mu\text{g m}^{-3}$)

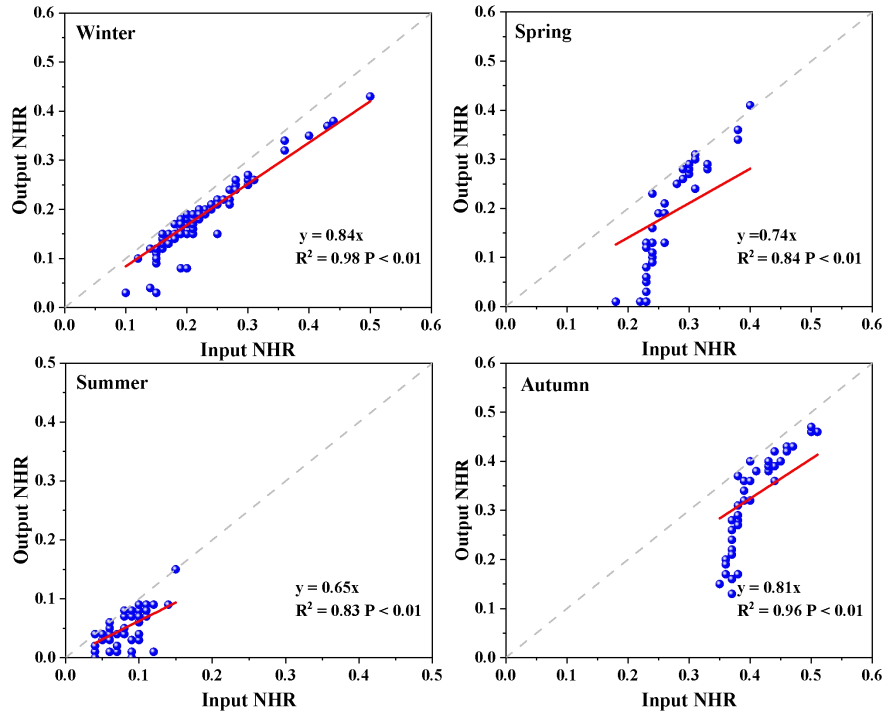


Fig. S3 Correlation between daily mean input and output NHR from the ISORROPIA-II

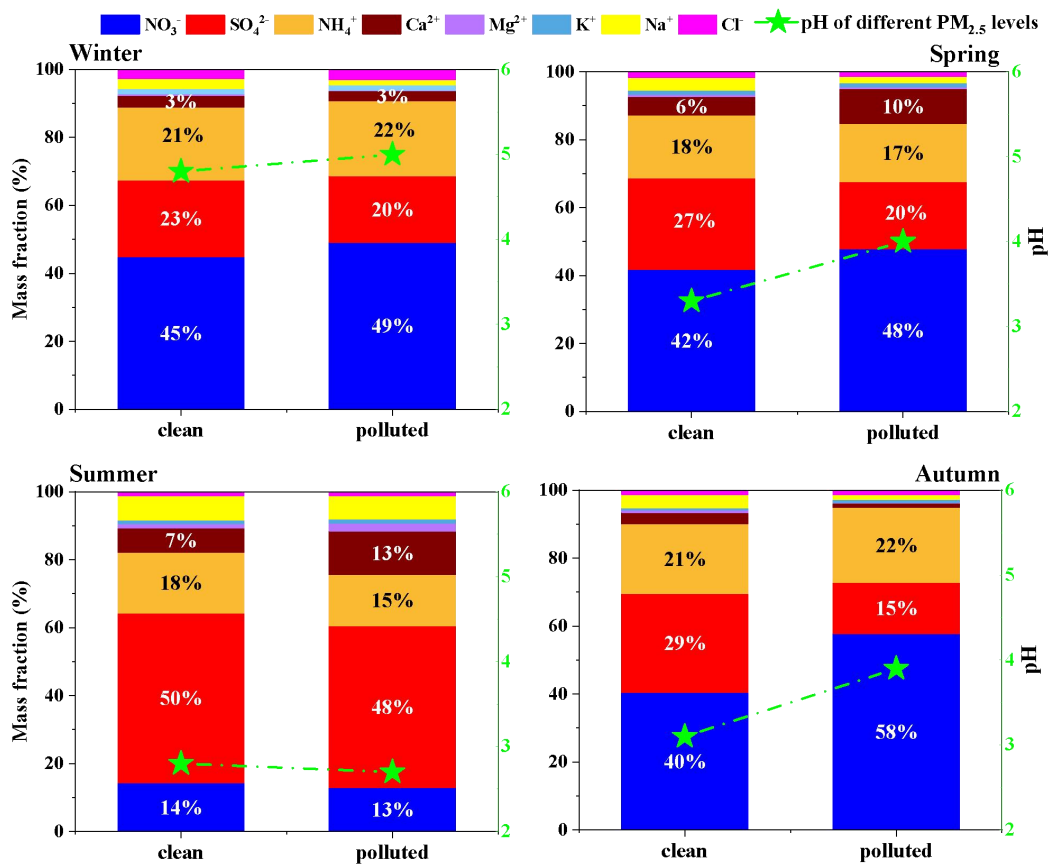


Fig. S4 Percentage change in aerosol pH and major WSIs across different $PM_{2.5}$ concentration bins. The asterisk represents the pH

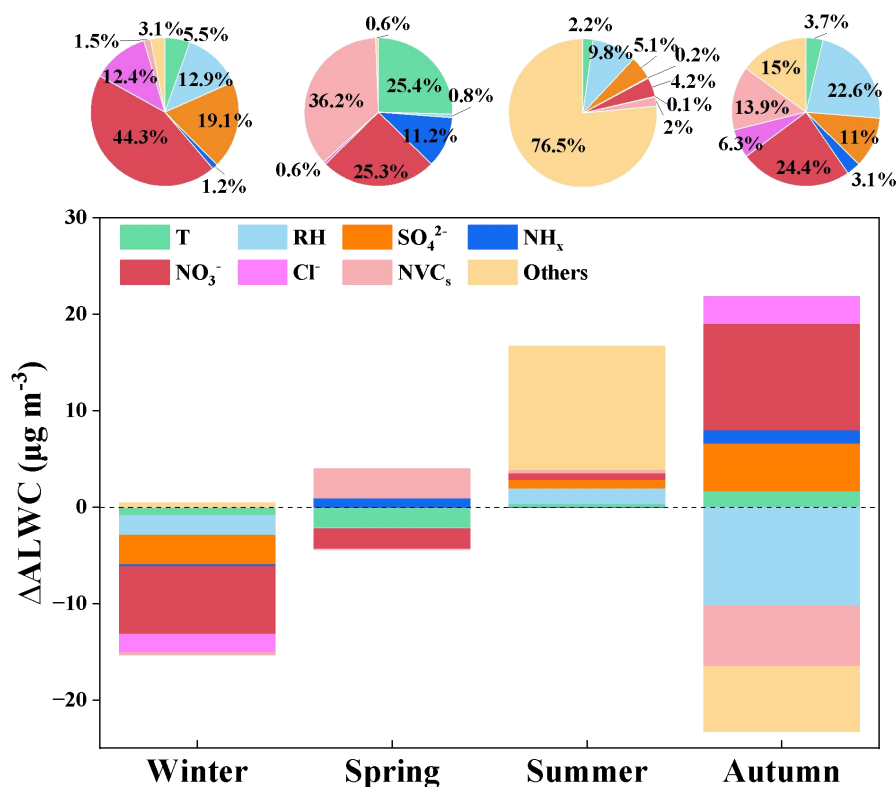


Fig. S5 The contribution of various influencing factors to the seasonal ALWC. The pie chart shows the relative contributions of various influencing factors to the seasonal ALWC (absolute values of ALWC was taken for pie chart).

Reference:

Ding, J., Zhao, P., Su, J., Dong, Q., Du, X., and Zhang, Y.: Aerosol pH and its driving factors in Beijing, *Atmos. Chem. Phys.*, 19(12), 7939–7954, <https://doi.org/10.5194/acp-19-7939-2019>, 2019.

Fu, Z., Cheng, L., Ye, X., Ma, Z., Wang, R., Duan, Y., Tao, J., and Cheng, J.: Characteristics of aerosol chemistry and acidity in shanghai after PM_{2.5} satisfied national guideline: Insight into future emission control. *Sci. Total Environ.*, 827, 154319, <http://dx.doi.org/10.1016/j.scitotenv.2022.154319>, 2022.

Jia, S., Chen, W., Zhang, Q., Krishnan, P., Mao, J., Zhong, B., Huang, M., Fan, Q., Zhang, J., Chang, M., Yang, L., and Wang, X.: A quantitative analysis of the driving factors affecting seasonal variation of aerosol pH in Guangzhou, China. *Sci. Total Environ.*, 725, 138228, <https://doi.org/10.1016/j.scitotenv.2020.138228>, 2020.

Liu, M., Song, Y., Zhou, T., Xu, Z., Yan, C., Zheng, M., Wu, Z., Hu, M., Wu, Y., and Zhu, T.: Fine particle pH during severe haze episodes in northern China. *Geophys. Res. Lett.*, 44(10), 5213–5221, <https://doi.org/10.1002/2017GL073210>, 2017.

Liu, Y., Guo, X., Zhang, Y., Cao, Y., Jiang, Y., Qi, W., Shen, M., Li, L., Wang, Q., Dai, W., and Li, J.: Chemical characteristics of wintertime PM_{2.5} in background region of northwest China during urban emission reduction. *Iscience*, 28(10), 113528, <https://doi.org/10.1016/j.isci.2025.113528>, 2025.

Tan, T., Hu, M., Li, M., Guo, Q., Wu, Y., Fang, X., Gu, F., Wang, Y., and Wu, Z.: New insight into PM_{2.5} pollution patterns in Beijing based on one-year measurement of chemical compositions. *Sci. Total Environ.*, 621, 734–743, <https://doi.org/10.1016/j.scitotenv.2017.11.208>, 2018.

Shi, G., Xu, J., Shi, X., Liu, B., Bi, X., Xiao, Z., Chen, K., Wen, J., Dong, S., Tian, Y., Feng, Y., Yu, H., Song, S., Zhao, Q., Gao, J., and Russell, A. G.: Aerosol pH dynamics during haze periods in an urban environment in China: use of detailed, hourly, speciated observations to study the role of ammonia availability and secondary aerosol formation and urban environment. *J. Geophys. Res.: Atmos.*, 124(16), 9730–9742, <https://doi.org/10.1029/2018JD029976>, 2019.

Wu, C.: Seasonal variation of atmospheric acid and alkali substances and gas-solid phase distribution characteristics in typical cities of Guanzhong. University of Chinese Academy of Sciences, Beijing, China, 2018.

Xu, K., Yin, L., Chen, Q., Liao, D., Ji, X., Zhang, K., Wu, Y., Xu, L., Li, M., Fan, X., Zhang, F., Huang, Z., Chen, J., and Hong, Y.: Quantitative analysis of influencing factors to aerosol pH and its responses to PM_{2.5} and O₃ pollution in a coastal city. *J. Environ. Sci.*, 151, 284–297, <https://doi.org/10.1016/j.jes.2024.03.044>, 2025.