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Measurement Report: Quantitative analysis of aerosol acidity and its driving factors in Guanzhong area, Northwest China

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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 ΔpH-total and the independent contribution of each factor.

	ΔpH -total	ΔpH -T	ΔpH-RH	ΔpH-SO_4^{2-}	ΔpH-NH_x	ΔpH-NO_3^-	ΔpH-Cl^-	ΔpH-NVCs	ΔpH-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 ΔpH-others represents the residual change of pH not captured by these single-factor replacements)

Table. S3 The numbers of $PM_{2.5}$, PM_{10} and O_3 pollution days in different seasons

	Winter	Spring	Summer	Autumn
$PM_{2.5}$(μg m^{-3})	67	17	2	10
PM_{10}(μg m^{-3})	44	7	0	9
O_3 (μg 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	295.93	P < 0.01	0.88	0.77	0.082
SO_4^{2-}	-0.003	-5.531	0.000					
NO_3^-	0.006	15.476	0.000					
K^+	0.023	4.297	0.000					
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	219.02	P < 0.01	0.83	0.69	0.044
SO_4^{2-}	0.006	12.774	0.000					
NO_3^-	0.005	15.513	0.000					
K^+	-0.018	-2.745	0.006					
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	339.18	P < 0.01	0.82	0.67	0.045
SO_4^{2-}	0.007	18.481	0.000					
NO_3^-	0.006	14.972	0.000					
K^+	0.010	0.864	0.388					
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	537.31	P < 0.01	0.86	0.74	0.057
SO_4^{2-}	0.006	16.318	0.000					
NO_3^-	0.003	15.854	0.000					
K^+	-0.003	-0.637	0.524					
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**	**SO_4^{2-}**	**NO_3^-**	**K^+**	**Mg^{2+}**	**Ca^{2+}**	**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**	**SO_4^{2-}**	**NO_3^-**	**K^+**	**Mg^{2+}**	**Ca^{2+}**	**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**	**SO_4^{2-}**	**NO_3^-**	**K^+**	**Mg^{2+}**	**Ca^{2+}**	**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**	**SO_4^{2-}**	**NO_3^-**	**K^+**	**Mg^{2+}**	**Ca^{2+}**	**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 NO_3, SO_4^{2-}, NH_4^+, $PM_{2.5}$, 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})	**SO_4^{2-}** (μg m^{-3})	**NO_3^-** (μg m^{-3})	**NH_4^+** (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	**$PM_{2.5}$**	**SO_4^{2-}**	**NO_3^-**	**NH_4^+**	**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	**$PM_{2.5}$**	**SO_4^{2-}**	**NO_3^-**	**NH_4^+**	**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	**$PM_{2.5}$**	**SO_4^{2-}**	**NO_3^-**	**NH_4^+**	**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 SO_4^{2-}, NH_x, NO_3^-, Cl^-, Ca^{2+}, 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

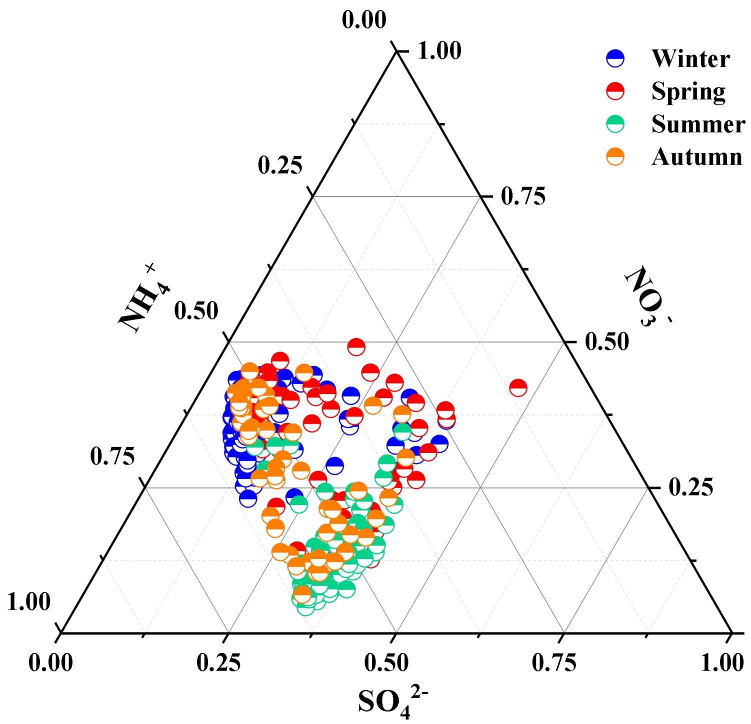

Fig. S1 Ternary diagram of molar concentration ratio of SO_4^{2-}、NO_3^- and NH_4^+ in each season

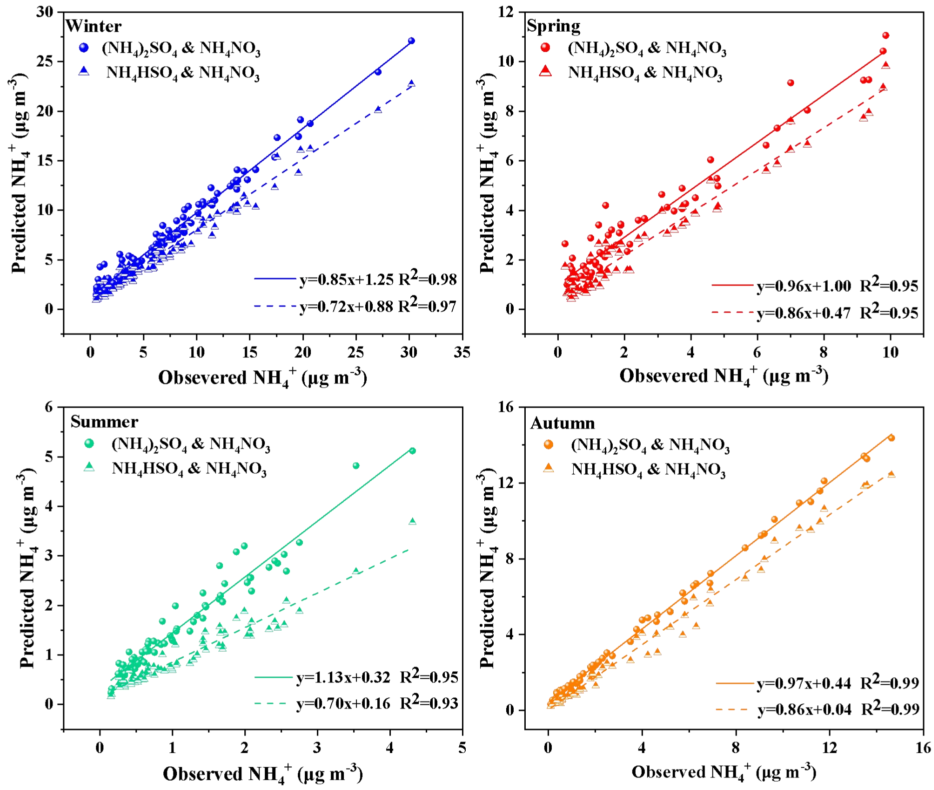

Fig. S2 Linear relationship between observed and predicted values of NH_4^+

(When NH_4^+, SO_4^{2-}, and NO_3^- exist in the atmosphere as $(NH_4)_2SO_4$ and NH_4NO_3, the predicted NH_4^+ concentration is calculated as:$[NH_4^+]=[NO_3^-]\times18/62+[SO_4^{2-}]\times36/96$; When exist as NH_4HSO_4 and NH_4NO_3, it is calculated as:$[NH_4^+]=[NO_3^-]\times18/62+[SO_4^{2-}]\times18/96$, μg m^{-3})

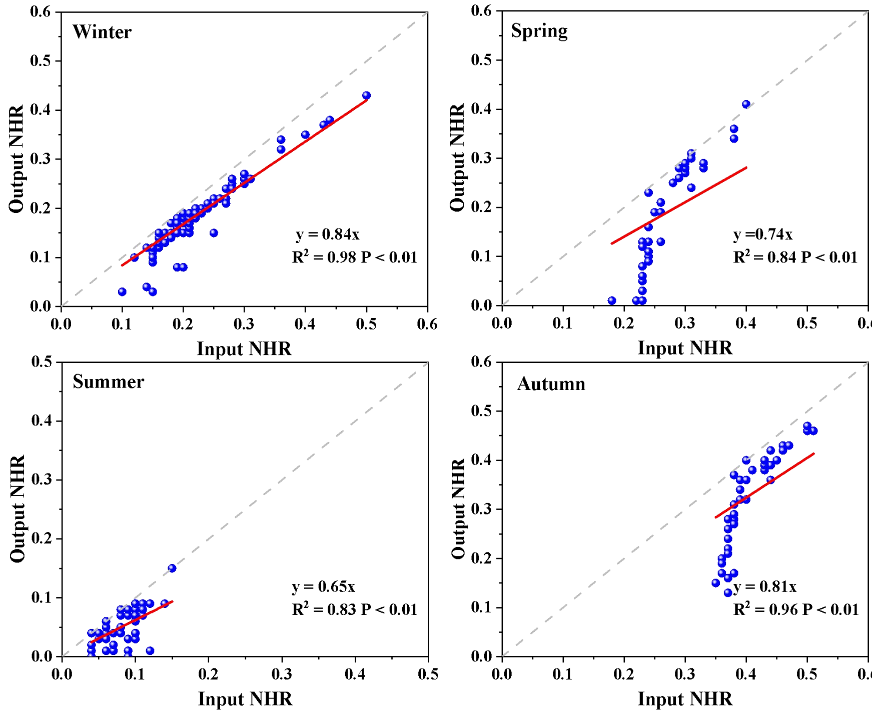

Fig. S3 Correlation between daily mean input and output NHR from the ISORROPIA-II

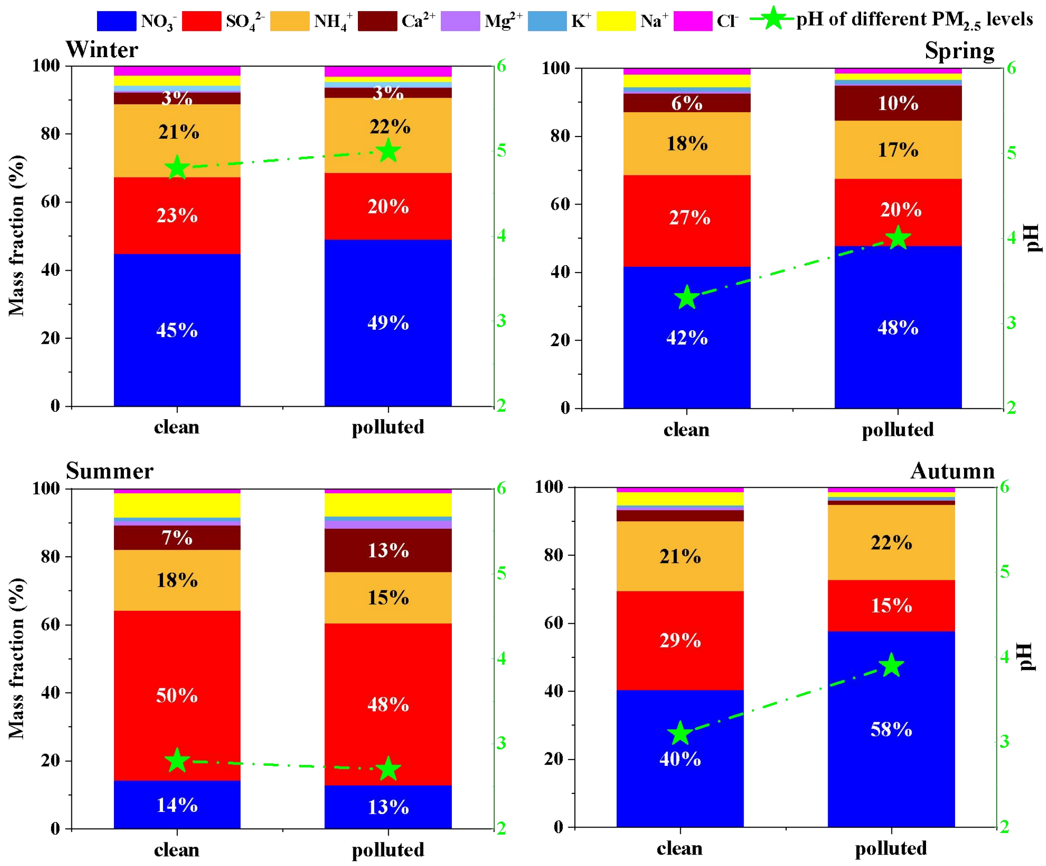

Fig. S4 Percentage change in aerosol pH and major WSIIs across different $PM_{2.5}$ concentration bins. The asterisk represents the pH

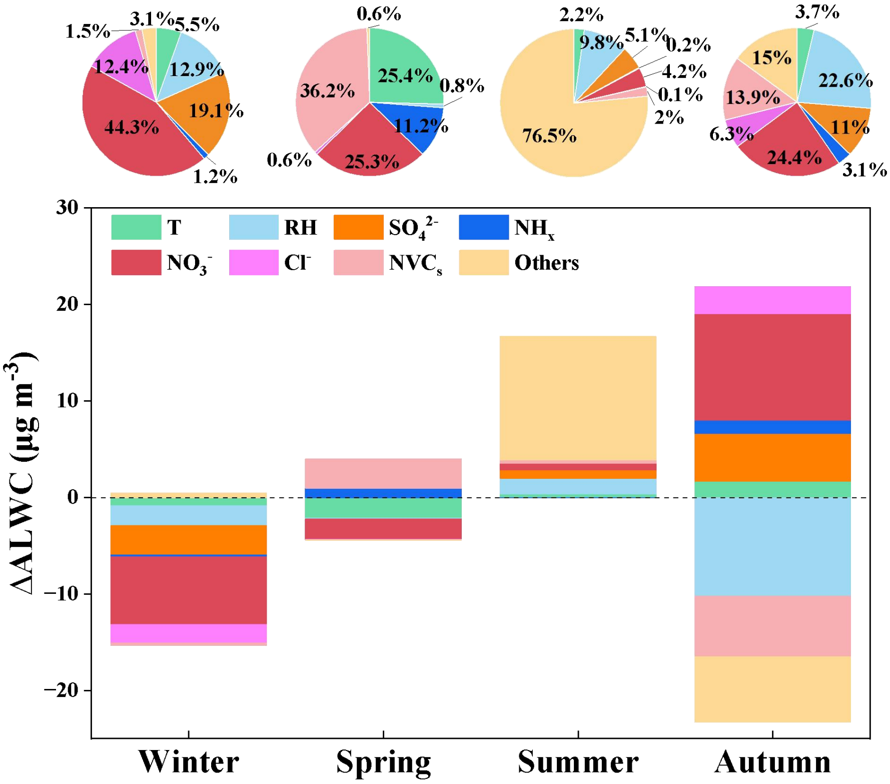

Fig. S5 The contribution of various influencing factors to the seasonal ALWC. The pie chart shows the relative contributions of various influencing factors to the seasonal ALWC (absolute values of ALWC was taken for pie chart).

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