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Dust pollution substantially weakens the impact of ammonia emission reduction on particulate nitrate formation

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Sect. S1 Metrics and Parameters in Machine Learning.

The performance of the model was evaluated using seven metrics. The calculation formulas for these metrics are as follows:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|x_i - y_i| \qquad \text{Eq (S1)}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(x_i - y_i)^2}{n}} \qquad \text{Eq (S2)}$$

$$NMSE = \frac{1}{n}\sum_{i=1}^{n}\frac{MSE}{VAR(x_i)} \qquad \text{Eq (S3)}$$

$$MB = \frac{1}{n}\sum_{i=1}^{n}(x_i - y_i) \qquad \text{Eq (S4)}$$

$$NMB = \frac{\sum_{i=1}^{n}(x_i - y_i)}{\sum_{i=1}^{n} y_i} \times 100\% \qquad \text{Eq (S5)}$$

$$IOA = 1 - \frac{\sum_{i=1}^{n}(x_i - y_i)^2}{\sum_{i=1}^{n}(|x_i - \bar{y}| + |y_i - \bar{y}|)^2} \qquad \text{Eq (S6)}$$

$$R = \frac{\sum_{i=1}^{n}(y_i - \bar{y})(x_i - \bar{x})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \qquad \text{Eq (S7)}$$

In the equations, x_i represents the observed concentration in the test dataset, y_i represents the predicted concentration, and $\bar{x}\ and\ \bar{y}$ are the mean values of the observed and predicted concentrations, respectively. The MAE represents the average absolute error between the predicted and observed concentrations, reflecting the average bias in the model's predictions. The smaller the value, the better the model's performance. RMSE is the square root of the average of the squared differences between the predicted and observed concentrations. NMSE is the ratio of the mean squared error to the variance of the observed data. Normalization allows for a more reasonable comparison of errors across different datasets. MB is the average difference between the predicted and actual values, indicating the systematic bias of the model. NMB is used to assess the deviation between the predicted and actual values, providing a measure of the model's bias. The IOA is a consistency index that ranges from 0 to 1. A value closer to 1 indicates a higher degree of agreement between the model predictions and observations. The correlation coefficient represents the linear correlation between the predicted and actual values.

Sect. S2. Correlation of cations and anions in MARGA sampling data from eight cities in Jiangsu affected by dust.

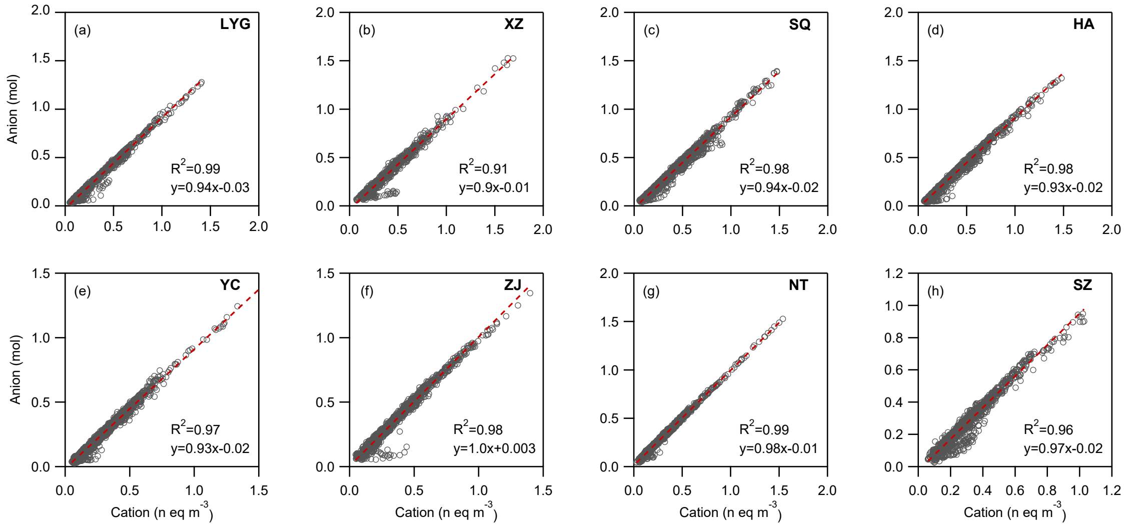

Fig. S1. The correlation between anions and cations of water-soluble inorganic ions in eight cities of Jiangsu during the observation period.

Sect. S3. Simulation of the effects of atmospheric dilution and dispersion on SO_4^{2-} and NO_3^- using a random forest model.

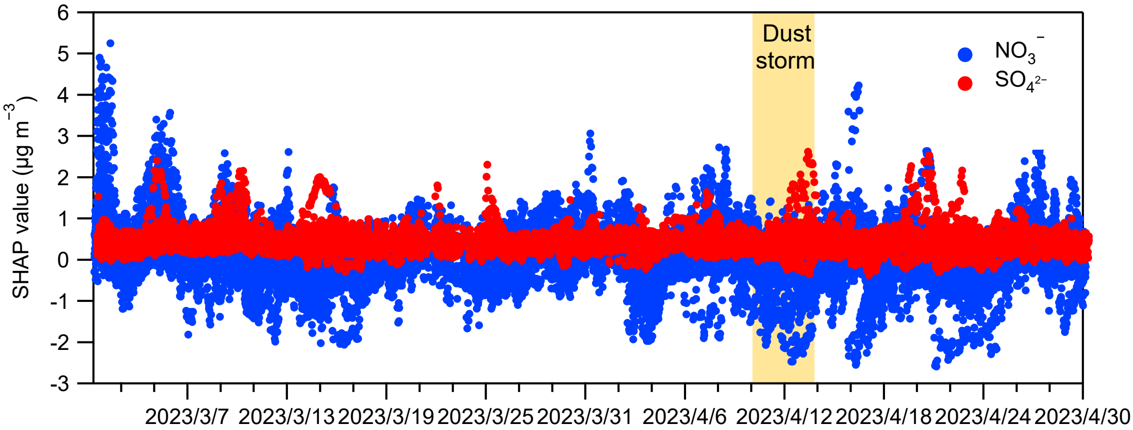

Fig. S2. Time series of the effects of atmospheric dilution and dispersion on NO_3^- and SO_4^{2-}. The y-axis represents the SHAP values of 12 factors simulated using a random forest model (detailed factors are in Table S4). Blue and red dots indicate the contributions of atmospheric dilution and dispersion effects to NO_3^- and SO_4^{2-}, respectively.

Sect. S4. Thermodynamic model validation: comparisons of predicted and observed NH_3, NO_3^-, NH_4^+ and Cl^- in three cities.

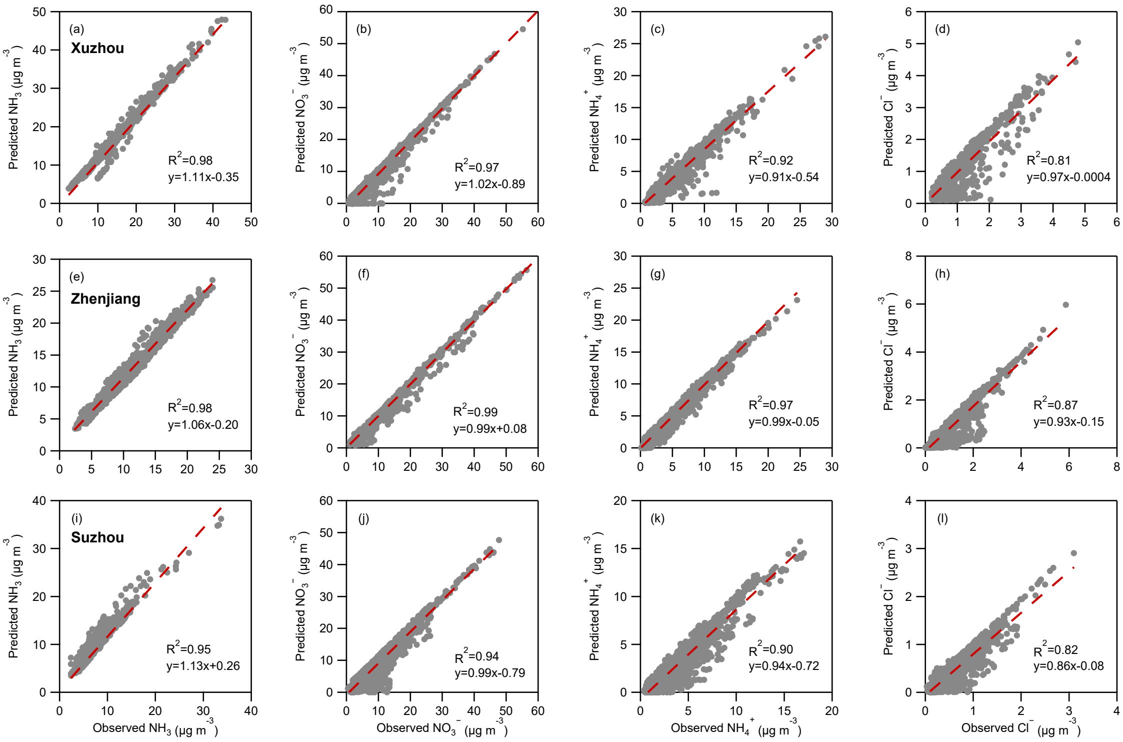

Fig. S3. Comparison of the correlation between the MARGA measured values and the ISORROPIA-II model predicted values in Xuzhou (a-d), Zhenjiang (e-h), and Suzhou (i-l) during the spring of 2023.

Sect. S5. Response of aerosol pH to variations in various factors(TNO_3, Ca^{2+}, TNH_x, SO_4^{2-}, RH and T).

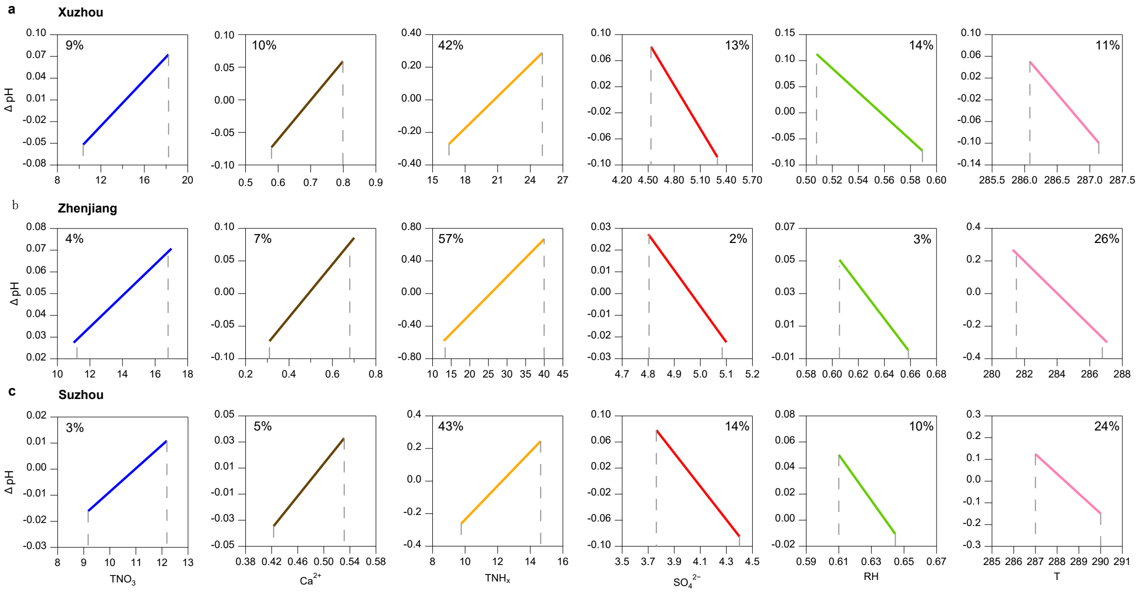

Fig. S4. Quantification of the effects of various factors, including TNO_3 ($TNO_3 = HNO_3 + NO_3^-$), Ca^{2+}, TNH_x ($TNH_x = NH_3 + NH_4^+$), SO_4^{2-}, RH, and T, on pH, with percentages representing the contribution of each factor. The first row (a) corresponds to Suzhou, the second row (b) to Zhenjiang, and the third row (c) to Suzhou. The two gray lines represent values obtained based on data from different months.

Sect. S6. Performance validation results of machine learning : Comparison of predicted and observed pH and ε(NO_3^-) in three cities.

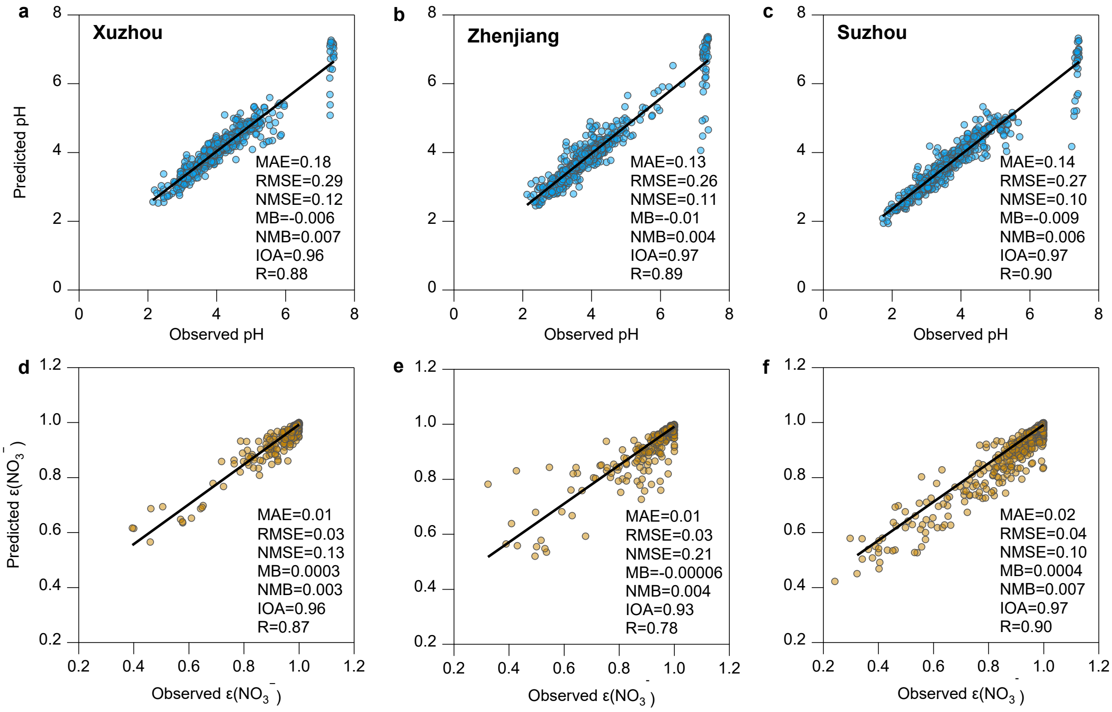

Fig. S5. Correlation between predicted and observed values for (a) – (c) pH and (d) – (f) ε(NO_3^-) in Xuzhou, Zhenjiang, and Suzhou.

Sect. S7. Summary of thermodynamic modeling and machine learning inputs and outputs in Xuzhou, Zhenjiang and Suzhou.

Table. S1 Concentrations (mean ± standard deviation) of water-soluble inorganic ions, gaseous precursors, temperature, relative humidity, and pH measured in Xuzhou during the spring of 2023 across different periods. The unit for T is K, RH is %, and the unit for particulate and gaseous inorganic ions is μg m^{-3}.

Xuzhou	Observation period	Dust strom	Local dust
HCl	0.31±0.09	0.25±0.05	0. 30±0.09
NH_3	14.70±6.32	13.32±4.92	13.24±4.28
HNO_3	1.13±1.63	0.70±0.28	0.76±0.24
Na^+	0.16±0.09	0.29±0.11	0.14±0.05
Ca^{2+}	0.62±0.67	2.00±1.66	0.47±0.36
K^+	0.34±0.21	0.37±0.12	0.38±0.20
Mg^{2+}	0.10±0.08	0.22±0.12	0.08±0.07
NH_4^+	6.37±4.06	2.37±1.78	5.97±2.61
Cl^-	1.11±1.17	0.59±0.16	1.10±0.88
SO_4^{2-}	5.16±2.42	3.25±2.03	4.66±1.42
NO_3^-	13.37±10.17	4.68±2.44	12.49±7.91
T	287.23±5.26	290.96±3.12	284.82±4.27
RH	0.63±0.18	0.53±0.14	0.65±0.18
pH	4.11±0.78	5.50±1.65	4.12±0.52

Table. S2 Concentrations (mean ± standard deviation) of water-soluble inorganic ions, gaseous precursors, temperature, relative humidity, and pH measured in Zhenjiang during the spring of 2023 across different periods. The unit for T is K, RH is %, and the unit for particulate and gaseous inorganic ions is μg m^{-3}.

Zhenjiang	Observation period	Dust strom	Local dust
HCl	0.13±0.14	0.19±0.08	0.11±0.15
NH_3	9.96±4.54	8.18±6.01	9.27±3.99
HNO_3	1.01±0.33	0.96±0.32	0.90±0.25
Na^+	0.12±0.14	0.09±0.06	0.13±0.15
Ca^{2+}	0.49±0.55	1.69±1.41	0.30±0.23
K^+	0.17±0.14	0.07±0.06	0.18±0.13
Mg^{2+}	0.10±0.07	0.18±0.10	0.08±0.06
NH_4^+	5.42±3.98	1.85±2.34	5.06±3.26
Cl^-	1.03±0.83	0.60±0.63	1.00±0.76
SO_4^{2-}	5.03±2.57	3.08±2.48	4.60±2.18
NO_3^-	13.23±10.41	5.20±4.68	12.59±8.47
T	287.48±5.23	290.72±3.47	284.89±3.61
RH	0.66±0.17	0.55±0.16	0.67±0.17
pH	3.87±0.67	5.44±1.69	3.92±0.32

Table. S3 Concentrations (mean ± standard deviation) of water-soluble inorganic ions, gaseous precursors, temperature, relative humidity, and pH measured in Suzhou during the spring of 2023 across different periods. The unit for T is K, RH is %, and the unit for particulate and gaseous inorganic ions is μg m^{-3}.

Suzhou	Observation period	Dust strom	Local dust
HCl	0.06±0.04	0.07±0.03	0.06±0.05
NH_3	6.91±3.43	8.20±3.17	6.16±3.51
HNO_3	0.63±0.48	0.57±0.45	0.85±0.56
Na^+	0.34±0.30	0.43±0.13	0.35±0.33
Ca^{2+}	0.48±0.32	0.92±0.52	0.35±0.26
K^+	0.21±0.11	0.22±0.08	0.19±0.08
Mg^{2+}	0.07±0.05	0.11±0.05	0.06±0.05
NH_4^+	4.57±3.16	2.03±1.35	4.62±2.95
Cl^-	0.62±0.46	0.45±0.21	0.67±0.45
SO_4^{2-}	4.09±2.17	3.06±1.95	3.96±2.29
NO_3^-	10.09±8.13	4.37±2.09	9.90±6.97
T	288.05±5.12	291.64±3.41	285.97±3.22
RH	0.64±0.15	0.57±0.15	0.66±0.15
pH	3.67±0.84	5.30±1.67	3.74±0.69

Table. S4 List of input meteorological parameters for simulating the effects of atmospheric dilution and dispersion on SO_4^{2-} and NO_3^- using a random forest model.

Variable Abbreviation	Full Variable Name	Unit
U10	10m u-component of wind	$m\ s^{-1}$
V10	10m v-component of wind	$m\ s^{-1}$
U850	850hPa u-component of wind	$m\ s^{-1}$
V850	850hPa v-component of wind	$m\ s^{-1}$
W850	850hPa w-component of wind	$m\ s^{-1}$
U650	650hPa u-component of wind	$m\ s^{-1}$
V650	650hPa v-component of wind	$m\ s^{-1}$
W650	650hPa w-component of wind	$m\ s^{-1}$
U500	500hPa u-component of wind	$m\ s^{-1}$
V500	500hPa v-component of wind	$m\ s^{-1}$
W500	500hPa w-component of wind	$m\ s^{-1}$
BLH	Boundary layer height	m