atmosphere

MDPI

Supplementary Materials:

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S1. Model evaluation

Several statistical indicators were computed to evaluate the models' abilities to reproduce observed $PM_{2.5}$ concentrations (so-called baseline scenario SC1). Considering M as the modelled values, O as the observations, n as the number of model–observation pairs, $\bar{M} = \frac{\sum_{i=1}^{n} M_i}{n}$ as the averaged modelled value and $\bar{O} = \frac{\sum_{i=1}^{n} O_i}{n}$ as the averaged observed value, the following metrics are used for evaluation:

$$NMB = \frac{\sum_{i=1}^{n} M_i - O_i}{\sum_{i=1}^{n} O_i} \quad \text{(S1)}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - M_i)^2} \quad \text{(S2)}$$

$$R = \frac{\sum_{i=1}^{n}(M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^{n}(M_i - \bar{M})^2}\sqrt{\sum_{i=1}^{n}(O_i - \bar{O})^2}} \quad \text{(S3)}$$

In addition, the model quality indicator (MQI), i.e., the statistical indicator of MQO, can be defined as follows:

$$MQI = \frac{1}{n}\frac{RMSE}{RMS_U} \quad \text{(S4)}$$

where RMS_U is the root mean square of the measurement uncertainty as defined by [86,87].

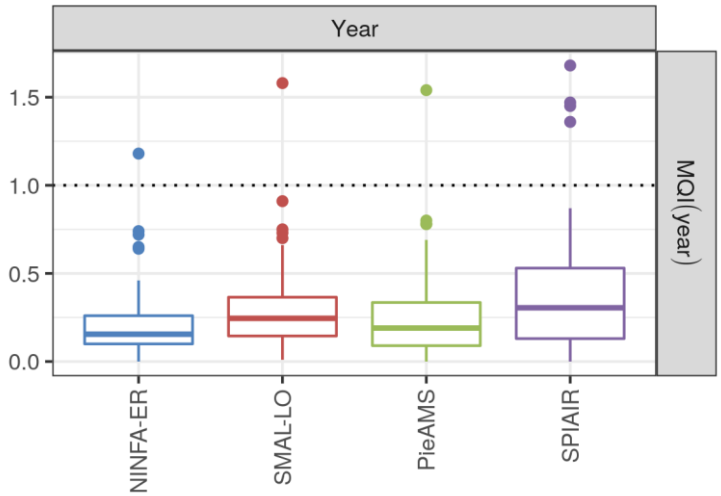

Figure S1. Model quality indicator (MQI) computed for yearly average $PM_{2.5}$ model results. The horizontal lines in a box indicate the median; the lower and upper ends of a box indicate the 25th and 75th percentiles, respectively. The upper whisker extends from the hinge to the largest value no further than 1.5 * inter-quartile range from the hinge. The lower whisker extends from the hinge

to the smallest value at most 1.5 * IQR of the hinge. Data beyond the end of the whiskers are plotted individually.

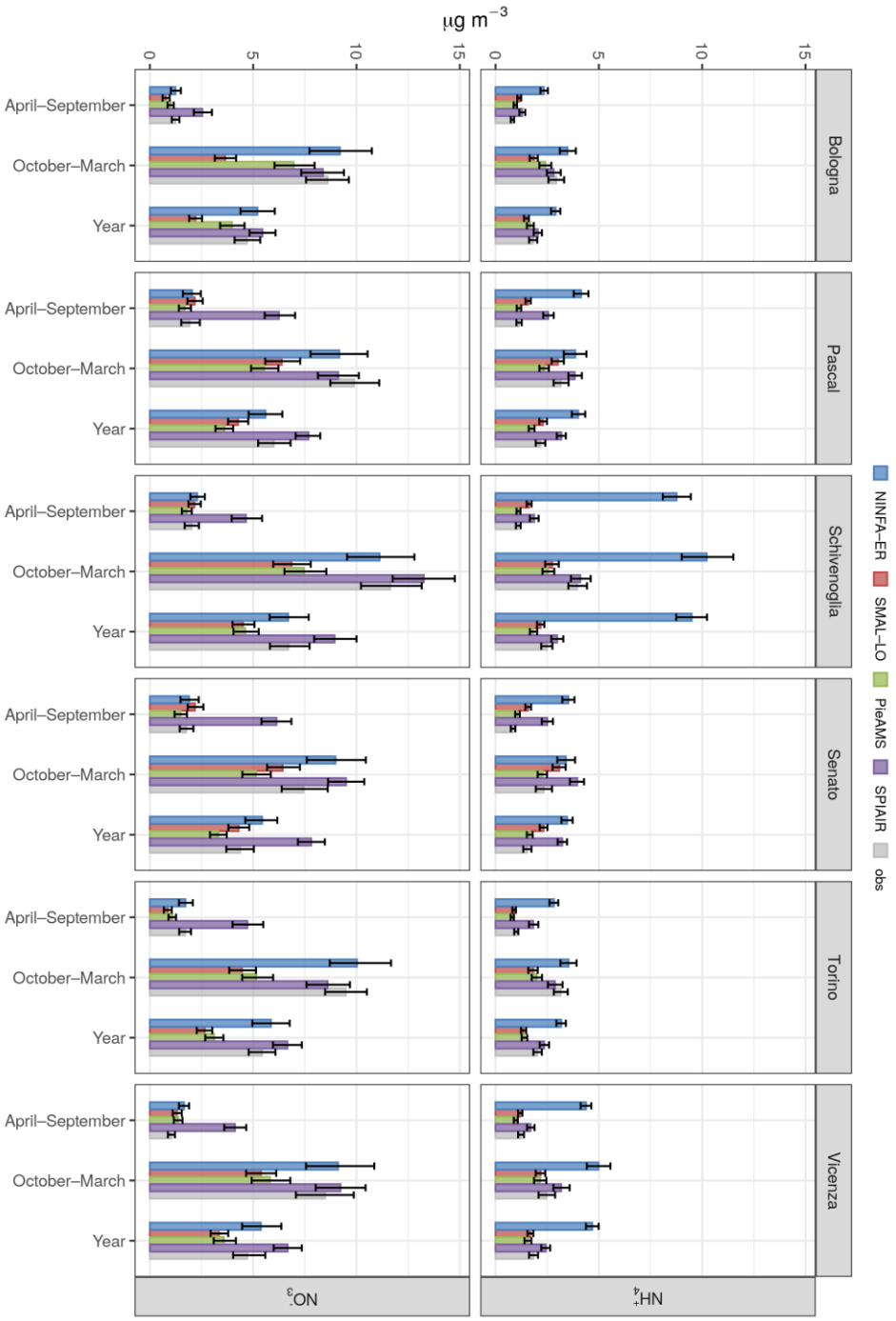

Figure S2. Comparison between modelled and observed total ammonium (NH_4^+, panels at the top) and total nitrate (NO_3^-, panels at the bottom) with related confidence interval at 95% level for winter, summer and yearly average.

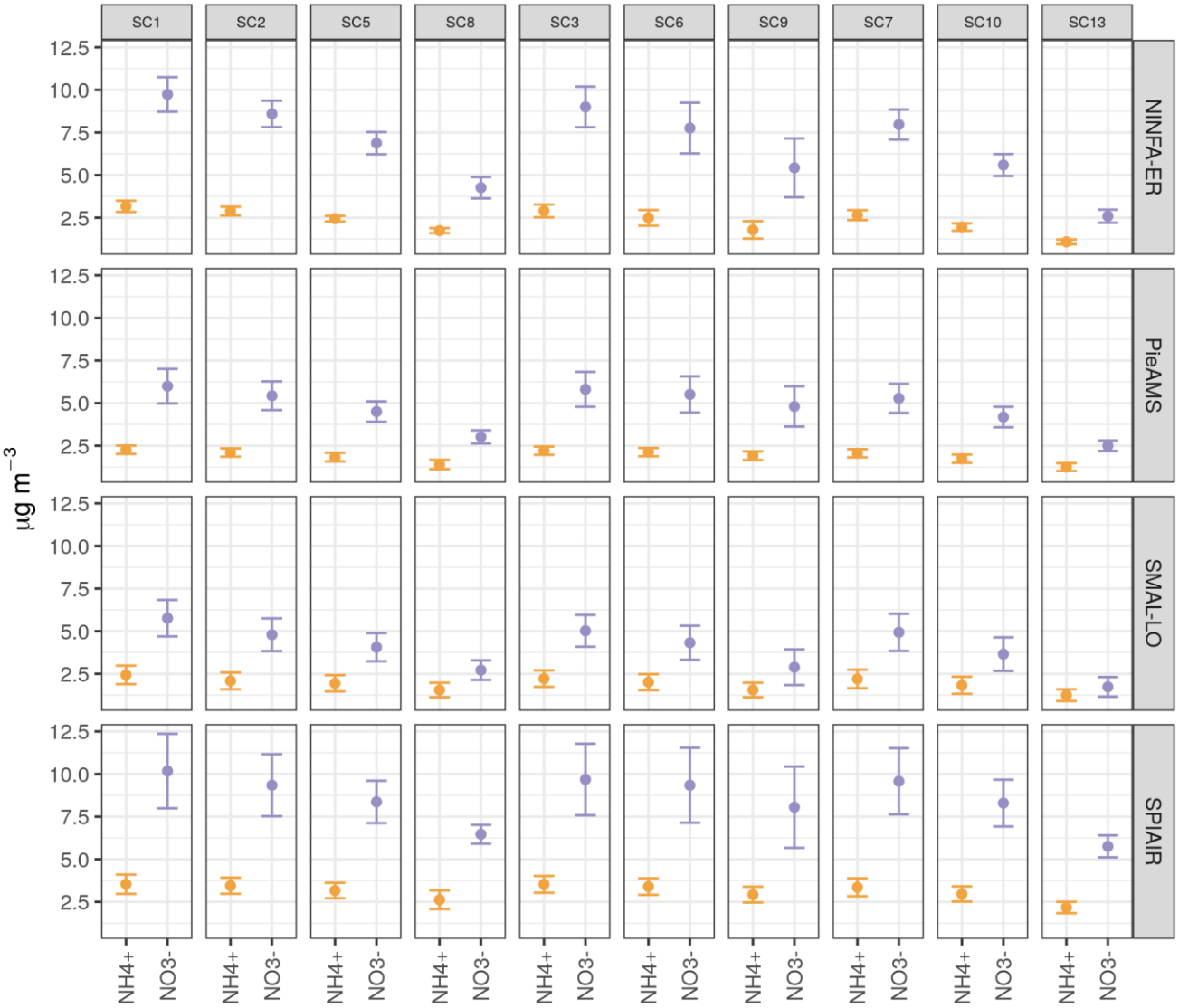

Figure S3. Winter (October–March) concentrations of total ammonium (NH_4^+, orange color) and total nitrate (NO_3^-, blue color) extracted at super-site locations (mean ± the standard deviation).

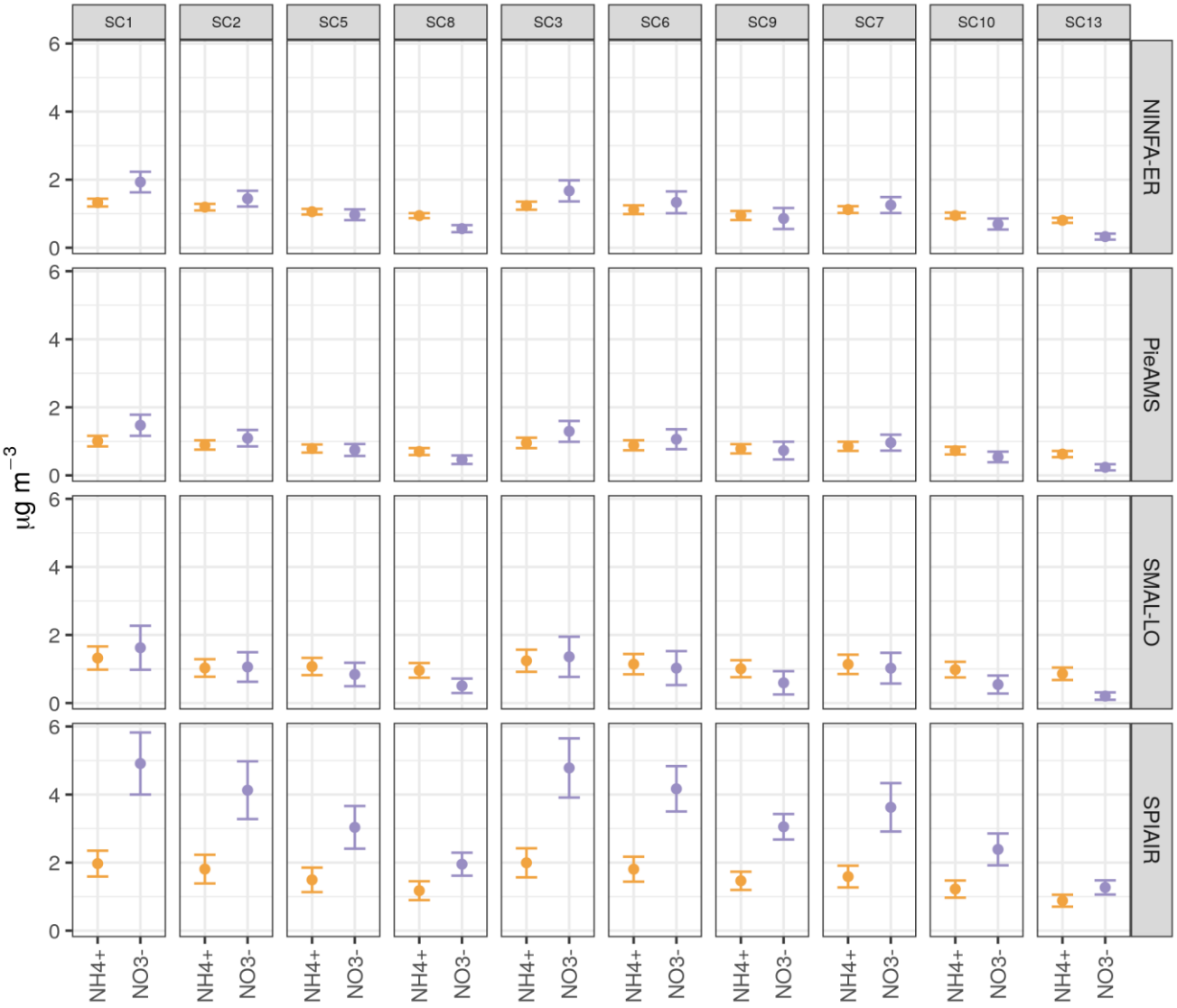

Figure S4. Summer (April–September) concentrations of total ammonium (NH_4^+, orange color) and total nitrate (NO_3^-, blue color) extracted at super-site locations (mean ± the standard deviation).

In order to compare the reduction efficiency of total ammonium and total nitrate between modeling systems, we computed the potential impacts (PI) of these components. Generally, PI are calculated using total PM concentrations, but in this particular context (Figure S5 and S6), the total PM concentrations are replaced with the concentrations of total ammonium and total nitrate, respectively. Eq. 1 in the main text is changed as follows (Eq. S5):

$$\Delta C_{NH4+} = C^0_{NH4+} - C^\alpha_{NH4+}$$
$$\Delta C_{NO3-} = C^0_{NO3-} - C^\alpha_{NO3-} \quad \text{(S5)}$$

where C^0_{NH4+} and C^0_{NO3-} represent, respectively, the concentrations of total ammonium and nitrate in SC1, and C^α_{NH4+} and C^α_{NO3-} are the concentrations of total ammonium and nitrate produced by an emission reduction of α from SC1. Eq. S5 is then used to calculate Eq. 2 and 3 as reported in the main text.

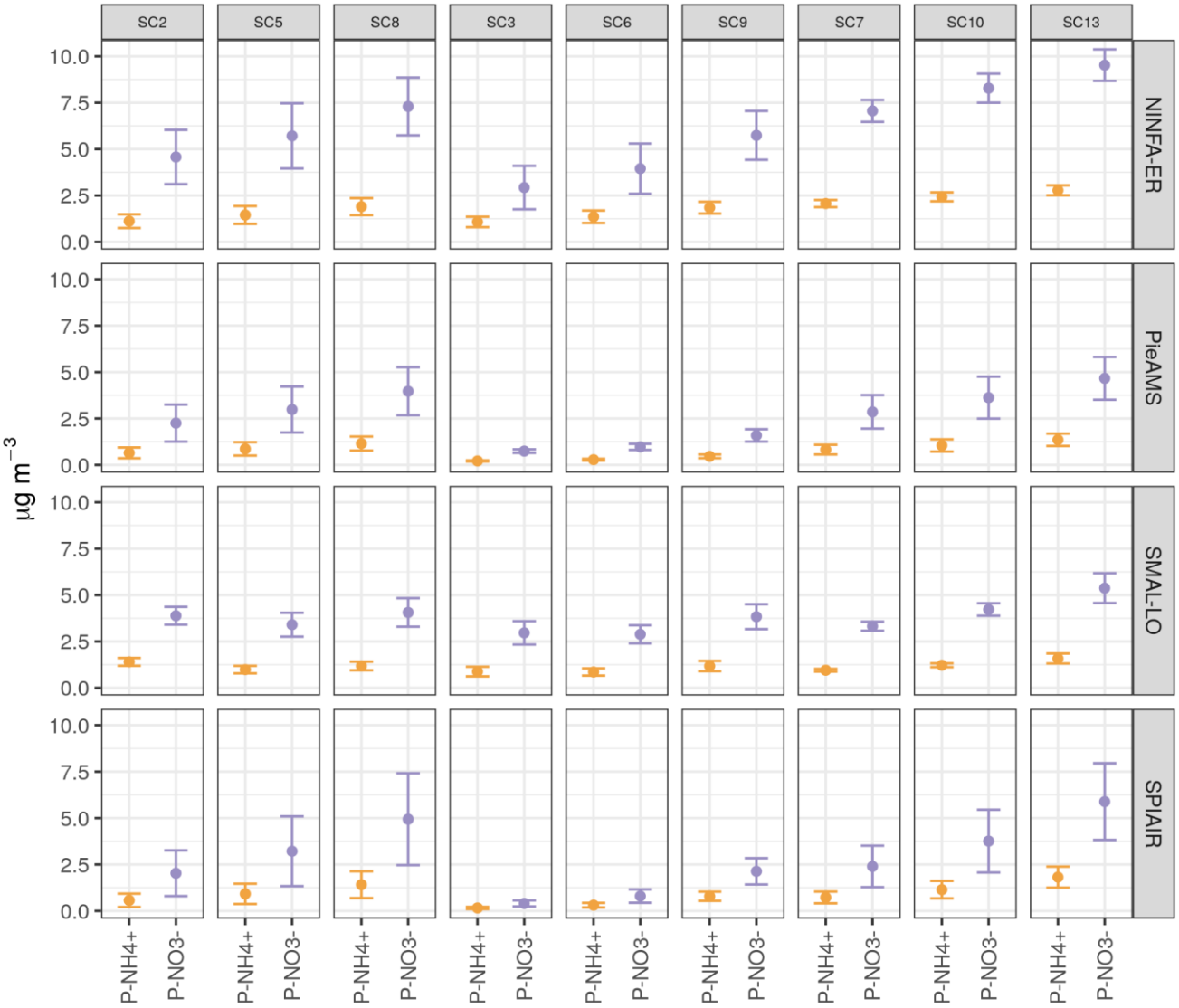

Figure S5. Winter (October–March) PI values of total ammonium (P-NH_4^+, orange color) and total nitrate (P-NO_3^-, blue color) extracted at super-site locations (mean ± the standard deviation).

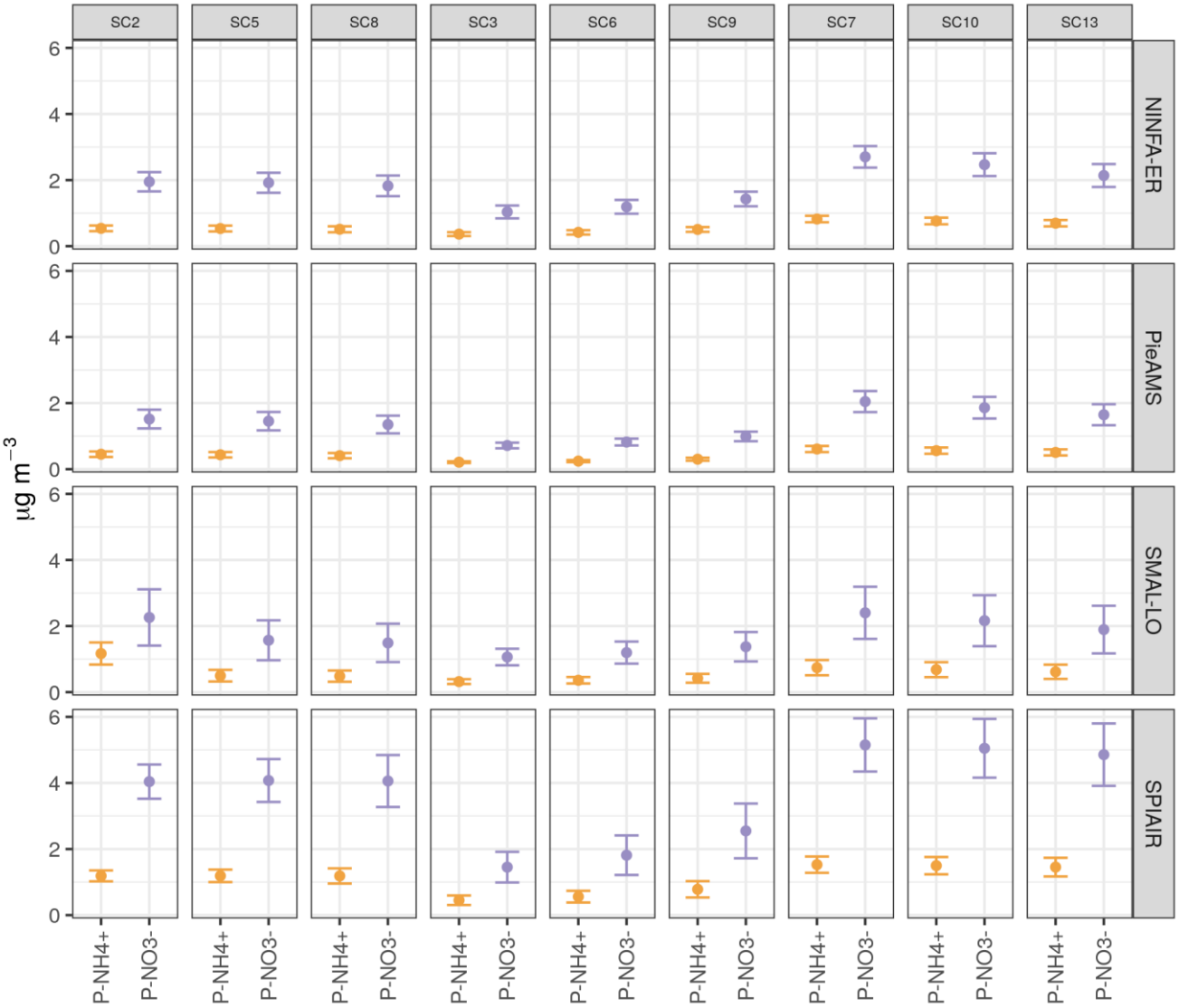

Figure S6. Summer (April–September) PI values of total ammonium (P-NH_4^+, orange color) and total nitrate (P-NO_3^-, blue color) extracted at super-site locations (mean ± the standard deviation).

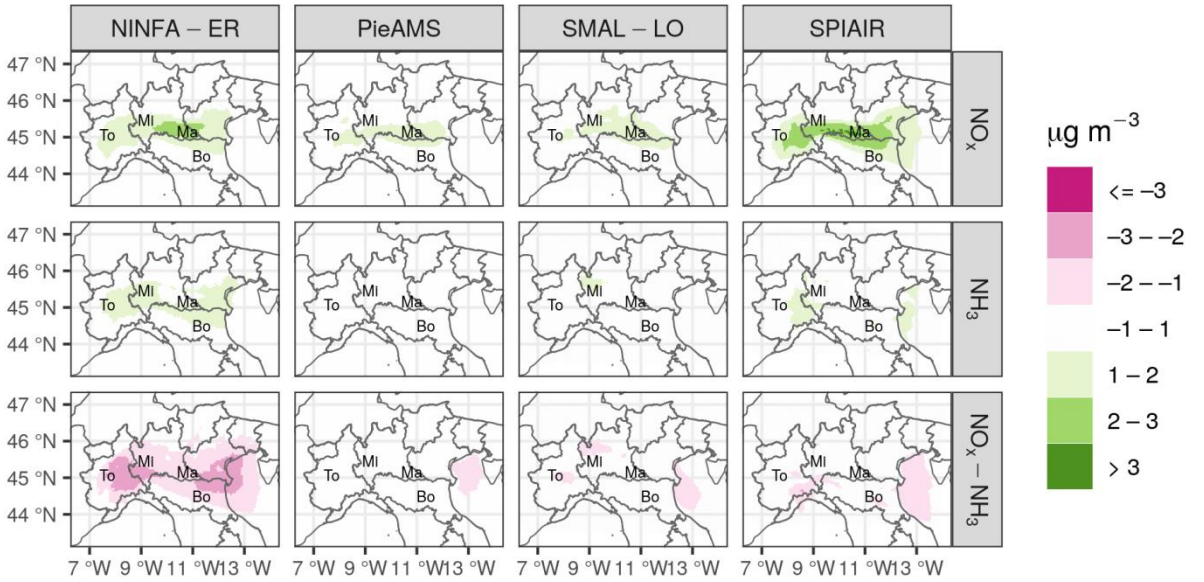

Figure S7. Winter maps of the components of the total non-linearity, expressed as PI (µg m^{-3}) between 25% and 50% emission reduction. Panels at the top show the single NO_x non-linearity term, panels in the center show the single NH_3 non-linearity term and panels at the bottom report the NO_x – NH_3 interaction term.

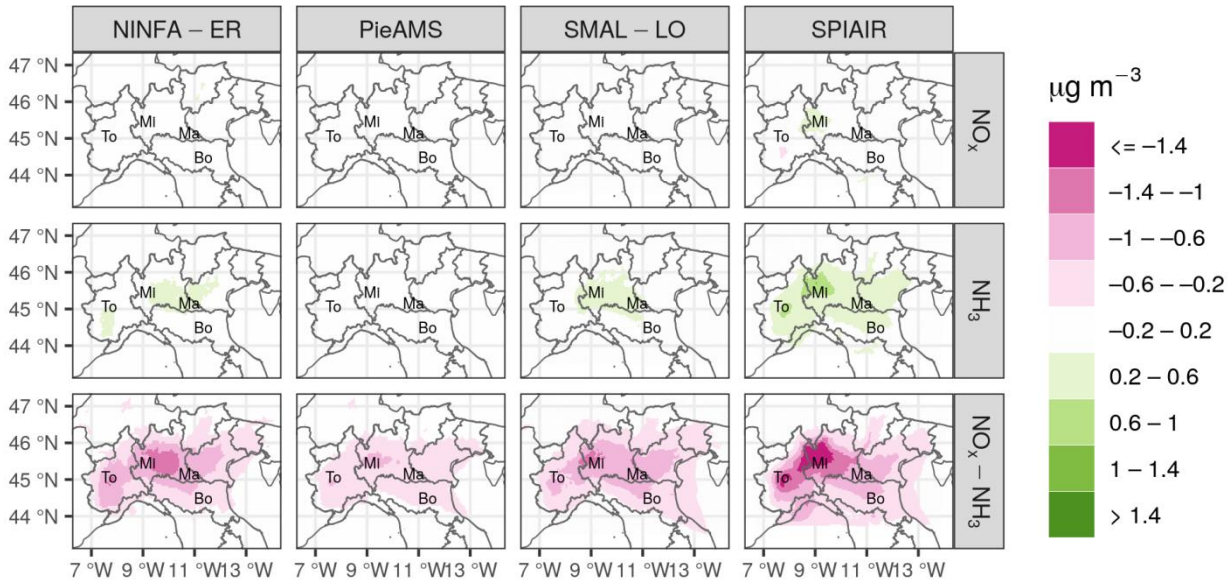

Figure S8. Same as Figure S7 but for summer. Please note the different scale with respect to Figure S7.

Section S1: Models evaluation [86,87]; Figure S1: Model Quality Indicator (MQI) computed for yearly average $PM_{2.5}$ model results; Figure S2: Comparison between modelled and observed total ammonium and total nitrate with related confidence interval at 95% level for wintertime, summertime and yearly average; Figure S3: Winter-averaged concentrations of total ammonium and total nitrate extracted at super-site locations for each simulated scenario; Figure S4: Summer-averaged concentrations of total ammonium and total nitrate extracted at super-site locations for each simulated scenario; Figure S5: Winter-averaged PI of total ammonium and nitrate extracted at super-site locations for each simulated scenario; Figure S6: Summer-averaged PI of total ammonium and nitrate extracted at super-site locations for each simulated scenario; Figure S7: Wintertime

maps of the components of the total non-linearity, expressed as PI (μg m^{-3}) between 25% and 50% emission reduction; Figure S8: Summertime maps of the components of the total non-linearity, expressed as PI (μg m^{-3}) between 25% and 50% emission reduction.

References

86. Thunis, P.; Pederzoli, A.; Pernigotti, D. Performance Criteria to Evaluate Air Quality Modeling Applications. *Atmos. Environ.* **2012**, *59*, 476–482, doi:10.1016/j.atmosenv.2012.05.043.
87. Pernigotti, D.; Gerboles, M.; Belis, C.A.; Thunis, P. Model Quality Objectives Based on Measurement Uncertainty. Part II: NO2 and PM10. *Atmos. Environ.* **2013**, *79*, 869–878, doi:10.1016/j.atmosenv.2013.07.045.