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Supplement of

Effectiveness of emission controls on atmospheric oxidation capacity and air pollutant concentrations: uncertainties due to chemical mechanisms and inventories

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Table S1. Comparison of CS07, S11 and S18 mechanisms.

Mechanism	# of species	# of reaction	Remarks
CS07	85	286	CS07 is a condensed version of SAPRC-07 comparable in size to CB05. It incorporates the condensed, approximate peroxy radical lumped operator method used in SAPRC99, CB4, and CB05. CS07 provides predictions of ozone (O_3), total peroxy radicals (PANs), and hydroxyl (OH) radicals that closely resemble those of the uncondensed mechanism.
S11	174	478	SAPRC-11 (S11) is a partial update of the standard SAPRC-07 mechanism to improve the representation of the aromatics reactions to better fit the chamber data.
S18	491	1779	The SAPRC-18 (S18) mechanism is the first full update since SAPRC-07/11, featuring an expanded mechanism generator with more compounds, new reaction types (e.g., peroxy radical auto-oxidation), and improved estimation methods. It is larger due to additional model species for emitted organics and their oxidation products, enabling more accurate predictions of secondary products, NOx recycling, and SOA precursor formation.

Table S2. Weekday emissions of NO_x ($NO+NO_2$), SO_2, ethene (ETHENE), formaldehyde (HCHO), higher alkenes OLE (OLE1+OLE2, lumped alkene species of different OH reactivity with propylene and trans-2-pentene as representative compounds), isoprene (ISOPRENE), and monoterpenes (TRP1) in municipalities and provinces based on MEIC and the S11 mechanism for July 2017. Units are kmoles d^{-1}.

Province	NOx	SO_2	ETHENE	HCHO	OLE	ISOPRENE	TRP1
Beijing	1.47E+04	1.73E+03	1.16E+03	2.09E+02	2.73E+03	1.42E+01	2.40E+01
Tianjin	1.72E+04	4.01E+03	1.35E+03	1.79E+02	2.79E+03	8.45E+00	1.25E+01
Shanghai	2.20E+04	6.92E+03	2.14E+03	6.87E+02	3.98E+03	1.53E+01	2.22E+01
Chongqing	2.15E+04	2.00E+04	1.55E+03	3.18E+02	2.08E+03	1.28E+01	3.28E+01
Hebei	1.02E+05	3.38E+04	6.56E+03	7.73E+02	7.25E+03	3.53E+01	1.76E+02
Henan	7.92E+04	2.10E+04	4.70E+03	8.99E+02	6.88E+03	3.76E+01	1.02E+02
Hubei	4.22E+04	2.47E+04	3.85E+03	7.19E+02	5.28E+03	2.87E+01	8.61E+01
Hunan	3.97E+04	2.39E+04	3.62E+03	5.08E+02	4.56E+03	2.69E+01	6.20E+01
Shandong	1.40E+05	5.27E+04	8.46E+03	1.26E+03	1.19E+04	6.95E+01	2.57E+02
Shanxi	6.22E+04	4.61E+04	5.40E+03	3.40E+02	3.86E+03	1.39E+01	2.45E+01
Anhui	6.11E+04	9.74E+03	3.57E+03	8.06E+02	4.84E+03	3.05E+01	1.01E+02
Jiangsu	9.57E+04	2.02E+04	5.56E+03	1.08E+03	1.14E+04	4.62E+01	2.16E+02
Zhejiang	5.40E+04	1.21E+04	3.05E+03	7.34E+02	9.23E+03	3.63E+01	1.41E+02
Jiangxi	2.88E+04	1.00E+04	1.95E+03	3.48E+02	2.89E+03	1.62E+01	5.41E+01
Fujian	3.09E+04	7.92E+03	2.28E+03	4.53E+02	3.71E+03	1.78E+01	5.25E+01
Guangdong	7.28E+04	2.46E+04	5.51E+03	1.37E+03	1.44E+04	7.30E+01	1.14E+02
Inner Mongolia	7.60E+04	2.81E+04	3.06E+03	2.96E+02	3.24E+03	1.29E+01	3.61E+01
Heilongjiang	3.97E+04	8.68E+03	2.89E+03	4.17E+02	3.36E+03	1.80E+01	5.52E+01
Jilin	3.30E+04	9.20E+03	2.15E+03	2.44E+02	2.29E+03	1.18E+01	3.67E+01
Liaoning	7.05E+04	2.28E+04	4.19E+03	7.09E+02	5.18E+03	2.63E+01	5.80E+01
Gansu	2.09E+04	6.98E+03	1.74E+03	2.17E+02	1.84E+03	8.44E+00	1.76E+01
Ningxia	1.49E+04	8.11E+03	7.31E+02	6.45E+01	1.02E+03	2.75E+00	6.74E+00
Shaanxi	3.30E+04	1.65E+04	3.23E+03	3.51E+02	3.28E+03	1.54E+01	2.75E+01
Xinjiang	3.64E+04	1.07E+04	2.74E+03	2.48E+02	2.81E+03	9.61E+00	1.83E+01
Qinghai	6.75E+03	1.98E+03	3.94E+02	6.01E+01	5.14E+02	2.13E+00	3.49E+00
Xizang	3.13E+03	5.27E+01	7.78E+01	3.56E+01	1.24E+02	4.48E-01	1.04E+00
Sichuan	4.63E+04	1.90E+04	3.96E+03	9.14E+02	6.46E+03	4.17E+01	1.08E+02
Yunnan	2.51E+04	1.54E+04	2.51E+03	3.60E+02	3.22E+03	1.75E+01	3.25E+01
Guangxi	2.44E+04	1.16E+04	2.31E+03	4.51E+02	3.33E+03	2.40E+01	6.62E+01
Guizhou	2.26E+04	2.86E+04	3.14E+03	2.48E+02	2.66E+03	1.84E+01	2.49E+01
Hainan	5.85E+03	1.97E+03	5.24E+02	1.30E+02	9.07E+02	7.54E+00	1.65E+01

Table S3. Weekday emissions of NO_x ($NO+NO_2$), SO_2, ETHENE, HCHO, OLE (OLE1+OLE2, lumped alkene species with propylene and trans-2-pentene as representative compounds), ISOPRENE, and TRP1 in municipalities and provinces based on REAS and the S11 mechanism for July 2017. Units are kmoles d^{-1}.

Province	NO_x	SO_2	ETHENE	HCHO	OLE	ISOPRENE	TRP1
Beijing	1.59E+04	2.62E+03	1.15E+03	6.17E+02	1.16E+03	7.40E+00	1.15E+01
Tianjin	1.59E+04	4.79E+03	1.18E+03	4.57E+02	1.14E+03	1.30E+01	1.15E+01
Shanghai	1.36E+04	4.10E+03	1.08E+03	4.29E+02	1.09E+03	7.55E+00	1.32E+01
Chongqing	2.27E+04	2.27E+04	1.28E+03	3.82E+02	1.33E+03	4.19E+01	1.68E+01
Hebei	1.08E+05	4.21E+04	7.00E+03	2.83E+03	6.46E+03	9.69E+01	5.27E+01
Henan	7.73E+04	3.45E+04	7.71E+03	3.14E+03	7.19E+03	1.24E+02	6.04E+01
Hubei	5.53E+04	3.90E+04	2.94E+03	8.84E+02	3.03E+03	9.05E+01	3.71E+01
Hunan	4.70E+04	3.38E+04	2.85E+03	9.97E+02	2.96E+03	8.19E+01	3.60E+01
Shandong	1.35E+05	6.51E+04	6.85E+03	2.52E+03	6.70E+03	1.30E+02	6.76E+01
Shanxi	6.09E+04	3.22E+04	3.08E+03	9.06E+02	2.84E+03	5.33E+01	3.05E+01
Anhui	5.22E+04	1.94E+04	3.38E+03	9.11E+02	3.55E+03	1.26E+02	4.53E+01
Jiangsu	7.39E+04	2.32E+04	5.93E+03	2.19E+03	5.80E+03	9.08E+01	6.03E+01
Zhejiang	4.55E+04	1.51E+04	3.94E+03	1.71E+03	3.78E+03	4.06E+01	3.41E+01
Jiangxi	2.64E+04	1.77E+04	1.68E+03	5.96E+02	1.72E+03	4.46E+01	2.00E+01
Fujian	3.03E+04	1.23E+04	1.78E+03	6.62E+02	1.82E+03	3.25E+01	2.06E+01
Guangdong	7.00E+04	2.86E+04	6.37E+03	2.38E+03	6.49E+03	1.38E+02	7.38E+01
Inner Mongolia	9.16E+04	4.11E+04	2.64E+03	1.05E+03	2.49E+03	3.90E+01	2.36E+01
Heilongjiang	4.56E+04	1.27E+04	2.07E+03	6.82E+02	2.14E+03	6.12E+01	2.60E+01
Jilin	2.99E+04	8.86E+03	2.18E+03	8.89E+02	2.11E+03	3.95E+01	2.03E+01
Liaoning	6.48E+04	2.67E+04	3.03E+03	1.05E+03	2.97E+03	5.52E+01	3.44E+01
Gansu	2.29E+04	1.33E+04	1.70E+03	5.41E+02	1.59E+03	3.27E+01	1.65E+01
Ningxia	1.15E+04	1.11E+04	8.45E+02	2.78E+02	7.36E+02	7.40E+00	6.67E+00
Shaanxi	3.40E+04	3.28E+04	2.43E+03	8.30E+02	2.35E+03	5.26E+01	2.56E+01
Xinjiang	5.49E+04	2.04E+04	1.75E+03	5.94E+02	1.66E+03	3.02E+01	1.74E+01
Qinghai	9.67E+03	3.03E+03	5.15E+02	2.61E+02	4.65E+02	4.60E+00	2.81E+00
Xizang	7.57E+03	1.87E+03	1.06E+02	4.67E+01	1.60E+02	2.28E+00	6.39E+01
Sichuan	5.43E+04	3.81E+04	4.75E+03	1.32E+03	4.94E+03	1.79E+02	6.09E+01
Yunnan	3.03E+04	3.24E+04	2.84E+03	1.04E+03	2.81E+03	7.41E+01	2.81E+01
Guangxi	3.21E+04	3.55E+04	3.86E+03	1.00E+03	4.08E+03	1.58E+02	5.21E+01
Guizhou	3.40E+04	6.35E+04	2.20E+03	5.44E+02	2.25E+03	8.30E+01	2.86E+01
Hainan	5.75E+03	2.22E+03	4.95E+02	1.72E+02	5.04E+02	1.36E+01	5.73E+00

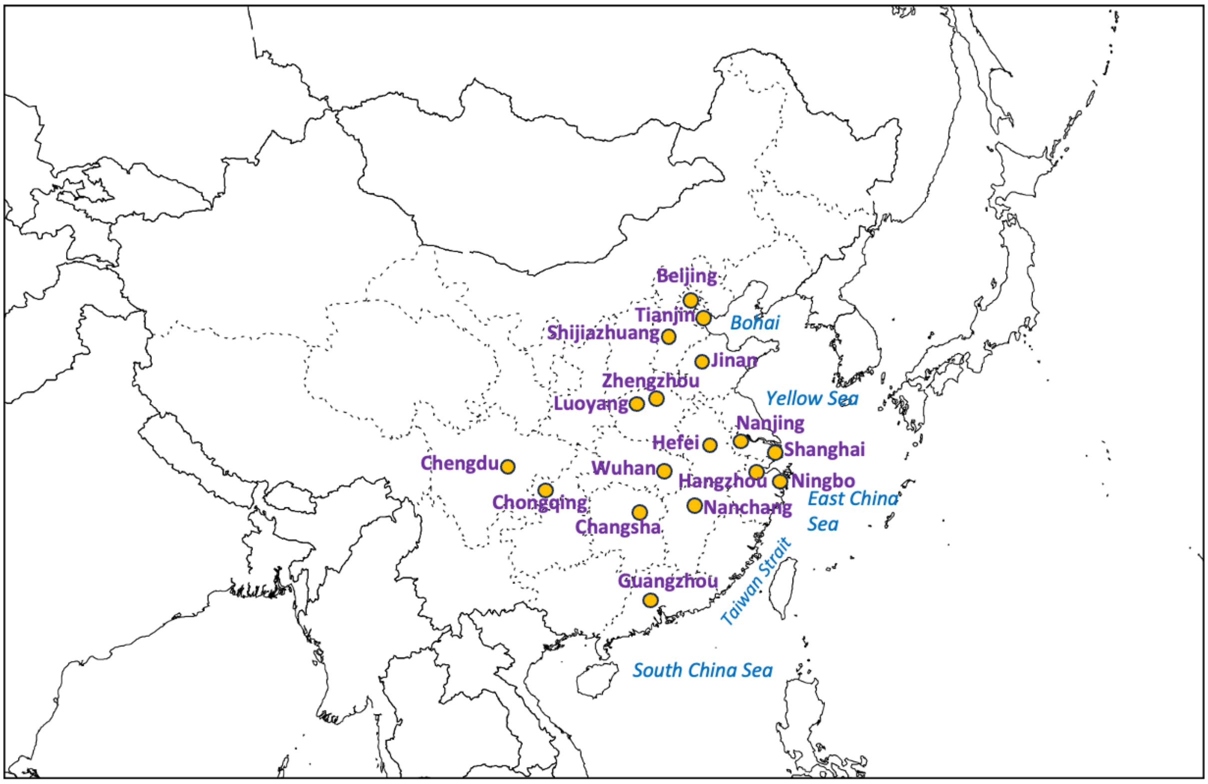

Figure S1. Model domain. Orange filled circles show the locations of cities mentioned in the manuscript.

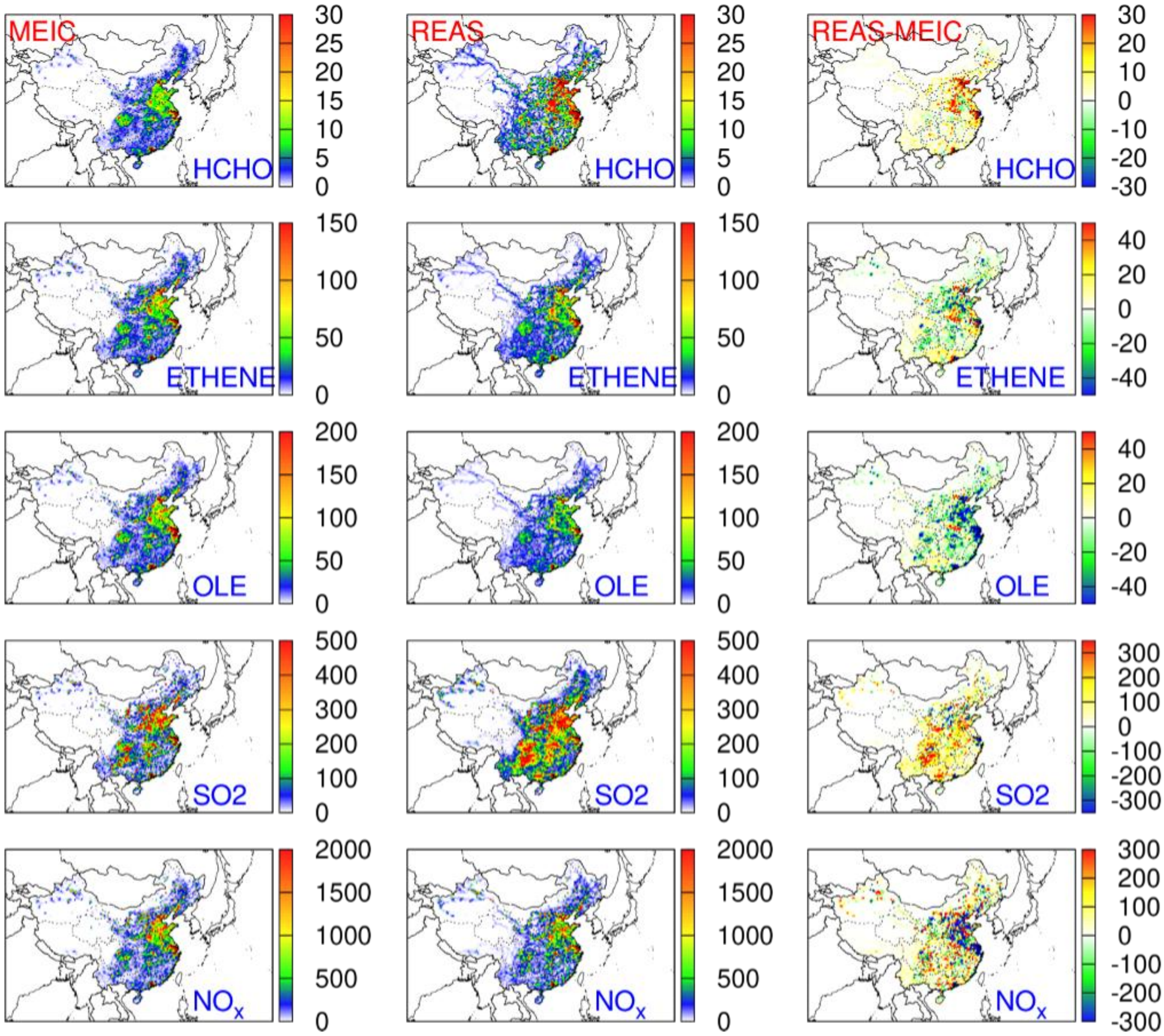

Figure S2. Weekday emissions of formaldehyde (HCHO), ethene (ETHENE), higher alkenes (OLE) (OLE1+OLE2, lumped alkene species of different OH reactivity with propylene and trans-2-pentene as representative compounds), SO_2, and NO_x ($NO+NO_2$) calculated from MEIC and REAS for July 2017, and the absolute differences between these two emission inventories are also calculated. Units are kmoles d^{-1}.

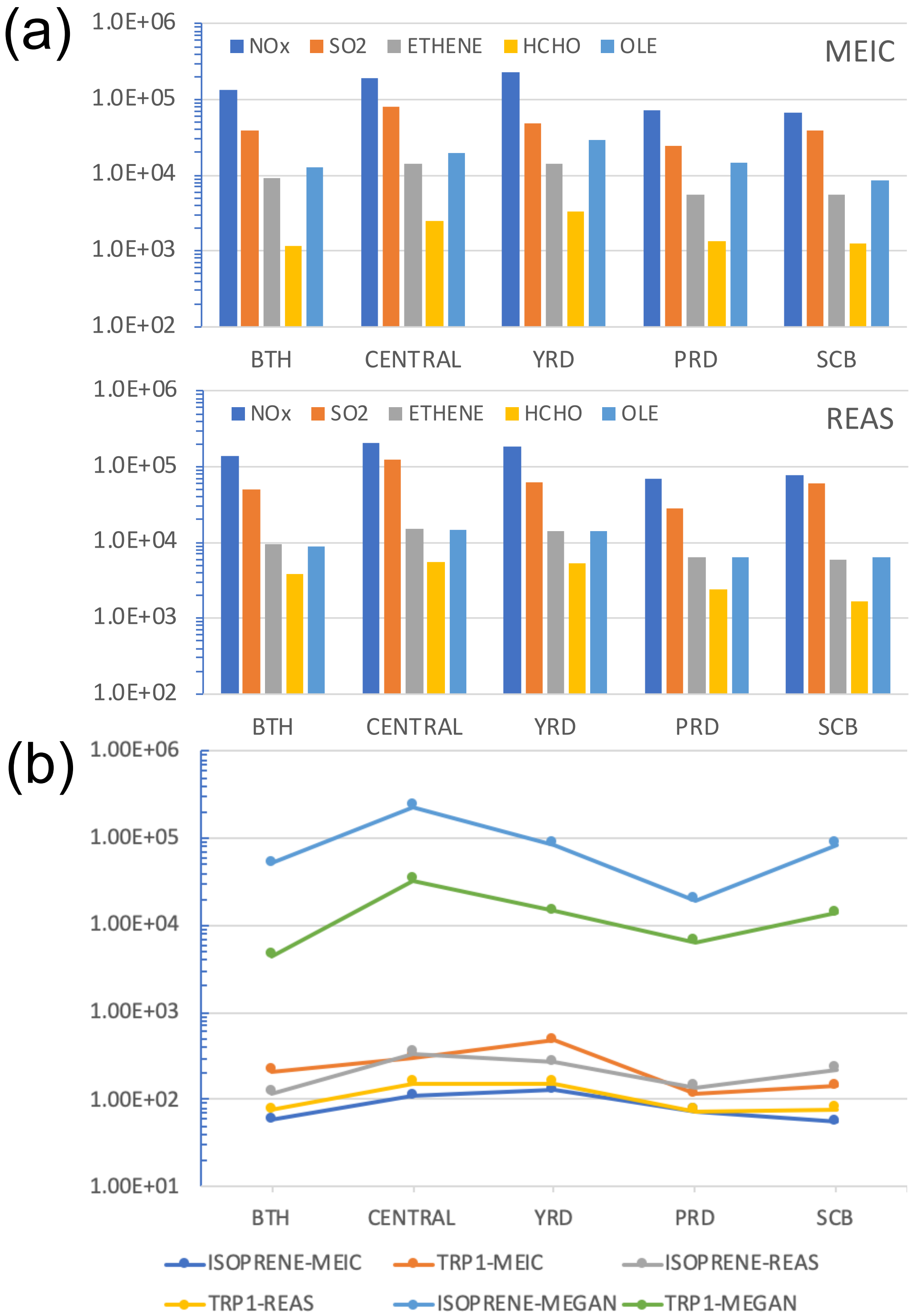

Figure S3. Weekday emissions of (a) NO_x ($NO+NO_2$), SO_2, ETHENE, HCHO, and OLE (OLE1+OLE2, lumped alkene species with propylene and trans-2-pentene as representative compounds) calculated from MEIC and REAS inventories for July 2017, and (b) isoprene and monoterpenes (TRP1) of MEIC, REAS and MEGAN in major regions of China in July 2017. BTH: Beijing, Tianjin, and Hebei provinces; CENTRAL: Henan, Hubei, Hunan, and Jiangxi; YRD: Shanghai, Anhui, Jiangsu, and Zhejiang; PRD: Guangdong; SCB: Chongqing and Sichuan. Units are kmoles d^{-1}.

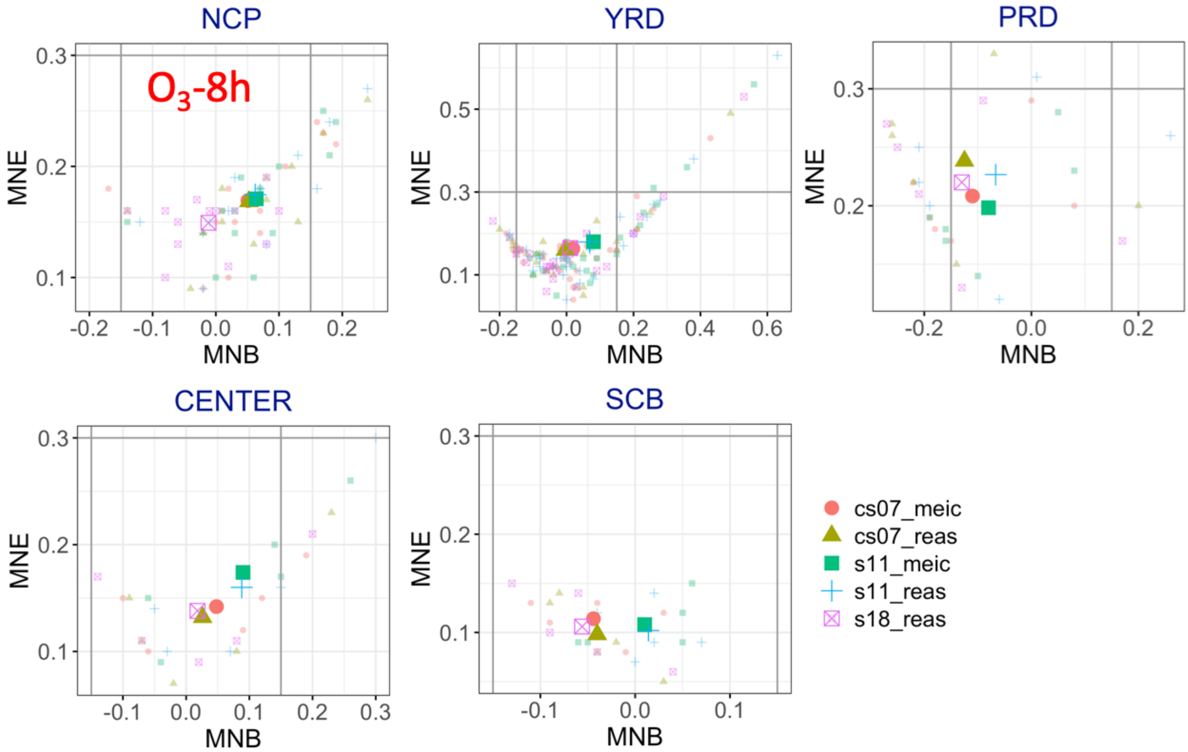

Figure S4. Comparison of daily maximum O_3-8h model performance across different mechanisms and emission inventories in major regions in July 2017. MNB is mean normalized bias, and MNE is mean normalized error. A concentration cutoff of 60 ppb was chosen when calculating MNB and MNE values. The averages of MNB and MNE values for each region are also displayed in the plot with larger icons. The performance criteria for O_3 are ±0.15 for MNB and 0.3 for MNE (Emery et al., 2017).

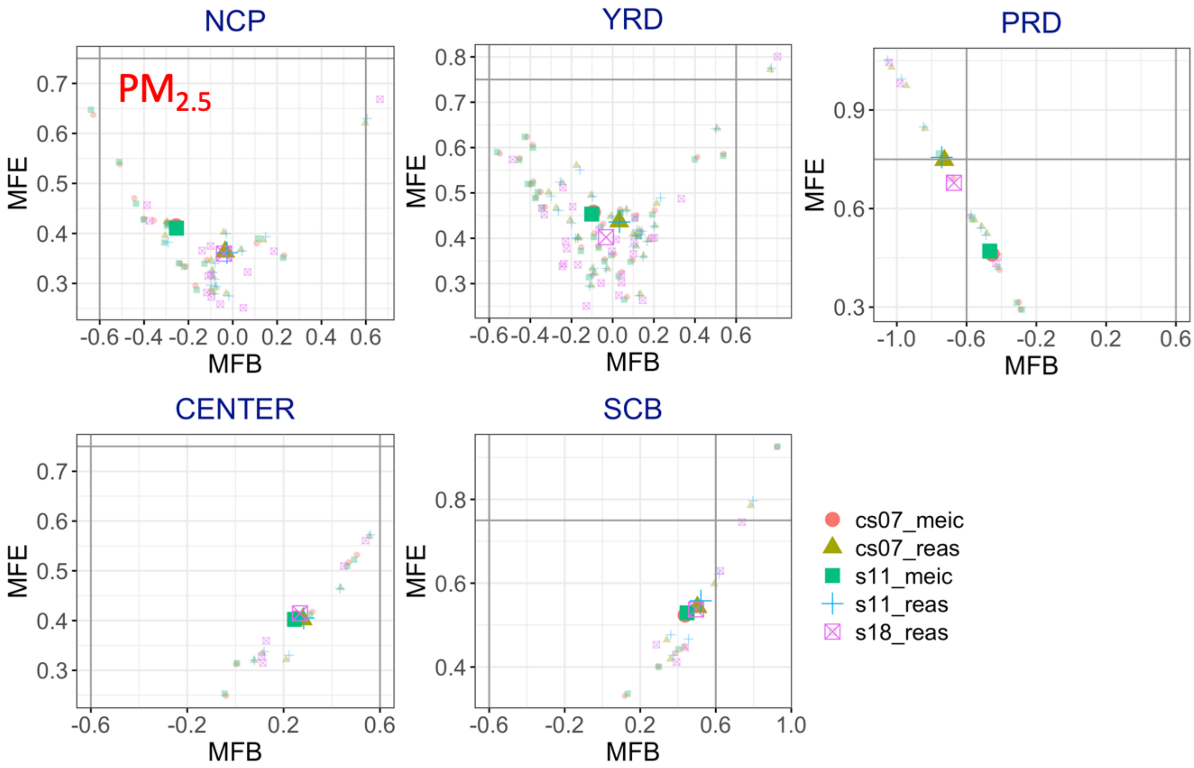

Figure S5. Comparison of $PM_{2.5}$ model performance across different mechanisms and emission inventories in major regions in July 2017. MFB is mean fractional bias, and MFE is mean fractional error. The averages of MFB and MFE values for each region are also plotted with larger icons. The performance criteria for $PM_{2.5}$ are ±0.6 for MFB and 0.75 for MFE, respectively (Boylan and Russell, 2006).

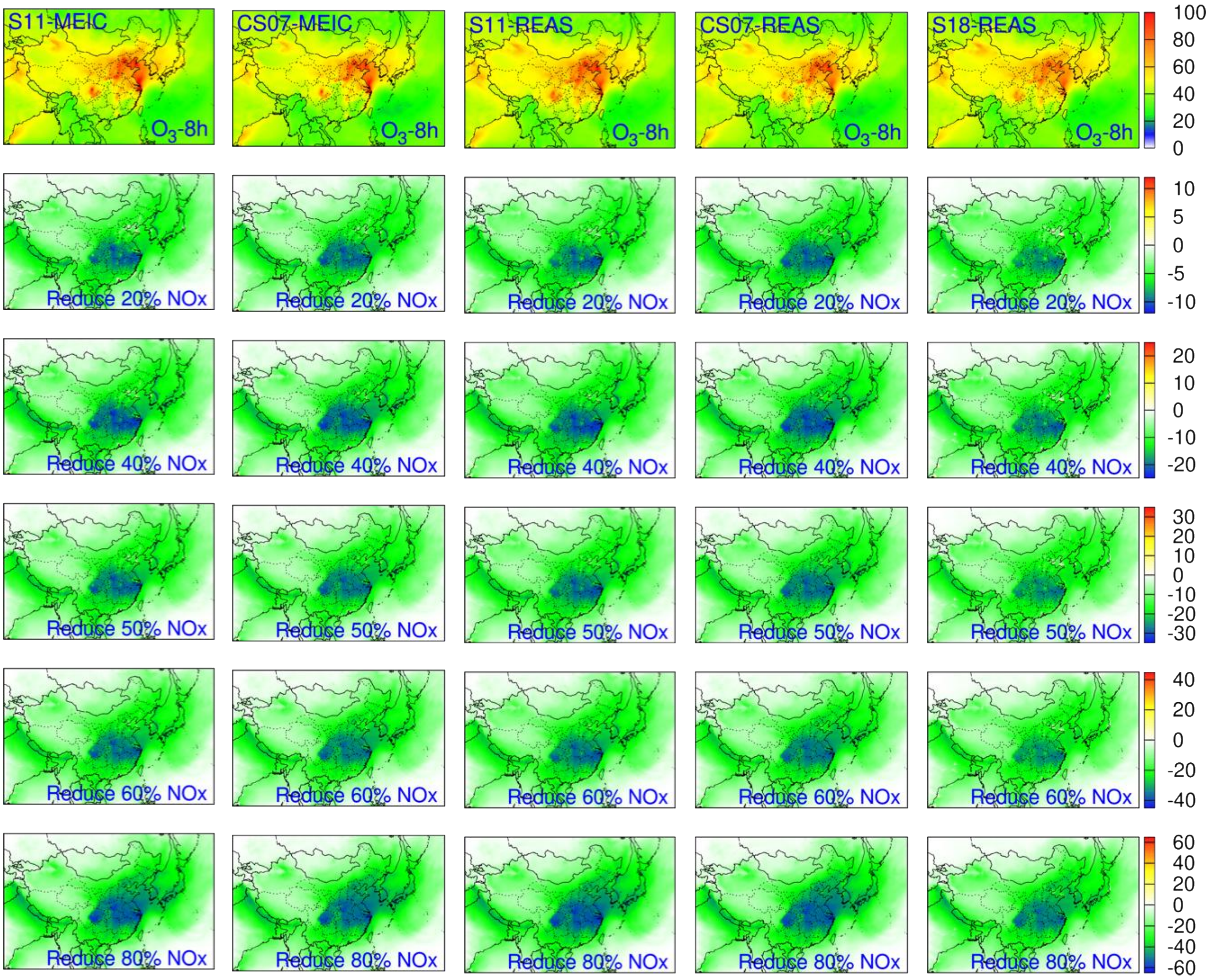

Figure S6. Predicted monthly average O_3-8h concentrations in July 2017 using different photochemical mechanisms and emission inventories (first row; units are ppb), and the percentage changes of O_3-8h due to 20%, 40%, 50%, 60%, and 80% reductions in NO_x emissions.

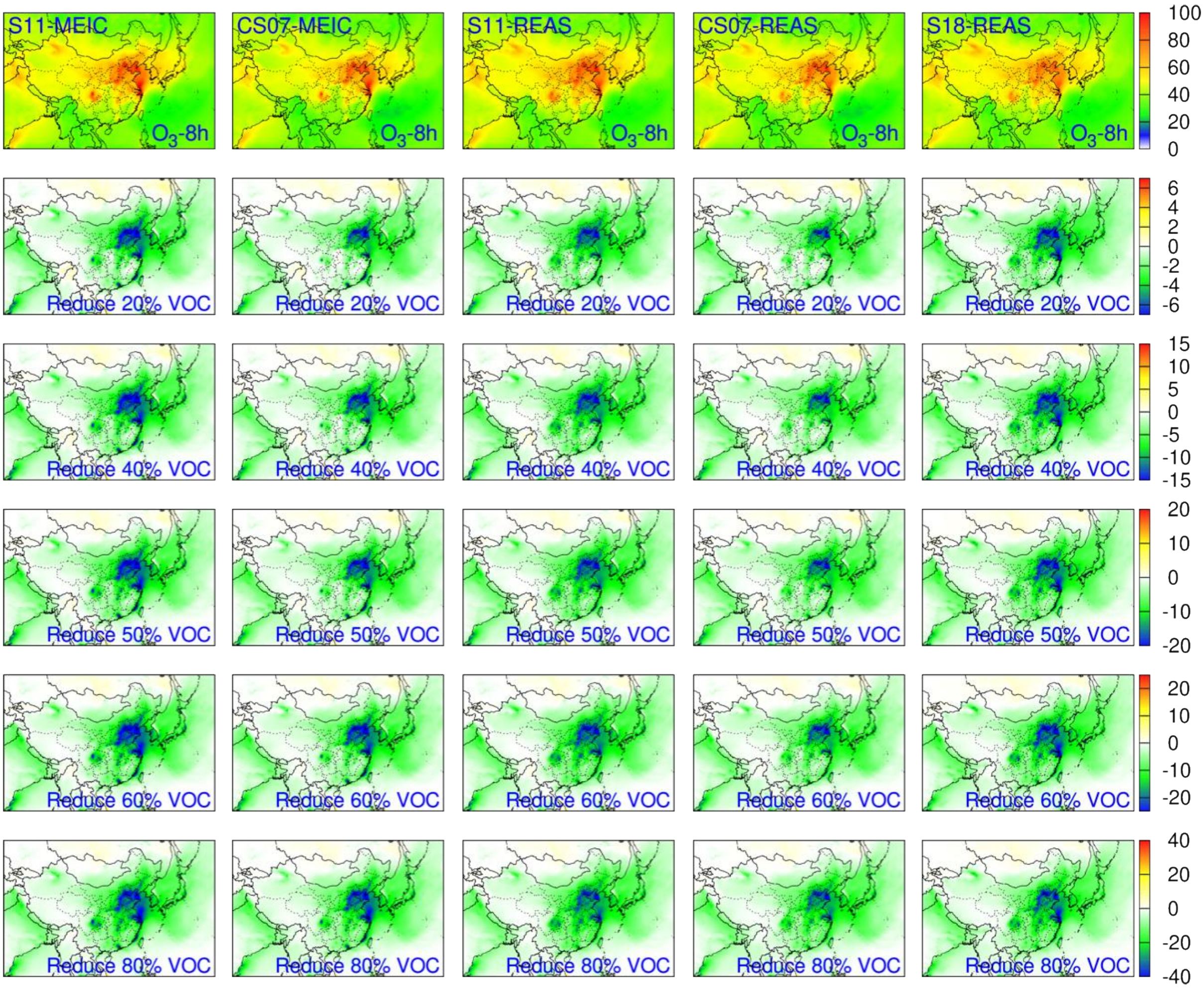

Figure S7. Predicted monthly average O_3-8h concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppb), and percentage changes of O_3-8h due to 20%, 40%, 50%, 60%, and 80% reductions in VOC emissions.

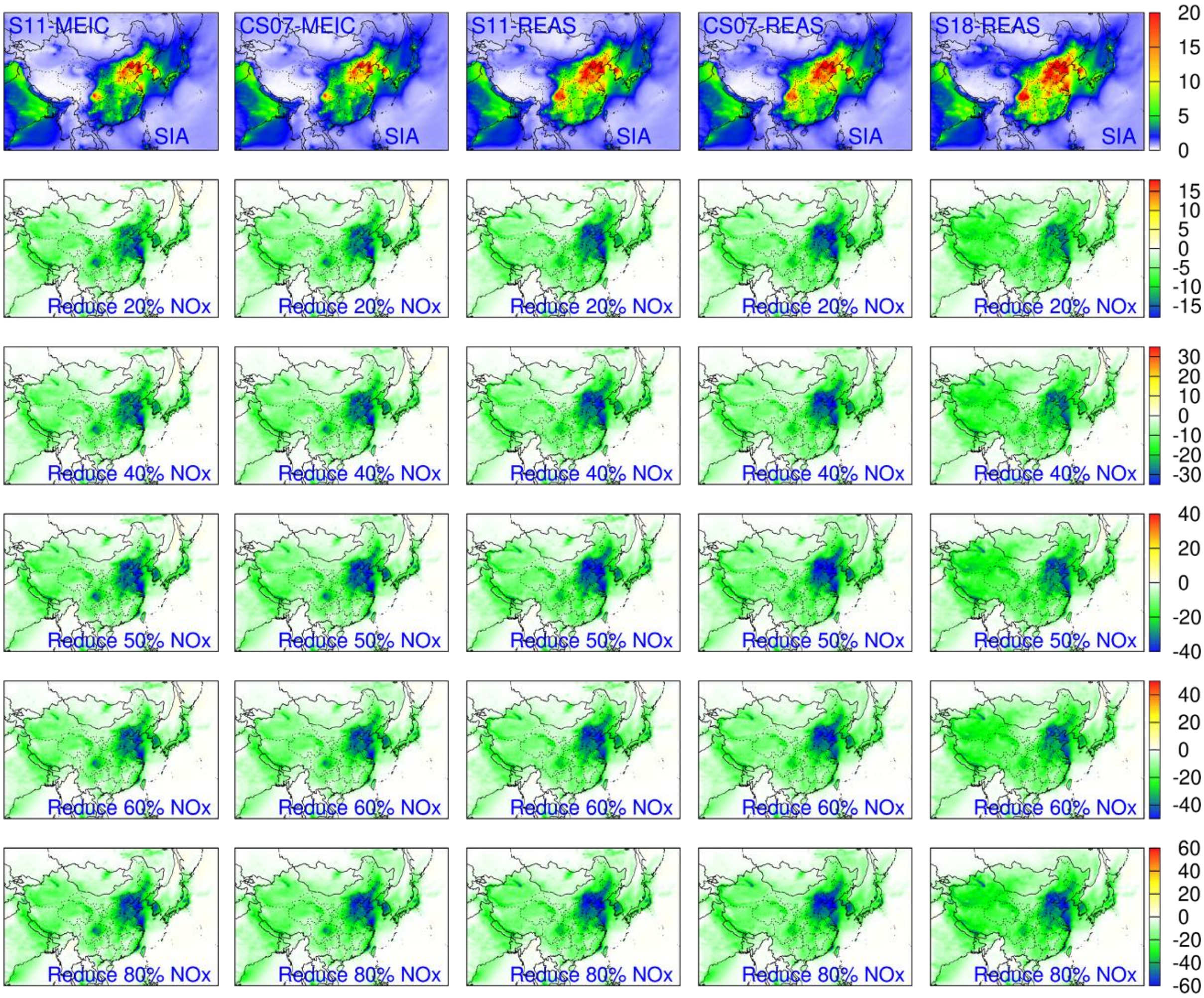

Figure S8. Predicted monthly average secondary inorganic aerosol (SIA, including nitrate + sulfate + ammonium ion) concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are μg m^{-3}), and the relative changes of SIA due to 20%, 40%, 50%, 60%, and 80% reductions in NO_x emissions.

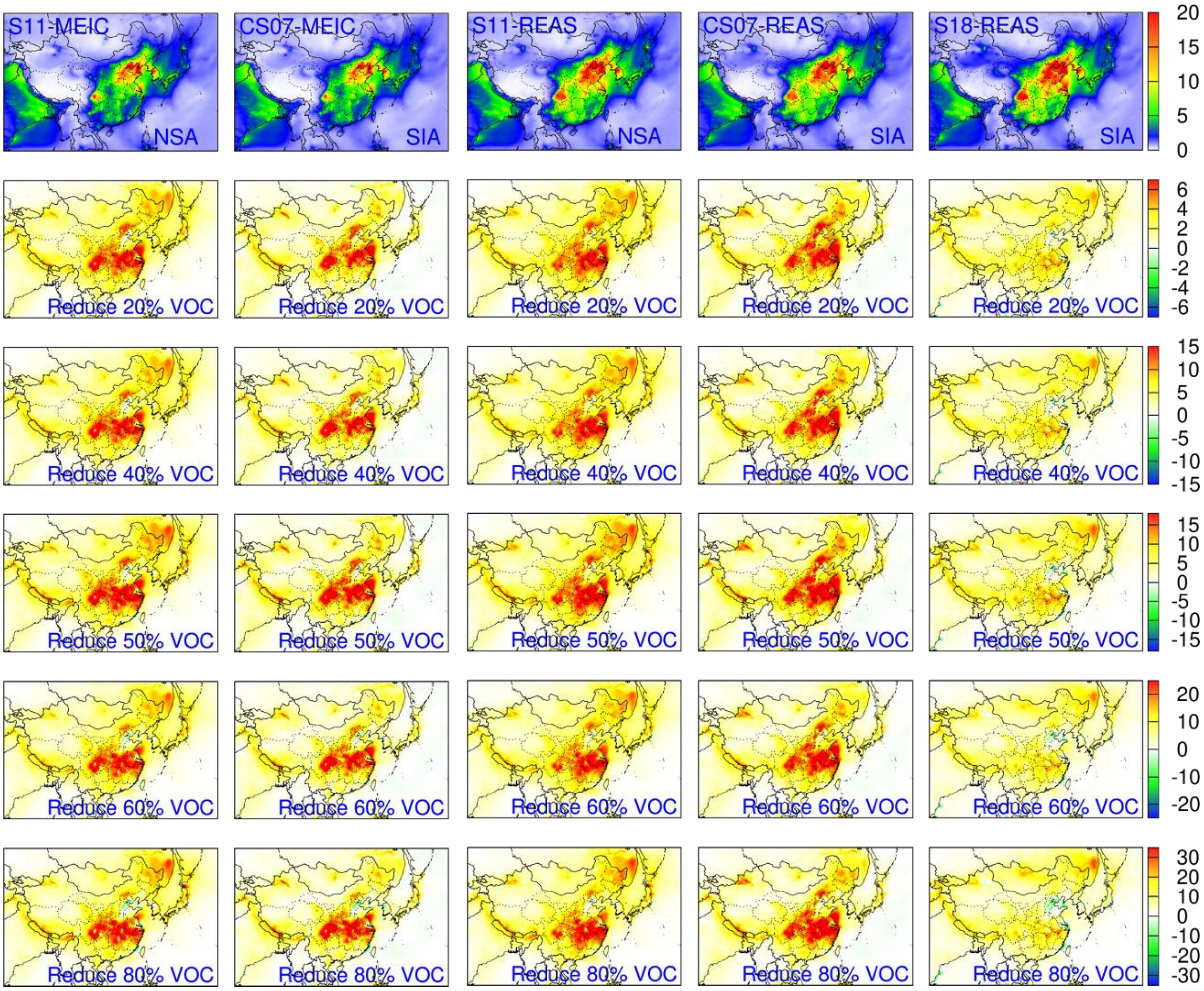

Figure S9. Predicted monthly average secondary inorganic aerosol (SIA, including nitrate + sulfate + ammonium ion) concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are μg m^{-3}), and the percentage changes of SIA due to 20%, 40%, 50%, 60%, and 80% reductions in VOC emissions.

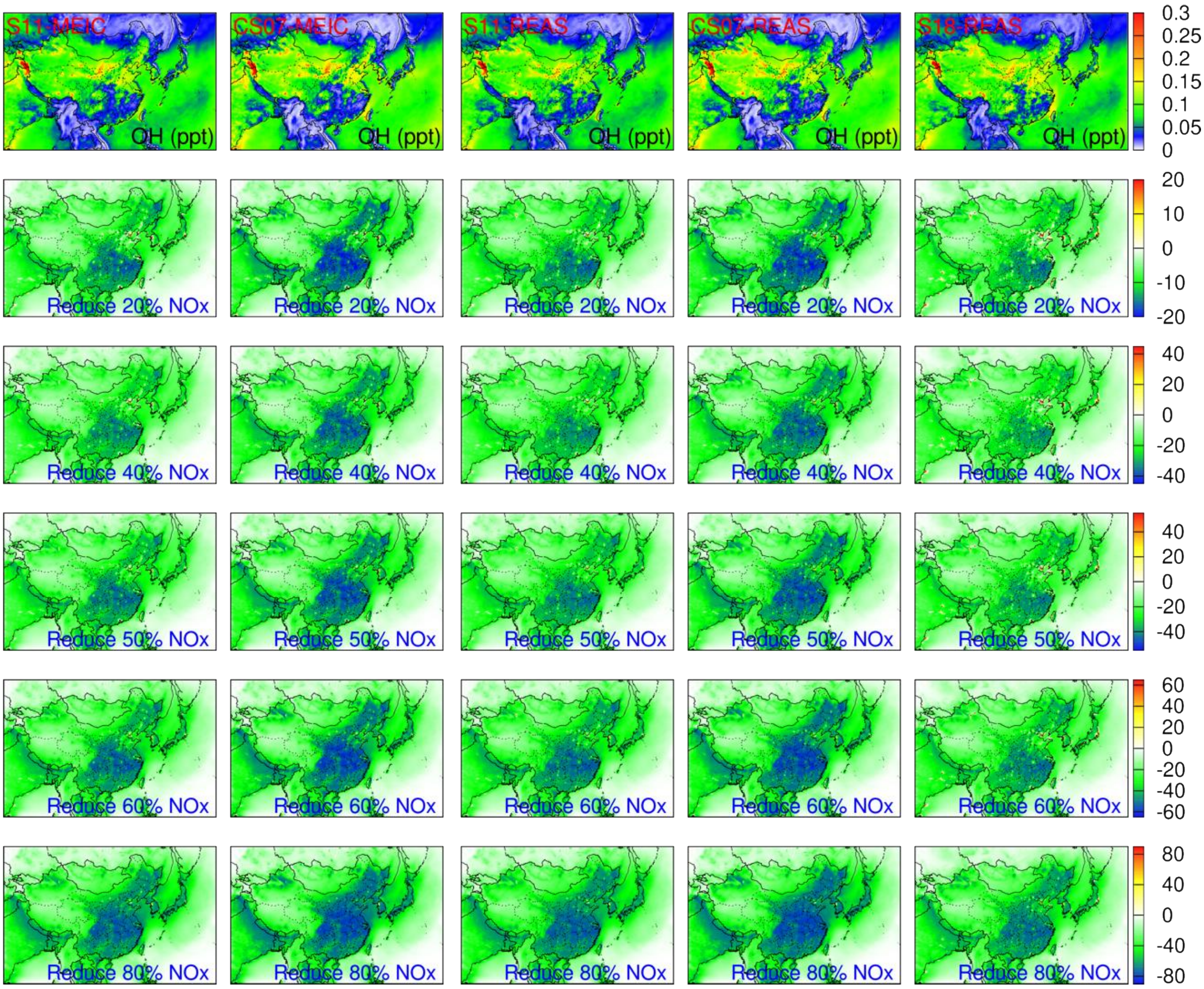

Figure S10. Predicted monthly average OH radical concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppt), and the percentage changes of OH due to 20%, 40%, 50%, 60%, and 80% reductions in NO_x emissions.

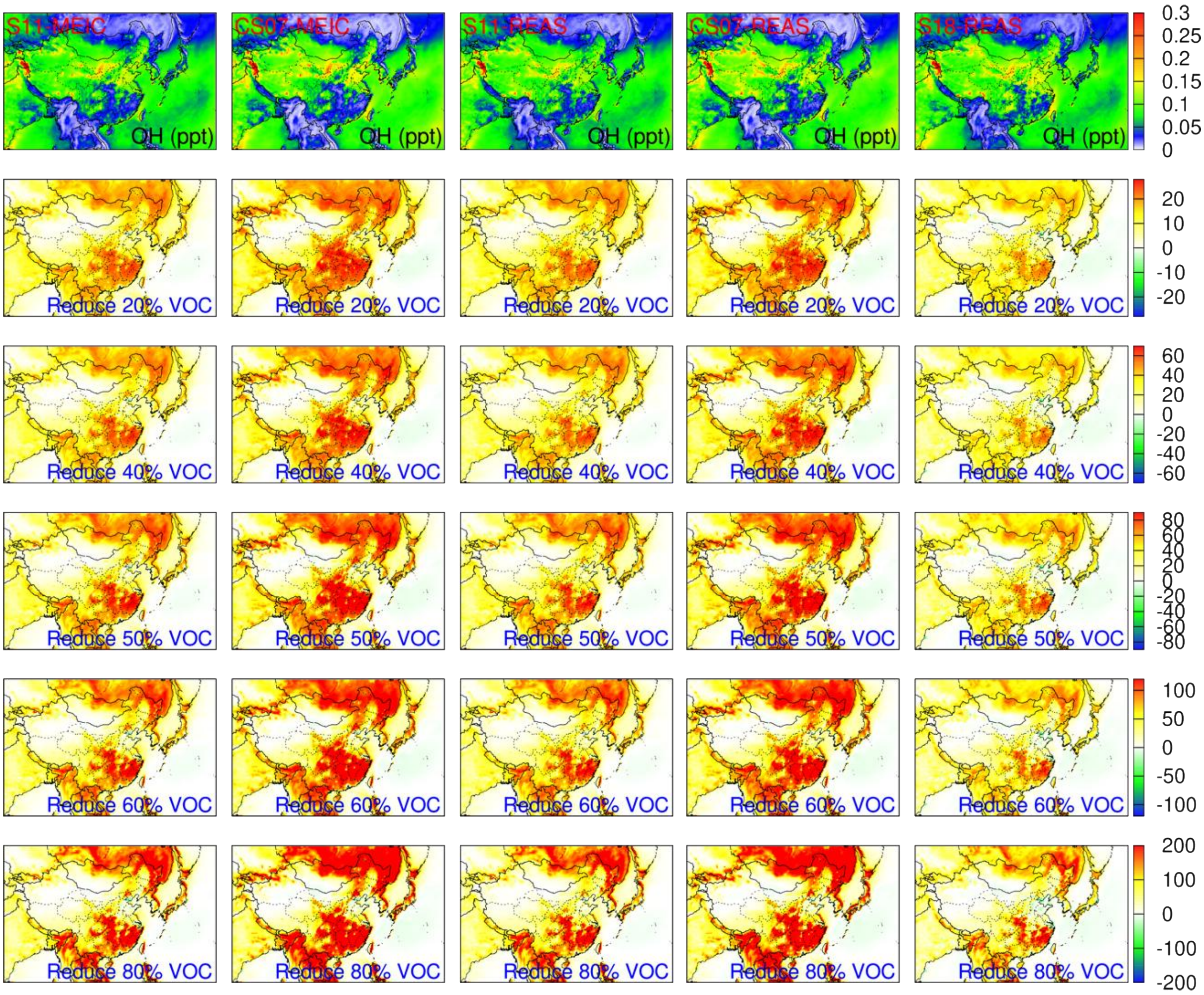

Figure S11. Predicted monthly average OH radical concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppt), and the percentage changes of OH due to 20%, 40%, 50%, 60%, and 80% reductions in VOC emissions.

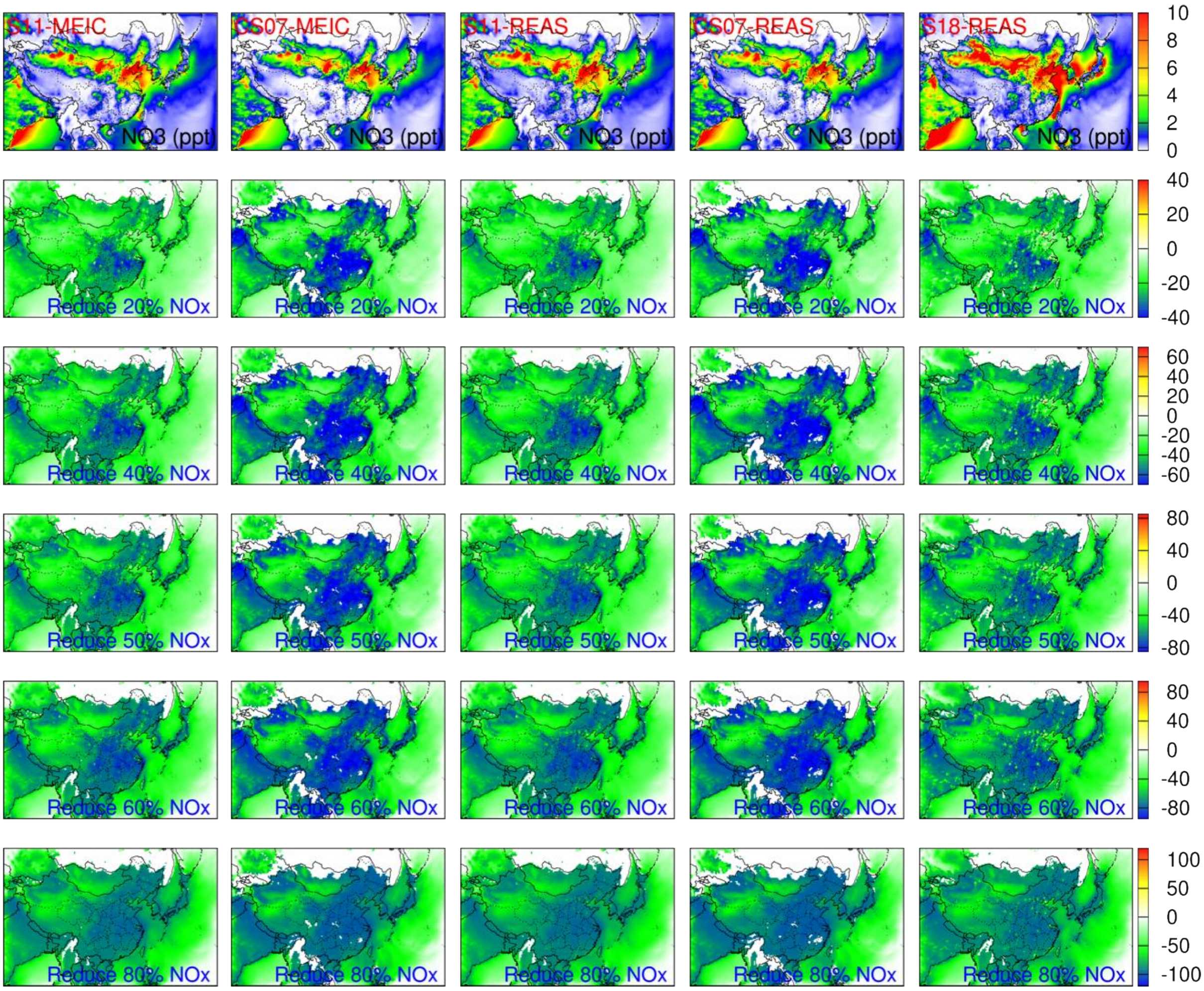

Figure S12. Predicted monthly average NO_3 radical concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppt), and the percentage changes of NO_3 due to 20%, 40%, 50%, 60%, and 80% reductions in NO_x emissions.

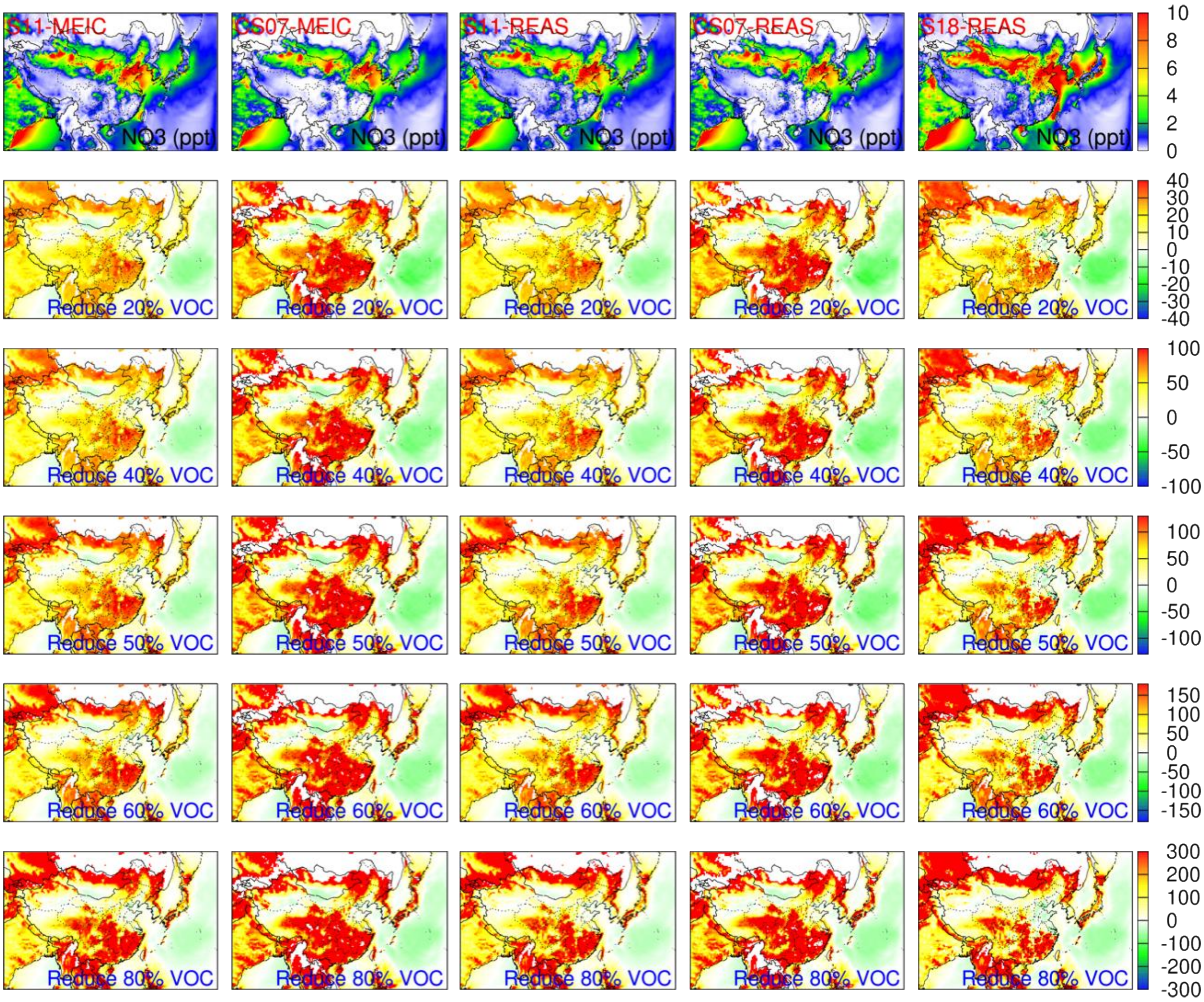

Figure S13. Predicted monthly average NO_3 radical concentrations in July 2017 using different photochemical mechanisms and emission inventories (first row; units are ppt), and the percentage changes of NO_3 due to 20%, 40%, 50%, 60%, and 80% reductions in VOC emissions.

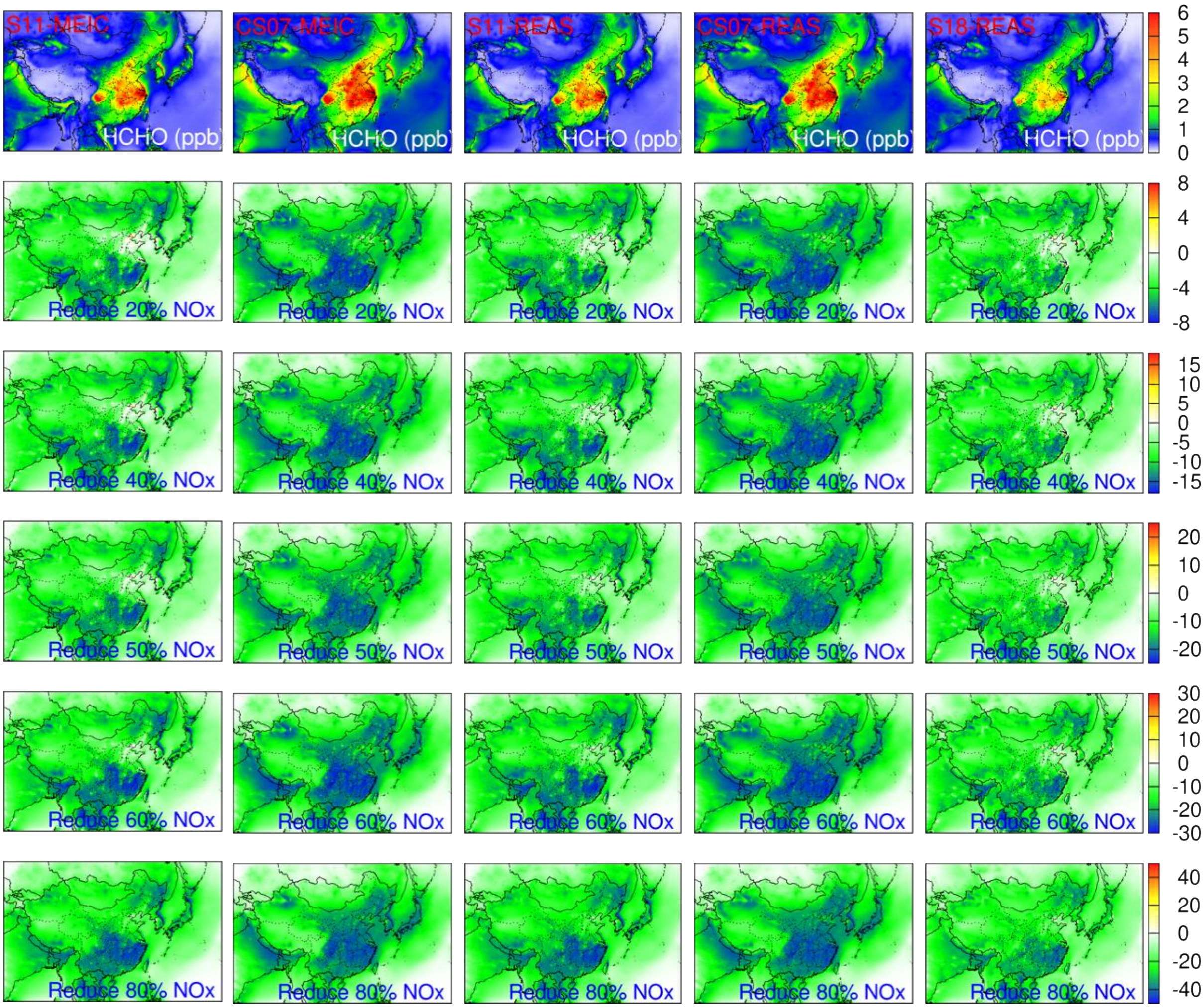

Figure S14. Predicted monthly average HCHO concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppb), and the percentage changes of HCHO due to 20%, 40%, 50%, 60%, and 80% reductions in NO_x emissions.

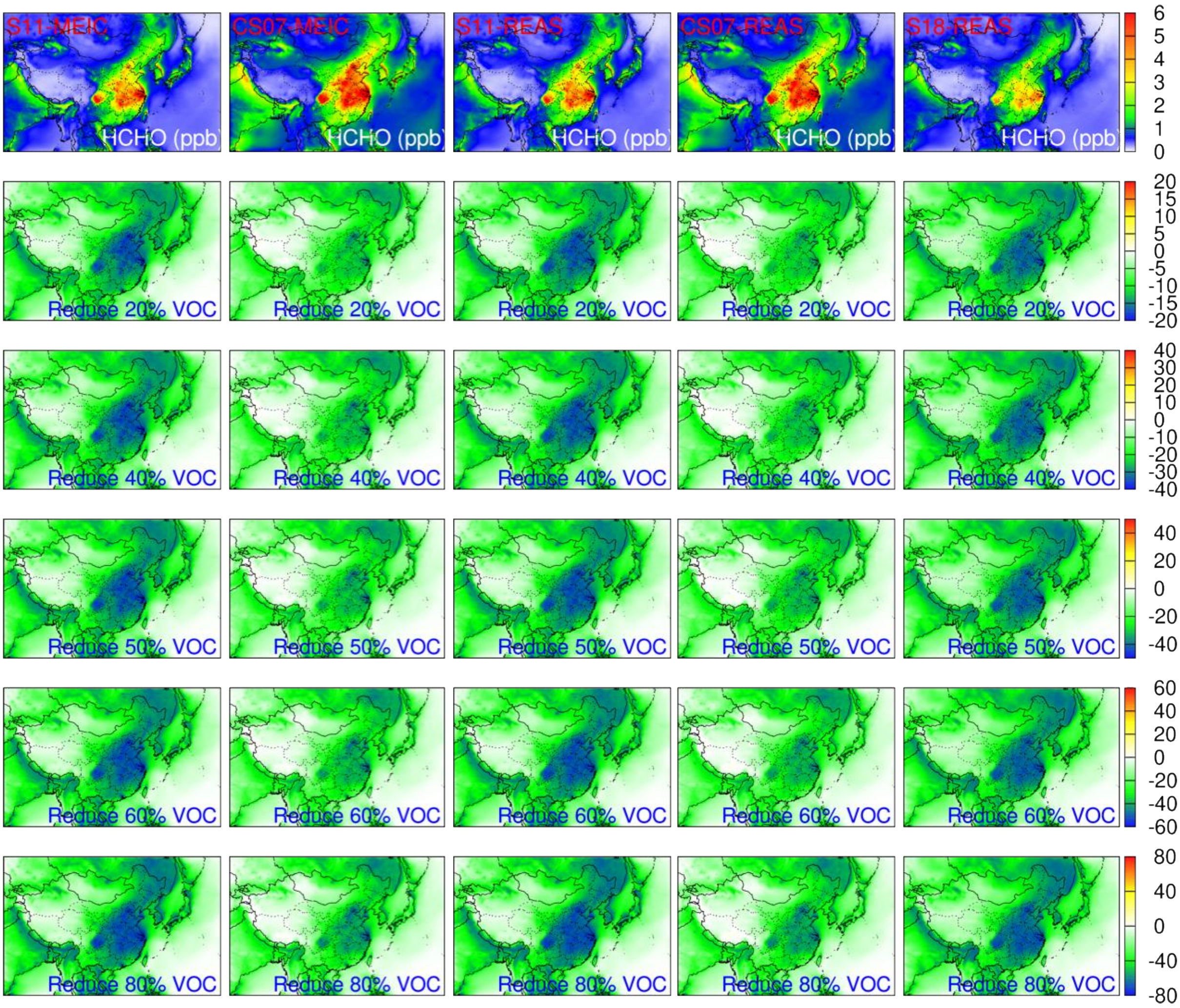

Figure S15. Predicted monthly average HCHO concentrations using different photochemical mechanisms and emission inventories in July 2017 (first row; units are ppb), and the percentage changes of HCHO due to 20%, 40%, 50%, 60%, and 80% reductions in VOC emissions.

Reference:

Boylan, J. W. and Russell, A. G.: PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models, Atmospheric Environment, 40, 4946–4959, https://doi.org/10.1016/j.atmosenv.2005.09.087, 2006.

Emery, C., Liu, Z., Russell, A. G., Odman, M. T., Yarwood, G., and Kumar, N.: Recommendations on statistics and benchmarks to assess photochemical model performance, Journal of the Air & Waste Management Association, 67, 582–598, https://doi.org/10.1080/10962247.2016.1265027, 2017.