

Supplement of
**A Comprehensive Global Modelling Assessment of Nitrate
Heterogeneous Formation on Desert Dust**

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S1 Model emissions, size bins and alkalinity calculations

Table S1. Total emissions (anthropogenic, biogenic and biomass burning) for 2018 used in this study.

Species	Emission (Tgy-1)
NO	75.93
NO2	17.86
HONO	0.51
NH3	61.81
SO2	104.40
PM2.5SO4	0.53

Table S2: Density, volumetric radius, effective radius, pm2.5 and pm10 fractions of each bin of the studied species

DUST									
	units	bin 1	bin 2	bin 3	bin 4	bin 5	bin 6	bin 7	bin 8
Density	kgm-3	2500	2500	2500	2500	2650	2650	2650	2650
Radius vol.	μm	0.15	0.25	0.47	0.8	1.36	2.29	3.93	7.24
Radius eff.	μm	0.15	0.25	0.45	0.78	1.32	2.24	3.80	7.11
PM2.5 frac.		1	1	1	1	0.38	0	0	0
PM10 frac.		1	1	1	1	1	1	0.87	0
SEA_SALT									
	units	bin 1	bin 2	bin 3	bin 4	bin 5	bin 6	bin 7	bin 8
Density	kgm-3	2160	2160	2160	2160	2160	2160	2160	2160
Radius vol.	μm	0.15	0.25	0.47	0.81	1.40	2.37	4.30	9.23
Radius eff.	μm	0.14	0.24	0.45	0.79	1.36	2.32	4.13	8.64
PM2.5 frac.		1	1	1	1	0.32	0	0	0
PM10 frac.		1	1	1	1	1	1	0.75	0
NO3									
	units	bin 1	bin 2						
Density	kgm-3	1700	2380						
Radius vol.	μm	0.35	2.23						
Radius eff.	μm	0.24	1.79						
PM2.5 frac.		1	0.2						
PM10 frac.		1	1						
NH4									
	units	bin 1	bin 2						
Density	kgm-3	1700	2380						
Radius vol.	μm	0.35	2.23						
Radius eff.	μm	0.24	1.79						
PM2.5 frac.		1	0.2						
PM10 frac.		1	1						
SO4									
	units	bin 1	bin 2						
Density	kgm-3	1700	2380						
Radius vol.	μm	0.35	2.23						
Radius eff.	μm	0.24	1.79						
PM2.5 frac.		1	0.2						
PM10 frac.		1	1						

Mineral	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Soluble in water?	Soluble in acids?	Assumed reactive?	Notes/References
Illite	8.5E-5	4.1E-4	3.1E-3	8.8E-3	2.2E-2	3.2E-2	5.5E-2	1.4E-2	no	yes	yes	1
Montmorillonite	6.2E-5	3.0E-4	2.2E-3	6.4E-3	1.6E-2	2.3E-2	4.0E-2	1.0E-2	-	yes	yes	2
Kaolinite	7.8E-5	3.7E-4	2.8E-3	8.0E-3	2.0E-2	2.9E-2	5.0E-2	1.3E-2	no	yes	no	3
Chlorite	1.2E-5	5.6E-5	4.2E-4	1.2E-3	4.8E-3	1.1E-2	2.6E-2	7.9E-3	no	-	no	4
Vermiculite	7.9E-6	3.8E-5	2.8E-4	8.1E-4	2.1E-3	2.9E-3	5.1E-3	1.3E-3	no	no	no	5
Feldspar	3.4E-6	1.6E-5	1.2E-4	3.5E-4	6.3E-3	2.2E-2	6.0E-2	1.9E-2	no	yes	yes	6
Quartz	1.2E-5	5.8E-5	4.4E-4	1.3E-3	1.9E-2	6.6E-2	1.8E-1	5.6E-2	no	no	no	7
Calcite	3.1E-5	1.5E-4	1.1E-3	3.2E-3	1.0E-2	1.9E-2	3.9E-2	1.1E-2	yes	yes	yes	8
Hematite	3.5E-6	1.7E-5	1.3E-4	3.6E-4	9.2E-4	1.3E-3	2.3E-3	5.9E-4	no	yes	no	9
Goethite	6.2E-6	2.9E-5	2.2E-4	6.3E-4	1.8E-3	3.1E-3	6.2E-3	1.8E-3	no	-	no	10
Gypsum	4.7E-7	2.2E-6	1.7E-5	4.8E-5	1.4E-4	2.5E-4	5.2E-4	1.5E-4	poor	yes	no	11
Mica	0.0E+0	0.0E+0	0.0E+0	0.0E+0	2.7E-3	1.0E-2	2.8E-2	9.0E-3	no	no	no	12
Total	3.0E-4	1.4E-3	1.1E-2	3.1E-2	1.1E-1	2.2E-1	4.9E-1	1.5E-1				

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Table S3. Globally-averaged mineral composition for each bin assumed from Journet et al. 2014 mineral database. References:

1. Assumed reactive because relatively soluble in acids Webmineral (2008f)
2. Assumed reactive because relatively soluble in acids Nutting (1941, 1932)
3. Assumed nonreactive because predominantly containing Al and Si. Yang (2008)
4. Assumed nonreactive because not soluble in water. Britannica, The Editors of Encyclopaedia (2018); Mindat.org (a)
5. Assumed nonreactive because not soluble. Huggett (2015); Schulze (2005); Bleam (2017)
6. Assumed reactive because relatively soluble in acids Blum (1994); Mindat.org (b)
7. Assumed nonreactive because not soluble. Usher et al. (2003)
8. Usher et al. (2003); Krueger et al. (2004); Hodzic et al. (2006)
9. Assumed nonreactive because iron is not considered in ISORROPIA-II. National Center for Biotechnology Information (2024a); Weast (1980)
10. Assumed nonreactive because not soluble, although lacking information if soluble in acids. Essington et al. (2005); National Center for Biotechnology Information. PubChem Compound Database (2024b)
11. Zhang and Muhammed (1989); National Center for Biotechnology Information. PubChem Compound Database (2024a); Krueger et al. (2004); Hodzic et al. (2006)
12. National Center for Biotechnology Information (2024b)

Mineral	Mineral Mw (g/mol)	Soluble element	Element Mw (g/mol)	Element fraction	Bin 1	Bin 2	Bin 3	Bin 4	Total fine	Bin 5	Bin 6	Bin 7	Bin 8	Total coarse	Total	References
Illite	389.34	K	39.10	0.10	2.84%	2.84%	2.84%	2.84%	2.84%	2.10%	1.45%	1.13%	0.99%	1.41%	2.20%	1
	389.34	Mg	24.31	0.06	1.76%	1.76%	1.76%	1.76%	1.76%	1.30%	0.90%	0.70%	0.62%	0.88%	1.37%	1
Montmorillonite	549.07	Ca	40.08	0.07	1.50%	1.50%	1.50%	1.50%	1.50%	1.11%	0.76%	0.59%	0.52%	0.75%	1.16%	2
	549.07	Na	22.99	0.04	0.86%	0.86%	0.86%	0.86%	0.86%	0.63%	0.44%	0.34%	0.30%	0.43%	0.67%	2
Feldspar - 1/3 Albite	263.02	Na (1/3)	22.99	0.03	0.03%	0.03%	0.03%	0.03%	0.03%	0.16%	0.27%	0.32%	0.35%	0.27%	0.14%	3
	277.41	Ca (1/3)	40.08	0.04	0.05%	0.05%	0.05%	0.05%	0.05%	0.26%	0.44%	0.53%	0.57%	0.45%	0.23%	4
- 1/3 Anorthite	278.33	K (1/3)	39.10	0.04	0.05%	0.05%	0.05%	0.05%	0.05%	0.25%	0.43%	0.52%	0.56%	0.44%	0.22%	5
	100.09	Ca	40.08	0.40	4.15%	4.15%	4.15%	4.15%	4.15%	3.76%	3.41%	3.23%	3.16%	3.39%	3.81%	6
Gypsum	172.20	Ca	40.08	0.23	0.04%	0.04%	0.04%	0.04%	0.04%	0.03%	0.03%	0.02%	0.02%	0.03%	0.03%	7
Total Ca					5.73%	5.73%	5.73%	5.73%	5.73%	5.15%	4.64%	4.39%	4.28%	4.61%	5.17%	
Total Na					0.89%	0.89%	0.89%	0.89%	0.89%	0.79%	0.71%	0.66%	0.65%	0.70%	0.79%	
Total K					2.88%	2.88%	2.88%	2.88%	2.88%	2.35%	1.88%	1.64%	1.55%	1.85%	2.37%	
Total Mg					1.76%	1.76%	1.76%	1.76%	1.76%	1.30%	0.90%	0.70%	0.62%	0.88%	1.32%	

Table S4. Size-resolved NVC content from globally-averaged mineralogy of Journet et al. 2014 for those minerals assumed to be soluble in water. References:

1. Webmineral (2008f)
2. Nutting (1941, 1932)
3. Webmineral (2008a)
4. Webmineral (2008b)
5. Webmineral (2008e)
6. Webmineral (2008c); National Center for Biotechnology Information. PubChem Compound Database (2024a)
7. Webmineral (2008d); Hulett and Allen (1902)

Mineral	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Soluble in water?	Soluble in acids?	Assumed reactive?	Notes/References
Illite	1.1E-04	5.4E-04	4.0E-03	1.2E-02	2.9E-02	4.2E-02	7.2E-02	1.9E-02	no	yes	yes	1
Montmorillonite	6.4E-05	3.0E-04	2.3E-03	6.5E-03	1.7E-02	2.4E-02	4.1E-02	1.1E-02	-	yes	yes	2
Kaolinite	7.6E-05	3.6E-04	2.7E-03	7.8E-03	2.0E-02	2.8E-02	4.8E-02	1.3E-02	no	yes	no	3
Calcite	1.3E-05	6.3E-05	4.7E-04	1.4E-03	5.2E-03	1.2E-02	2.7E-02	8.0E-03	yes	yes	yes	4
Quartz	2.0E-05	9.7E-05	7.3E-04	2.1E-03	2.4E-02	8.0E-02	2.1E-01	6.7E-02	no	no	no	5
Feldspar	8.1E-06	3.9E-05	2.9E-04	8.3E-04	8.5E-03	2.8E-02	7.3E-02	2.3E-02	no	yes	yes	6
Iron Oxide	4.6E-06	2.2E-05	1.6E-04	4.7E-04	1.6E-03	3.3E-03	7.3E-03	2.2E-03	-	-	no	7
Gypsum	3.4E-06	1.6E-05	1.2E-04	3.5E-04	1.3E-03	2.8E-03	6.3E-03	1.9E-03	poor	yes	no	8
Total	3.0E-04	1.4E-03	1.1E-02	3.1E-02	1.1E-01	2.2E-01	4.9E-01	1.4E-01				

6

Table S5. Globally-averaged mineral composition for each bin assumed from Claquin et al. (1999) mineral database. References:

1. Assumed reactive because relatively soluble in acids Webmineral (2008f)
2. Assumed reactive because relatively soluble in acids Nutting (1941, 1932)
3. Assumed nonreactive because predominantly containing Al and Si. Yang (2008)
4. Usher et al. (2003); Krueger et al. (2004); Hodzic et al. (2006)
5. Assumed nonreactive because not soluble. Usher et al. (2003)
6. Assumed reactive because relatively soluble in acids Blum (1994); Mindat.org (b)
7. Assumed nonreactive because iron is not considered in ISORROPIA-II. National Center for Biotechnology Information (2024a); Weast (1980)
8. Zhang and Muhammed (1989); National Center for Biotechnology Information. PubChem Compound Database (2024a); Krueger et al. (2004); Hodzic et al. (2006)

Mineral	Mineral Mw (g/mol)	Soluble element	Element Mw (g/mol)	Element fraction	Bin 1	Bin 2	Bin 3	Bin 4	Total fine	Bin 5	Bin 6	Bin 7	Bin 8	Total coarse	Total	References
Illite	389.340	K	39.10	0.10	3.76%	3.76%	3.76%	3.76%	3.76%	2.78%	1.92%	1.49%	1.31%	1.88%	2.92%	1
	389.340	Mg	24.31	0.06	2.34%	2.34%	2.34%	2.34%	2.34%	1.73%	1.19%	0.93%	0.82%	1.17%	1.82%	1
Montmorillonite	549.070	Ca	40.08	0.07	1.54%	1.54%	1.54%	1.54%	1.54%	1.14%	0.78%	0.61%	0.54%	0.77%	1.20%	2
	549.070	Na	22.99	0.04	0.88%	0.88%	0.88%	0.88%	0.88%	0.65%	0.45%	0.35%	0.31%	0.44%	0.69%	2
Feldspar - 1/3 Albite	263.020	Na (1/3)	22.99	0.03	0.07%	0.07%	0.07%	0.07%	0.07%	0.21%	0.33%	0.39%	0.42%	0.34%	0.19%	3
	277.410	Ca (1/3)	40.08	0.04	0.12%	0.12%	0.12%	0.12%	0.12%	0.35%	0.55%	0.65%	0.70%	0.56%	0.31%	4
- 1/3 Anorthite	278.330	K (1/3)	39.10	0.04	0.11%	0.11%	0.11%	0.11%	0.11%	0.34%	0.54%	0.63%	0.68%	0.55%	0.31%	5
	100.090	Ca	40.08	0.40	1.76%	1.76%	1.76%	1.76%	1.76%	1.95%	2.11%	2.19%	2.22%	2.12%	1.92%	6
Gypsum	172.200	Ca	40.08	0.23	0.26%	0.26%	0.26%	0.26%	0.26%	0.28%	0.30%	0.30%	0.31%	0.30%	0.28%	7
					3.68%	3.68%	3.68%	3.68%	3.68%	3.71%	3.74%	3.76%	3.76%	3.74%	3.71%	
Total Ca					0.95%	0.95%	0.95%	0.95%	0.95%	0.86%	0.78%	0.75%	0.73%	0.78%	0.87%	
Total Na					3.87%	3.87%	3.87%	3.87%	3.87%	3.12%	2.45%	2.13%	1.99%	2.42%	3.15%	
Total K					2.34%	2.34%	2.34%	2.34%	2.34%	1.73%	1.19%	0.93%	0.82%	1.17%	1.75%	
Total Mg																

Table S6. Size-resolved NVC content from globally-averaged mineralogy of Claquin et al. (1999) for those minerals assumed to be soluble in water. References:

1. Webmineral (2008f)
2. Nutting (1941, 1932)
3. Webmineral (2008a)
4. Webmineral (2008b)
5. Webmineral (2008e)
6. Webmineral (2008c); National Center for Biotechnology Information. PubChem Compound Database (2024a)
7. Webmineral (2008d); Hulett and Allen (1902)

S2 Spatial distributions

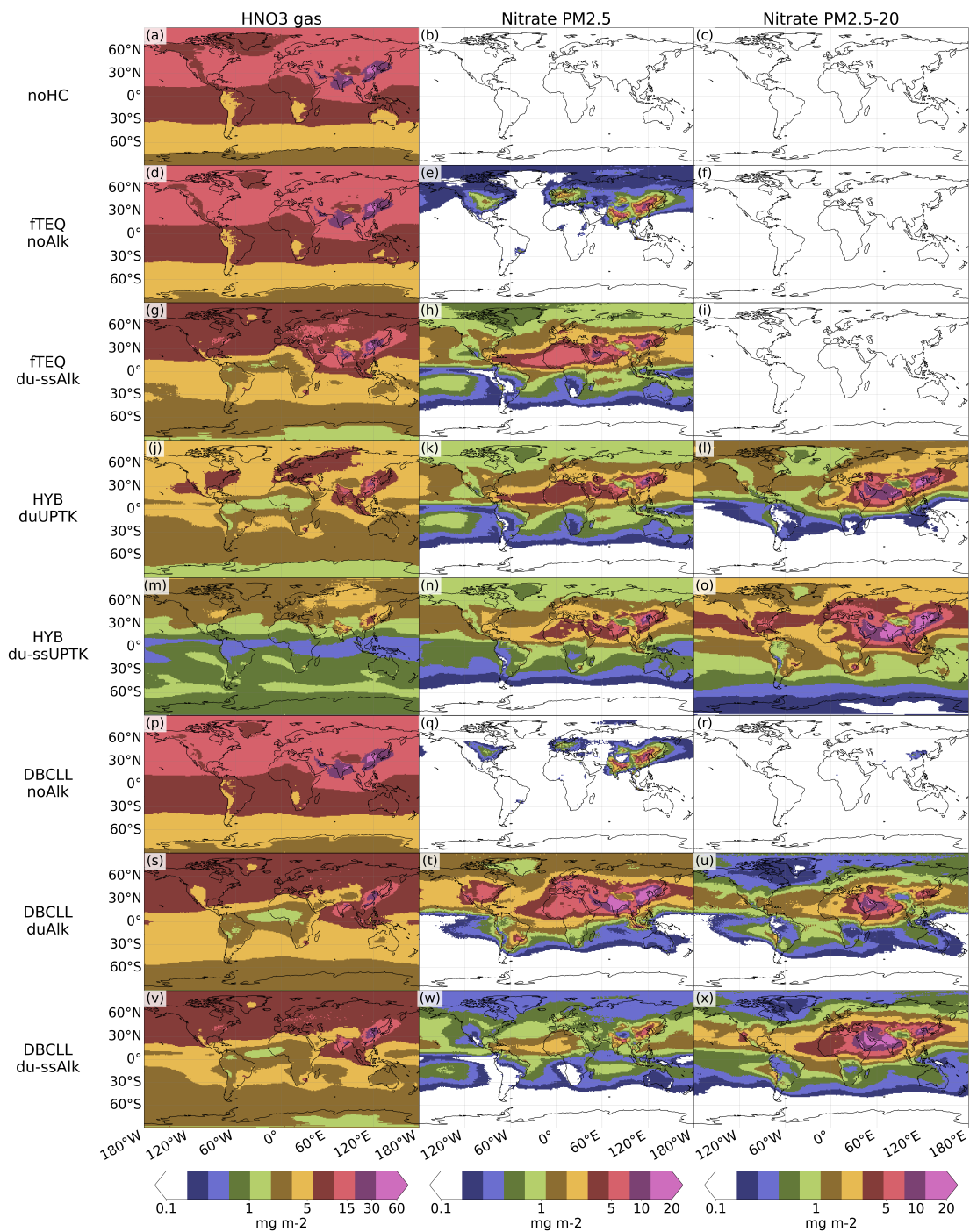


Figure S1. Column load (mg m^{-2}) of $\text{HNO}_3(\text{g})$, fine and coarse particulate nitrate simulated by the different mechanisms, averaged for 2018.

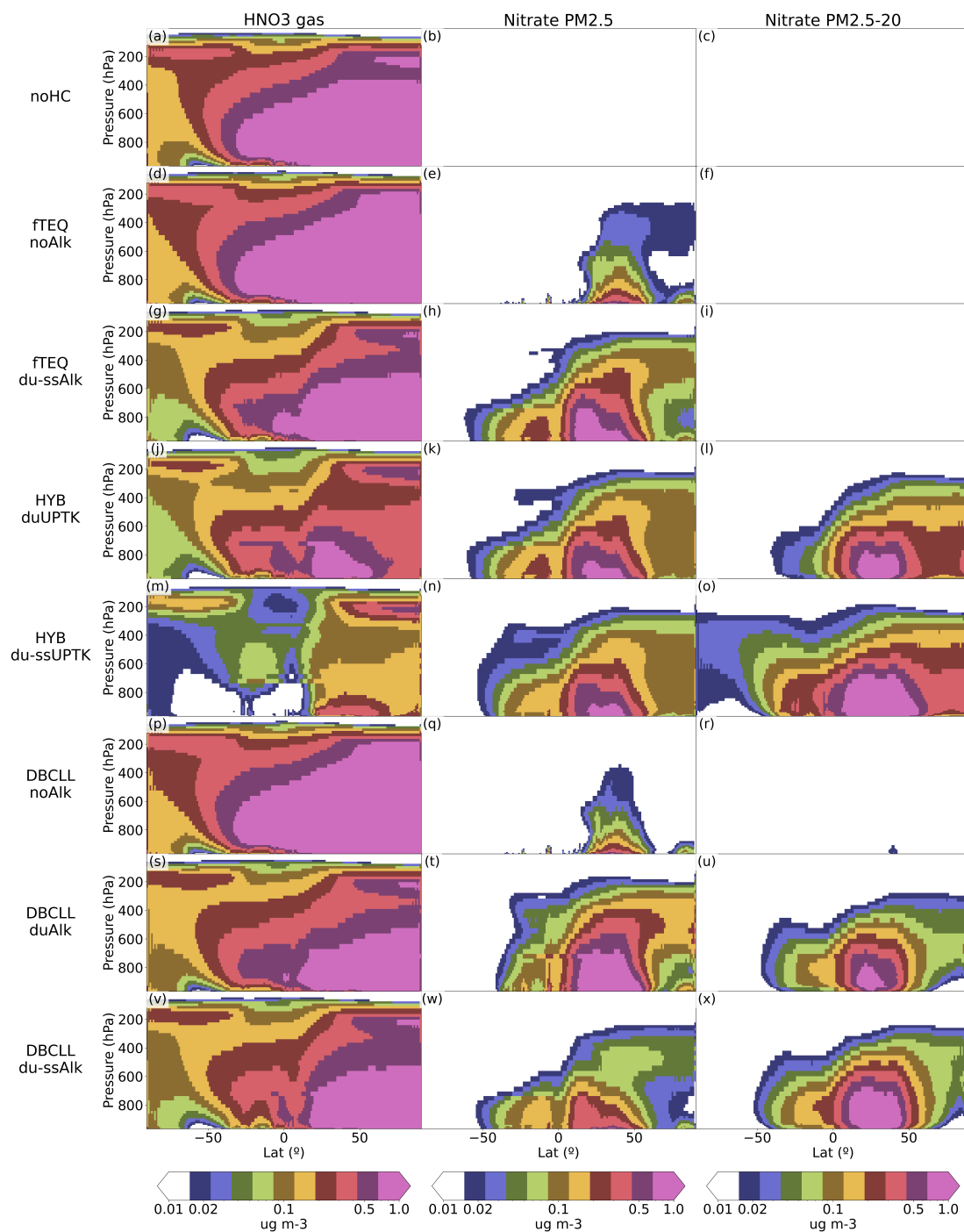


Figure S2. Zonal average concentration ($\mu\text{g m}^{-3}$) of HNO₃, fine and coarse particulate nitrate simulated by the different mechanisms in 2018.

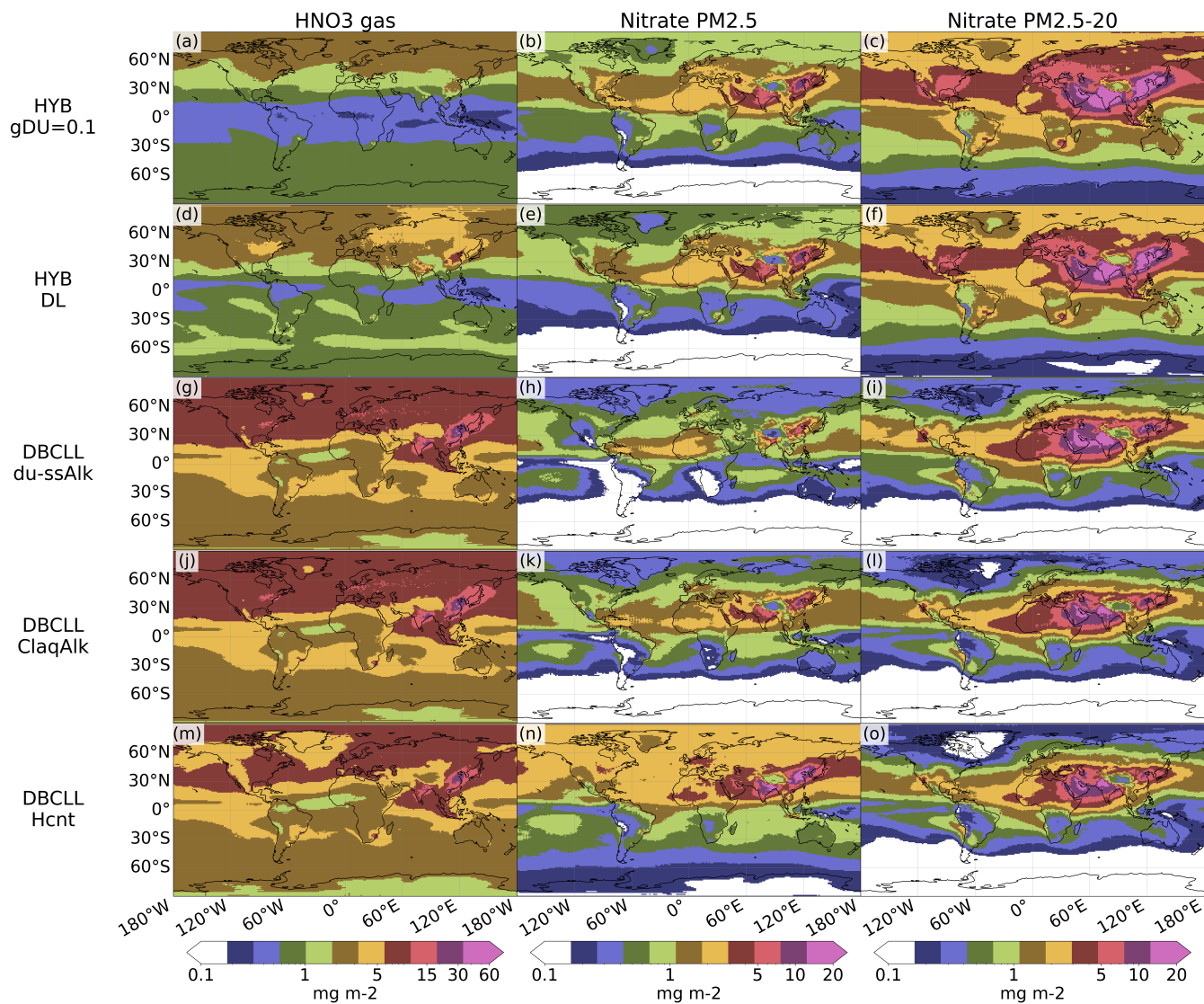


Figure S3. Column load ($mg\ m^{-2}$) of $HNO_3(g)$, fine and coarse particulate nitrate simulated by additional mechanisms, averaged for 2018.

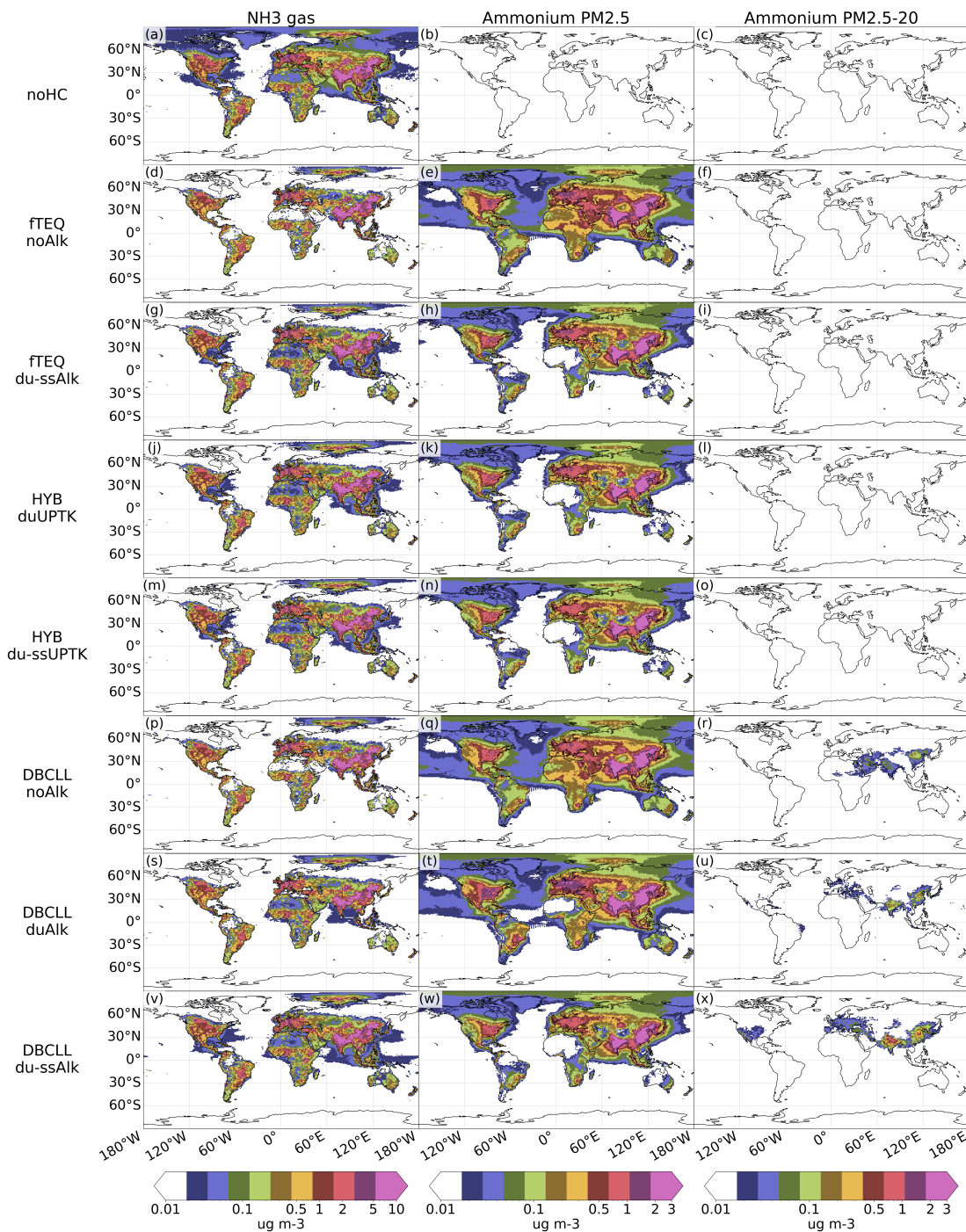


Figure S4. Surface concentration ($\mu\text{g m}^{-3}$) of $\text{NH}_3(\text{g})$, fine and coarse particulate ammonium simulated by the different mechanisms, averaged for 2018.

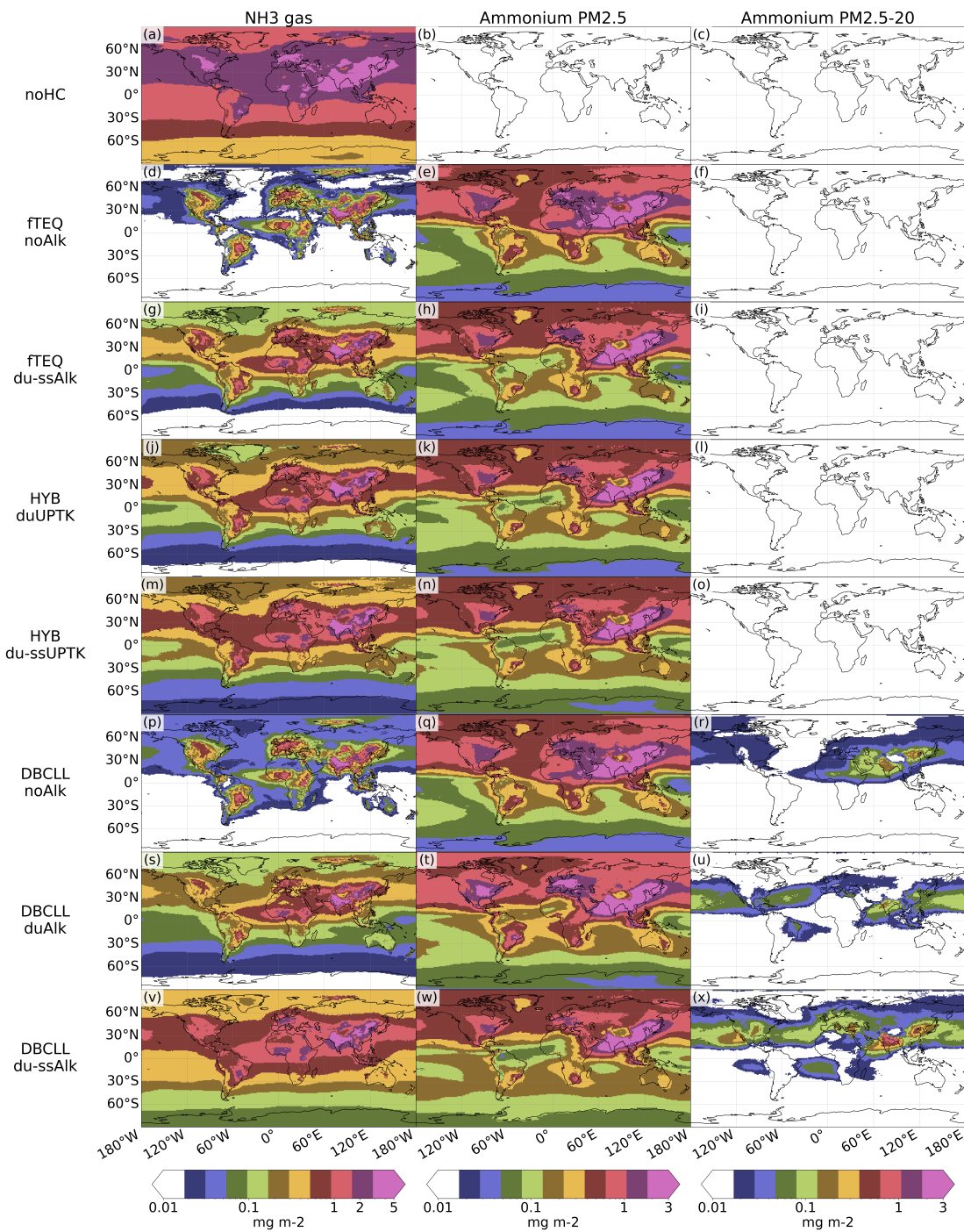


Figure S5. Column load (mg m^{-2}) of $\text{NH}_3(\text{g})$, fine and coarse particulate ammonium simulated by different mechanisms, averaged for 2018.

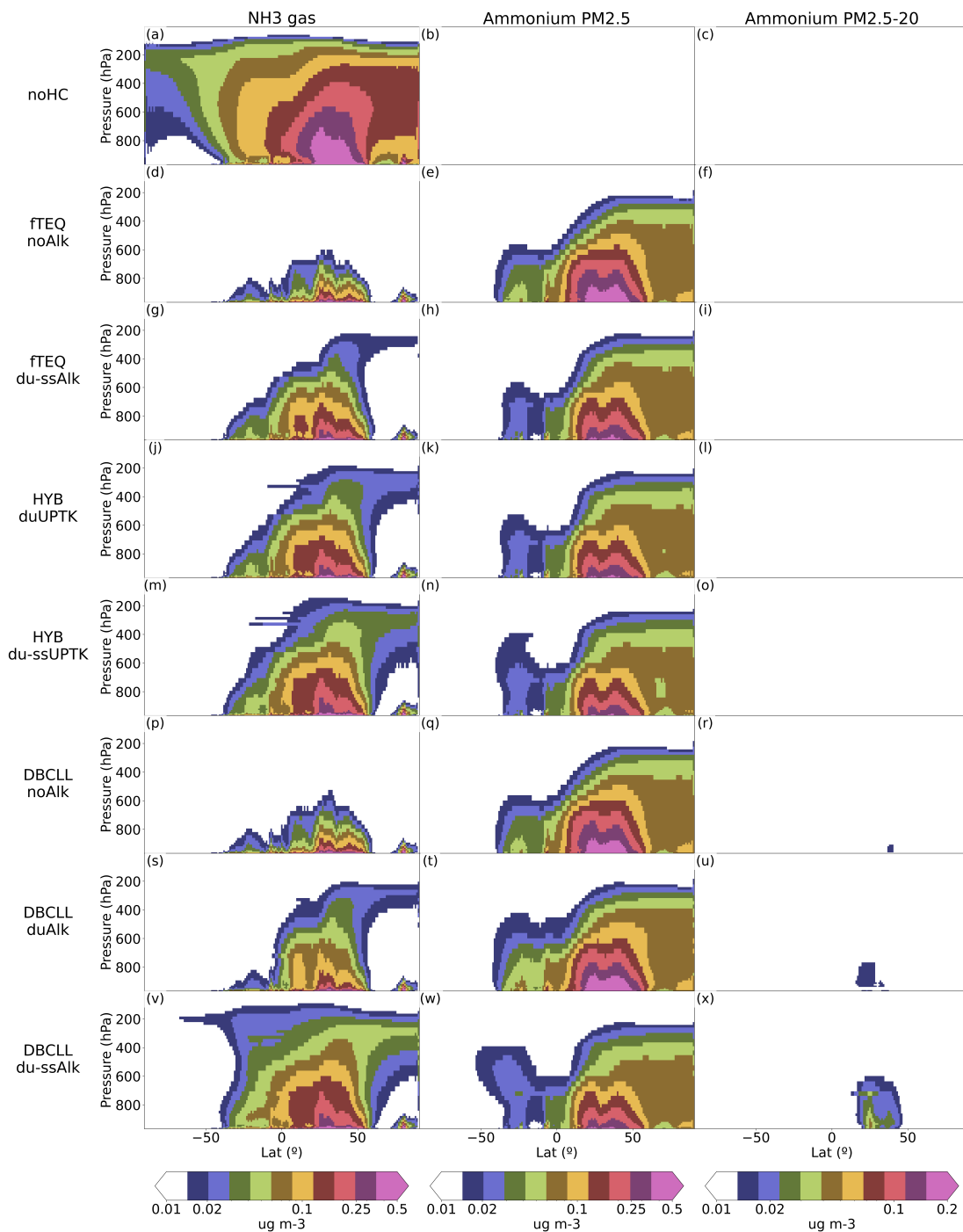


Figure S6. Zonal average concentration ($\mu\text{g m}^{-3}$) of $\text{NH}_3(\text{g})$, fine and coarse particulate ammonium simulated by the different mechanisms in 2018.

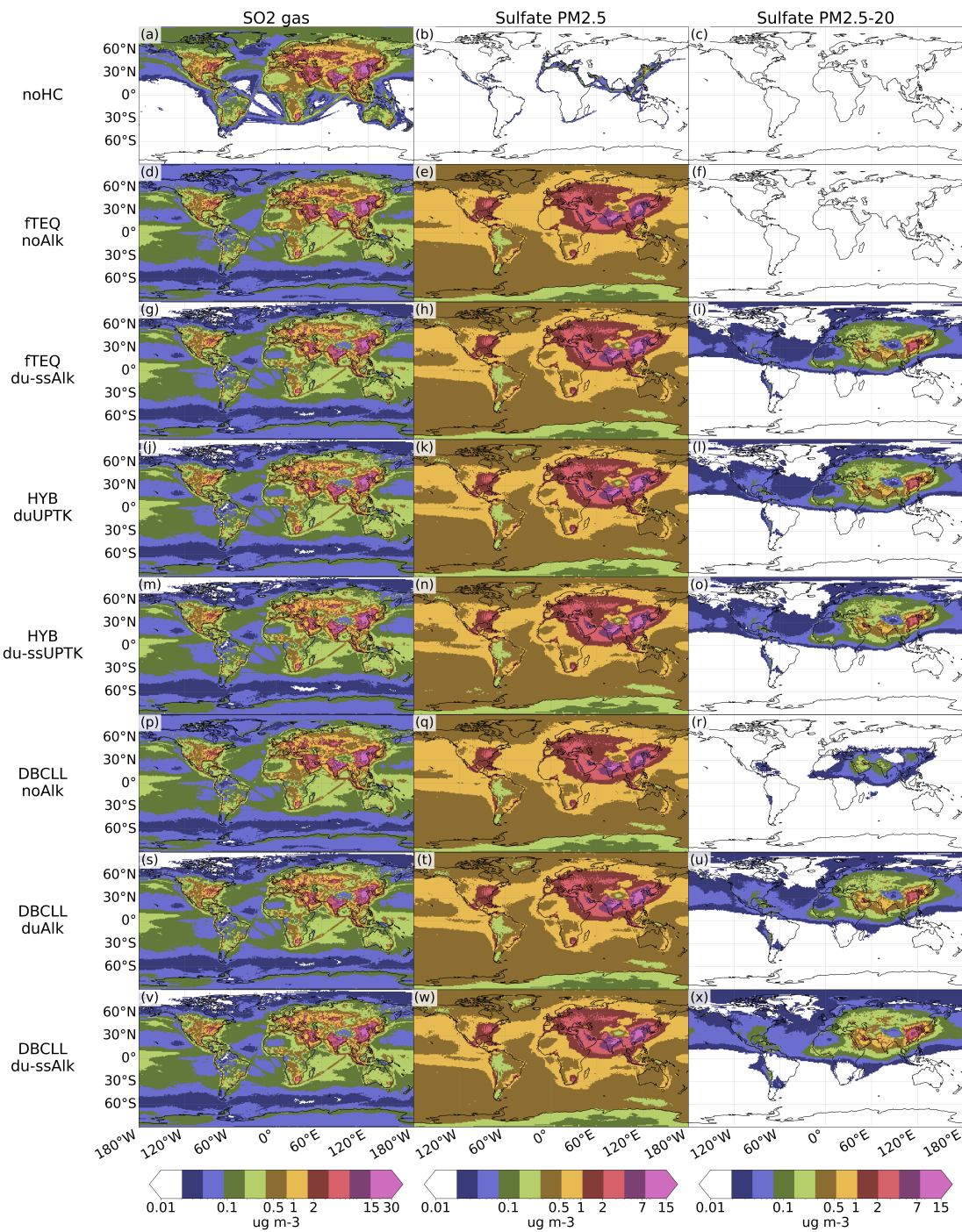


Figure S7. Surface concentration ($\mu\text{g m}^{-3}$) of $\text{SO}_2(\text{g})$, fine and coarse particulate sulfate simulated by the different mechanisms, averaged for 2018.

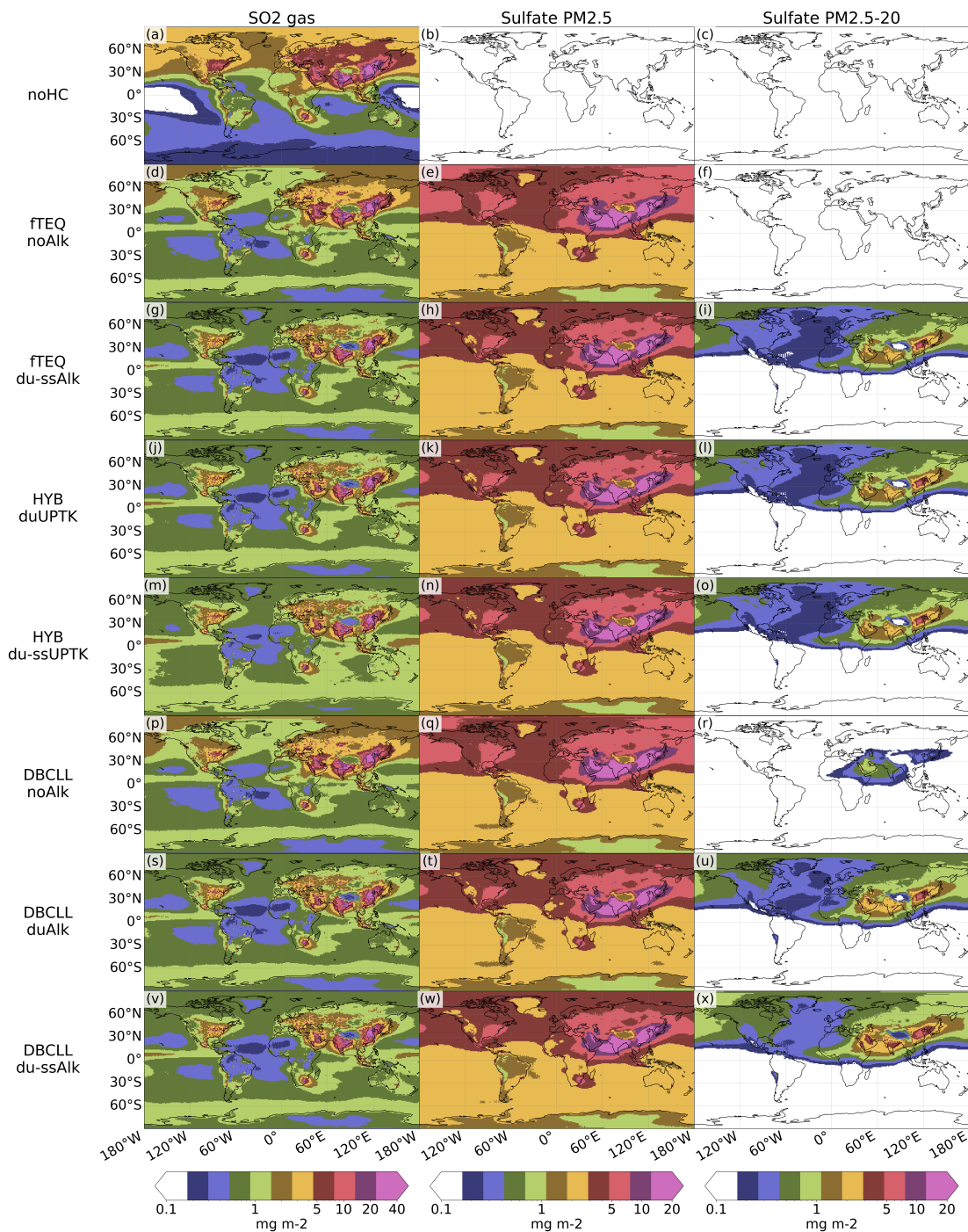


Figure S8. Column load (mg m^{-2}) of $\text{SO}_2(\text{g})$, fine and coarse particulate sulfate simulated by different mechanisms, averaged for 2018.

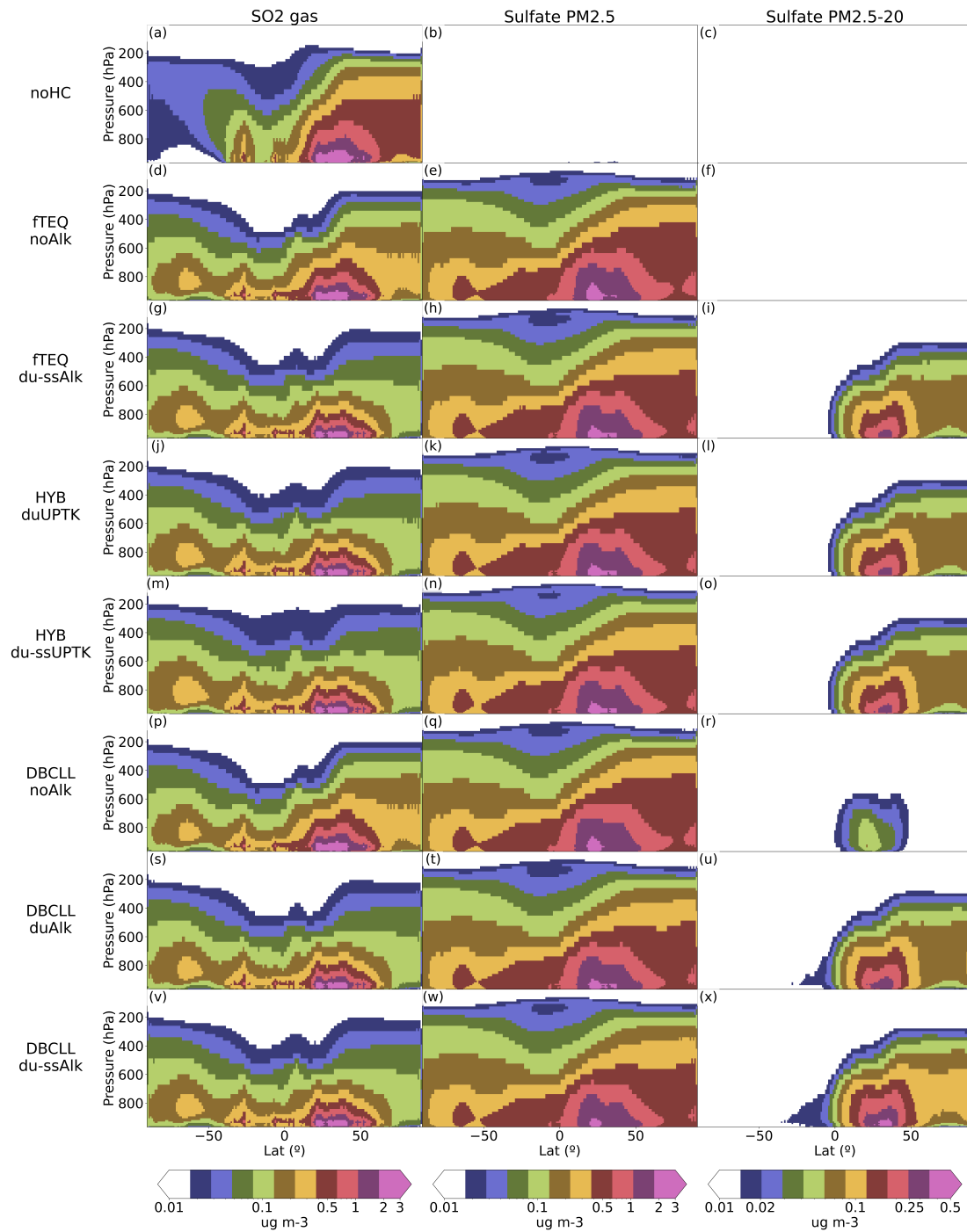


Figure S9. Zonal average concentration ($\mu\text{g m}^{-3}$) of $\text{SO}_2(\text{g})$, fine and coarse particulate sulfate simulated by the different mechanisms in 2018.

Column average concentration (20180101 to 20181231)

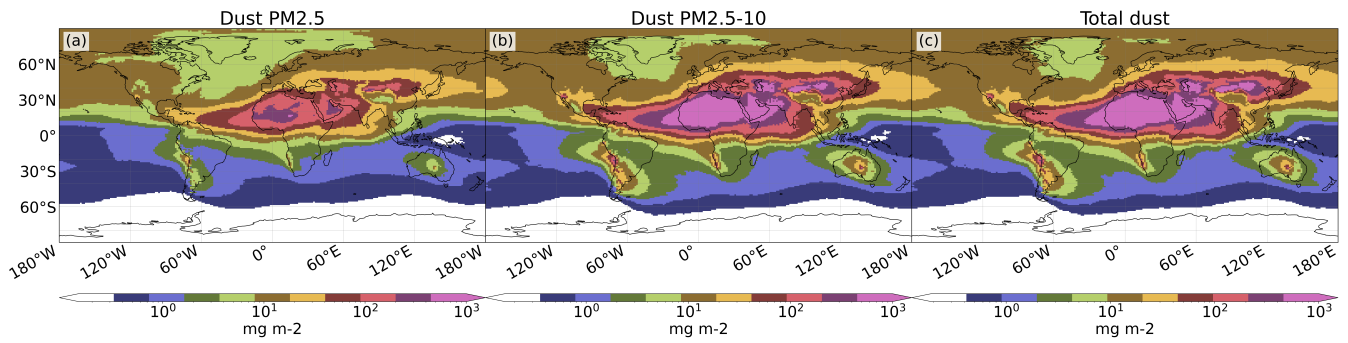


Figure S10. Dust average column load (mg m^{-2}) for 2018.

Column average concentration (20180101 to 20181231)

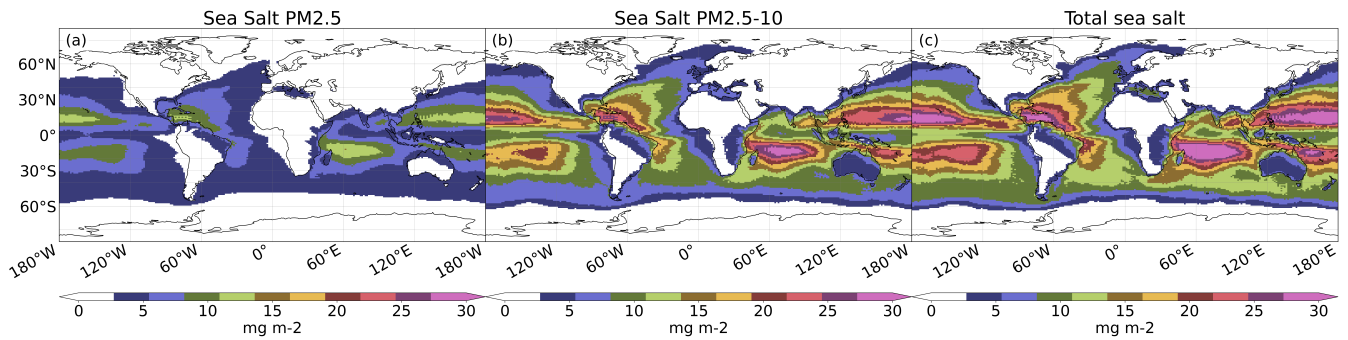


Figure S11. Sea salt average column load (mg m^{-2}) for 2018.

S3 Statistical metrics and supplementary evaluation results

Each experiment is evaluated against observations in terms of correlation coefficient (corr), mean bias (bias) and root mean square error (rmse), formulated as follows:

$$corr = \frac{\sum_{i=1}^N (S_i - \bar{S})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (S_i - \bar{S})^2} \sqrt{\sum_{i=1}^N (O_i - \bar{O})^2}} \quad (1)$$

$$bias = \frac{\sum_{i=1}^N (S_i - O_i)}{N} \quad (2)$$

$$rmse = \sqrt{\frac{\sum_{i=1}^N (S_i - O_i)^2}{N}} \quad (3)$$

Where S are the simulation results, O the observations and N the number of observations.

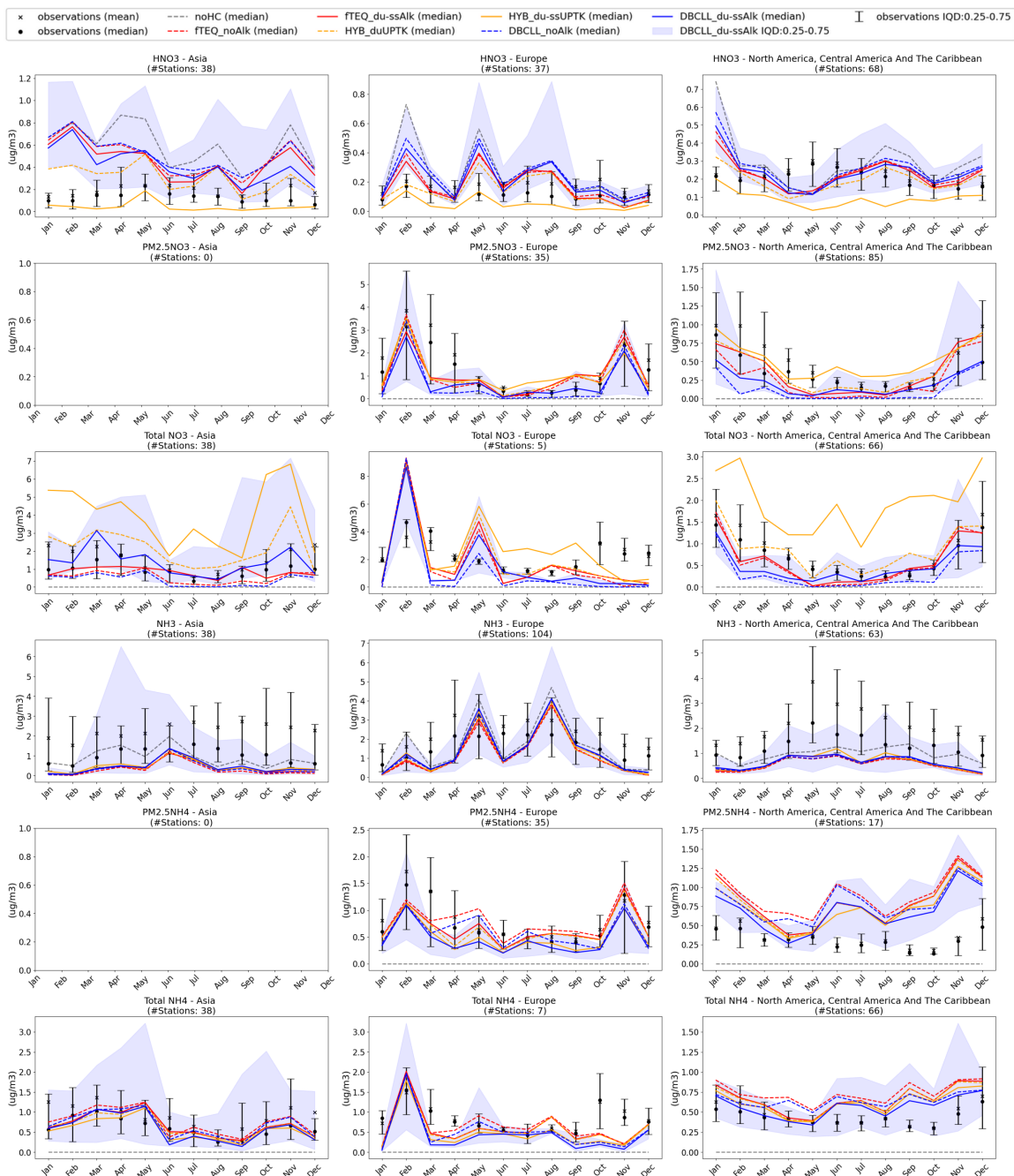


Figure S12. Yearly surface concentration evaluation for Asia, Europe and North-Central America continents. Species are in rows and continents in columns. Black solid dots and crosses represent observational mean and median, respectively. Error bars are the interquartile 0.25 to 0.75 distance. Coloured lines represent medians obtained from the most representative configurations. Blue shade is the interquartile 0.25 - 0.75 distance for the DBCLL_du-ssAlk simulation. Observational PM₁₀ from EANET (Asia) and US-EPA-CASTNET (North America) refers to total particle concentration, while GHOST data refers to data limited to PM₁₀.

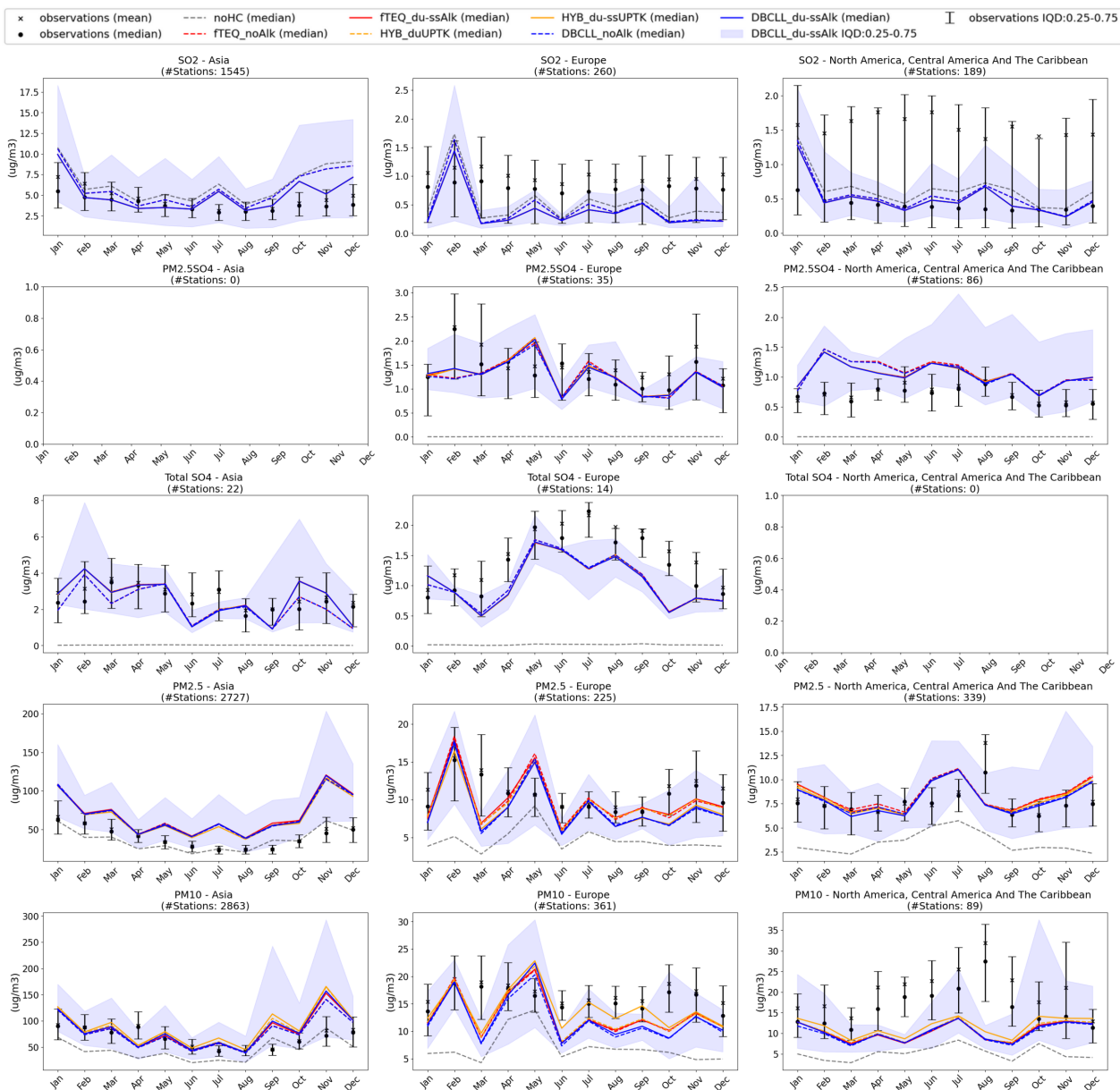


Figure S12. Yearly surface concentration evaluation for Asia, Europe and North-Central America continents. Species are in rows and continents in columns. Black solid dots and crosses represent observational mean and median, respectively. Error bars are the interquartile 0.25 to 0.75 distance. Coloured lines represent medians obtained from the most representative configurations. Blue shade is the interquartile 0.25 - 0.75 distance for the DBCLL_{du-ssAlk} simulation. Observational PM₁₀ from EANET (Asia) and US-EPA-CASTNET (North America) for sulfate refers to total particle concentration, while GHOST data refers to data limited to PM₁₀.

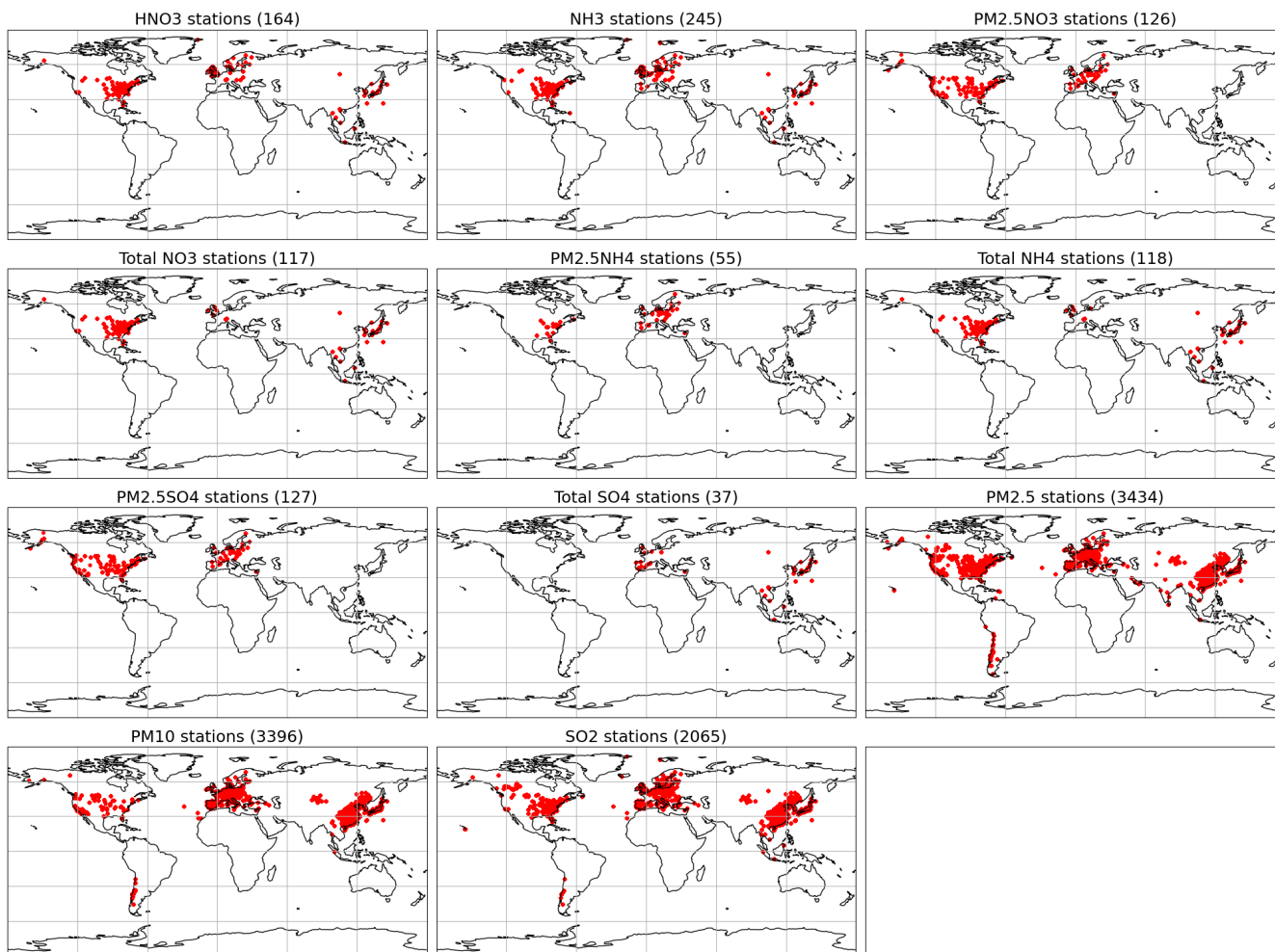


Figure S13. Stations used for each species in the observational evaluation from the main text Figure 5 and Supplement Figure S12.

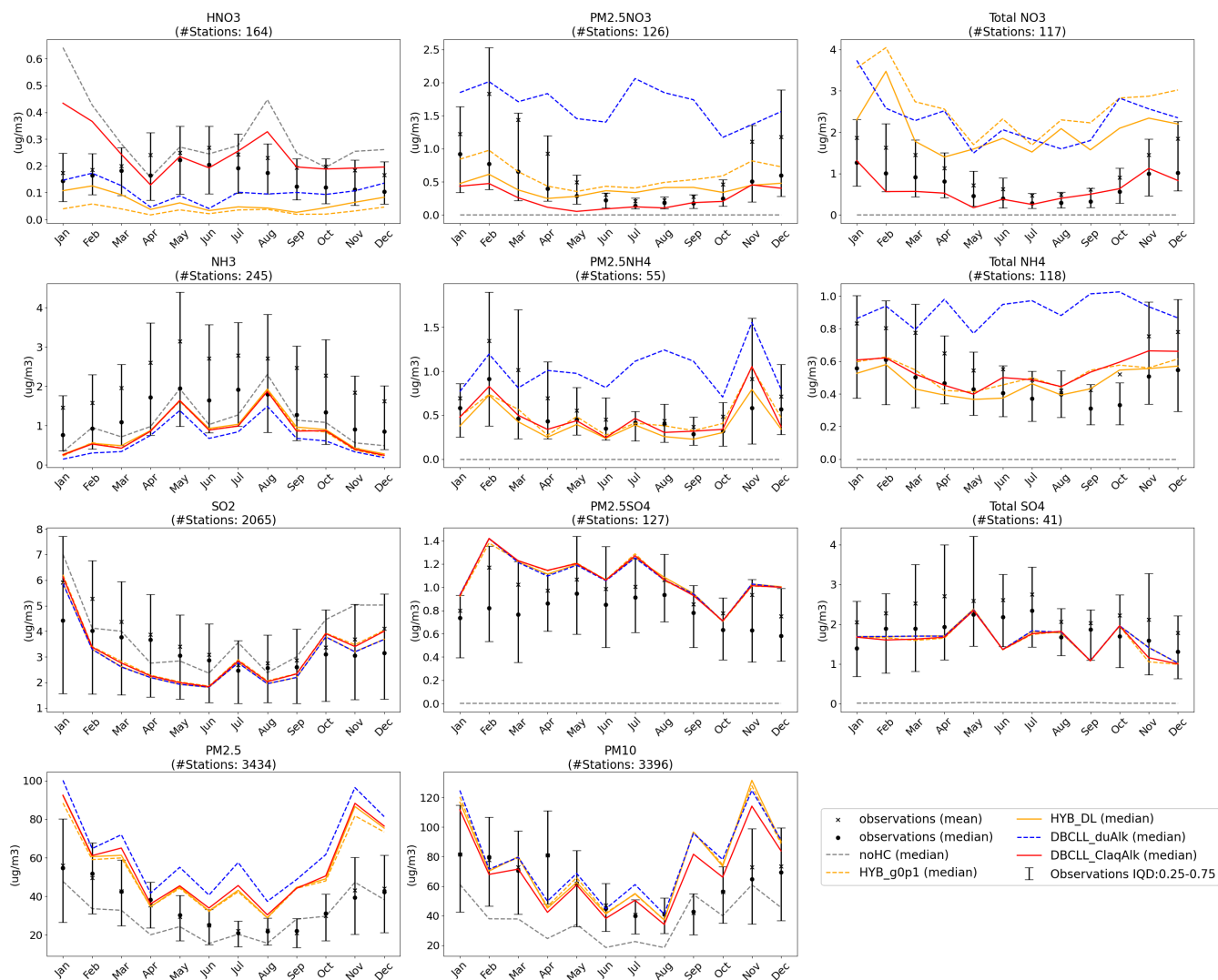


Figure S14. Observational evaluation of gas and particulate species. Black solid dots and crosses represent monthly mean and median of observations, respectively. Colour lines represent each configuration’s monthly median surface concentrations over observational points. Error bars are the observational interquartile 0.25 to 0.75 distance. For the Total NO_3 modes, data from Europe, Asia and North-Central America has been averaged, despite data from Asia and North-Central America refers to total particle concentration, while data from Europe is limited strictly to $10\mu\text{m}$ particle diameter.

Table S7: Correlation coefficients, bias and root mean square error (RMSE) of each configuration's results median with respect to observations' median for timeseries of Figure 5 from the main manuscript.

	HNO3			PM2.5NO3			Total NO3		
	corr	bias	rmse	corr	bias	rmse	corr	bias	rmse
noHC	0.03	0.15	0.20	0.00	-0.43	0.49	0.00	-0.70	0.77
HYB_g0p1	0.05	-0.13	0.13	0.83	0.18	0.23	0.81	1.96	2.01
HYB_DL	-0.08	-0.10	0.11	0.61	-0.03	0.21	0.53	1.32	1.40
DBCLL_duAlk	-0.34	-0.05	0.08	0.21	1.24	1.28	0.80	1.61	1.65
DBCLL_ClaqAlk	0.14	0.09	0.12	0.82	-0.18	0.24	0.81	-0.09	0.22
	NH3			PM2.5NH4			Total NH4		
	corr	bias	rmse	corr	bias	rmse	corr	bias	rmse
noHC	0.80	-0.29	0.44	0.00	-0.48	0.51	0.00	-0.45	0.46
HYB_g0p1	0.85	-0.53	0.59	0.64	0.01	0.16	0.47	0.07	0.11
HYB_DL	0.85	-0.49	0.56	0.77	-0.09	0.14	0.50	0.02	0.09
DBCLL_duAlk	0.88	-0.71	0.73	0.27	0.53	0.58	-0.46	0.46	0.48
DBCLL_ClaqAlk	0.85	-0.53	0.59	0.70	-0.01	0.16	0.50	0.09	0.12
	SO2			PM2.5SO4			Total SO4		
	corr	bias	rmse	corr	bias	rmse	corr	bias	rmse
noHC	0.61	0.65	1.24	0.59	-0.79	0.80	0.62	-1.91	1.93
HYB_g0p1	0.62	-0.12	0.94	0.59	0.29	0.32	0.53	-0.42	0.54
HYB_DL	0.63	-0.29	0.91	0.57	0.29	0.33	0.60	-0.39	0.50
DBCLL_duAlk	0.63	-0.29	0.91	0.55	0.29	0.32	0.59	-0.38	0.49
DBCLL_ClaqAlk	0.62	-0.16	0.94	0.57	0.29	0.33	0.55	-0.41	0.52
	PM2.5			PM10					
	corr	bias	rmse	corr	bias	rmse			
noHC	0.75	-5.62	9.55	0.40	-23.16	28.42			
HYB_g0p1	0.76	18.02	21.95	0.38	14.27	29.96			
HYB_DL	0.76	19.44	23.81	0.36	13.87	30.41			
DBCLL_duAlk	0.71	28.07	31.58	0.38	16.47	30.10			
DBCLL_ClaqAlk	0.76	20.75	24.88	0.43	7.45	24.20			

Table S8. GHOST quality flags used for the observational evaluation.

Code	Flag	Description
0	Missing Measurement	i.e. NaN.
1	Infinite Value	Value is infinite – occurs when data values are outside of the range that <i>float32</i> data type can handle (-3.4E+38 to +3.4E+38).
2	Negative Measurement	Measurement is negative in absolute terms.
6	Invalid Data Provider Flags - GHOST Decreed	Measurements are associated with data quality flags given by the data provider which have been decreed by the GHOST project architects as being associated with substantial uncertainty/bias.
8	No Valid Data to Average	After screening by key QA flags, no valid data remains to average in the temporal window.
20	Erroneous Primary Sampling	The primary sampling is not appropriate to prepare the specific parameter for subsequent measurement.
21	Erroneous Sample Preparation	The sample preparation is not appropriate to prepare the specific parameter for subsequent measurement.
22	Erroneous Measurement Methodology	The measurement methodology used is not known to be able to measure the specific parameter.
72	Below Preferential Lower Limit of Detection	Measurement is below or equal to the preferential lower limit of detection.
75	Above Preferential Upper Limit of Detection	Measurement is above or equal to the preferential upper limit of detection.
82	Insufficient Measurement Resolution - Preferential	The preferential resolution for the measurement is coarser than a set limit (variable by measured parameter).
83	Insufficient Measurement Resolution - Empirical	The resolution of the measurement is analysed month by month. If the minimum difference between observations is coarser than a set limit (variable by measured parameter), measurements are flagged.
110	Data Outlier - Exceeds Scientifically Decreed Lower/Upper Limit	The measured value is below or greater than scientifically feasible lower/upper limits (variable by parameter).
111	Data Outlier - Monthly Median Exceeds Scientifically Decreed Upper Limit	The median of the measurements in a month is greater than a scientifically feasible limit (variable by parameter).
112	Data Outlier - Network Decreed	Data has been reported to be an outlier through data flags by the network data reporters (and not manually checked and verified as valid).
113	Data Outlier - Manually Decreed	Data has been found and decreed manually to be an outlier.
115	Probable Data Outlier - Monthly Adjusted Boxplot	Measured value exceeds adjusted boxplot outer fence (lower or upper) of monthly data, therefore is a probable data outlier.
132	Systematic Inconsistent Monthly Distributions - 4/6 Months >= Zone 6	4 out of 6 months' distributions are classed as Zone 6 or higher, suggesting there are potentially systematic reasons for the inconsistent distributions across the 6 months.
133	Systematic Inconsistent Monthly Distributions - 8/12 Months >= Zone 6	8 out of 12 months' distributions are classed as Zone 6 or higher, suggesting there are potentially systematic reasons for the inconsistent distributions across the 12 months.

Table S9. Results for gas $\text{HNO}_{3(g)}$ obtained with the studied heterogeneous chemistry mechanisms. Results from the references are reported at the end of the Table: the average of all the participating models in the intercomparison AeroCom phase III nitrate experiment for 2008, specifying their standard deviation (*STD*), and results from the GMI model (using a similar HYB approach with UPTK reactions on dust and SS) and the EMAC model (*EMAC 2008*, that uses a similar approach to DBCLL_du-ssAlk). Also using the EMAC model, results obtained by the Karydis et al. (2016) study are reported as *EMAC 2005-2008*. Results from models using a similar approach to HYB_du-ssUPTK are reported as *IFS* for Rémy et al. (2022), *LMDz-INCA* for Hauglustaine et al. (2014) and *MetOffice UM* for Jones et al. (2021).

$\text{HNO}_{3(g)}$	Burden (Tg)	Wet Dep. (Tg y-1)	Dry Dep. (Tg y-1)	Total Dep. (Tg y-1)	Production (Tg y-1)	Lifetime (days)
noHC	4.79	47.1	110.4	157.5	158.3	5.5
fTEQ_noAlk	4.99	48.6	107.3	155.9	156.7	5.8
fTEQ_du-ssAlk	2.93	41.4	77.4	118.8	119.3	4.5
HYB_duUPTK	1.96	29.9	52.0	81.9	82.4	4.4
HYB_du-ssUPTK	0.69	7.2	13.7	20.9	21.4	5.9
HYB_gDU=0.1	0.46	5.9	5.9	11.8	12.2	7.1
HYB_DL	0.72	6.7	14.0	20.7	21.2	6.2
DBCLL_noAlk	5.13	49.1	109.1	158.2	159.0	5.9
DBCLL_duAlk	2.72	45.4	59.9	105.3	105.7	4.7
DBCLL_du-ssAlk	2.53	36.1	61.9	98.0	98.6	4.7
DBCLL_ClaqAlk	2.58	36.2	62.1	98.3	98.9	4.8
AeroCom	2.50	108.7	45.8	154.5	179.0	4.6
STD AeroCom	±1.83	±39.8	±13.0	±52.8	±89.9	±1.6
GMI	2.50	108.7	45.8	154.5	110.0	3.5
EMAC 2008¹	3.10	136.0	56.1	192.1	-	-
EMAC 2005-2008²	1.65	-	-	-	-	-
IFS	-	-	-	-	-	-
LMDz-INCA	1.35	76.6	66.0	142.6	218.3	2.3
MetOffice UM³	2.16	67.1	27.0	94.1	242.1	3.2

¹ From Bian et al. (2017).

² From Karydis et al. (2016).

³ Jones et al. (2021) performs two sensitivity tests to the accommodation coefficient used for NO_3^- formation in the fine mode: *FAST* with 0.193 and *SLOW* with 0.001. Here, results from the *FAST* test are reported on the basis that they present similar fine NO_3^- formation rates to our average fine nitrate results

Table S10. Results for gas $\text{NH}_{3(\text{g})}$ obtained with the studied heterogeneous chemistry mechanisms. Results from the references are reported at the end of the Table: the average of all the participating models in the intercomparison AeroCom phase III nitrate experiment for 2008, specifying their standard deviation (*STD*), and results from the GMI model (using a similar HYB approach with UPTK reactions on dust and SS) and the EMAC model (*EMAC 2008*, that uses a similar approach to DBCLL_du-ssAlk). Also using the EMAC model, results obtained by the Karydis et al. (2016) study are reported as *EMAC 2005-2008*. Results from models using a similar approach to HYB_du-ssUPTK are reported as *IFS* for Rémy et al. (2022), *LMDz-INCA* for Hauglustaine et al. (2014) and *MetOffice UM* for Jones et al. (2021).

$\text{NH}_{3(\text{g})}$	Emissions (Tg y-1)	Burden (Tg)	Wet Dep. (Tg y-1)	Dry Dep. (Tg y-1)	Total Dep. (Tg y-1)	Loss (Tg y-1)	Lifetime (days)
noHC	61.8	0.86	7.1	54.5	61.7	0.0	5.1
fTEQ_noAlk	61.8	0.05	1.3	39.6	40.9	-20.9	0.3
fTEQ_du-ssAlk	61.8	0.16	1.8	44.2	45.9	-15.9	0.9
HYB_duUPTK	61.8	0.21	1.9	44.7	46.6	-15.1	1.2
HYB_du-ssUPTK	61.8	0.26	2.2	45.6	47.8	-14.0	1.5
HYB_gDU=0.1	61.8	0.28	2.2	46.0	48.3	-13.5	1.7
HYB_DL	61.8	0.38	2.9	46.7	49.6	-12.1	2.2
DBCLL_noAlk	61.8	0.06	1.6	40.4	42.0	-19.8	0.4
DBCLL_duAlk	61.8	0.14	1.8	39.8	41.7	-20.2	0.8
DBCLL_du-ssAlk	61.8	0.35	2.8	45.9	48.6	-13.2	2.0
DBCLL_ClaqAlk	61.8	0.31	2.7	45.5	48.2	-13.6	1.8
AeroCom	62.9	0.20	13.4	18.7	32.1	-32.1	0.7
STD AeroCom	±3.9	±0.20	±5.1	±5.1	±10.2	±12.0	±0.3
GMI	60.4	0.85	1.1	8.7	9.8	-50.1	5.2
EMAC 2008¹	59.3	0.85	0.0	15.5	15.5	-	-
EMAC 2005-2008²	-	0.82	-	-	-	-	-
IFS	-	-	-	-	-	-	-
LMDz-INCA	61.3	0.11	13.4	25.9	39.3	-21.2	0.6
MetOffice UM³	64.7	0.05	6.9	21.1	28.0	-36.8	0.3

¹ From Bian et al. (2017).

² From Karydis et al. (2016).

³ Jones et al. (2021) performs two sensitivity tests to the accommodation coefficient used for NO_3^- formation in the fine mode: *FAST* with 0.193 and *SLOW* with 0.001. Here, results from the *FAST* test are reported on the basis that they present similar fine NO_3^- formation rates to our average fine nitrate results.

Table S11. Results for particle NH_4^+ obtained with the studied heterogeneous chemistry mechanisms. Results from the references are reported at the end of the Table: the average of all the participating models in the intercomparison AeroCom phase III nitrate experiment for 2008, specifying their standard deviation (*STD*), and results from the GMI model (using a similar HYB approach with UPTK reactions on dust and SS) and the EMAC model (*EMAC 2008*, that uses a similar approach to DBCELL_du-ssAlk). Also using the EMAC model, results obtained by the Karydis et al. (2016) study are reported as *EMAC 2005-2008*. Results from models using a similar approach to HYB_du-ssUPTK are reported as *IFS* for Rémy et al. (2022), *LMDz-INCA* for Hauglustaine et al. (2014) and *MetOffice UM* for Jones et al. (2021).

Experiment	Burden (Tg)			Wet Dep. (Tg y ⁻¹)			Dry Dep. (Tg y ⁻¹)			Total Dep. (Tg y ⁻¹)			Production (Tg y ⁻¹)			Lifetime (days)		
	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total
<i>fTEQ_noAlk</i>	0.30	0.00	0.30	19.2	0.0	19.2	3.0	0.0	3.0	22.2	0.0	22.2	22.2	0.0	22.2	2.5	0.0	2.5
<i>fTEQ_du-ssAlk</i>	0.21	0.00	0.21	14.9	0.0	14.9	2.0	0.0	2.0	16.9	0.0	16.9	16.9	0.0	16.9	2.3	0.0	2.3
<i>HYB_duUPTK</i>	0.21	0.00	0.21	14.3	0.0	14.3	1.9	0.0	1.9	16.2	0.0	16.2	16.2	0.0	16.2	2.3	0.0	2.3
<i>HYB_du-ssUPTK</i>	0.20	0.00	0.20	13.2	0.0	13.2	1.7	0.0	1.7	15.0	0.0	15.0	15.0	0.0	15.0	2.4	0.0	2.4
<i>HYB_gDU=0.1</i>	0.19	0.00	0.19	12.9	0.0	12.9	1.6	0.0	1.6	14.5	0.0	14.5	14.5	0.0	14.5	2.4	0.0	2.4
<i>HYB_DL</i>	0.19	0.00	0.19	11.7	0.0	11.7	1.6	0.0	1.6	13.3	0.0	13.3	13.3	0.0	13.3	2.7	0.0	2.7
<i>DBCELL_noAlk</i>	0.29	0.01	0.30	17.8	0.3	18.1	2.8	0.2	2.9	20.5	0.5	21.0	20.5	0.5	21.0	2.6	3.1	2.6
<i>DBCELL_duAlk</i>	0.30	0.01	0.31	18.9	0.3	19.2	3.1	0.2	3.3	22.1	0.4	22.5	22.1	0.4	22.5	2.5	4.1	2.5
<i>DBCELL_du-ssAlk</i>	0.20	0.02	0.22	12.6	0.2	12.7	1.8	0.1	1.9	14.3	0.3	14.6	14.3	0.3	14.6	2.6	10.8	2.8
<i>DBCELL_ClaqAlk</i>	0.22	0.02	0.23	12.9	0.2	13.1	1.8	0.2	2.0	14.7	0.4	15.1	14.7	0.4	15.1	2.7	7.7	2.8
<i>AeroCom</i>	-	-	0.32	-	-	24.4	-	-	5.8	-	-	30.2	-	-	30.4	-	-	4.3
<i>STD AeroCom</i>	-	-	±0.20	-	-	±10.0	-	-	±5.8	-	-	±15.8	-	-	±4.3	-	-	±2.6
<i>GMI</i>	-	-	0.48	-	-	50.7	-	-	1.9	-	-	52.6	-	-	53.0	-	-	3.4
<i>EMAC 2008¹</i>	-	-	0.19	-	-	44.5	-	-	3.6	-	-	48.1	-	-	-	-	-	-
<i>EMAC 2005-2008²</i>	-	-	0.17	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
<i>IFS³</i>	-	-	0.15	-	-	17.4	-	-	1.4	-	-	18.8	-	-	18.6	-	-	2.9
<i>LMDz-INCA</i>	-	-	0.28	-	-	19.2	-	-	3.2	-	-	22.4	-	-	22.4	-	-	4.5
<i>MetOffice UM⁴</i>	-	-	0.54	-	-	32.1	-	-	7.4	-	-	32.1	-	-	39.2	-	-	5.0

1. From Bian et al. (2017).

2. From Karydis et al. (2016).

3. Fine NO_3^- reported from neutralization of nitric acid, ammonia and sulfate. Coarse nitrate from heterogeneous chemistry (Rémy et al., 2022).

4. Jones et al. (2021) performs two sensitivity tests to the accommodation coefficient used for NO_3^- formation in the fine mode: *FAST* with 0.193 and *SLOW* with 0.001. Here, results from the *FAST* test are reported on the basis that they present similar fine NO_3^- formation rates to our average fine nitrate results

Table S12. Results for particle SO_4^{2-} obtained with the studied heterogeneous chemistry mechanisms. Results from the references are reported at the end of the Table: the average of all the participating models in the intercomparison AeroCom phase III nitrate experiment for 2008, specifying their standard deviation (*STD*), and results from the GMI model (using a similar HYB approach with UPTK reactions on dust and SS) and the EMAC model (*EMAC 2008*, that uses a similar approach to DBCELL_du-ssAlk). Also using the EMAC model, results obtained by the Karydis et al. (2016) study are reported as *EMAC 2005-2008*. Results from models using a similar approach to HYB_du-ssUPTK are reported as *IFS* for Rémy et al. (2022), *LMDz-INCA* for Hauglustaine et al. (2014) and *MetOffice UM* for Jones et al. (2021).

Experiment	SO4 Emissions (Tg.y-1)		SO2 Emissions (Tg.y-1)		SO4 Burden (Tg)		SO4 Wet Dep. (Tg.y-1)		SO4 Dry Dep. (Tg.y-1)		SO4 Total Dep. (Tg.y-1)		SO4 Production (Tg.y-1)		SO4 Lifetime (days)				
	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	Fine	Coarse	Total	
noHC	0.5	0.0	104.4	4.4E-3	0.00	0.00	0.5	0.0	0.5	0.1	0.0	0.1	0.5	0.0	0.5	0.0	0.0	0.0	3.0
fTEQ_noAlk	0.5	0.0	104.4	1.98	0.00	1.98	126.9	0.0	126.9	13.5	0.0	13.5	140.5	0.0	140.5	139.9	0.0	139.9	2.6
fTEQ_du-ssAlk	0.5	0.0	104.4	1.82	0.14	1.96	116.7	6.9	123.6	13.0	3.5	16.5	129.7	10.4	140.1	129.1	10.4	139.5	2.6
HYB_duUPTK	0.5	0.0	104.4	1.82	0.14	1.96	116.5	7.0	123.5	13.0	3.5	16.4	129.4	10.5	139.9	128.9	10.5	139.3	2.6
HYB_du-ssUPTK	0.5	0.0	104.4	1.85	0.14	1.98	116.4	7.1	123.5	12.9	3.5	16.4	129.3	10.6	139.9	128.7	10.6	139.3	2.6
HYB_gDU=0.1	0.5	0.0	104.4	1.87	0.12	1.99	117.8	6.1	124.0	12.7	2.9	15.7	130.6	9.1	139.7	130.0	9.0	139.1	2.6
HYB_DL	0.5	0.0	104.4	1.85	0.14	1.99	116.4	7.1	123.5	12.9	3.5	16.4	129.3	10.6	139.9	128.7	10.6	139.3	2.6
DBCELL_noAlk	0.5	0.0	104.4	1.94	0.04	1.98	124.4	2.0	126.4	13.2	0.9	14.0	137.6	2.9	140.5	137.0	2.9	139.9	2.6
DBCELL_duAlk	0.5	0.0	104.4	1.78	0.16	1.94	114.8	8.4	123.1	12.7	4.1	16.8	127.5	12.4	139.9	126.9	12.4	139.3	2.6
DBCELL_du-ssAlk	0.5	0.0	104.4	1.76	0.20	1.96	114.9	8.3	123.2	12.7	4.1	16.8	127.6	12.4	140.0	127.1	12.3	139.4	2.5
DBCELL_ClaqAlk	0.5	0.0	104.4	1.84	0.13	1.97	117.0	6.9	123.8	12.8	3.3	16.1	129.8	10.1	139.9	129.2	10.1	139.3	2.6
AeroCom	-	-	122.0	-	-	1.80	-	-	140.0	-	-	14.3	-	-	154.3	-	-	151.0	-
STD AeroCom	-	-	±12.0	-	-	±0.81	-	-	±65.3	-	-	±163.3	-	-	±228.6	-	-	±56.0	-
GMI	-	-	122.0	-	-	3.30	-	-	140.0	-	-	14.3	-	-	154.3	-	-	151.0	-
EMAC 2008 ¹	-	-	138.0	-	-	1.90	-	-	302.0	-	-	504.0	-	-	806.0	-	-	187.0	-
EMAC 2005-2008 ²	-	-	-	-	-	1.78	-	-	-	-	-	-	-	-	-	-	-	-	-
IFS ³	-	-	70.3	-	-	0.367	-	-	39.7	-	-	1.9	-	-	39.7	-	-	41.4	-
LMDz-INCA	-	-	-	-	-	1.26	-	-	-	-	-	-	-	-	-	-	-	-	-
MetOffice UM ⁴	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

1. From Bian et al. (2017).

2. From Karydis et al. (2016).

3. Fine NO_3^- reported from neutralization of nitric acid, ammonia and sulfate. Coarse nitrate from heterogeneous chemistry (Rémy et al., 2022).

4. Jones et al. (2021) performs two sensitivity tests to the accommodation coefficient used for NO_3^- formation in the fine mode: *FAST* with 0.193 and *SLOW* with 0.001. Here, results from the *FAST* test are reported on the basis that they present similar fine NO_3^- formation rates to our average fine nitrate results

Table S13. Nitrogen burdens (TgN) for each experiment and species.

Nitrogen burdens	fTEQ		HYB		HYB		HYB		HYB		DBCLL		DBCLL	
	noHC	noAlk	du-ssAlk	duUPTK	du-ssUPTK	gDU=0.1	DL	noAlk	duAlk	du-ssAlk	noAlk	duAlk	du-ssAlk	ClaqAlk
HNO _{3(g)}	1.06	1.11	0.65	0.44	0.15	0.1	0.16	1.14	0.6	0.56	1.14	0.6	0.56	0.57
NH _{3(g)}	0.71	0.04	0.13	0.17	0.21	0.23	0.31	0.05	0.11	0.28	0.05	0.11	0.28	0.25
NO _(g)	0.14	0.18	0.14	0.13	0.11	0.1	0.11	0.19	0.14	0.14	0.19	0.14	0.14	0.14
NO _{2(g)}	0.24	0.27	0.22	0.2	0.17	0.17	0.17	0.28	0.22	0.22	0.28	0.22	0.22	0.22
N ₂ O _{5(g)}	0.04	0.03	0.02	0.02	0.01	0.01	0.01	0.03	0.02	0.02	0.03	0.02	0.02	0.02
NTR _(g)	0.44	0.47	0.48	0.48	0.47	0.47	0.47	0.47	0.47	0.48	0.47	0.47	0.48	0.48
PNA _(g)	0.04	0.03	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.03	0.02	0.02	0.02
PAN _(g)	0.8	0.64	0.53	0.49	0.42	0.41	0.42	0.65	0.52	0.52	0.65	0.52	0.52	0.52
PAN _{x(g)}	0.16	0.13	0.11	0.11	0.09	0.09	0.09	0.14	0.11	0.11	0.14	0.11	0.11	0.11
PM _{2.5} NO _{3(aer)}	0	0.02	0.15	0.13	0.12	0.11	0.09	0.01	0.22	0.06	0.01	0.22	0.06	0.09
PM _{2.5-10} NO _{3(aer)}	0	0	0	0.13	0.27	0.32	0.29	0	0.11	0.18	0	0.11	0.18	0.14
PM _{2.5} NH _{4(aer)}	0	0.23	0.17	0.16	0.15	0.15	0.15	0.22	0.24	0.16	0.22	0.24	0.16	0.17
PM _{2.5-10} NH _{4(aer)}	0	0	0	0	0	0	0	0.01	0.01	0.01	0.01	0.01	0.01	0.01
NO _(g) + NO _{2(g)} + NO _{3(g)}	0.39	0.46	0.36	0.33	0.28	0.28	0.28	0.47	0.37	0.36	0.47	0.37	0.36	0.36
NTR _(g) + PNA _(g) + PAN _(g) + PAN _{x(g)}	1.44	1.28	1.14	1.09	1.01	0.99	1	1.29	1.13	1.13	1.29	1.13	1.13	1.13
Aerosol nitrate + ammonium	0	0.25	0.31	0.42	0.55	0.58	0.53	0.24	0.57	0.41	0.24	0.57	0.41	0.42
Total nitrogen	3.63	3.15	2.62	2.48	2.19	2.18	2.29	3.22	2.79	2.76	3.22	2.79	2.76	2.74

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