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Supplement of

Implementation of the ISORROPIA-lite aerosol thermodynamics model into the EMAC chemistry climate model (based on MESSy v2.55): implications for aerosol composition and acidity

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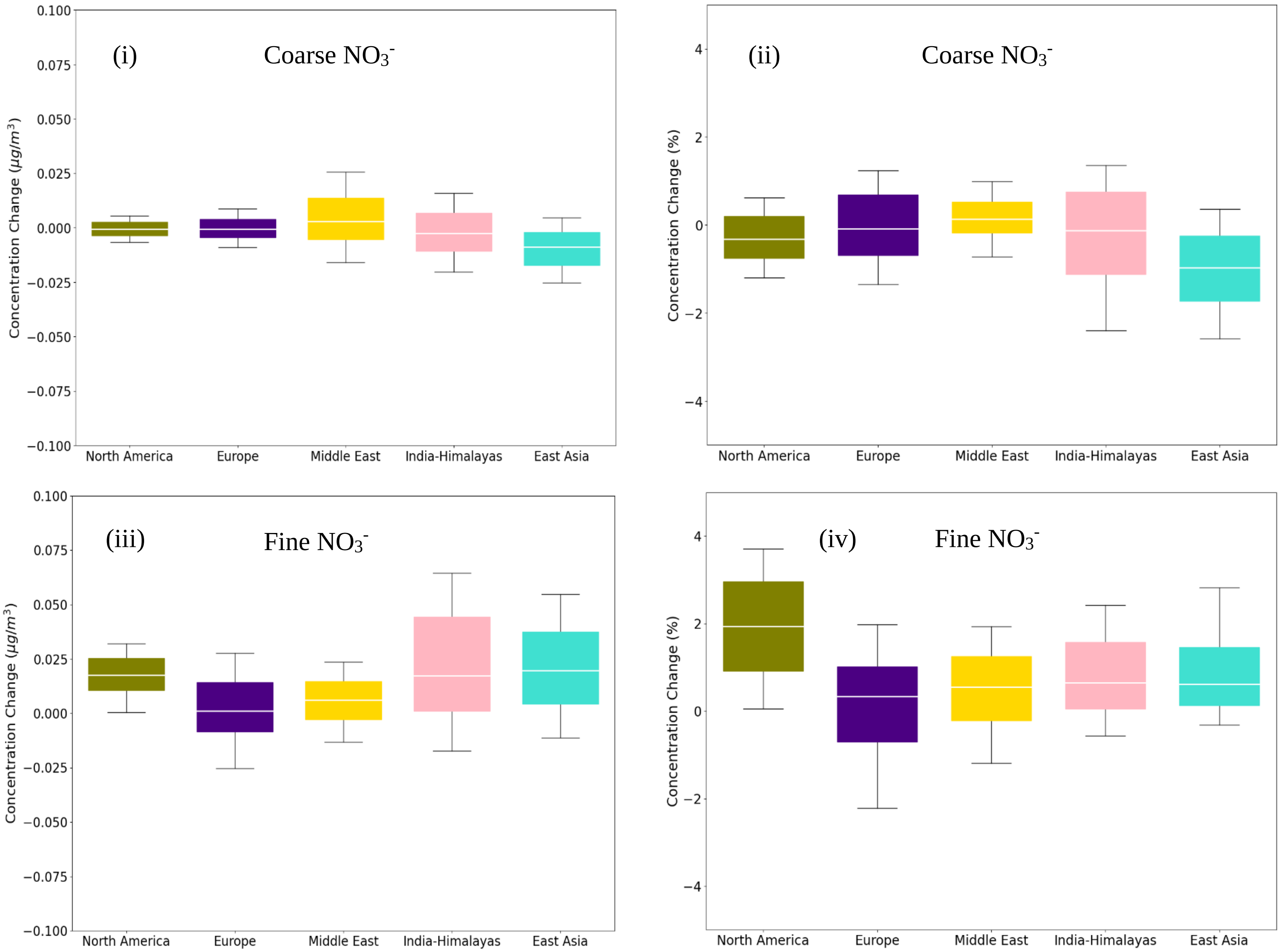

Figure S1: Bar chart plots depicting the 25th, 50th and 75th percentiles (box) of the difference in the global daily mean surface concentrations of i) coarse and ii) fine aerosol NO_3^- for the regions of North America, Europe, Middle East, India-Himalayas and East Asia, as predicted by EMAC using ISORROPIA II v1 and ISORROPIA II v2.3. The fractional differences in global daily mean surface concentrations of iii) coarse and iv) fine aerosol NO_3^- for the same regions are also shown. Both models assume that the aerosol is at its stable state at low RH and a positive change corresponds to higher concentrations by ISORROPIA II v1.

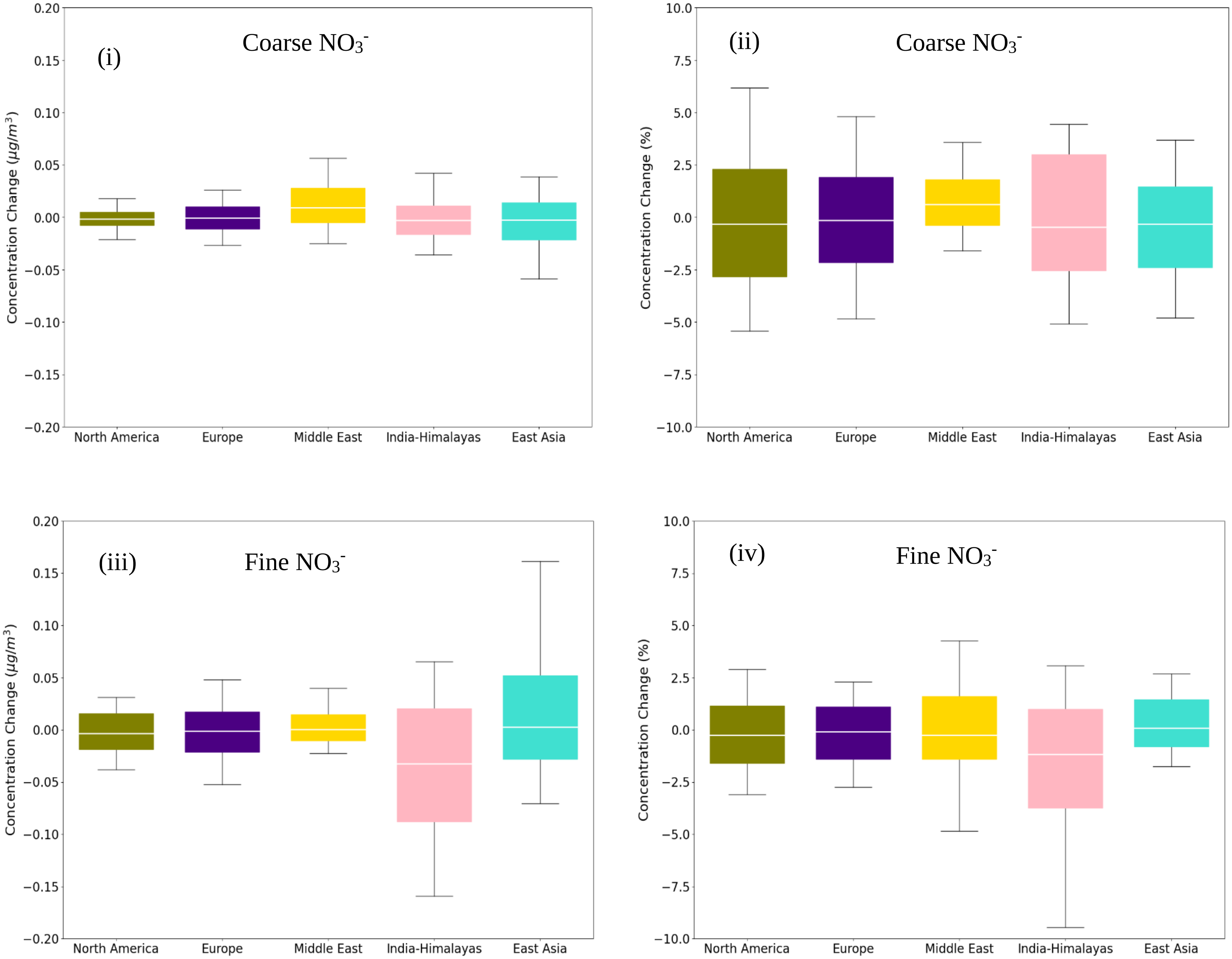

Figure S2: Bar chart plots depicting the 25th, 50th and 75th percentiles (box) of the difference in the global daily mean surface concentrations of i) coarse and ii) fine aerosol NO_3^- for the regions of North America, Europe, Middle East, India-Himalayas and East Asia, as predicted by EMAC using ISORROPIA-lite and ISORROPIA II. The fractional differences in global daily mean surface concentrations of iii) coarse and iv) fine aerosol NO_3^- for the same regions are also shown. Both models assume that the aerosol is at its metastable state at low RH and a positive change corresponds to higher concentrations by ISORROPIA-lite.

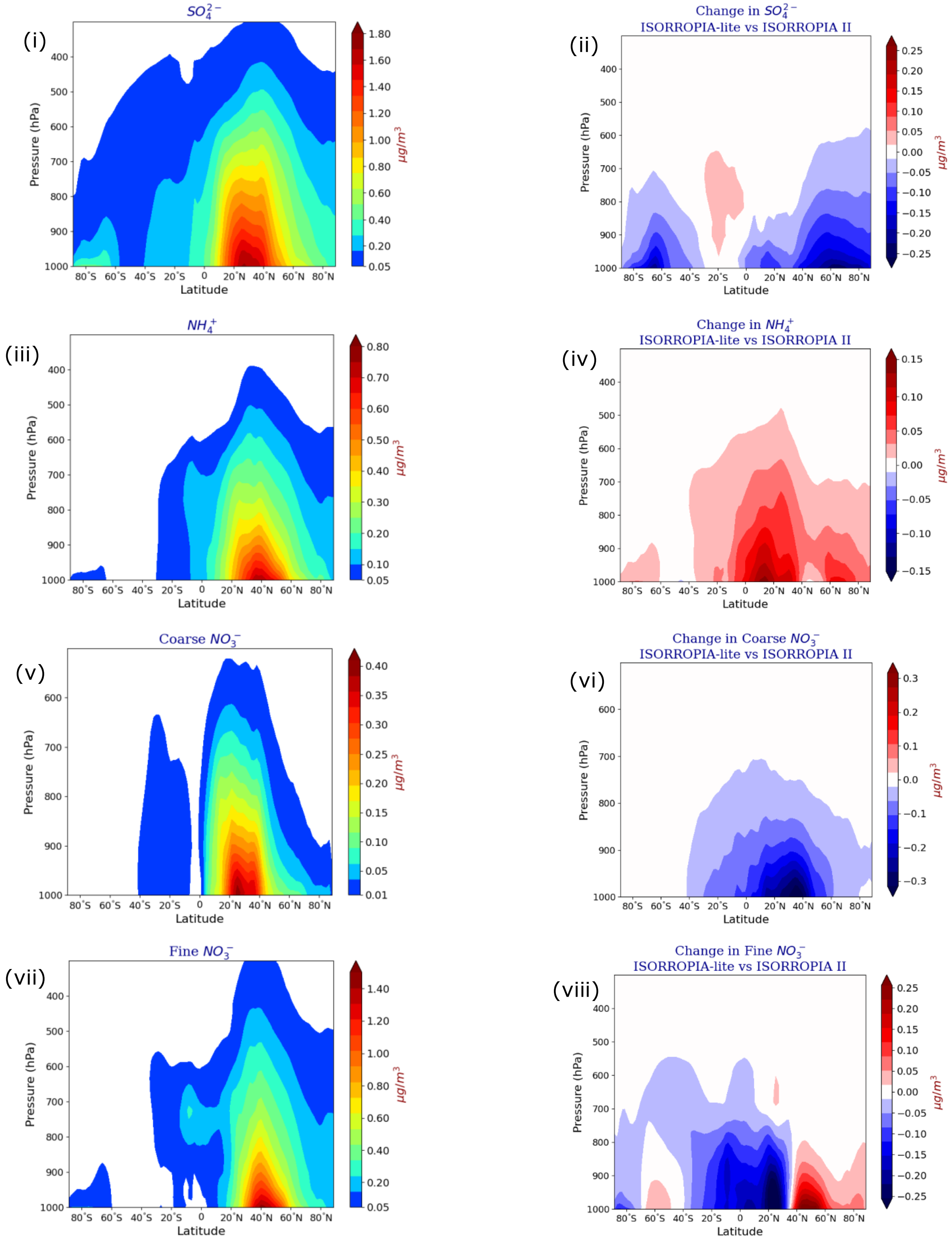

Figure S3 : Annually averaged zonal concentrations of i) SO_4^{2-} and ii) NH_4^+ in TSP, iii) coarse and iv) fine aerosol NO_3^- as predicted by EMAC using ISORROPIA-lite. Change of the annually averaged EMAC-simulated zonal concentration of v) NH_4^+ and vi) SO_4^{2-} in TSP, vii) coarse and viii) fine aerosol NO_3^- after employing ISORROPIA II. Positive values in red indicate higher concentrations by ISORROPIA-lite. The models assume different aerosol states.

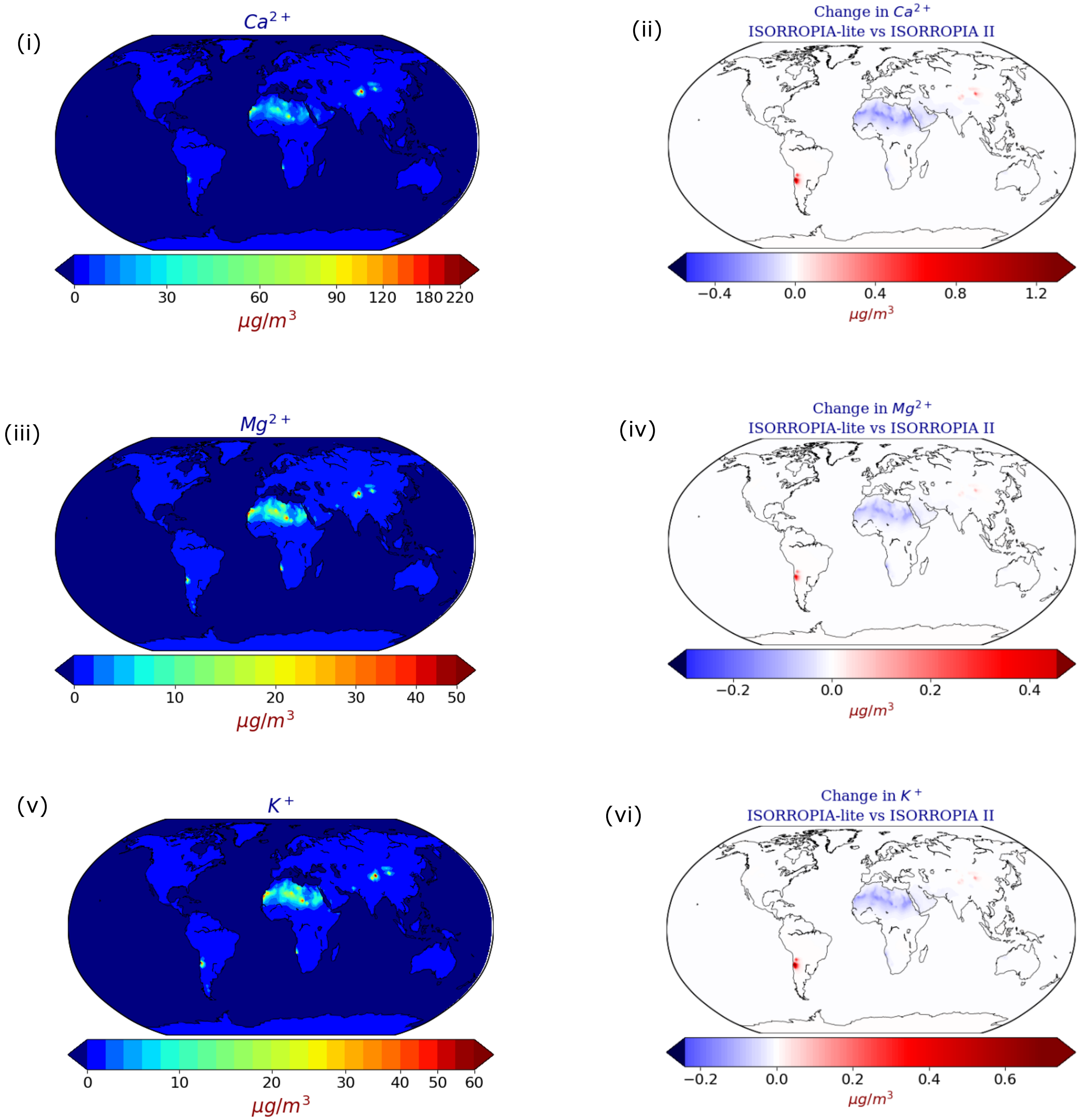

Figure S4: Annual mean surface concentrations of i) Ca^{2+}, ii) Mg^{2+} and iii) K^{+} in TSP as predicted by EMAC using ISORROPIA-lite. Change of the annual mean EMAC-simulated surface concentration of iv) Ca^{2+}, v) Mg^{2+} and vi) K^{+} in TSP after employing ISORROPIA II. Positive values in red indicate higher concentrations by ISORROPIA-lite. The models assume different aerosol states.

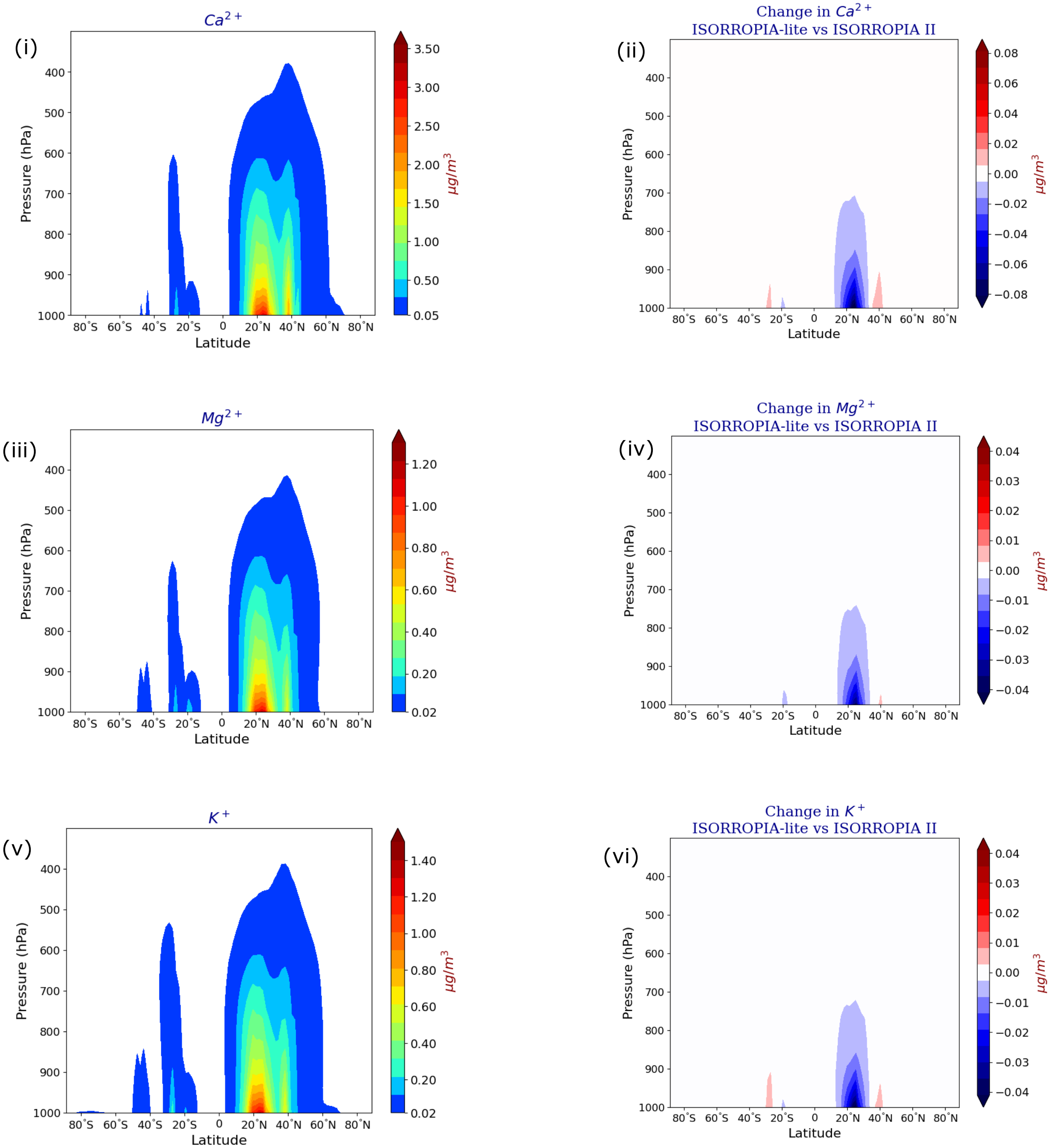

Figure S5: Annually averaged zonal concentrations of i) Ca^{2+}, ii) Mg^{2+} and iii) K^{+} in TSP as predicted by EMAC using ISORROPIA-lite. Change of the annually averaged EMAC-simulated zonal concentration of iv) Ca^{2+}, v) Mg^{2+} and vi) K^{+} in TSP after employing ISORROPIA II. Positive values in red indicate higher concentrations by ISORROPIA-lite. The models assume different aerosol states.

Table S1: Seasonal statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ SO_4^{2-} using ISORROPIA II in stable mode against observations during 2010.

Network	**Season**	**Number of datasets**	**Mean Observed** (μg m^{-3})	**Mean Predicted** (μg m^{-3})	**MAGE** (μg m^{-3})	**MB** (μg m^{-3})	**NME** (%)	**NMB** (%)	**RMSE** (μg m^{-3})
EPA	Winter	148	2.15	1.08	1.11	-1.06	51.73	-49.52	1.57
	Spring	290	1.99	1.68	0.57	-0.31	28.52	-15.44	0.73
	Summer	287	2.64	1.18	1.48	-1.46	55.88	-55.33	1.76
	Autumn	294	1.87	1.49	0.49	-0.37	26.33	-19.9	0.63
IMPROVE	Winter	116	0.92	0.72	0.57	-0.2	61.48	-21.67	1.26
	Spring	233	0.99	1.09	0.38	0.1	38.11	10.16	0.5
	Summer	193	1.35	0.79	0.68	-0.56	50.41	-41.55	1.05
	Autumn	214	0.94	0.99	0.31	0.04	33.1	4.61	0.42
EMEP	Winter	7	2.82	1.74	1.08	-1.08	38.28	-38.28	1.42
	Spring	18	1.62	1.2	0.75	-0.42	46.52	-25.74	0.88
	Summer	18	2.24	1.15	1.09	-1.09	48.62	-48.44	1.28
	Autumn	17	1.73	1.21	0.76	-0.53	43.91	-30.4	0.89
EANET	Winter	30	3.72	1.27	2.68	-2.45	72.04	-65.83	4.0
	Spring	60	3.79	1.77	2.3	-2.02	60.73	-53.34	3.42
	Summer	61	2.66	1.38	1.56	-1.28	58.7	-48.17	2.15
	Autumn	61	2.28	1.27	1.31	-1.01	57.49	-44.16	1.92

Table S2: Seasonal statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ NH_4^+ using ISORROPIA II in stable mode against observations during 2010.

Network	**Season**	**Number of datasets**	**Mean Observed** ($\mu g\ m^{-3}$)	**Mean Predicted** ($\mu g\ m^{-3}$)	**MAGE** ($\mu g\ m^{-3}$)	**MB** ($\mu g\ m^{-3}$)	**NME** (%)	**NMB** (%)	**RMSE** ($\mu g\ m^{-3}$)
EPA	Winter	137	1.52	1.56	0.57	0.04	37.73	2.66	0.94
	Spring	269	0.98	1.69	0.79	0.71	80.17	72.58	0.97
	Summer	265	0.82	0.41	0.43	-0.41	51.71	-49.8	0.56
	Autumn	273	0.65	0.55	0.19	-0.11	29.33	-16.39	0.29
EMEP	Winter	6	2.07	2.8	0.84	0.74	40.56	35.63	1.27
	Spring	14	1.24	2.17	0.99	0.93	79.77	74.9	1.19
	Summer	14	0.84	0.43	0.41	-0.41	48.61	-48.61	0.45
	Autumn	13	0.83	1.16	0.41	0.34	49.7	40.67	0.53
EANET	Winter	27	1.39	1.38	0.94	-0.02	67.29	-1.12	1.81
	Spring	59	1.07	1.7	1.22	0.63	114.5	58.75	1.78
	Summer	58	0.69	0.56	0.33	-0.14	47.43	-19.85	0.47
	Autumn	58	0.54	0.48	0.38	-0.06	69.24	-11.74	0.58

Table S3: Seasonal statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ NO_3^- using ISORROPIA II in stable mode against observations during 2010.

Network	Season	Number of datasets	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	NME (%)	NMB (%)	RMSE ($\mu g\ m^{-3}$)
EPA	Winter	144	2.82	3.83	1.97	1.01	70.0	35.87	2.61
	Spring	291	1.41	3.2	1.9	1.79	135.16	127.11	2.35
	Summer	280	0.5	0.28	0.28	-0.22	55.11	-44.42	0.69
	Autumn	290	0.66	0.54	0.36	-0.12	54.07	-18.01	0.58
IMPROVE	Winter	116	0.81	2.16	1.41	1.34	173.76	164.76	1.77
	Spring	233	0.5	1.81	1.35	1.32	272.05	266.11	1.78
	Summer	193	0.2	0.29	0.18	0.09	89.7	48.07	0.25
	Autumn	214	0.21	0.37	0.25	0.16	119.85	77.91	0.35
EMEP	Winter	7	3.35	5.27	2.81	1.92	83.9	57.38	4.13
	Spring	18	1.63	2.47	1.56	0.83	95.71	50.94	2.14
	Summer	18	0.27	0.58	0.43	0.31	158.9	114.1	0.63
	Autumn	17	0.8	1.5	0.85	0.7	106.94	87.44	1.35
EANET	Winter	30	2.03	2.88	2.01	0.85	99.01	41.67	3.03
	Spring	59	1.85	2.43	1.97	0.58	106.59	31.6	3.05
	Summer	59	0.63	0.64	0.61	0.01	96.31	1.3	0.91
	Autumn	59	0.77	0.83	0.69	0.06	89.49	7.92	1.08

Table S4: Seasonal statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ SO_4^{2-} using ISORROPIA-lite against observations during 2010.

Network	**Season**	**Number of datasets**	**Mean Observed** (μg m^{-3})	**Mean Predicted** (μg m^{-3})	**MAGE** (μg m^{-3})	**MB** (μg m^{-3})	**NME** (%)	**NMB** (%)	**RMSE** (μg m^{-3})
EPA	Winter	148	2.15	1.05	1.14	-1.09	52.91	-50.9	1.59
	Spring	290	1.99	1.68	0.57	-0.31	28.53	-15.67	0.73
	Summer	287	2.64	1.19	1.47	-1.46	55.7	-55.16	1.75
	Autumn	294	1.87	1.48	0.49	-0.38	26.53	-20.53	0.64
IMPROVE	Winter	116	0.92	0.7	0.57	-0.22	61.55	-24.25	1.26
	Spring	233	0.99	1.09	0.38	0.1	38.04	9.99	0.49
	Summer	193	1.35	0.79	0.68	-0.56	50.32	-41.67	1.04
	Autumn	214	0.94	0.99	0.31	0.04	33.1	4.61	0.42
EMEP	Winter	7	2.82	1.72	1.1	-1.1	39.06	-39.06	1.44
	Spring	18	1.62	1.2	0.74	-0.42	45.99	-25.96	0.87
	Summer	18	2.24	1.15	1.1	-1.09	48.93	-48.83	1.29
	Autumn	17	1.73	1.2	0.77	-0.54	44.58	-30.91	0.91
EANET	Winter	30	3.72	1.24	2.7	-2.48	72.49	-66.6	4.03
	Spring	60	3.79	1.79	2.28	-1.99	60.18	-52.68	3.4
	Summer	61	2.66	1.38	1.56	-1.28	58.74	-48.13	2.15
	Autumn	61	2.28	1.28	1.3	-1.0	57.08	-43.97	1.91

Table S5: Seasonal Statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ NH_4^+ using ISORROPIA-lite against observations during 2010.

Network	Season	Number of datasets	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	NME (%)	NMB (%)	RMSE ($\mu g\ m^{-3}$)
EPA	Winter	137	1.52	1.54	0.56	0.02	37.09	1.47	0.93
	Spring	269	0.98	1.72	0.8	0.74	81.38	74.93	0.98
	Summer	265	0.82	0.42	0.42	-0.4	50.71	-48.66	0.56
	Autumn	273	0.65	0.58	0.19	-0.07	29.08	-10.72	0.28
EMEP	Winter	6	2.07	2.77	0.82	0.71	39.47	34.09	1.25
	Spring	14	1.24	1.97	0.84	0.73	67.16	58.72	1.02
	Summer	14	0.84	0.46	0.38	-0.38	44.76	-44.76	0.42
	Autumn	13	0.83	1.18	0.43	0.35	51.57	42.76	0.54
EANET	Winter	27	1.39	1.35	0.93	-0.05	66.56	-3.36	1.81
	Spring	59	1.07	1.56	1.07	0.49	100.22	45.52	1.63
	Summer	58	0.69	0.59	0.32	-0.1	45.81	-14.62	0.46
	Autumn	58	0.54	0.52	0.37	-0.02	67.43	-4.4	0.56

Table S6: Seasonal statistical evaluation of EMAC predicted surface concentrations of $PM_{2.5}$ NO_3^- using ISORROPIA-lite against observations during 2010.

Network	Season	Number of datasets	Mean Observed ($\mu g\ m^{-3}$)	Mean Predicted ($\mu g\ m^{-3}$)	MAGE ($\mu g\ m^{-3}$)	MB ($\mu g\ m^{-3}$)	NME (%)	NMB (%)	RMSE ($\mu g\ m^{-3}$)
EPA	Winter	144	2.82	3.76	1.91	0.94	67.68	33.49	2.54
	Spring	291	1.41	3.26	1.96	1.85	139.4	131.61	2.36
	Summer	280	0.5	0.29	0.27	-0.21	54.12	-41.95	0.69
	Autumn	290	0.66	0.63	0.38	-0.03	56.94	-4.81	0.6
IMPROVE	Winter	116	0.81	2.15	1.41	1.34	172.65	164.36	1.74
	Spring	233	0.5	1.86	1.39	1.36	279.62	275.01	1.79
	Summer	193	0.2	0.3	0.18	0.1	92.3	53.19	0.26
	Autumn	214	0.21	0.42	0.28	0.21	137.09	102.38	0.39
EMEP	Winter	7	3.35	5.22	2.79	1.87	83.37	55.94	4.09
	Spring	18	1.63	2.55	1.58	0.92	96.88	56.11	2.1
	Summer	18	0.27	0.64	0.48	0.37	174.65	134.53	0.69
	Autumn	17	0.8	1.6	0.92	0.8	115.23	100.3	1.42
EANET	Winter	30	2.03	2.88	2.01	0.85	98.65	41.9	3.03
	Spring	59	1.85	2.38	1.9	0.53	103.14	28.86	2.98
	Summer	59	0.63	0.69	0.64	0.06	100.43	8.81	0.95
	Autumn	59	0.77	0.87	0.69	0.1	89.82	13.14	1.08