

IMPACTS OF EAST MEDITERRANEAN MEGACITY EMISSIONS ON AIR QUALITY

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Model Evaluation - statistics

Correlation coefficient (r ; eq.1), bias (eq. 2), mean normalized bias (MNB, eq. 3), root mean square error (RMSE; eq. 4), index of agreement (IOA; eq. 5) and mean absolute gross error (MAGE; eq. 6) values have been calculated in order to compare the model calculations (P) with observations (O).

$$r = \left[\frac{\frac{1}{N} \sum_{i=1}^N (O_i - \bar{O})(P_i - \bar{P})}{\sigma_O \sigma_P} \right] \quad (\text{Eq. 1})$$

$$BIAS = \frac{1}{N} \sum_{i=1}^N (P_i - O_i) \quad (\text{Eq. 2})$$

$$MNB = \frac{1}{N} \sum_{i=1}^N \left(\frac{P_i - O_i}{O_i} \right) \quad (\text{Eq. 3})$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2} \quad (\text{Eq. 4})$$

$$1 \quad IOA = 1 - \frac{\sum_{i=1}^N (P_i - O_i)^2}{\sum_{i=1}^N \left(|P_i - \bar{O}| + |O_i - \bar{O}| \right)^2} \quad (\text{Eq. 5})$$

$$2 \quad MAGE = \frac{1}{N} \sum_{i=1}^N |P_i - O_i| \quad (\text{Eq. 6})$$

3 where O_i and P_i stand for observations and predictions at each time step, \bar{O} and \bar{P}
 4 stand for the daily mean of observations and predictions, σ stands for standard
 5 deviation and N is the number of pairs (observations, predictions) that are compared.

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Table S1 Winter (December 2008) and summer (July 2008) sectoral contributions (in %) to the anthropogenic emissions in GIA and GAA. Only contributions higher than or equal to ~1% are reported.

		Heating	Industry*	Road	Non-Road	Maritime	Solvent	Other**
GIA								
CO	Winter	17	4	78				1
	Summer	2	4	93				1
NO _x	Winter	4	6	78	1	10		1
	Summer		5	83	1	10		1
SO ₂	Winter	19	61	2		17		1
	Summer	4	64	3		27		2
NMVOC	Winter	4		42	1	1	28	24
	Summer			46	1	1	30	22
PM ₁₀	Winter	10	67	15		6		2
	Summer	2	67	20		8		3
GAA								
CO	Winter	21		56	23			
	Summer			67	31	2		
NO _x	Winter	9	5	49	16	21		
	Summer		4	51	22	23		
SO ₂	Winter	28	37		4	22		9
	Summer		45		8	37		10
NMVOC	Winter	6	2	37	43		9	3
	Summer		2	38	50	2	6	2
PM ₁₀	Winter	60	7	11	6	6		10
	Summer		16	31	24	18		11

6 * Industry includes energy, industrial combustion and industrial processes

7 ** Others include agriculture, waste management, coal extraction and fuel distribution

Table S2 Country-based IIASA mitigation factors (ratios of 2030 mitigated emissions to the reference year emissions) applied in the mitigation scenario (Mitig).

	SO ₂	NO _x	NMVOG	CO	PM _{2.5}	BC	OC
Albania	0.985	0.658	0.787	0.836	0.579	0.392	0.516
Bosnia	0.976	0.875	0.825	0.797	0.645	0.423	0.534
Bulgaria	0.990	0.950	0.874	0.897	0.815	0.431	0.568
Croatia	0.996	0.859	0.907	0.944	0.733	0.493	0.653
Greece	1.000	0.958	0.869	0.934	0.707	0.549	0.564
Italy	1.000	0.913	0.921	0.585	0.862	0.638	0.759
Former Yugoslavian Republic of Macedonia	0.987	0.707	0.914	0.948	0.867	0.520	0.811
Romania	1.000	0.976	0.812	0.885	0.726	0.363	0.505
Serbia	0.912	0.826	0.767	0.827	0.609	0.326	0.494
Turkey	0.986	0.836	0.770	0.686	0.822	0.533	0.531

Table S3. Measurement stations in GIA, GAA and at FKL: Geographical information and pollutants measured during the simulation periods of this study. In GIA, all measurement stations correspond to the same model grid whereas in GAA, the stations correspond to two different model grids and have been accordingly grouped in GAA1, GAA2, and GAA3 for grid boxes 1, 2 and 3 shown in Figure 1.

Station	Lat (°)	Lon (°)	Alt (m)	Pollutants
Greater Istanbul Area GIA (9 stations)				
Alibeykoy	41.07	28.95	60	NO ₂ , CO, SO ₂ , PM ₁₀
Besiktas	41.05	29.01	94	NO ₂ , CO, SO ₂ , PM ₁₀
Esenler	41.04	28.89	59	NO ₂ , CO, SO ₂ , PM ₁₀
Kadikoy	40.99	29.03	6	NO ₂ , CO, SO ₂ , PM ₁₀
Sariyer	41.70	29.05	103	CO, SO ₂ , PM ₁₀
Uskudar	41.02	29.03	70	CO, SO ₂ , PM ₁₀
Yenibosna	40.59	28.49	23	CO, SO ₂ , PM ₁₀
ESC (Bogazici University)	41.09	29.05	80	Aerosol chemical composition (PM ₁₀)
Kandilli	41.06	29.06	125	O ₃
Greater Athens Area (GAA)				
GAA1				
Ag. Paraskevi)	38.00	23.82	290	O ₃ , PM ₁₀
Aristotelous	37.99	23.73	95	O ₃ , PM ₁₀
Athinas	37.98	23.73	100	O ₃ , NO ₂ , CO, SO ₂
Lykovrysi	38.07	23.78	210	O ₃ , NO ₂ , PM ₁₀
Marousi	38.03	23.79	145	O ₃ , PM ₁₀
Patision	38.00	23.73	105	O ₃ , NO ₂ , CO, SO ₂
Thrakomakedones	38.14	23.76	550	O ₃ , NO ₂ , PM ₁₀
Penteli	37.58	23.43	107	Aerosol chemical composition (PM _{2.5})
GAA2				
Geoponiki	37.98	23.71	50	O ₃ , NO ₂ , CO, SO ₂ , Aerosol chemical composition (PM _{2.5})
Liosia	38.08	23.70	165	O ₃ , NO ₂ , SO ₂
Elefsina	38.05	23.58	20	O ₃ , NO ₂ , SO ₂
Smyrni	37.93	23.72	50	O ₃ , NO ₂ , CO, SO ₂
Peristeri	38.02	23.70	80	O ₃
Pireas	37.94	23.65	20	O ₃ , NO ₂ , SO ₂ , PM ₁₀
GAA3				
Aegina (Tourlos)	37.75	23.55	15	PM ₁ , PM _{2.5} , Aerosol chemical composition
FINOKALIA (FKL)	35.20	25.40	250	O ₃ , PM ₁₀ , Aerosol chemical composition (PM _{2.5} , PM _{2.5-10})

Table S4. Winter (December 2008) and summer (July 2008) changes (%) in surface concentrations of the main pollutants in GIA and GAA, at FKL and in the whole simulation domain due to an increase by 50% of the boundary conditions of all pollutants for which boundary conditions are used. Values are calculated as $[100 \cdot (\text{'Boundaries'}/\text{'Base'}) - \text{'Base'}]$. Those greater than or equal to 50% are marked in bold.

	Winter								Summer							
	GIA			GAA			FKL	Dom.	GIA			GAA			FKL	Dom.
	Urb.	Rur.	Ext.	Urb.	Rur.	Ext.			Urb.	Rur.	Ext.	Urb.	Rur.	Ext.		
O ₃	82	56	61	69	57	58	46	49	51	38	41	37	32	33	28	31
NO _x	-1	-3	-2	-3	-7	-5	-14	-12	-3	-12	-4	-2	-4	-4	-7	-7
CO	18	33	27	16	31	27	48	45	26	44	36	16	39	27	43	44
PAN	54	53	53	54	53	54	54	53	60	54	56	38	36	36	35	40
HNO ₃	20	33	28	40	47	39	23	29	29	32	32	22	24	21	14	20
PM _{2.5}	3	8	5	3	8	6	18	19	10	22	16	10	18	14	18	20
nss-SO ₄ ²⁻	15	22	20	14	22	20	27	28	30	30	30	23	23	22	23	24
NO ₃ ⁻	3	16	8	11	12	10	13	25	8	13	11	8	8	6	3	5
OC	1	5	3	1	4	3	20	18	5	19	10	13	20	17	18	19
EC	1	4	3	4	7	7	19	18	5	21	11	9	19	14	21	23

Table S5. Domain-mean winter (December 2008) and summer (July 2008) surface concentrations and chemical indicators from the ‘Base’ case simulation (S0), ‘NoBiog’ (S1), ‘NoAnth’ (S2), ‘NoIst’ (S3), ‘NoAth’ (S4), ‘NoIstAth’ (S5), and ‘Mitig’ (S6), averaged over the simulation periods.

	Winter							Summer						
	S0	S1	S2	S3	S4	S5	S6	S0	S1	S2	S3	S4	S5	S6
O ₃ (ppbv)	33.3	33.2	34.6	33.6	33.4	33.7	33.6	62.9	60.4	52.4	62.6	62.8	62.4	62.3
NO _x (ppbv)	2.9	2.9	0.2	2.3	2.8	2.3	2.5	2.0	2.0	0.2	1.8	2.0	1.8	1.9
CO (ppbv)	147.4	147.3	134.3	146.3	146.5	145.3	144.2	124.0	120.3	116.6	123.0	122.9	121.9	122.1
PAN (ppbv)	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.2	0.2	0.3	0.3	0.3	0.3
HNO ₃ (ppbv)	0.7	0.7	0.2	0.7	0.7	0.7	0.6	1.6	1.8	0.5	1.5	1.6	1.5	1.5
NMVO _C /NO _x	8.1	8.0	60.2	8.2	8.1	8.2	8.2	8.8	4.4	67.4	8.9	8.8	8.8	9.2
CO/NO _x	51.4	51.4	767.3	62.3	52.6	64.1	56.7	61.2	59.4	627.9	66.9	62.3	68.3	64.4
PM _{2.5} (µg m ⁻³)	2.9	3.0	1.4	2.8	2.9	2.8	2.6	6.1	6.3	3.2	5.9	6.1	5.8	5.8
nss-SO ₄ ²⁻ (µg m ⁻³)	1.0	1.0	0.5	1.0	1.0	0.9	1.0	3.3	3.6	1.8	3.2	3.3	3.2	3.2
NO ₃ ⁻ (µg m ⁻³)	0.6	0.6	0.3	0.6	0.6	0.6	0.6	1.6	1.6	0.4	1.5	1.6	1.4	1.5
OC (µg m ⁻³)	0.5	0.5	0.3	0.5	0.5	0.4	0.4	0.8	0.8	0.4	0.8	0.8	0.8	0.7
EC (µg m ⁻³)	0.2	0.2	0.1	0.2	0.2	0.2	0.2	0.4	0.4	0.2	0.3	0.4	0.3	0.3

Table S6 Winter (December 2008) and summer (July 2008) changes (%) in surface concentrations of the main pollutants and chemical indicators in GIA and GAA, at FKL and in the whole simulation domain compared to the base case simulations when assuming country-based mitigation of anthropogenic emissions (Mitig). Values are calculated as $[100 \cdot (\text{Mitig} - \text{Base}) / \text{Base}]$.

	Winter								Summer							
	GIA			GAA			FKL	Dom.	GIA			GAA			FKL	Dom.
	Urb.	Rur.	Ext.	Urb.	Rur.	Ext.			Urb.	Rur.	Ext.	Urb.	Rur.	Ext.		
O ₃	13.4	3.6	5.4	2.4	1.3	1.4	0.3	1.0	7.0	0.6	2.2	0.1	-0.6	-0.4	-0.8	-0.8
NO _x	-16.3	-16.3	-16.3	-4.4	-4.5	-4.4	-3.6	-11.3	-16.3	-13.0	-16.0	-4.5	-3.1	-4.5	-3.4	-6.4
CO	-20.1	-10.5	-14.5	-4.6	-2.6	-3.1	-0.5	-2.2	-13.9	-2.2	-7.4	-4.6	-1.2	-3.1	-1.1	-1.5
PAN	-0.1	-0.2	-0.2	-0.5	-0.5	-0.5	-0.3	-0.4	1.7	-0.4	0.4	-3.4	-2.8	-3.4	-3.9	-3.1
HNO ₃	-20.6	-11.4	-15.4	-12.3	-9.1	-8.2	-5.1	-7.8	-6.6	-2.6	-4.5	-5.9	-5.1	-5.0	-6.8	-5.6
NMVOC/NO _x	0.8	2.6	2.8	-6.8	-2.2	-3.3	1.6	2.2	3.4	6.1	6.3	-5.1	0.4	-1.7	-1.3	5.1
CO/NO _x	-4.4	7.0	2.3	-0.2	2.0	1.4	3.2	10.3	3.0	12.5	10.3	-0.1	2.0	1.5	2.3	5.2
PM _{2.5}	-29.6	-24.9	-27.2	-20.2	-16.9	-17.7	-4.9	-10.3	-24.3	-7.0	-16.7	-9.5	-6.1	-7.9	-4.9	-5.7
nss-SO ₄ ²⁻	-9.3	-5.2	-6.8	-15.7	-9.1	-10.2	-2.8	-2.2	-2.3	-0.6	-1.4	-4.2	-2.7	-3.4	-1.9	-2.5
NO ₃ ⁻	-0.7	-2.6	-1.7	1.5	-2.6	-1.1	-3.2	-2.7	2.7	0.2	1.0	-1.0	-0.9	-0.7	-5.1	-3.4
OC	-44.3	-38.1	-41.7	-41.4	-38.2	-38.6	-6.7	-16.0	-39.6	-17.0	-31.9	-25.1	-15.9	-19.7	-14.0	-11.6
EC	-44.7	-39.4	-42.4	-40.6	-36.7	-36.9	-17.8	-25.3	-40.2	-19.1	-33.1	-36.1	-25.7	-30.7	-18.0	-15.1

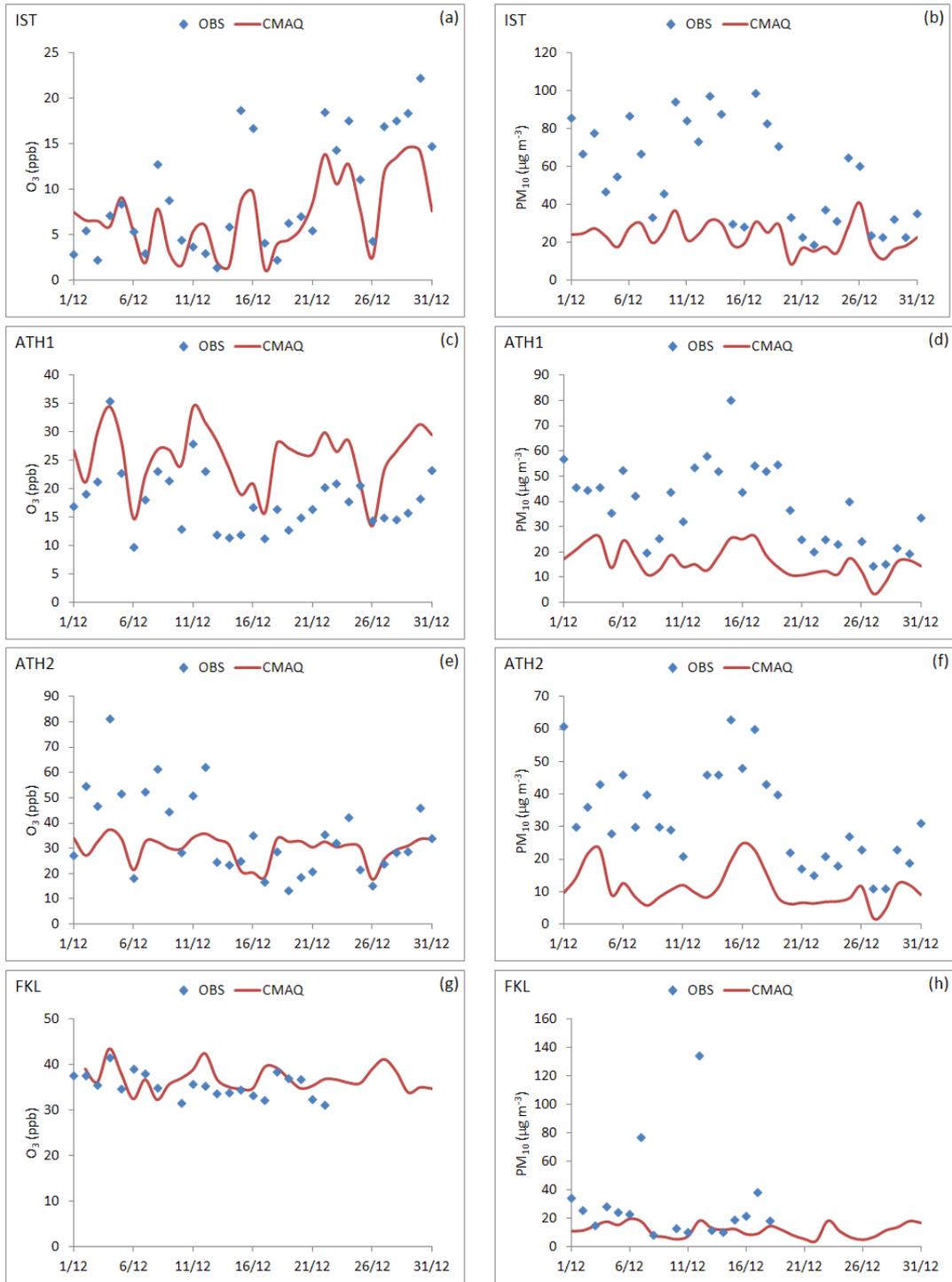


Fig. S1. Observed (diamonds) and modeled (line) wintertime (December 2008) daily mean surface O₃ (left panel) and PM₁₀ (right panel) levels at IST (a,b), ATH1 (c,d), ATH2 (e,f) and FKL (g,h) for the base case simulation.

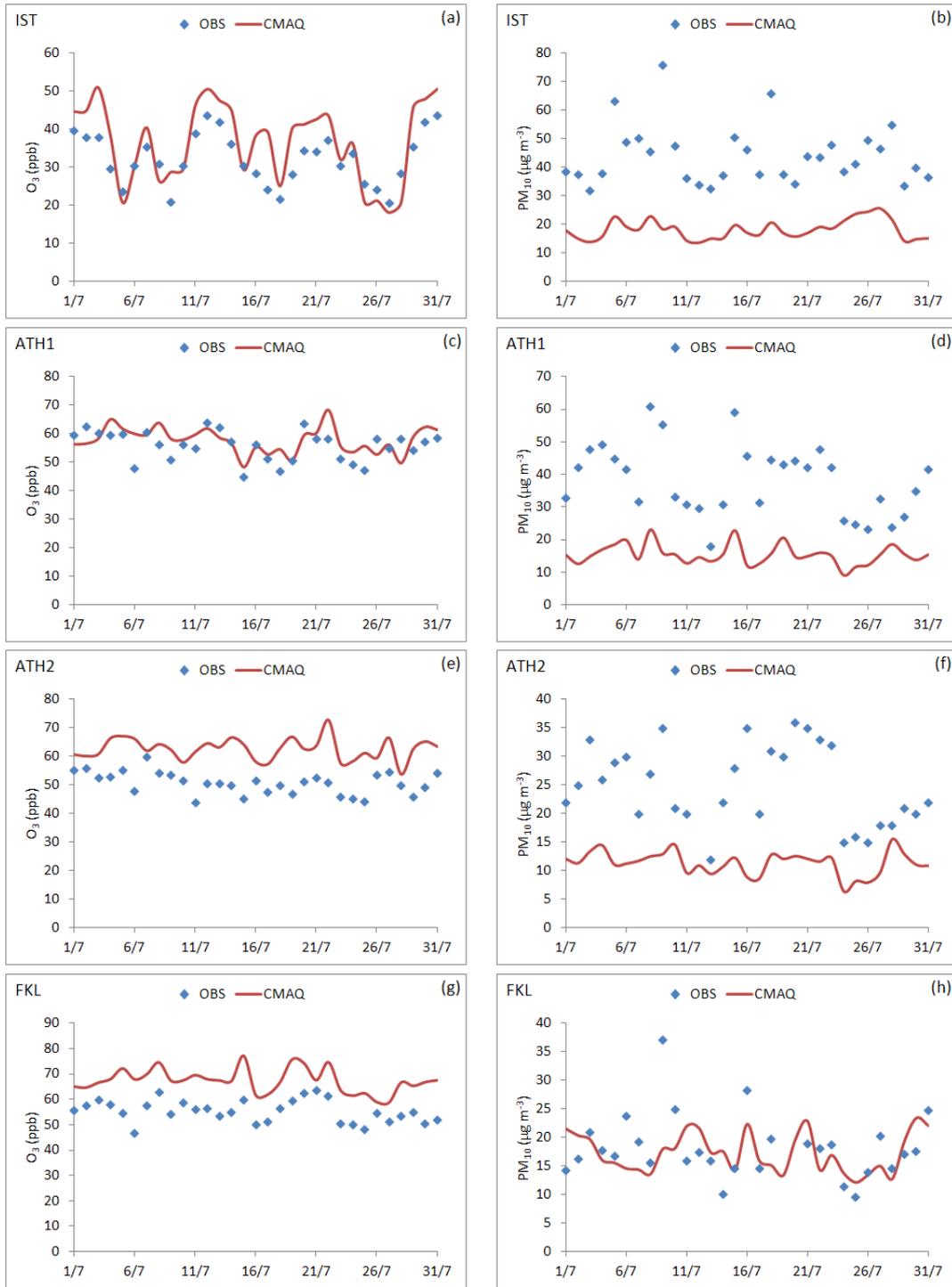


Fig. S2. Observed (diamonds) and modeled (line) summertime (July 2008) daily mean surface O₃ (left panel) and PM₁₀ (right panel) levels at IST (a,b), ATH1 (c,d), ATH2 (e,f) and FKL (g,h) for the base case simulation.

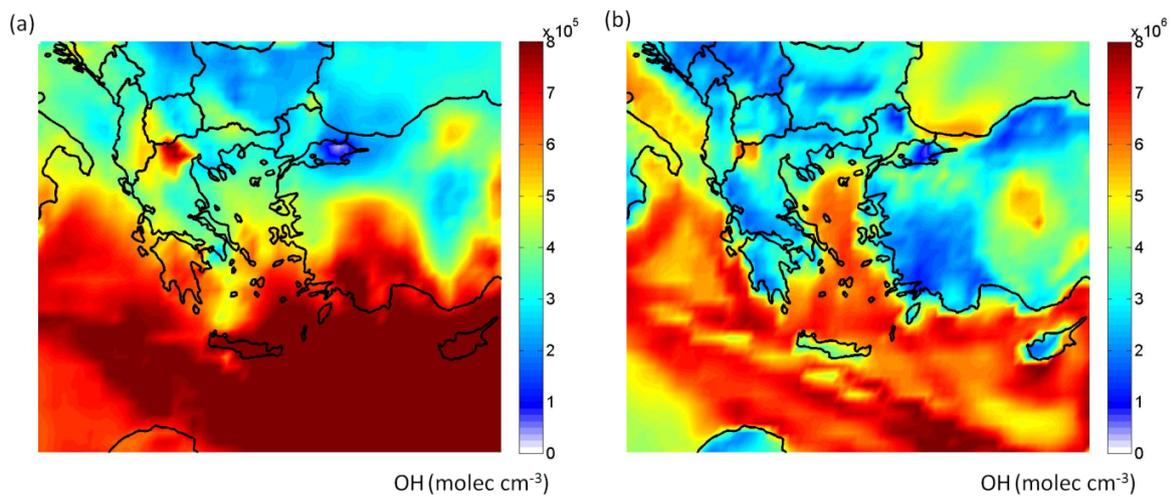


Fig. S3. Surface OH levels averaged over each 31-day simulation period: a) in winter (December 2008) in $10^5 \text{ molec cm}^{-3}$ and b) in summer (July 2008) in $10^6 \text{ molec cm}^{-3}$.

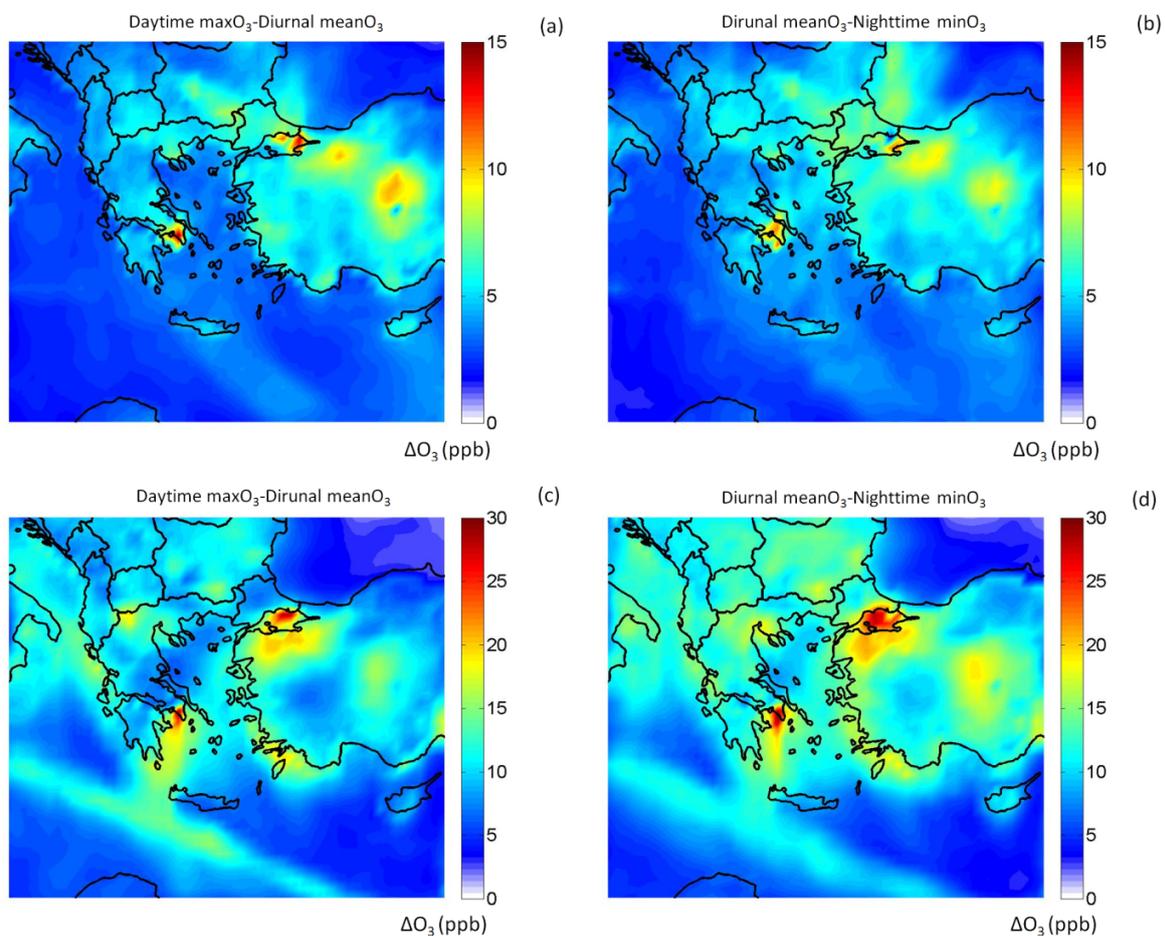


Fig. S4 Differences in daytime maximum and diurnal mean (maxO₃-meanO₃; a,c) and diurnal mean and nighttime minimum (meanO₃-minO₃; b,d) surface O₃ levels averaged over the wintertime (December 2008; a,b) and summertime (July 2008; c,d) simulations.

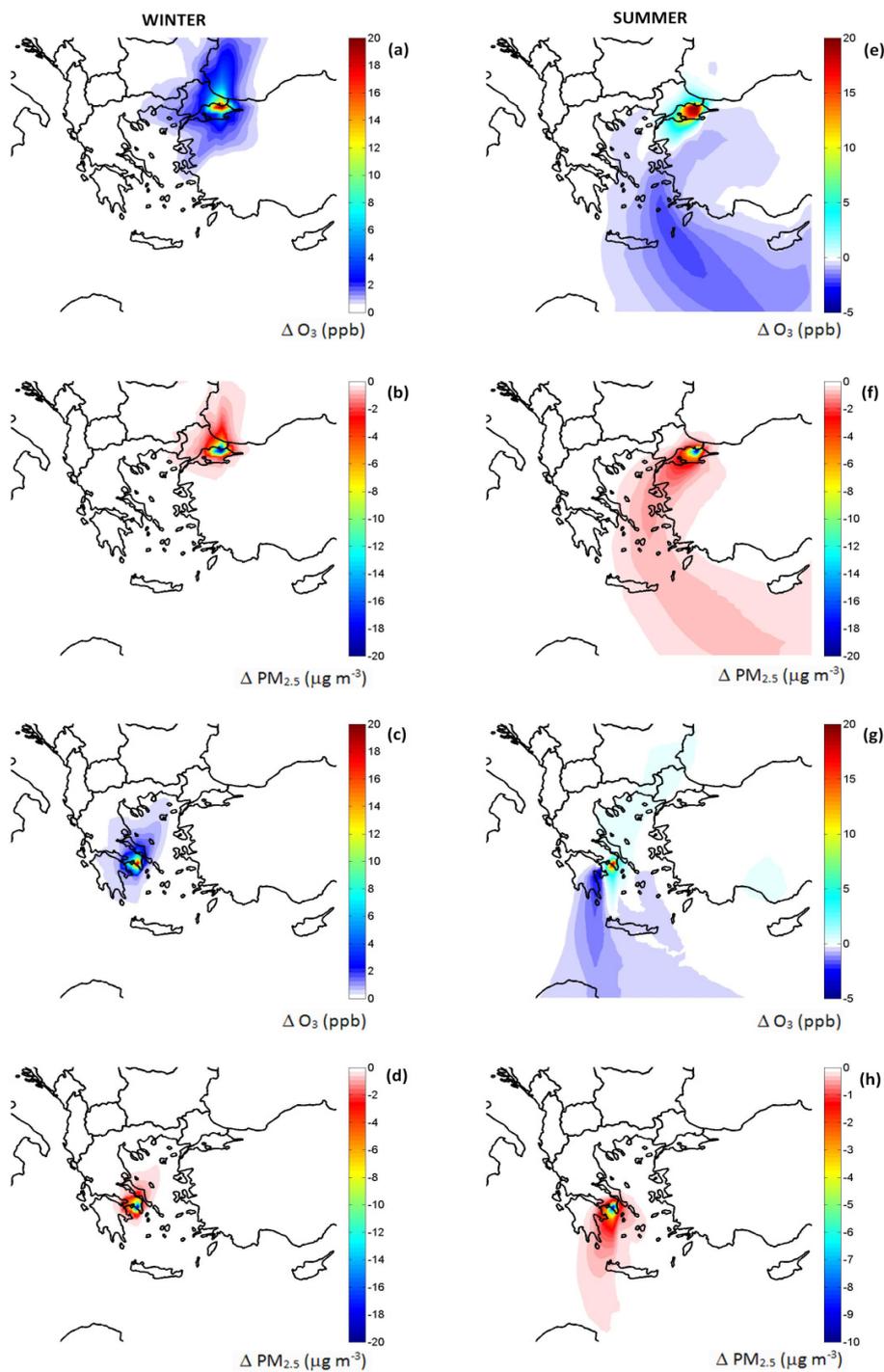


Fig. S5. Regional impacts of 'NoIst' and 'NoAth' scenarios on surface O_3 and $PM_{2.5}$ in winter (December 2008) and in summer (July 2008), averaged over each one-month simulation period. ΔO_3 in ppb: (a) 'NoIst' winter, (e) 'NoIst' summer, (e) 'NoAth' winter, (g) 'NoAth' summer; $\Delta PM_{2.5}$ in $\mu g \cdot m^{-3}$ (b) 'NoIst' winter, (d) 'NoIst' summer, (f) 'NoAth' winter, (h) 'NoAth' summer.

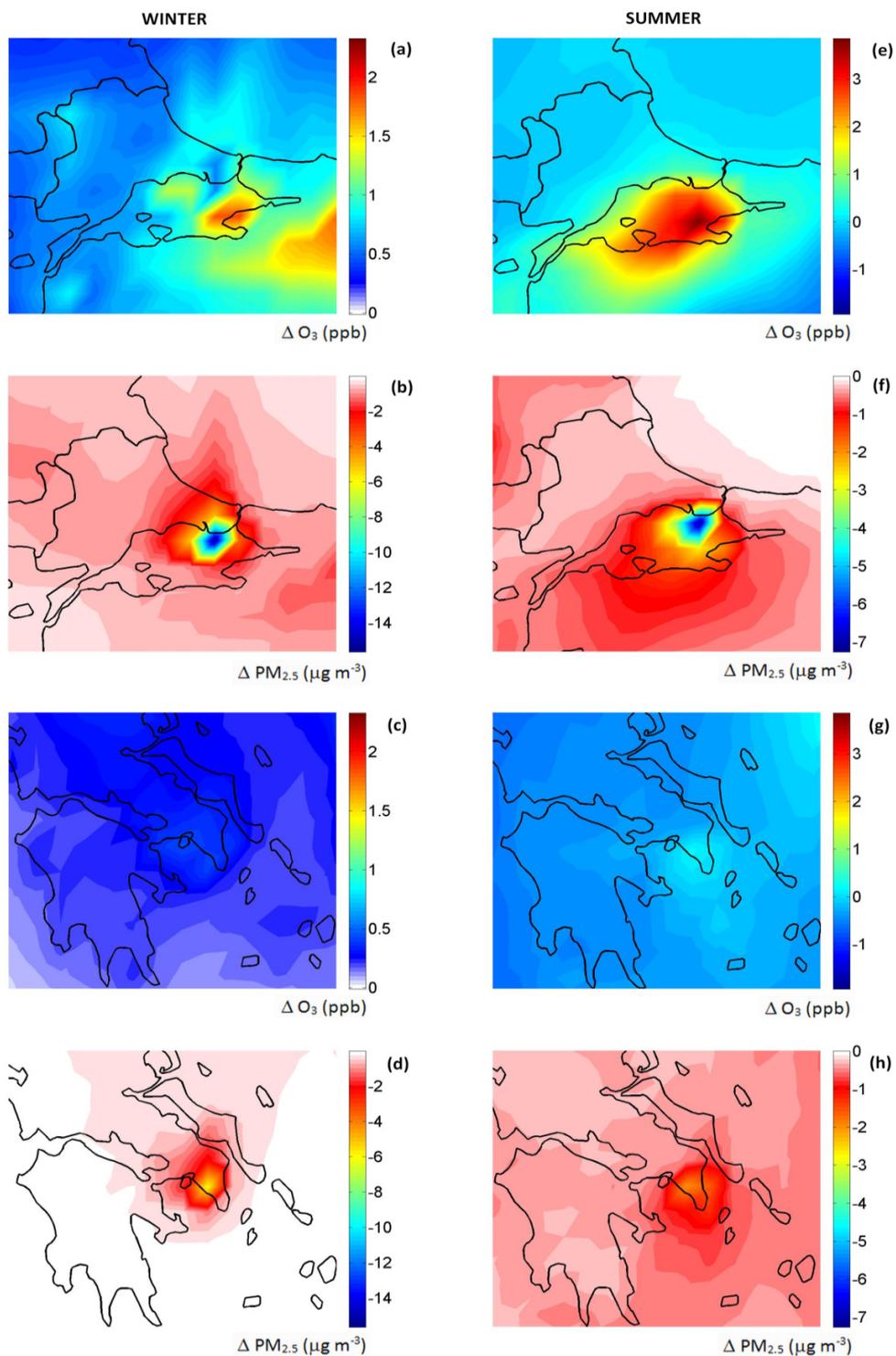


Fig. S6. Changes in surface O₃ (a, c, e, g) and PM_{2.5} (b, d, f, h) levels over Istanbul and Athens due to the mitigation of anthropogenic emissions (Mitig) averaged over each one-month simulation period in winter (left column; December 2008) and in summer (right column; July 2008). Units are ppbv for ΔO₃ and μg m⁻³ for ΔPM_{2.5}.