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Modelling the impacts of emission changes on O_3 sensitivity, atmospheric oxidation capacity, and pollution transport over the Catalonia region

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1 Observations

1.1 Air quality

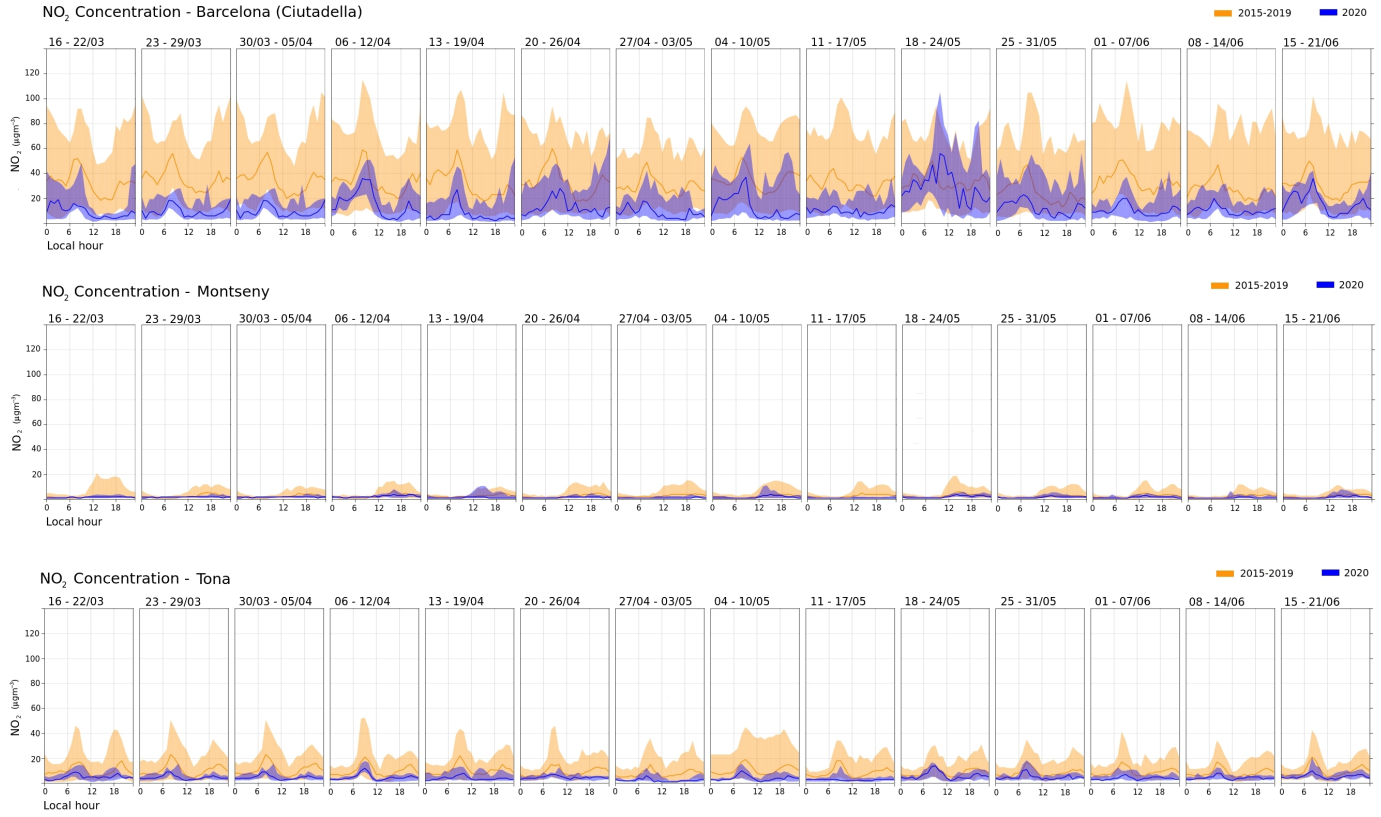

Figure S1. Variation for NO_2 concentrations during COVID-19 confinement and phase-out weeks (in blue) and the same month for the year 2019 (orange), observed at Eixample air quality monitoring station (as part of the Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica, XVPCA). Blue and orange lines show the medians (50th percentile) and shaded zones show the 10th/90th percentiles.

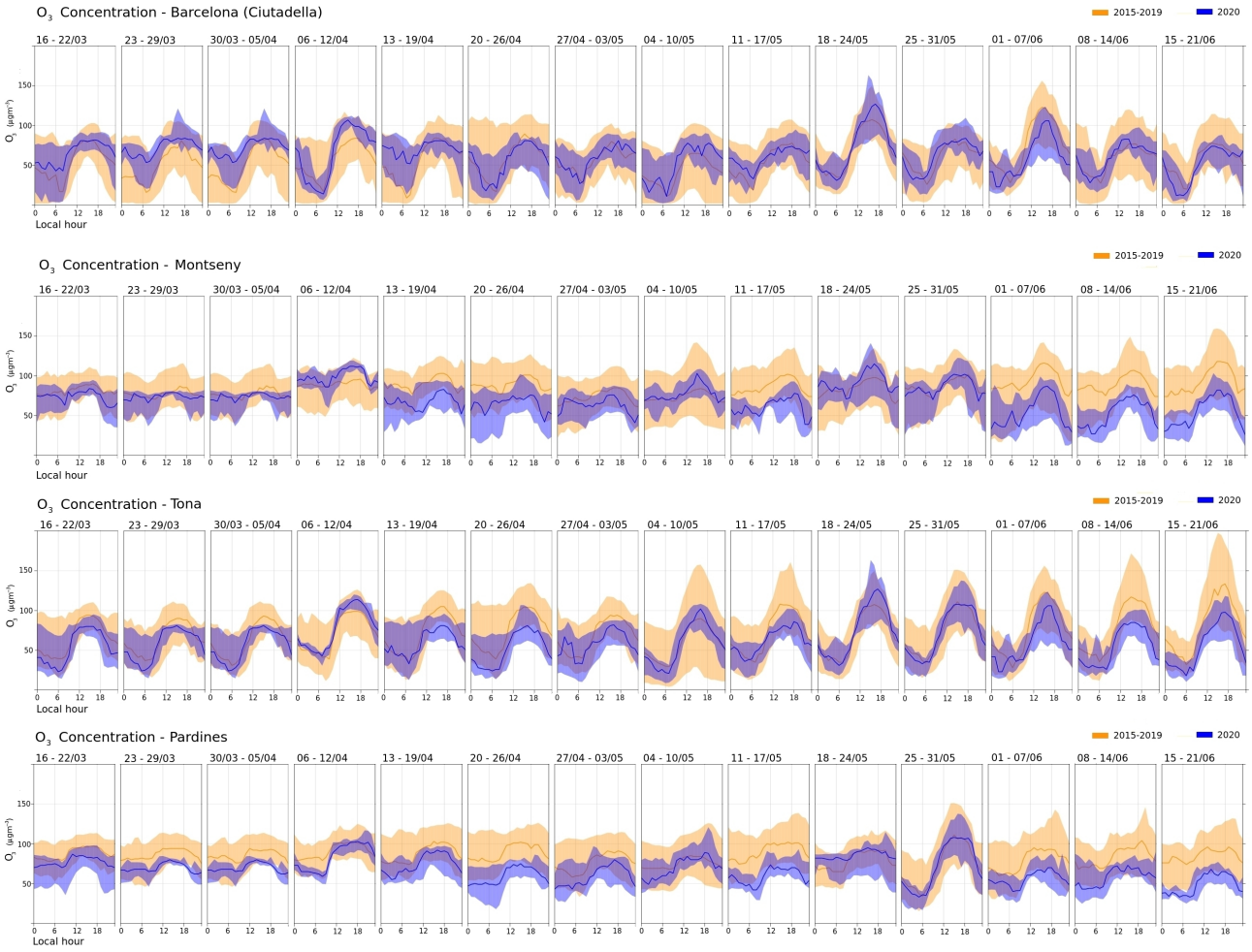

Figure S2. Variation for O_3 concentrations during COVID-19 confinement and phase-out weeks (in blue) and the same month for the year 2019 (orange), observed at diferent air quality monitoring stations (as part of the Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica, XVPCA). Blue and orange lines show the medians (50th percentile) and shaded zones show the 10th/90th percentiles.

Table S1. Ozone levels for 3rd and 6th of April 22 and 26 of May in Barcelona-Ciutadella, Montseny, Tona and, Pardines , observed at Eixample air quality monitoring station (as part of the Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica, XVPCA).

	Ciutadella	**Montseny**	**Tona**	**Pardines**	**Ciutadella**	**Montseny**	**Tona**	**Pardines**
	Min O_3 (μg m^3)				**Max O_3 (μg m^3)**			
3 April	3	54	15	52	88	92	86	81
6 April	14	75	41	64	111	112	115	107
22 May	2	68	25	60	87	143	174	123
26 May	63	20	49	12	127	143	87	103
	Mean O_3 (μg m^3)				**8 max h-mean O_3 (μg m^3)**			
3 April	53.58	70.96	49.92	70.50	76.6	81	77.3	75.4
6 April	66.91	95.33	78.29	87.13	103	109.63	110.5	104.88
22 May	41.54	100.13	81.71	86.71	64.13	119.63	135.25	105.88
26 May	91.54	71.25	66.42	58.75	114.75	114.63	80.75	99.13

1.2 Meteorology

Table S2. Meteorological conditions for 3 and 6 of April 22 and 26 of May near the sites of Barcelona-Ciutadella (Raval), Montseny (Viladrau), Tona (Muntanyola) and Pardines (Núria). Data is from the Servei Meteorològic de Catalunya (SMC), 2020.

	Raval	**Viladrau**	**Muntanyola**	**Núria**	**Raval**	**Viladrau**	**Muntanyola**	**Núria**
	Mean temperature (ºC)				**Pressure at surface level (hPa)**			
3 April	13.5	6.5	6.9	0.3	1015.7	1015	1015.5	1016.2
6 April	14.5	8.7	10.5	3.6	1023.9	1022.7	1023.3	1023.4
22 May	24.4	19.1	21.6	12.5	1022.5	1021.8	1022	1022.9
26 May	23.1	16.2	19.1	9.8	1024.9	1024.5	1024.6	1025.5
	Precipitation acumulated (mm)				**Mean relative humidity (%)**			
3 April	0	0	0	0	61	87	76	63
6 April	0	0	0	0	66	64	51	66
22 May	0	0	0	2.9	54	64	53	68
26 May	0	0	0	0	53	68	57	64
	Max. Wind speed at 2m (km/h)				**Max. Wind direction at 2m (º)**			
3 April	31.7	30.2	33.1	45.4	225	263	254	45
6 April	18.7	20.9	24.8	18.7	151	76	227	206
22 May	27	22.3	25.2	19.1	207	75	232	211
26 May	25.9	26.3	26.6	31	213	84	112	30
	Solar irradiance (MJ/m2)							
3 April	21.5	20.6	24.2	24.3				
6 April	22.6	23.8	23	19.2				
22 May	30.1	29	29.6	23.2				
26 May	29.8	27.1	28.2	28.6				

2 Model validation

2.1 Meteorology

Table S3. Statistical evaluation of the model chemistry results, COVID simulation, over the Metropolitan Area of Barcelona (AMB) and Catalonia (CAT) for the 30 March - 12 April 2020 from observations in hourly basis. The number of stations are shown in parenthesis on the second column for AMB and CAT, respectively. The observation mean (OM), model mean (MM), mean bias (MB), normalised mean bias (NMB), root-mean-square error (RMSE), correlation (R) and the index of agreement (IOA) and are calculated between simulated and observed concentrations.

Variable	Type	OM		MM		MB		NMB [0,1]		RMSE		R[0,1]		IOA [0,1]	
		AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT
T (ºC)	urban (5/6)	12.94	12.88	13.36	13.20	0.42	0.31	0.04	0.03	1.35	1.37	0.93	0.94	0.94	0.95
	rural (2/19)	12.95	8.93	13.89	9.17	0.94	0.24	0.07	0.27	1.48	1.68	0.95	0.94	0.95	0.94
RH (%)	urban (5/6)	70.82	70.25	68.80	68.97	-2.02	-1.28	-0.03	-0.02	10.47	10.26	0.71	0.75	0.80	0.82
	rural (2/19)	73.34	73.70	68.14	75.08	-5.21	1.38	-0.07	0.02	10.25	12.75	0.79	0.82	0.82	0.84
WS (m/s)	urban (4/5)	2.43	2.38	2.83	2.93	0.40	0.55	0.36	0.39	1.91	1.88	0.79	0.81	0.74	0.76
	rural (1/11)	1.99	1.81	3.23	3.67	1.24	1.86	0.62	1.28	2.39	2.74	0.62	0.48	0.66	0.50

Table S4. Same as Table 2 for the 18 to 30 May.

Variable	Type	OM		MM		MB		NMB [0,1]		RMSE		R [0,1]		IOA [0,1]	
		AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT
T (ºC)	urban (5/6)	21.14	21.20	21.30	21.22	0.16	0.03	0.01	0.00	1.46	1.49	0.90	0.92	0.93	0.94
	rural (2/19)	21.07	17.55	21.96	17.71	0.90	0.16	0.04	-0.00	1.60	1.90	0.93	0.94	0.94	0.94
RH (%)	urban (5/6)	64.36	63.88	65.91	66.04	1.55	2.16	0.03	0.04	10.50	10.31	0.75	0.78	0.84	0.85
	rural (2/19)	69.15	67.02	65.34	71.60	-3.80	4.59	-0.055	0.073	9.37	13.35	0.82	0.82	0.88	0.84
WS (m/s)	urban (4/5)	2.18	2.09	2.19	2.24	0.01	0.15	0.12	0.18	1.42	1.38	0.66	0.69	0.71	0.74
	rural (1/11)	2.08	1.76	2.52	3.08	0.44	1.32	0.21	0.94	1.25	2.27	0.71	0.49	0.82	0.51

2.2 Air quality

Table S5. Statistical evaluation of the modelled chemistry (COVID simulation), over the Metropolitan Area of Barcelona (AMB) and Catalonia (CAT) for the 30 March - 12 April 2020 in hourly basis. The number of stations are shown in parenthesis on the second column for AMB and CAT, respectively. The observation mean (OM), model mean (MM), mean bias (MB), normalised mean bias (NMB), root-mean-square error (RMSE), correlation (R) and the index of agreement (IOA) and are calculated between simulated and observed concentrations. Stations are classified into urban background, urban traffic, suburban background, and rural background.

Specie	Type	OM (μg m^{-3})		MM (μg m^{-3})		MB (μg m^{-3})		NMB [0,1]		RMSE (μg m^{-3})		R [0,1]		IOA [0,1]	
		AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT		
NO_2	urban b. (8/13)	14.28	13.81	13.16	11.56	-1.12	-2.25	-0.06	-0.15	14.05	13.55	0.45	0.43	0.43	0.39
	urban t. (5/9)	16.65	16.10	11.02	9.92	-5.63	-6.18	-0.37	-0.42	15.46	15.09	0.44	0.4	0.45	0.41
	suburb. b. (5/13)	10.73	9.60	8.21	5.80	-2.52	-3.8	-0.26	-0.45	9.16	8.55	0.39	0.39	0.41	0.34
	rural b. (-/4)	-	3.23	-	1.09	-	-2.14	-	-0.63	-	2.88	-	0.32	-	0.15
O_3	urban b.(4/7)	71.57	71.88	85.67	84.51	13.63	12.63	0.20	0.17	25.12	25.19	0.73	0.70	0.48	0.50
	urban t. (2/8)	65.94	68.96	83.63	88.16	17.69	19.20	0.26	0.28	31.96	30.55	0.61	0.62	0.50	0.51
	suburb. b. (4/8)	83.93	74.74	101.6	93.73	17.67	18.99	0.22	0.26	22.43	25.19	0.73	0.66	0.51	0.46
	rural b. (-/)		76.06	-	92.43	-	16.37	-	0.22	-	27.81	-	0.42	-	0.42

Table S6. Same as Table 3 for the 18 to 30 May.

Specie	Type	OM (μg m^{-3})		MM (μg m^{-3})		MB (μg m^{-3})		NMB [0,1]		RMSE (μg m^{-3})		R[0,1]		IOA [0,1]	
		AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT	AMB	CAT		
NO_2	urban b. (-/12)	19.50	17.91	16.44	13.59	-3.05	-4.32	-0.15	-0.24	18.38	16.58	0.23	0.27	0.41	0.38
	urban t. (5/9)	30.22	23.3	20.4	10.25	-9.82	-13.05	-0.32	-0.6	24.94	21.27	0.20	0.23	0.33	0.25
	suburb. b. (5/13)	13.69	12.14	10.87	7.18	-2.81	-4.96	-0.26	-0.42	11.33	10.94	0.40	0.30	0.528	0.38
	rural b. (-/4)	-	3.23	-	1.09	-	-2.14	-	-0.66	-	2.96	-	0.24	-	0.26
O_3	urban b. (4/7)	66.18	68.14	78.83	79.14	12.65	11.01	0.21	0.17	28.18	27.98	0.62	0.60	0.54	0.55
	urban t. (2/8)	60.03	61.10	77.32	77.62	17.29	16.59	0.28	0.27	29.35	29.62	0.62	0.60	0.48	0.51
	suburb. b. (4/8)	79.00	69.38	88.00	84.87	9.01	15.49	0.13	0.24	28.43	32.31	0.51	0.49	0.52	0.49
	rural b. (-/12)	-	75.86	-	86.44	-	10.57	-	0.16	-	27.82	-	0.42	-	0.44

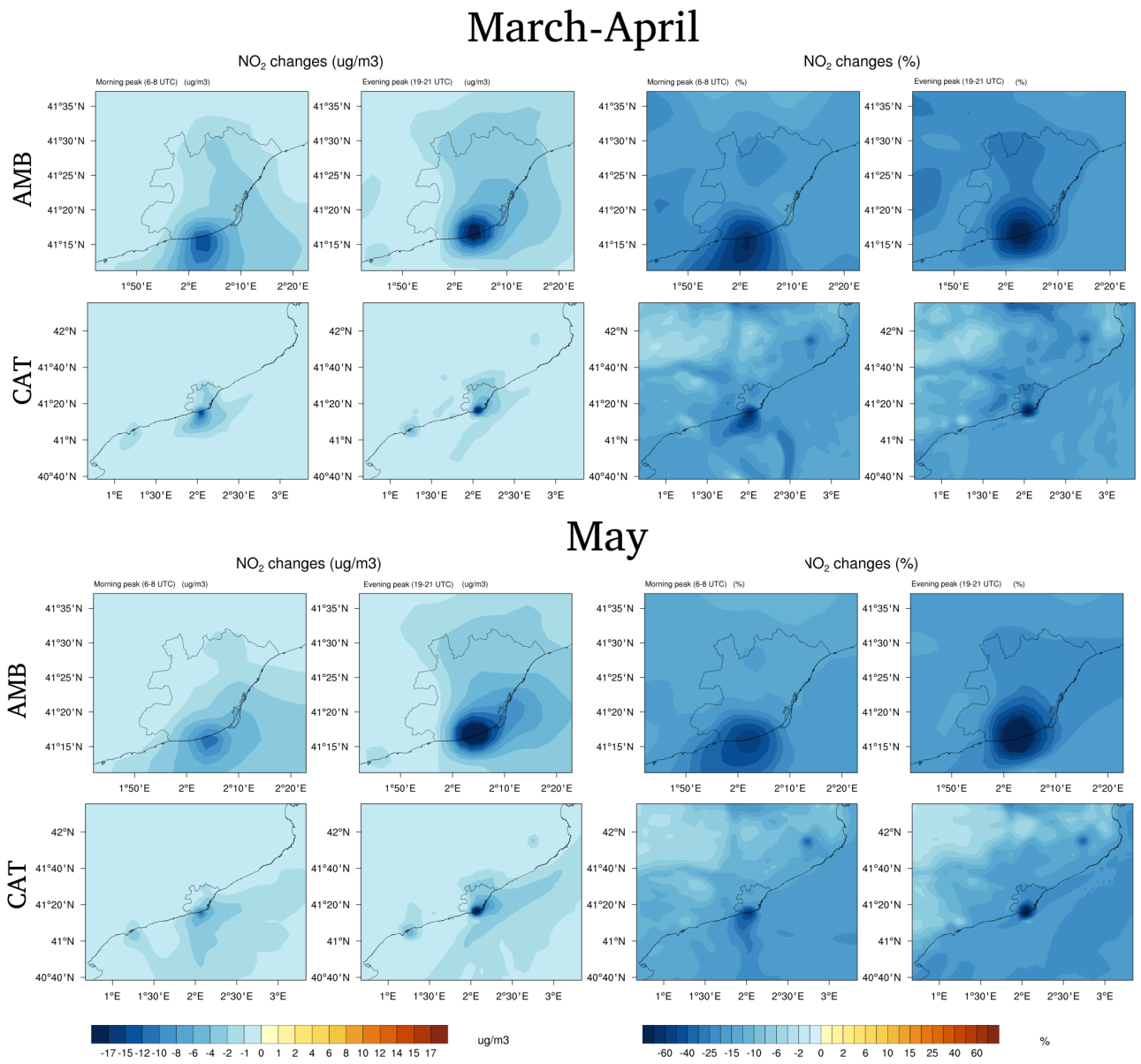

Figure S3. Averaged surface NO_2 changes over the Metropolitan Area of Barcelona (AMB) and the Catalonia region (CAT) during 30 March to 12 April (only weekdays) and 18 to 30 May (only weekdays) in absolute value (ug/m3) and relative change (%). Relative change (%) is calculated as (COVID-BAU)/BAU$\times$100.

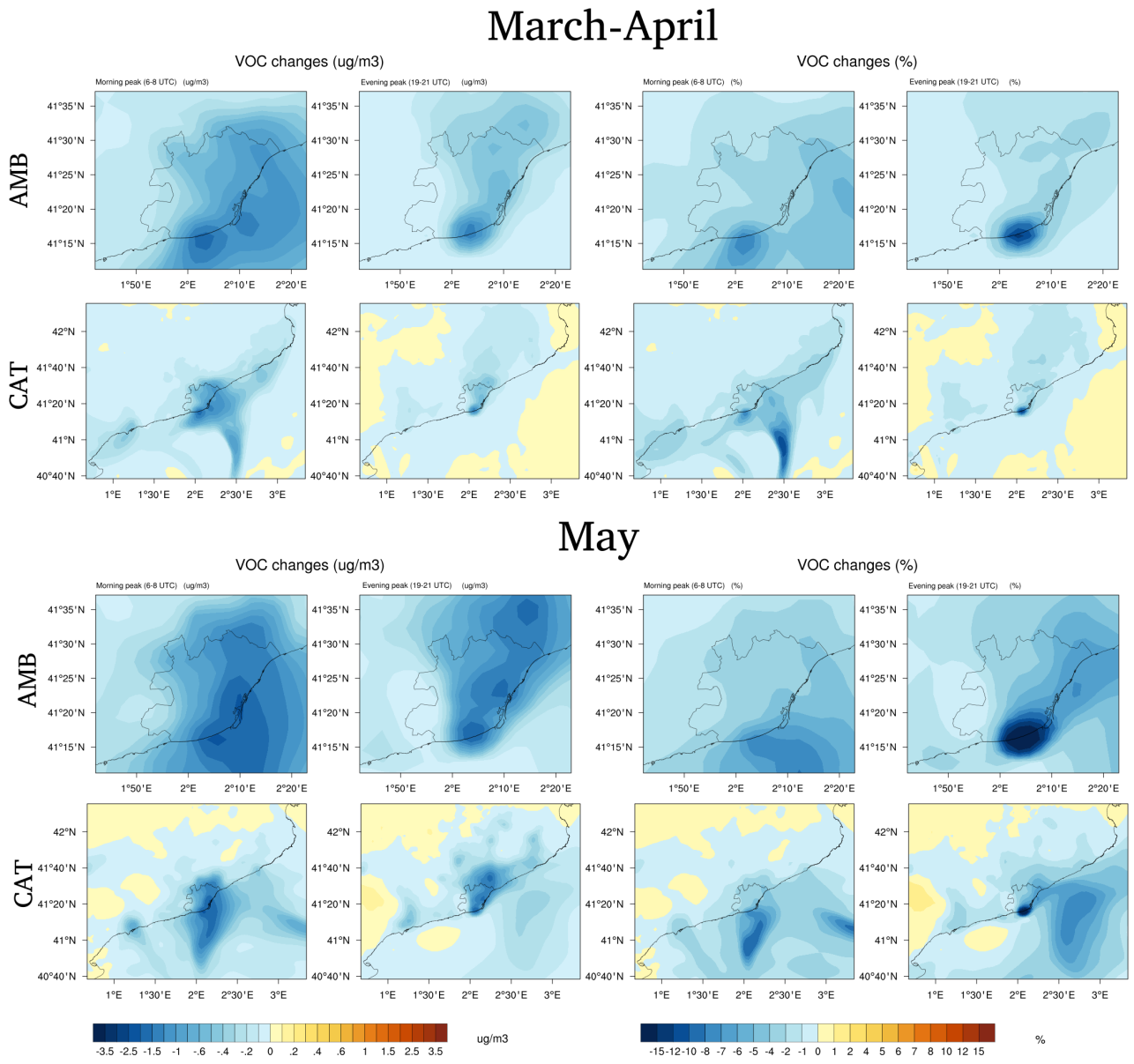

Figure S4. Same as Figure S3 for VOC changes.

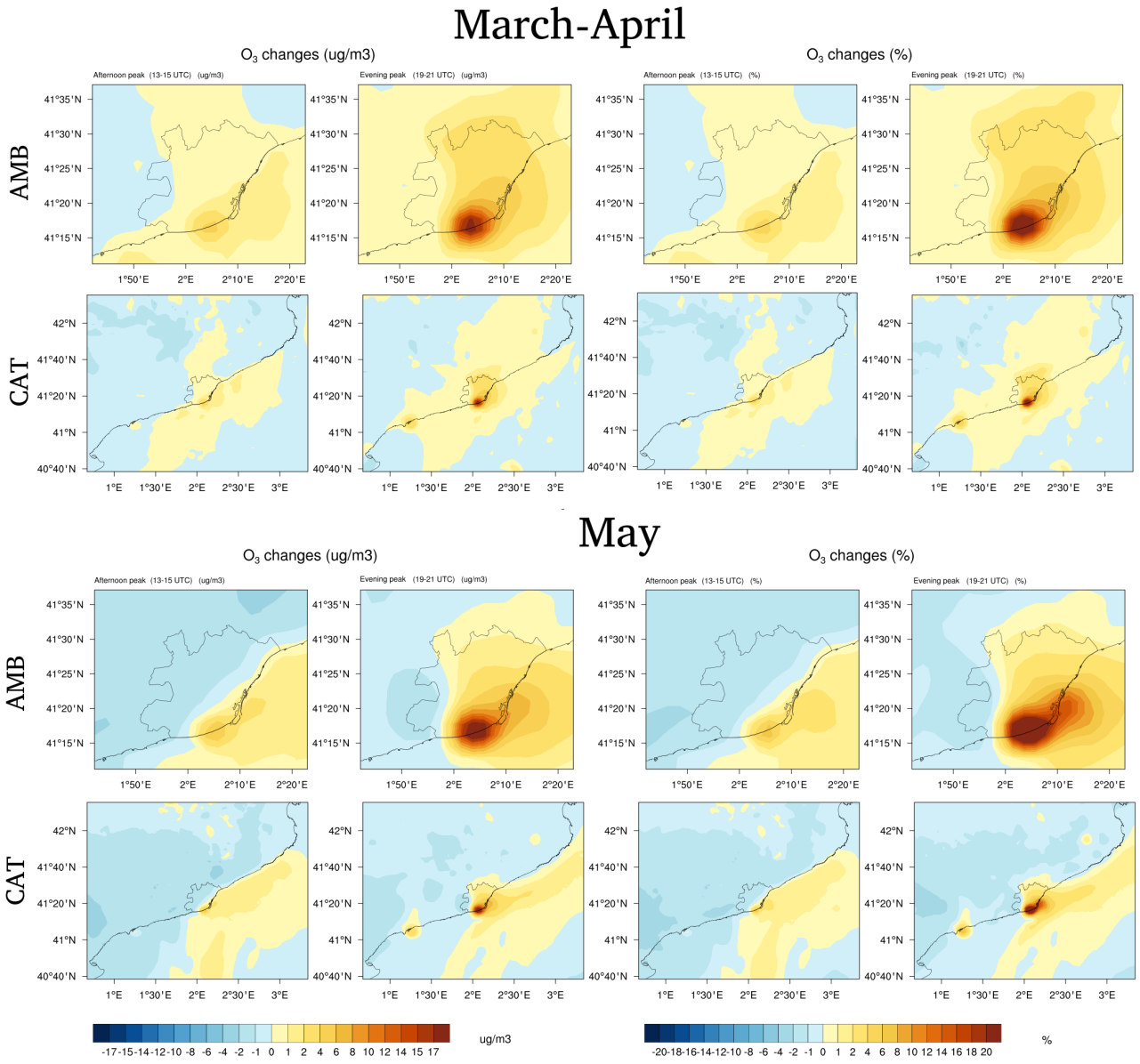

Figure S5. Same as Figure S3 for O_3 changes.

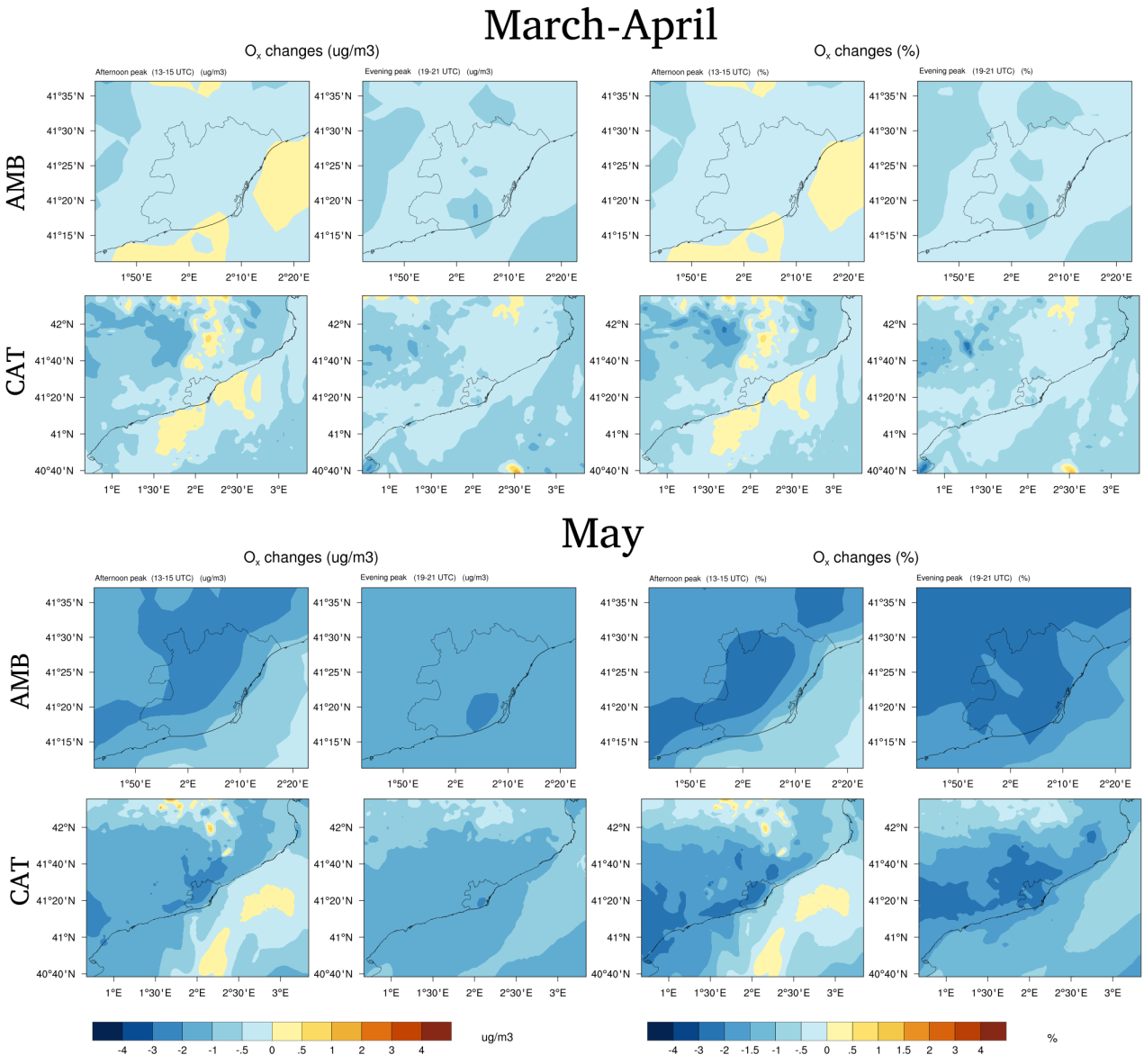

Figure S6. Same as Figure S3 for O_x changes.

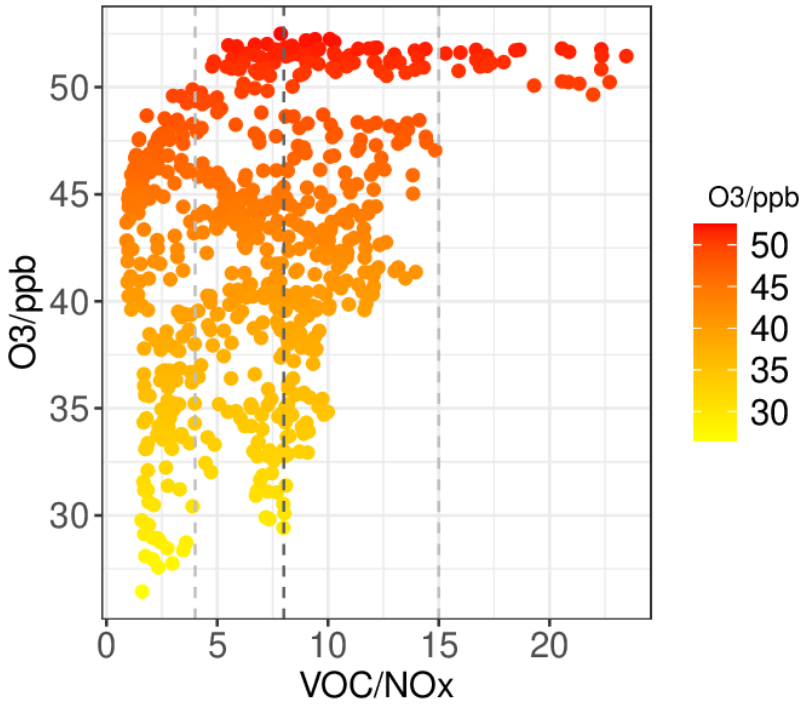

Figure S7. O_3 concentration as a function of VOC/NO_X concentration. Points are calculated with a 5 hours average concentration for the two periods using the BAU simulation. Dark vertical line separate the two photochemical regimes by the local O_3 maximum. Grey vertical lines separate the transitional regimes.

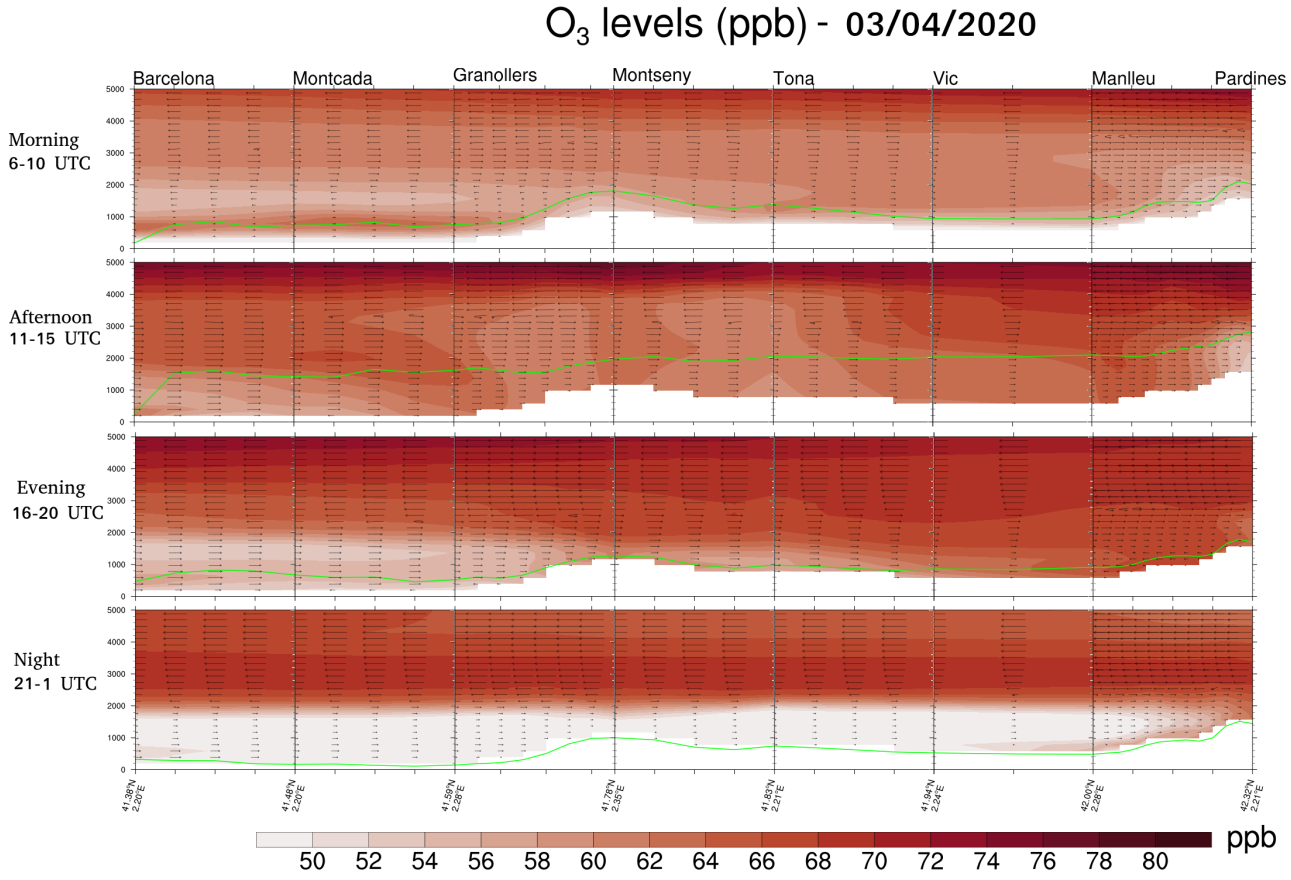

Figure S8. O_3 levels in BAU simulation along the atmospheric plume from the AMB to the Pyrenees for the 3rd of April. The modelled PBLH is shown with a green line. Black arrows are plotted for the the wind (u,v).

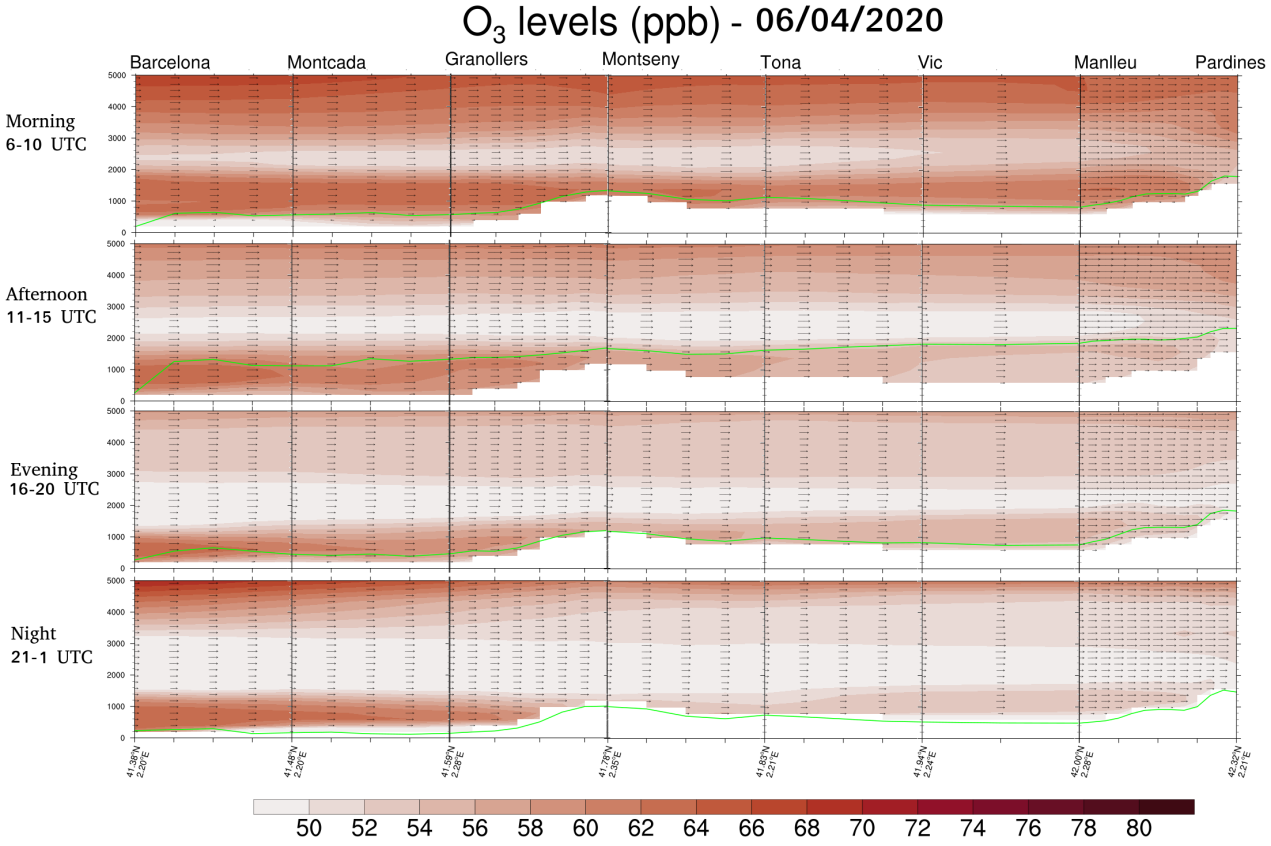

Figure S9. O_3 levels in BAU simulation along the atmospheric plume from the AMB to the Pyrenees for the 6rd of April. The modelled PBLH is shown with a green line. Black arrows are plotted for the the wind (u,v).

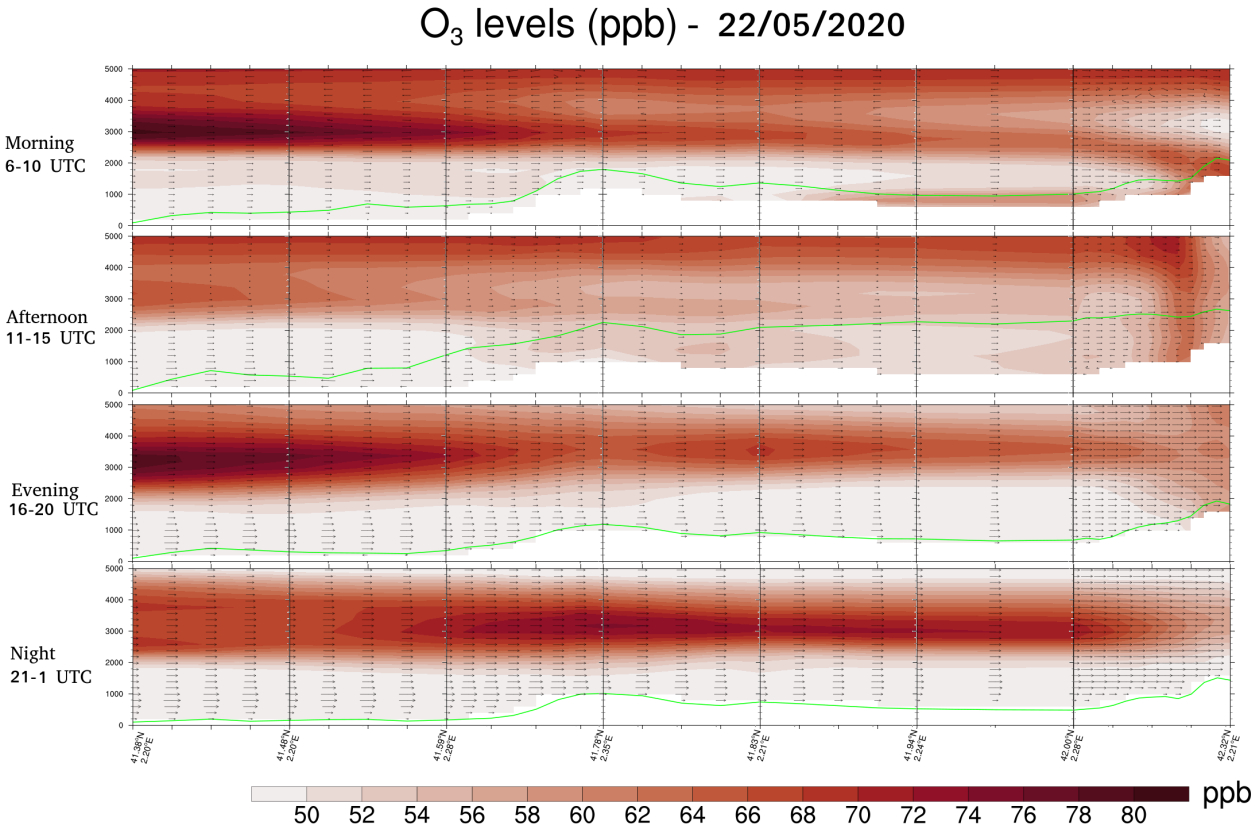

Figure S10. O_3 levels in BAU simulation along the atmospheric plume from the AMB to the Pyrenees for the 22nd of May. The modelled PBLH is shown with a green line. Black arrows are plotted for the the wind (u,v).

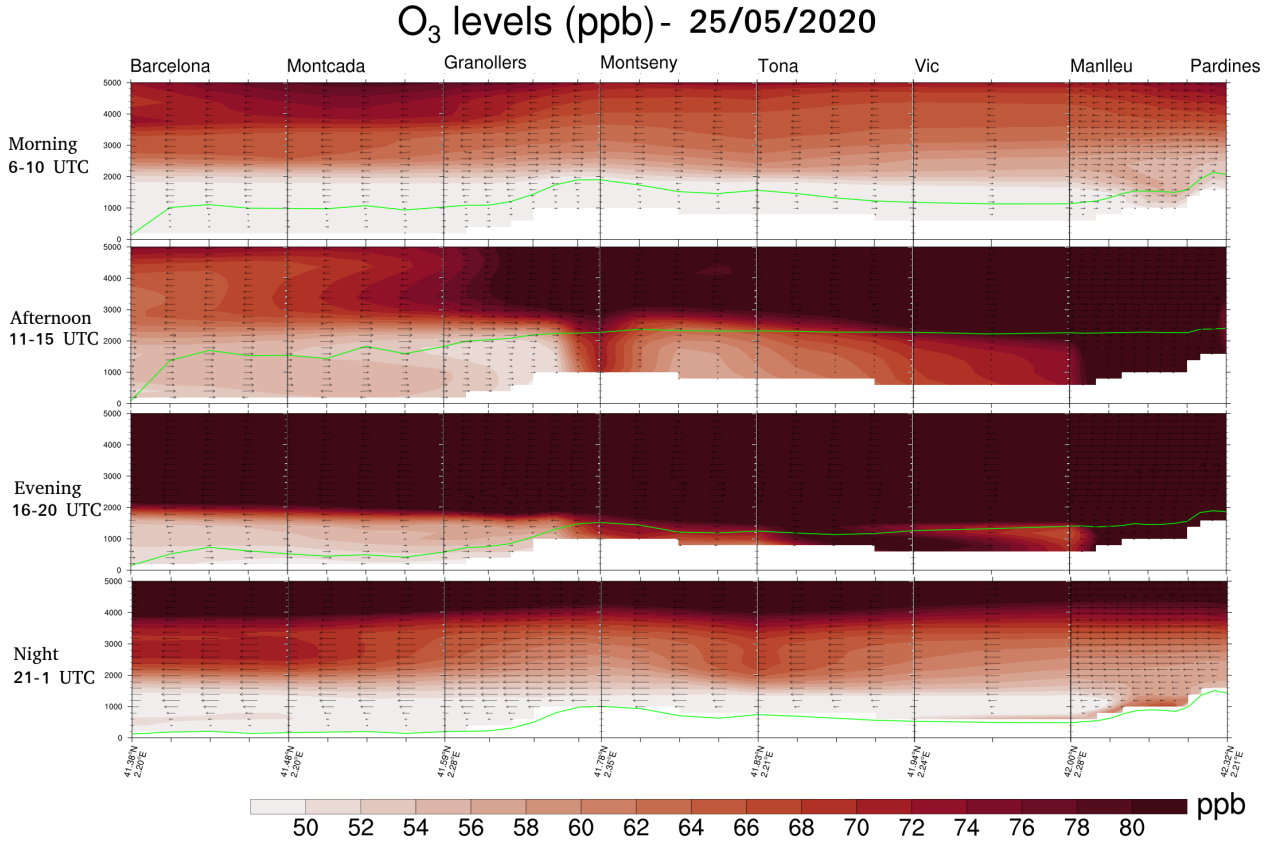

Figure S11. O_3 levels in BAU simulation along the atmospheric plume from the AMB to the Pyrenees for the 26th of May. The modelled PBLH is shown with a green line. Black arrows are plotted for the the wind (u,v).

Table S7. Average and relative change concentrations for NO_x, O_3 and VOCs during the 30 March to 12 April (only weekdays) in the morning (6-8 UTC), midday (13-15 UTC) and afternoon (19-21 UTC). Average concentrations are in ppb for NO_x and O_3 and ppbC for VOCs and the relative change (%) is calculated as (COVID-BAU)/BAU$\times$100.

Pollutant	Landuse	Morning			Afternoon			Evening		
		BAU	COVID	Change	BAU	COVID	Change	BAU	COVID	Change
NO_x	Forest	2.9	2.3	-20.5	1.0	0.8	-21.9	3.4	2.6	-23.7
	Natural Open	3.5	2.1	-40.4	1.3	0.9	-26.3	3.4	2.1	-36.4
	Agriculture	4.8	3.0	-37.1	1.5	1.0	-30.1	4.7	2.8	-40.3
	Water	10.2	7.8	-24.2	5.0	3.9	-22.3	9.4	6.9	-27.0
	Compact urban	8.8	7.2	-18.4	3.3	2.6	-19.2	9.0	6.9	-23.3
	Open urban	4.1	2.8	-30.9	1.5	1.1	-25.3	4.8	3.5	-26.7
	Industrial	6.1	4.8	-21.7	2.2	1.6	-25.6	6.8	4.7	-31.1
VOC	Forest	28.4	27.7	-2.1	13.7	13.6	-1.3	23.8	23.5	-1.3
	Natural Open	22.2	21.5	-3.3	11.9	11.7	-1.3	17.5	17.2	-1.7
	Agriculture	30.8	30.0	-2.6	13.2	13	-1.6	24.1	23.7	-1.7
	Water	40.8	38.9	-4.5	10.1	9.9	-2.4	13.3	12.9	-2.9
	Compact urban	53.0	51.8	-2.4	19.3	19	-1.8	38.2	37.5	-1.9
	Open urban	32.8	31.7	-3.3	13.9	13.6	-2.0	26.4	25.9	-1.8
	Industrial	40.9	39.9	-2.5	16.3	16	-1.9	31.7	31.1	-1.9
O_3	Forest	40.3	40.7	1.0	51.7	51.7	0.0	42.3	42.9	1.3
	Natural Open	42.8	43.9	2.5	51.7	51.9	0.3	45.4	46.4	2.1
	Agriculture	37.3	38.5	3.4	51	51.2	0.4	40.7	42.2	3.7
	Water	37	38.7	4.6	48.6	49.4	1.6	42.1	44.2	5.0
	Compact urban	35.8	36.9	2.9	52	52.3	0.6	40.4	42.2	4.3
	Open urban	39.4	40.4	2.4	52.6	52.8	0.3	42.6	43.6	2.4
	Industrial	36.8	37.7	2.3	52.2	52.5	0.5	40.1	41.8	4.2

Table S8. Same as Table S7 for the 18 to 30 May (only weekdays).

Pollutant	Landuse	Morning			Afternoon			Evening		
		BAU	COVID	Change	BAU	COVID	Change	BAU	COVID	Change
NO_x	Forest	2.6	2.2	-16	1.0	0.8	-25.3	4.0	3.2	-21.4
	Natural Open	3.5	2.4	-32.3	1.1	0.7	-34.7	3.4	2.2	-37.2
	Agriculture	4.5	3.2	-30.2	1.2	0.7	-39.7	5.1	3	-41.2
	Water	15.3	11.5	-24.8	8.0	5.9	-26.2	15	10.8	-27.9
	Compact urban	8.1	6.9	-15.5	3.5	2.7	-23.9	10.6	8.1	-24.0
	Open urban	3.9	2.9	-25.3	1.7	1.2	-27.5	5.5	4.1	-24.9
	Industrial	6.0	4.8	-20.0	2.2	1.5	-31.5	7.6	5.2	-31.7
VOC	Forest	34.2	33.3	-2.5	18.7	18.5	-0.9	28.7	27.9	-2.8
	Natural Open	28.7	27.7	-3.3	13.8	13.5	-2.2	17.5	17	-3.2
	Agriculture	36.8	35.6	-3.2	15.5	15.2	-1.7	26.5	25.5	-3.6
	Water	43.8	41.2	-5.9	10.1	8.9	-11.6	11.3	10.5	-7.9
	Compact urban	59.1	56.9	-3.8	22.4	21.6	-3.6	40.6	38.5	-5.1
	Open urban	38.7	37.3	-3.7	17.2	16.7	-2.7	28.8	27.5	-4.4
	Industrial	48.1	46.3	-3.6	20.5	19.9	-2.5	33.1	31.6	-4.6
O_3	Forest	36.9	36.7	-0.6	51.3	50.5	-1.6	37.7	37.6	-0.1
	Natural Open	37.0	37.3	0.6	48.9	48.3	-1.3	40.3	40.6	0.8
	Agriculture	33.3	33.8	1.4	50.5	49.9	-1.2	36.3	37.3	3.0
	Water	29.7	31.2	4.9	42.5	43.4	2.2	32.0	35	9.4
	Compact urban	33.6	33.9	1.0	50.8	50.4	-0.8	35.8	37.2	3.8
	Open urban	36.7	36.9	0.5	51.3	50.7	-1.1	38.2	38.6	1.1
	Industrial	34.3	34.6	0.9	52.1	51.6	-1.1	36.3	37.6	3.5

4 Land use categories

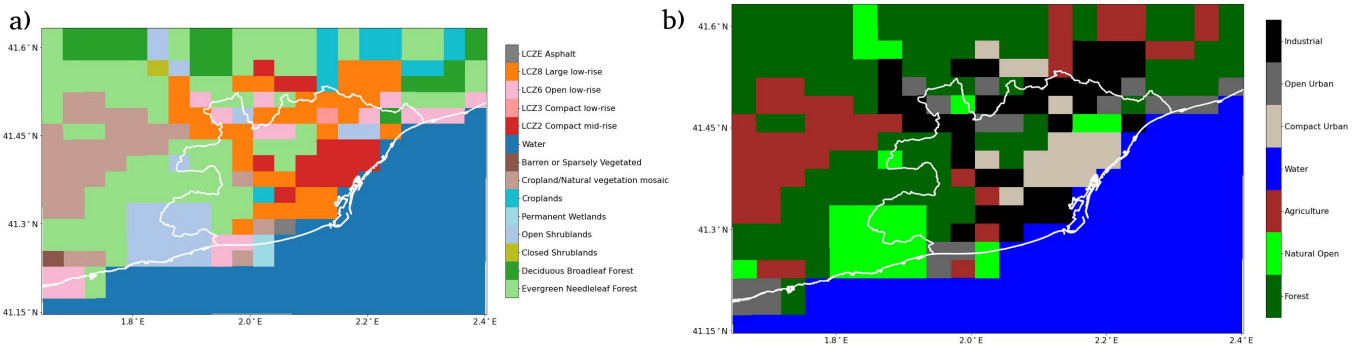

Figure S12. Land-use classification in the model (a) and for the model analysis (b). The white line define the AMB limits.

Table S9. Land-use classification for the model analysis

Model land-use	Land-use category for the model analysis
Evergreen Needleleaf Forest	Forests
Deciduous Broadleaf Forest	Forests
Mixed Forest	Forests
Closed Shrublands	Natural open areas
Open Shrublands	Natural open areas
Grassland	Natural open areas
Permanent Wetlands	Natural open areas
Croplands	Natural open areas
Barren or Sparsely Vegetated	Agricultural areas
Cropland/Nature Vegetation Mosaic	Agricultural areas
Water	Water
LCZ1 Compact high-rise	Compact urban areas
LCZ2 Compact mid-rise	Compact urban areas
LCZ3 Compact low-rise	Compact urban areas
LCZ5 Open mid-rise	Open urban areas
LCZ6 Open low-rise	Open urban areas
LCZ9 Sparely built	Open urban areas
LCZ8 Large low-rise	Industrial, commercial and airport areas
LCZ10 Heavy industry	Industrial, commercial and airport areas
LCZE Asphalt	Industrial, commercial and airport areas

10 References

Servei Meteorològic de Catalunya (SMC), .: Butlletí climàtic mensual (maig del 2020), Tech. rep., Departament de Territori i Sostenibilitat., 2020.