

Supplementary material

Table S1. Detail set up of the CALIOPE system in the present modelling study

Meteorological model	WRF-ARWv3.5.1
Initial and boundary meteorological conditions	GFS-FNL (1.5°x1.5°, 6h)
Meteorological spin-up period	12 hours
WRF mother domain 12-km resolution over Europe (nx, ny, nz)	480 x 400 x 38
WRF nested domain 4-km resolution over the Iberian Peninsula (nx, ny, nz)	399 x 399 x 38
WRF parametrizations	Boundary layer: YSU Microphysics scheme: WSM5 Cumulus scheme: no cumulus parametrization Land Surf physics: unified Noah land-surface model Long Wave: RRTM Short Wave: Dudhia Surface Layer: Revised MM5 Monin-Obukhov scheme
Emission model	HERMESv2
Base year of the emission	2009
Chemical Transport Model	CMAQv5.0.2
Chemical mechanism	cb05-TUCL-aero6
Chemical boundary conditions	MOZART4-GEOS5 forecast (1.7° x 2.5°, 6h)
CTM spin-up period	6 days
ISAM tracked species	O ₃ , NO _x , NMVOC
Mother domain 12-km resolution over Europe (nx, ny, nz)	478 x 398 x 15
Nested domain 4-km resolution over the Iberian Peninsula (nx, ny, nz)	397 x 397 x 15
CMAQ parametrizations	Horizontal advection scheme: Yamartino mass-conserving Vertical advection scheme: Piecewise Parabolic Method (PPM) Vertical diffusion: Asymmetric Convective Model v2 (ACM2) Eddy diffusivity approach Dry deposition routine: Models-3 + Cl species

Table S2. Absolute (μgm^{-3}) and normalized (%) contribution of tagged sources to surface O₃ concentration by receptor region: Center of the IP (CIP), Eastern IP (EIP), Ebro Valley (EV), Guadalquivir

Valley (GV), the Mediterranean Sea (MED), North-Eastern IP (NEIP), Northern IP (NIP), North-Western IP (NWIP), Southern IP (SIP) and Western IP (WIP). Regions are sorted by decrease BCON O₃ concentration.

Zone	Concentration ($\mu\text{g m}^{-3}$)						Percentage (%)					
	BCON	OTHR	SNAP1	SNAP34	SNAP7	SNAP8	BCON	OTHR	SNAP1	SNAP34	SNAP7	SNAP8
MED	77.6	2.4	2.0	1.8	9.5	8.4	76	2	2	2	9	8
EV	67.7	3.7	3.2	3.2	10.8	11.6	68	4	3	3	11	12
EIP	67.1	3.7	2.8	2.9	12.2	11.9	67	4	3	3	12	12
NEIP	62.2	5.2	2.6	4.0	16.3	13.5	60	5	2	4	16	13
CIP	59.3	5.8	2.1	4.1	17.3	10.3	60	6	2	4	18	10
WIP	59.2	5.7	2.5	3.5	12.8	9.8	63	6	3	4	14	11
SIP	58.7	4.5	3.5	2.6	14.8	19.2	57	4	3	3	14	19
NIP	56.3	5.4	2.6	4.6	14.4	11.8	59	6	3	5	15	12
NWIP	55.7	5.8	4.4	4.5	13.6	10.3	59	6	5	5	14	11
GV	49.2	8.3	5.2	6.4	18.9	18.3	46	8	5	6	18	17



FIGURE S1. CMAQ domains in the CALIOPE system for the present study. EU12 corresponds to the mother domain at 12-km horizontal resolution (black). IP4 depicts the Iberian Peninsula domain at 4-km horizontal resolution used to run ISAM (red).

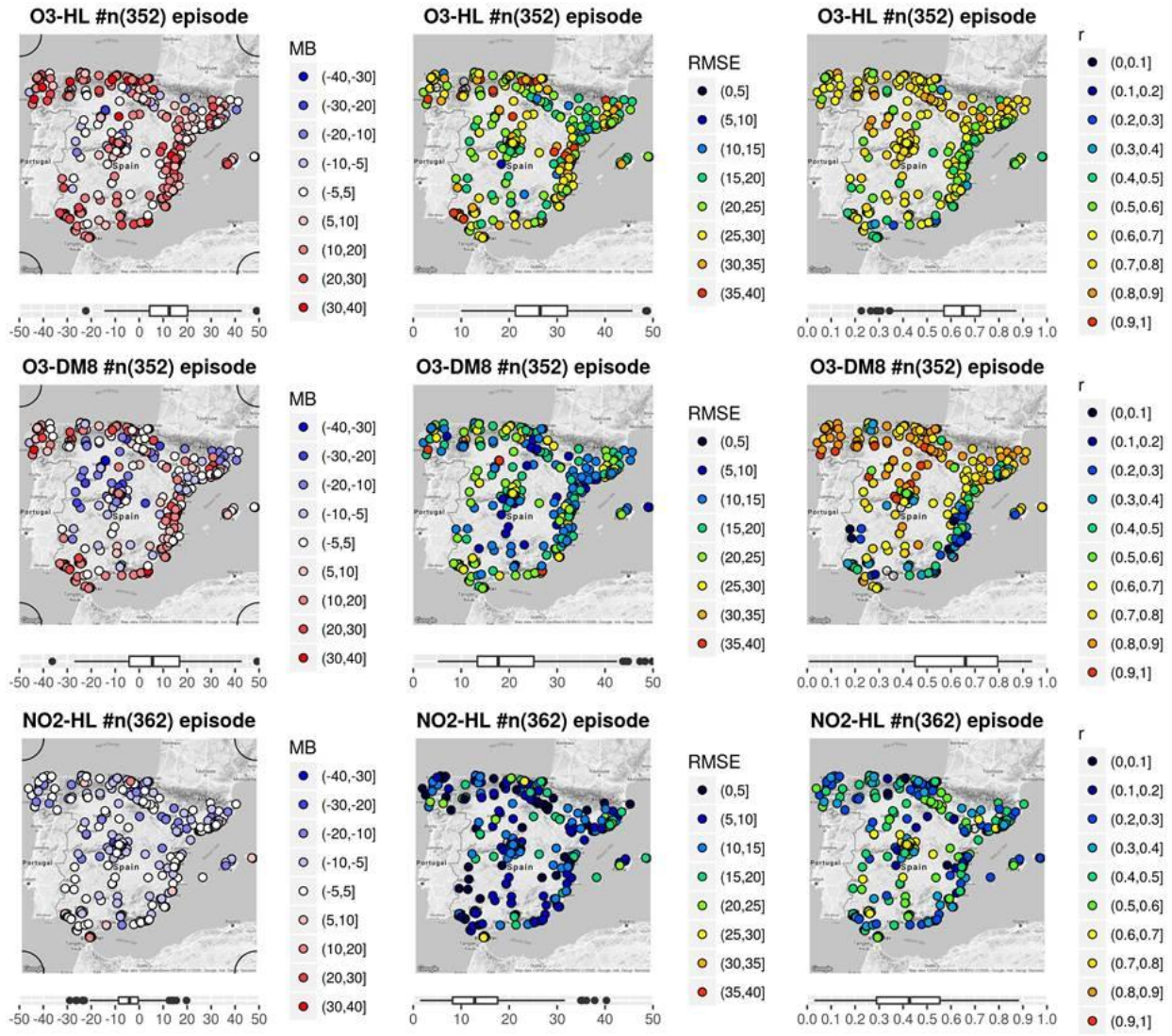


Figure S2. Mean bias (MB, in $\mu\text{g}/\text{m}^3$) (first column), Root Mean Squared Error (RMSE, in $\mu\text{g}/\text{m}^3$) (second column) and correlation coefficient (r) (third column) for HL O₃, MDA8 O₃ and HL NO₂ at the Spanish EIONET stations during the selected O₃ episode.

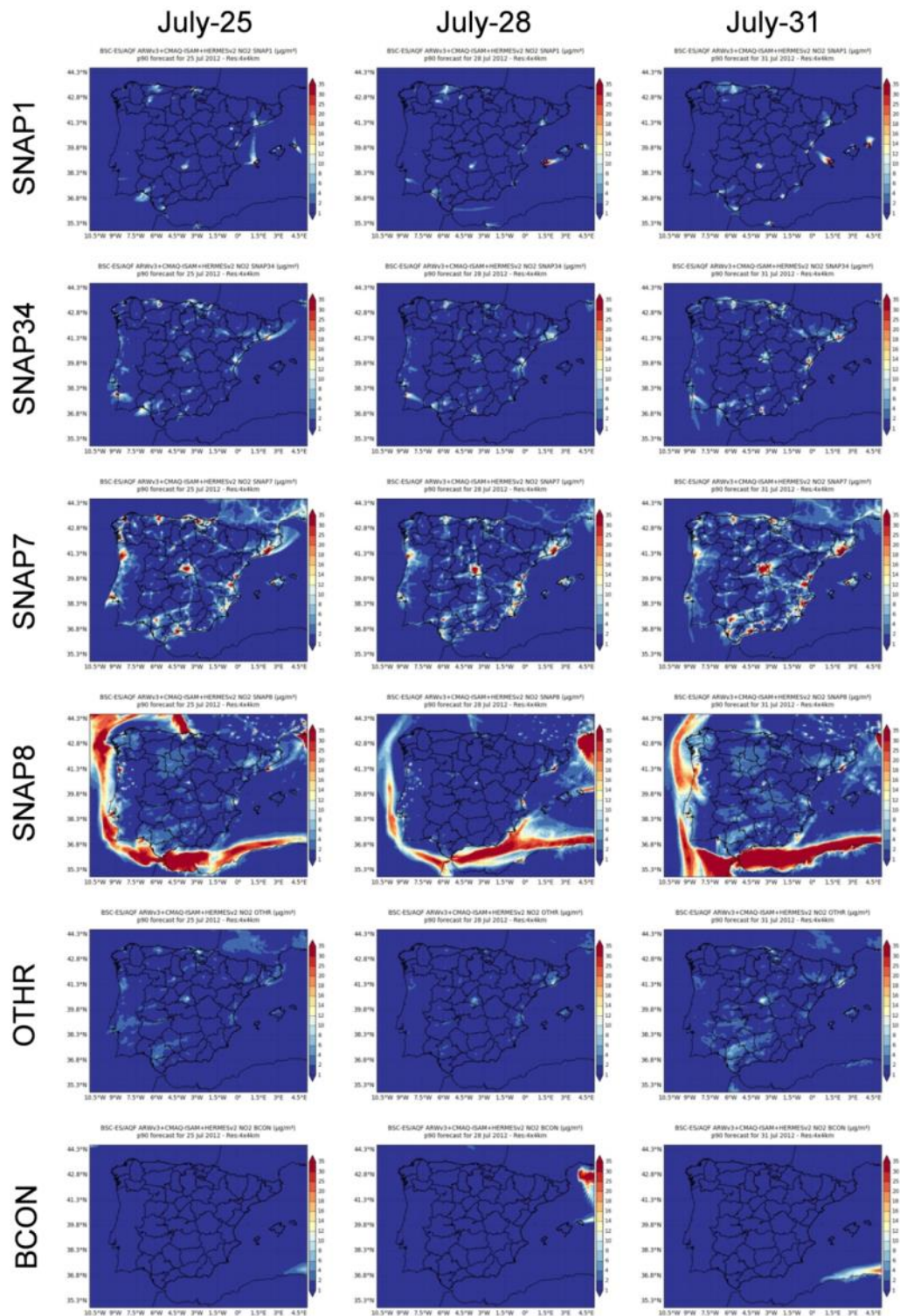


Figure S3. Tagged NO₂ concentrations (in $\mu\text{g}/\text{m}^3$) corresponding to the p90 of the hourly concentrations: SNAP1, SNAP34, SNAP7, SNAP8, OTHER, and BCON for July 25th (first column), 28th (second column) and 31st (third columns) in 2012

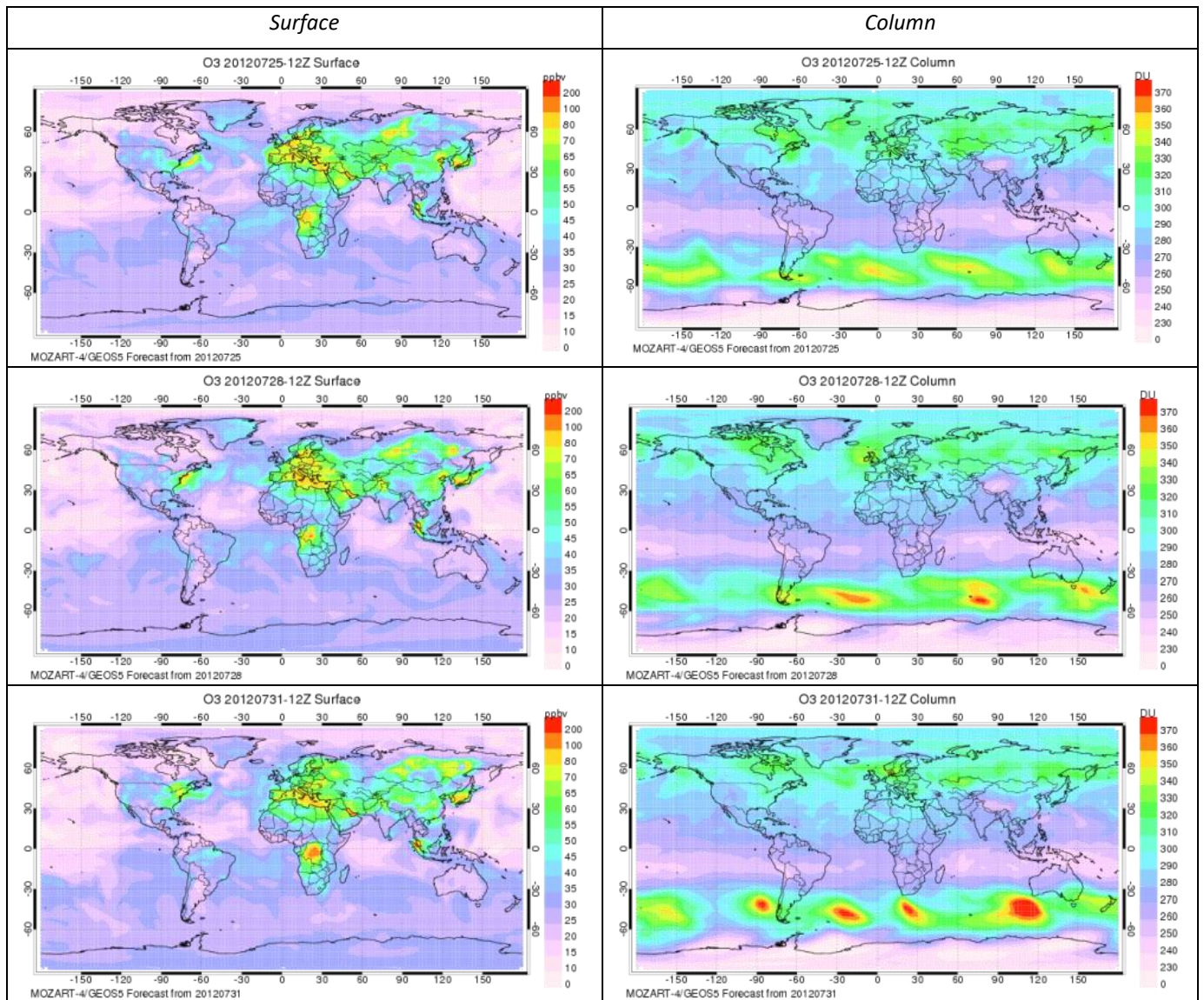


Figure S4. O₃ global maps for surface concentration (first column, in ppbv) and column (right column, in DU) for the July 25th (first row), 28th (second row) and 31st (third row) in 2012 for the MOZART-4 model used for CALIOPE boundary condition in the European domain (EU12). Source:

<http://www.acom.ucar.edu/acresp/forecast/>