Impact of external industrial sources on the regional and local air quality of Mexico Megacity

Supplementary Material

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In this supplement the corresponding Tables and Figures addressing Reviewers' comments are provided.

Table S1. Effect of including Multiscale FDDA in model simulations. Upper row: baseline case of our previous study. Bottom row: simulation with Multiscale FDDA corresponding to RPC configuration case.

| Station		RMSEvec (m/s)	WD IOA	BIAS (°)
CHA	(NE)	3.8	0.86	4.41
		1.29973	0.68699	1.29973
CUA	(SW)	2.99	0.75	0.2
		1.0032	0.78839	1.0032
EAC	(NW)	2.29	0.72	26.8
		0.94683	0.7184	0.94683
MER	(C)	2.45	0.75	-23.5
		0.84904	0.80453	0.84904
PLA	(SW)	2.22	0.81	-5.81
		0.79706	0.81221	0.79706
TAC	(NW)	2.21	0.68	6.27
		0.90808	0.85222	0.90808
TAH	(SE)	3.65	0.54	-0.16
		1.48058	0.70785	1.48058
TLA	(NW)	2.68	0.71	2.31
		0.99774	0.77368	0.99774
TPN	(SW)	3.93	0.63	27.64
		2.7928	0.5795	2.7928
VIF	(NE)	2.95	0.7	-35.61
		1.07771	0.81751	1.07771
XAL	(NE)	3.24	0.62	-11.54
		1.05576	0.71401	1.05576
T0		2.61	0.57	3.4
		0.84359	0.82871	0.84359
T1		3.38	0.81	-0.37
		1.10844	0.85306	1.10844
T2		3.6	0.88	9.53
		1.15227	0.89553	1.15227
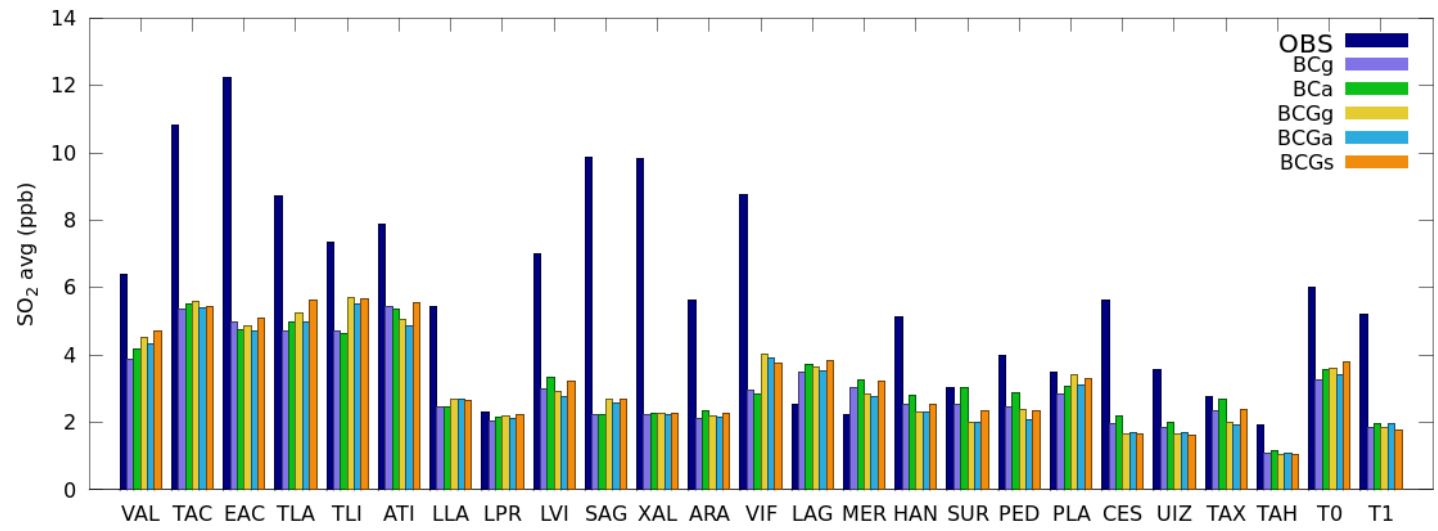
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2   **Figure 1. Average SO$_2$ concentration after including the aerosol phase.**
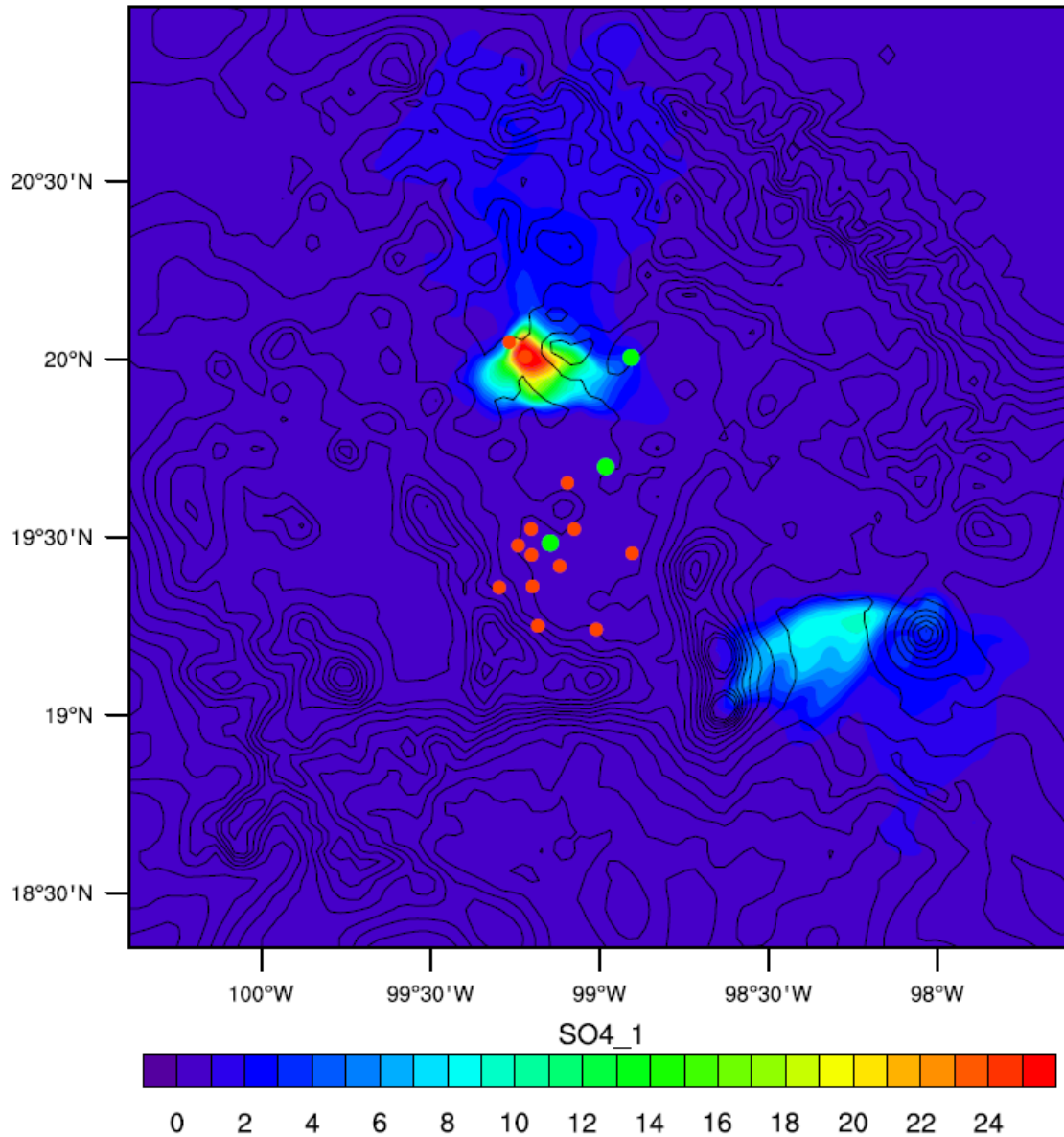
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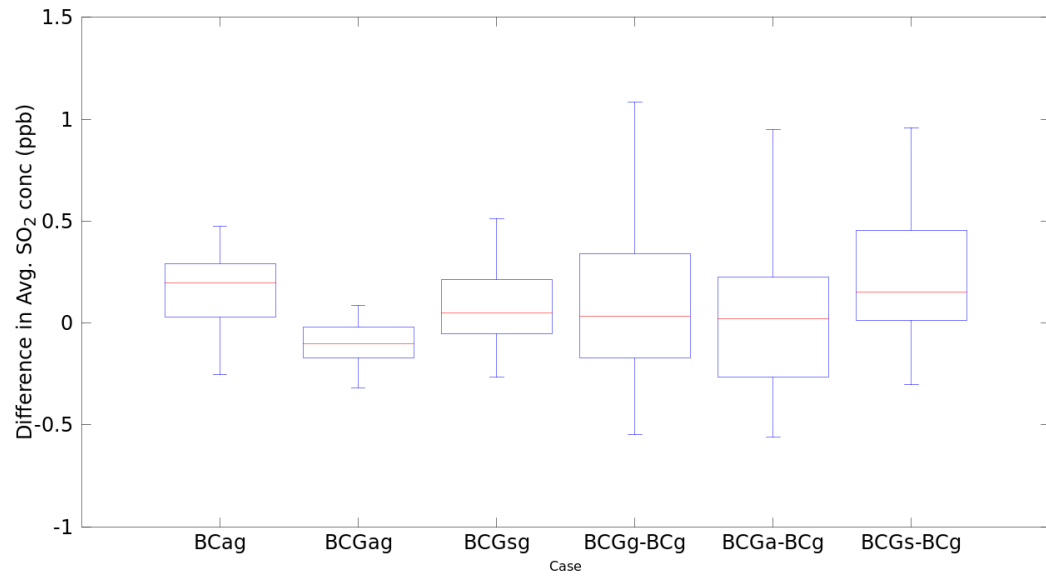
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3 **Figure 2. Boxplot of differences in the average SO$_2$ concentration for the considered**
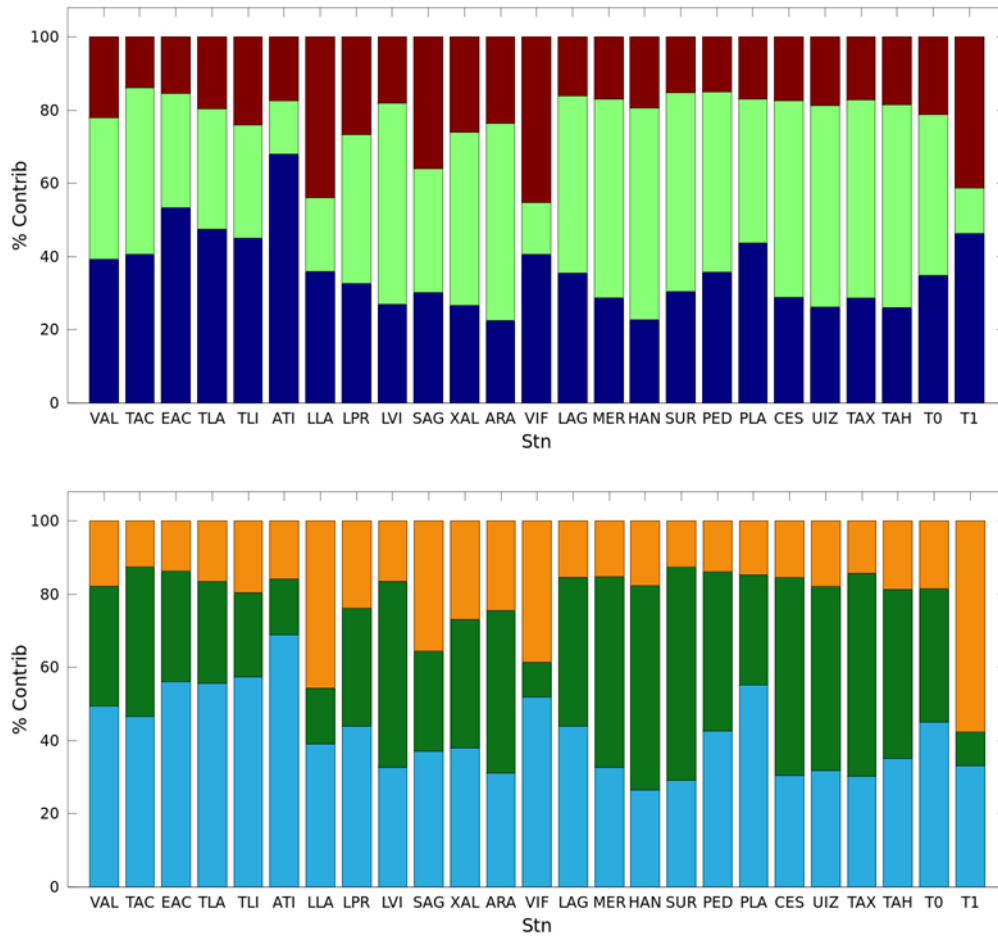4 **simulation cases.**
5
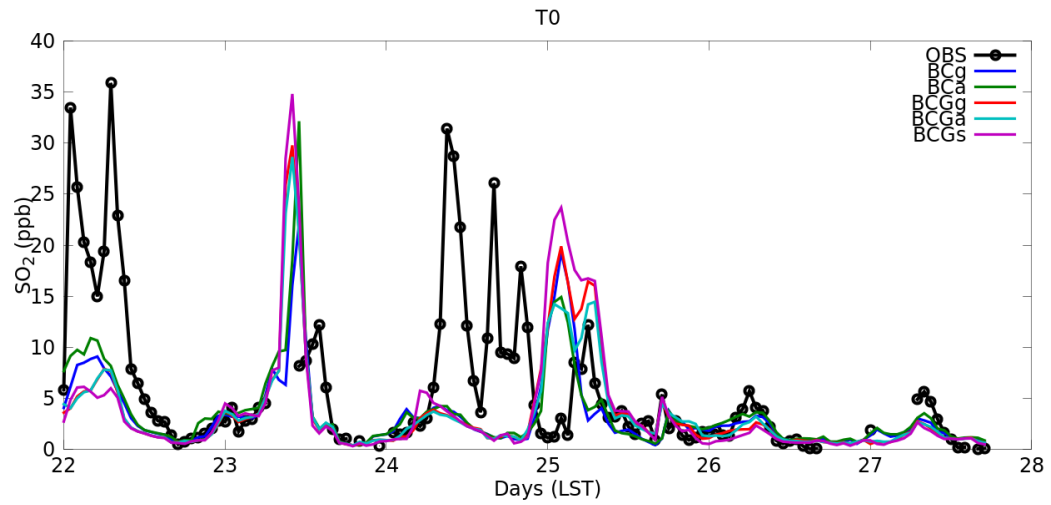
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2 **Figure 3. Time series of SO₂ concentration at T0 for the simulation cases considering**
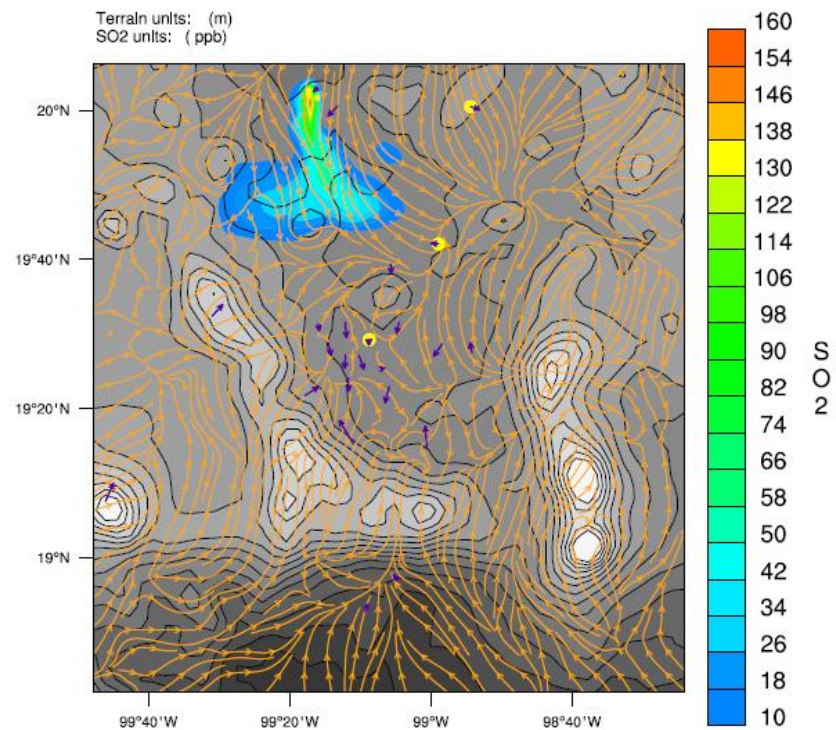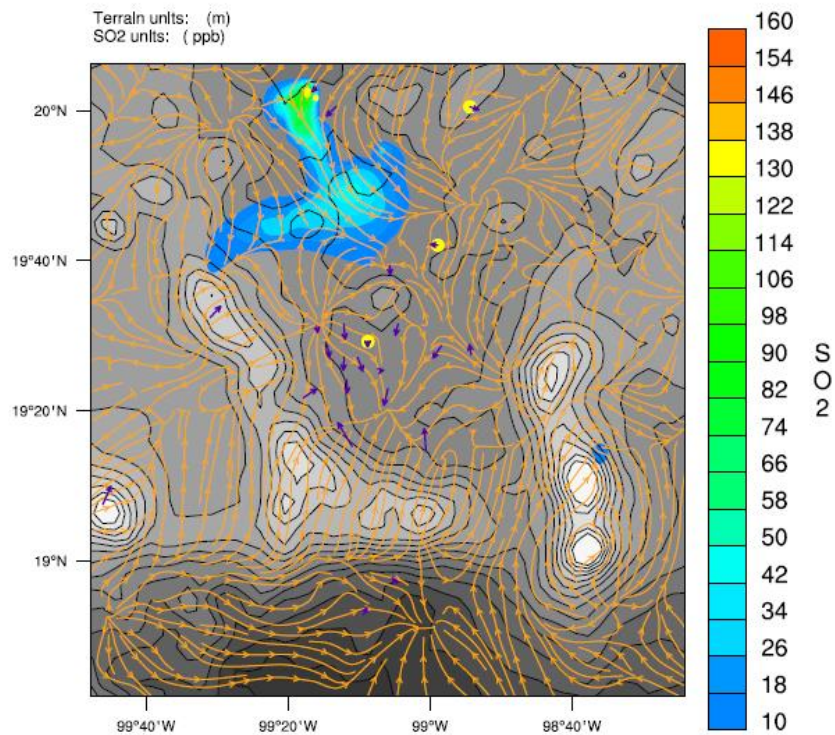3 **the aerosol phase.**
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Terrain units: (m)
SO4 units: (ug / m3)

SO4_1

Figure 4. PM₁ Sulfate concentration on 26 March at 16:00 LST after considering the direct and indirect aerosol effects. Monitoring sites (red dots); MILAGRO supersites (green dots).
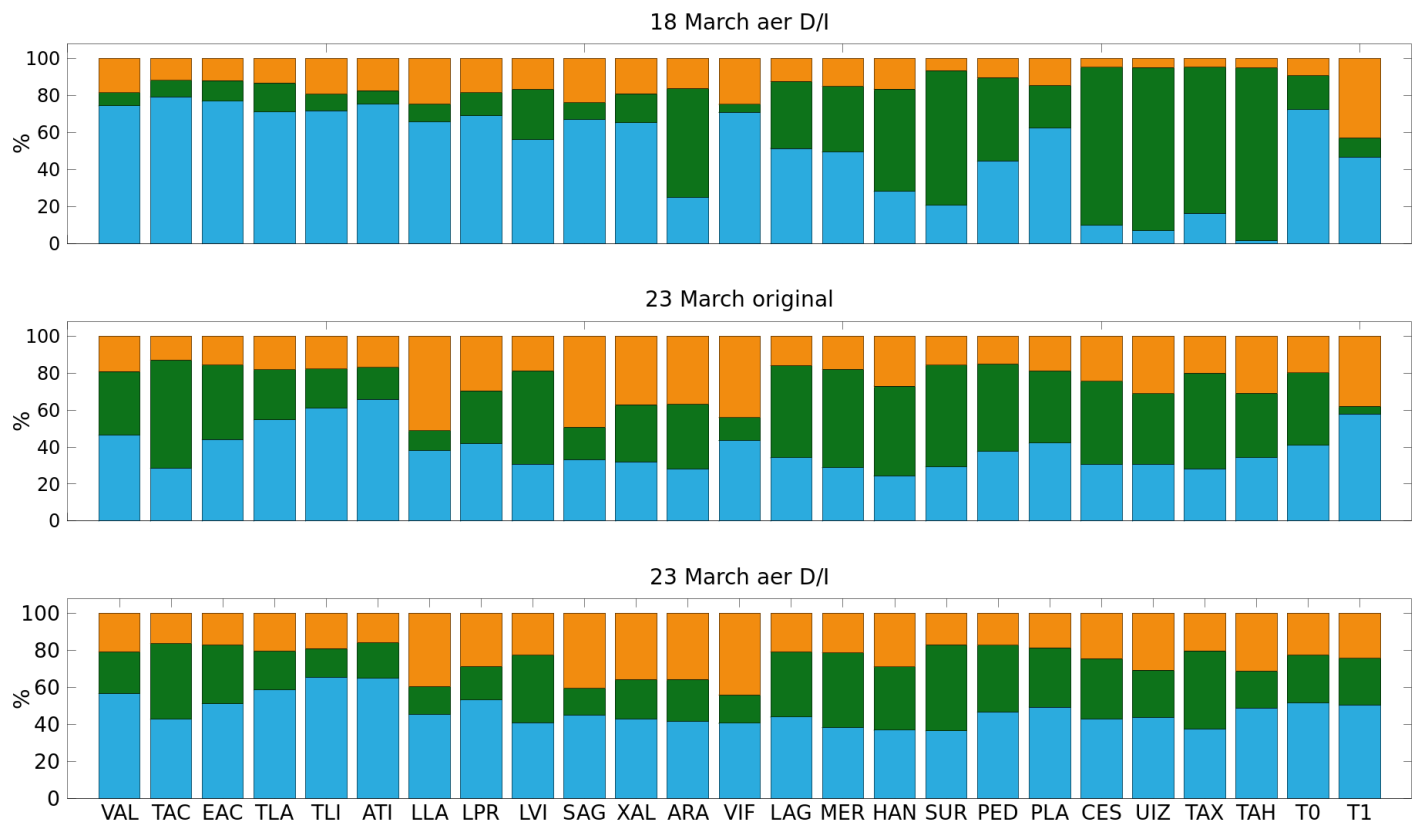
Figure 5. Contribution of TIC, MCMA and cement plants on average SO₂ concentration. Original results (top panel) and after including the aerosol chemistry with direct/indirect effects (bottom panel).

**Figure 6. Model convergence zone that prevented the transport to the south on 24 March at 17:00 LST: simulation with aerosol phase plus direct and indirect effect (left panel); original results with gas phase (right panel). These plots show the streamlines (orange), and the wind vectors of some monitoring stations (purple). The filled circles denote supersites location (yellow).**

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2 **Figure 7. Contribution of TIC, MCMA and cement plants on average SO₂ concentration for 18 March.**

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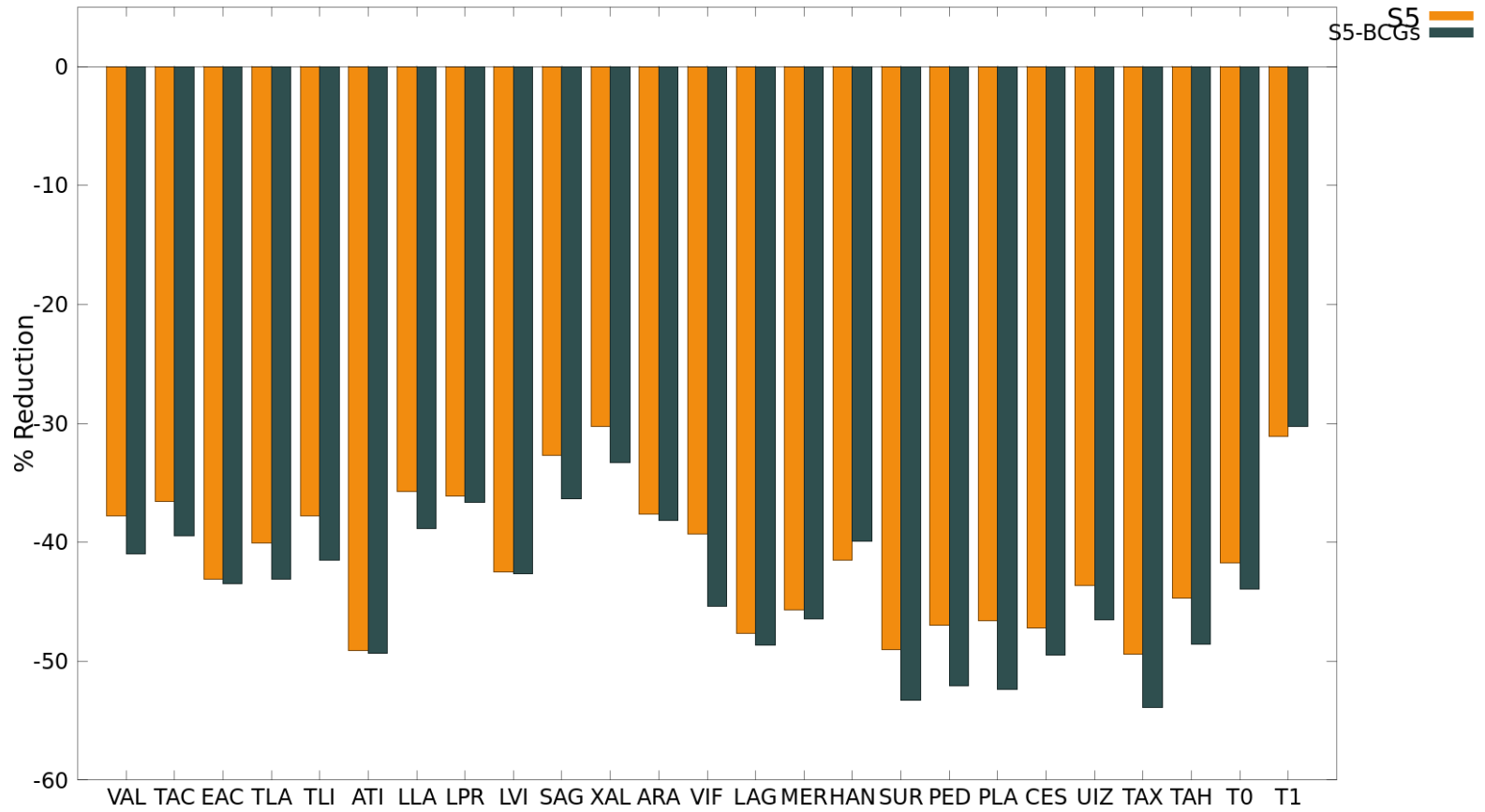
Figure 8. Reduction scenario S5 after the inclusion of the aerosol phase (dark green) compared with the original results (orange).

Terrain units: (m)
Ozone units: (ppb)

Terrain units: (m)
Ozone units: (ppb)

O3

O3
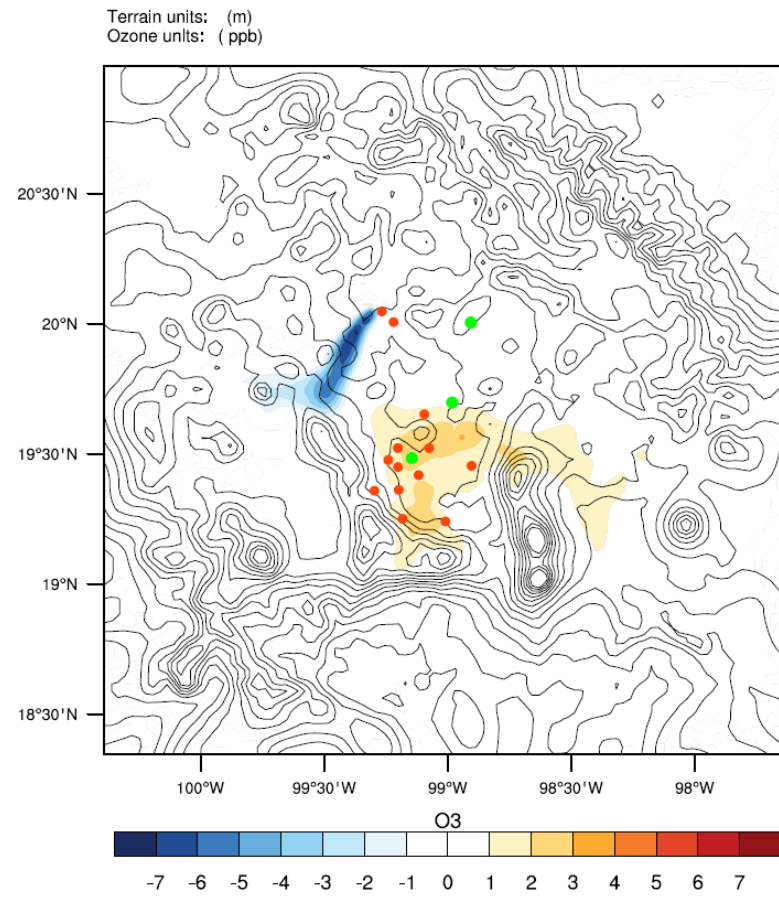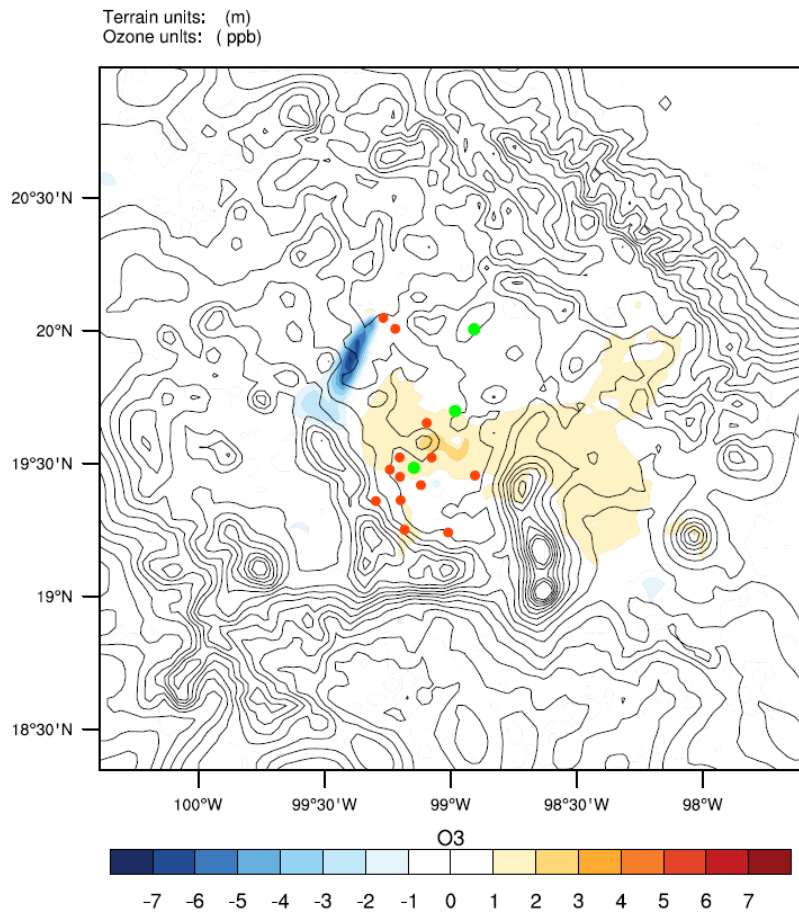
Figure 9. Ozone plume from TIC-generated precursors on 25 March at 20:00 LST. Baseline case for gas phase using Dudhia scheme (left); Baseline case for gas phase using Goddard scheme (right).

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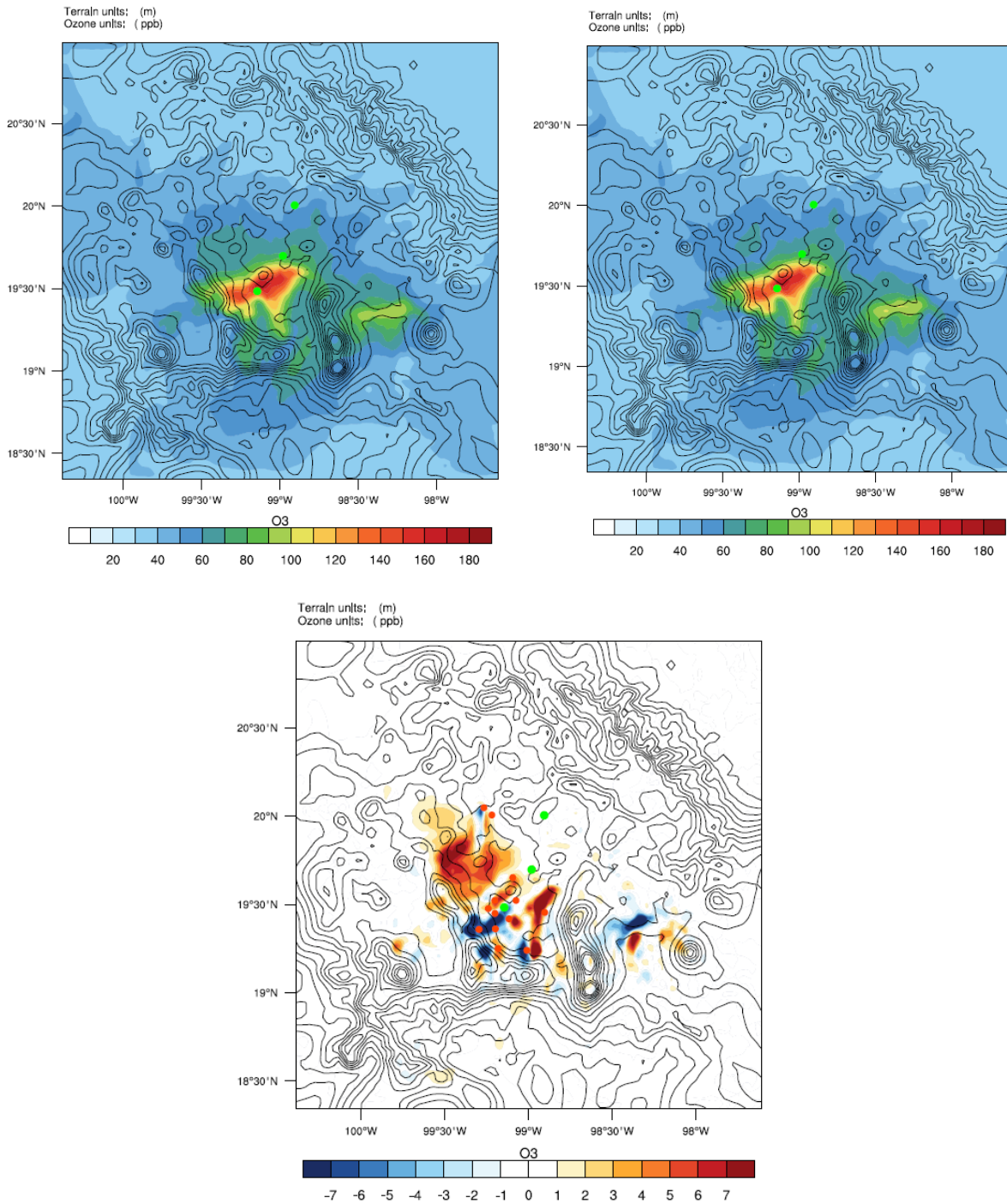
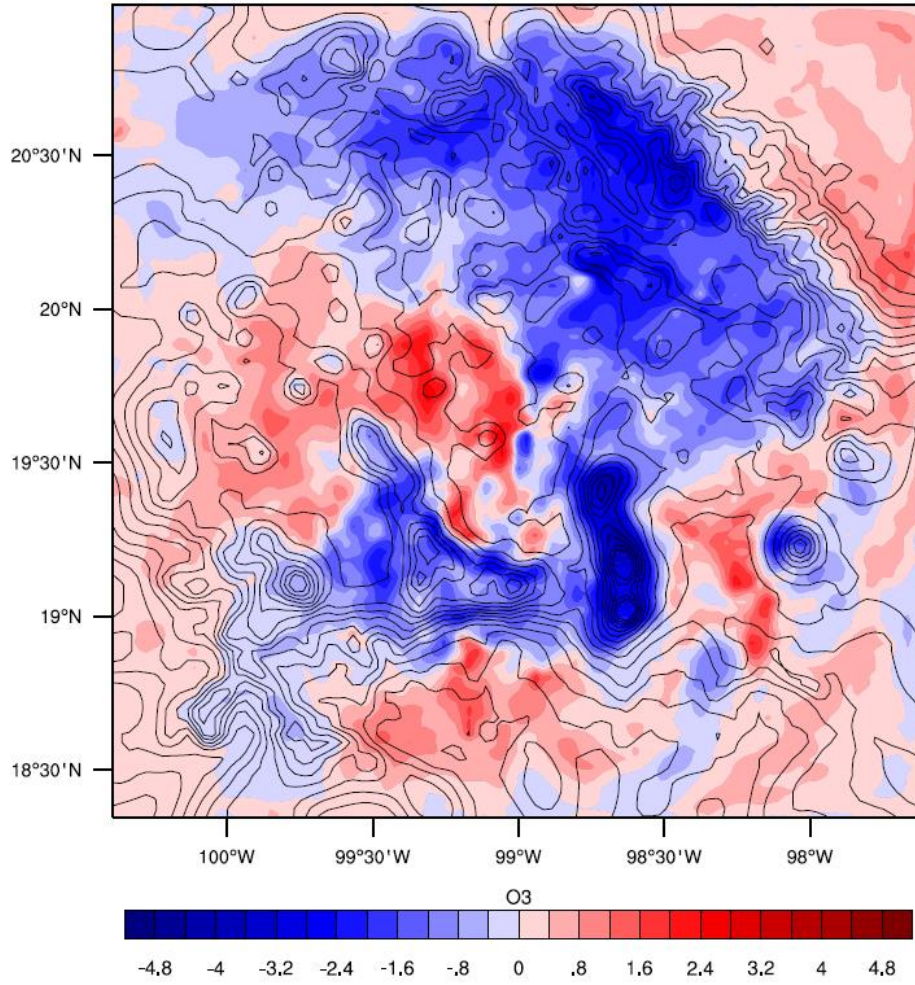Figure 10. Ozone plume from TIC-generated precursors after including the aerosol
phase plus the direct and indirect effects on 24 March at 15:00 LST. Baseline case
including all the anthropogenic sources (left); Simulation case with all the
anthropogenic sources but the TIC (right); Difference of concentration fields
(bottom).

Figure 11. Difference of the total average concentration for the entire simulation period.
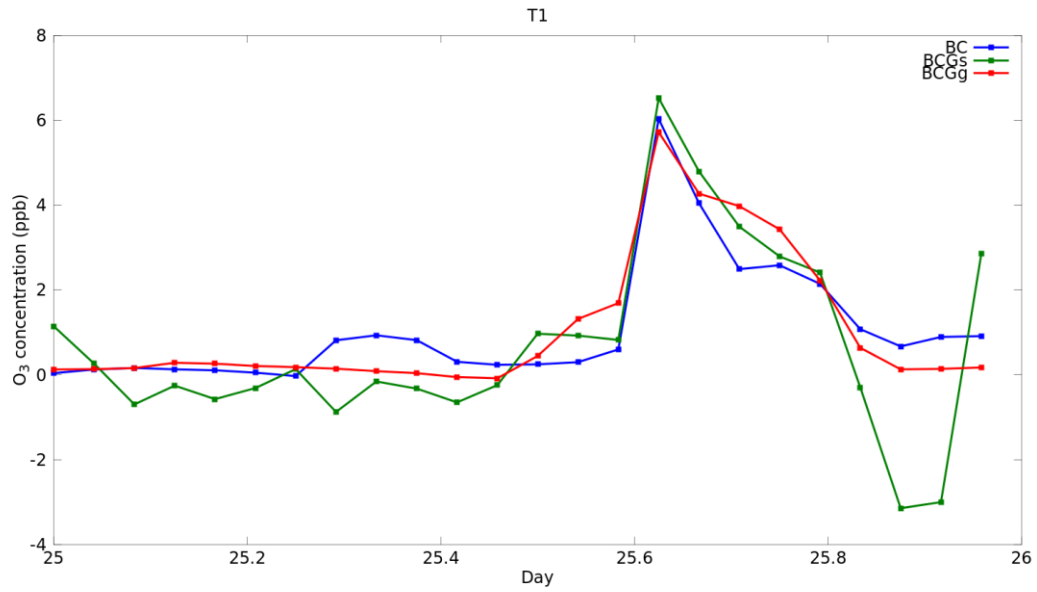
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2 **Figure 12. Ozone concentration on 25 March at T1. Original Baseline case with gas**
3 **phase (blue); Baseline case with Goddard scheme for gas phase (red); Baseline case**
4 **with Goddard scheme including the aerosol phase plus direct and indirect effects**
5 **(green).**
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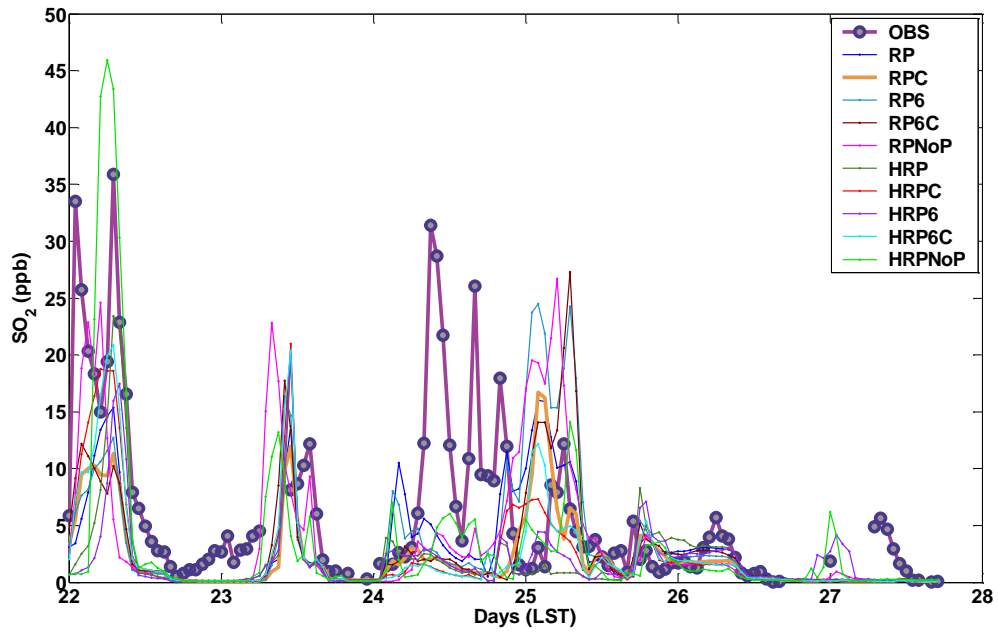
Figure 13. SO₂ time series at T0 supersite for each configuration of the sensitivity cases. RPC results are in gold.

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