

Supplementary Information (SI)

Tables:

SI-Table 1: Trace gas and aerosol total emission rates (Tons/day) over two modeling domains considered in this study.

Species	Coarse Domain ⁽³⁾	Fine Domain ⁽⁴⁾
CO ⁽¹⁾	17 411	8 889
NOx ⁽¹⁾	3 081	1 094
PM _{2.5} ⁽¹⁾	806	111
Anthropogenic VOC ⁽¹⁾	8 223	2 262
Isoprene ⁽²⁾	27 390	1 085
Monoterpenes ⁽²⁾	3 660	34

⁽¹⁾ Anthropogenic emissions from combined MCMA 2002 urban inventory and NEI 1999 regional inventory as described in Section 3.3.2. Stack industrial emissions (e.g. Tula) are included here.

⁽²⁾ Biogenic emissions as predicted by the MEGAN model (see Section 3.3.3). Values given here correspond to daily average emissions calculated for 11 March 2006.

⁽³⁾ Total emissions over the CHIMERE coarse-scale domain ranging between 115.4-82.2°W and 9.9-30.1°N.

⁽⁴⁾ Total emissions over the CHIMERE fine-scale domain ranging between 101.1-98.3°W and 18.6-21.1°N.

Figures

SI-Figure 1: Comparison of isoprene concentrations as observed by G1 airplane (black dots) and simulated by the CHIMERE model (red line) during the MILAGRO experiment.

SI-Figure 2: Time series (a) and diurnal profiles (b) of O_x (=O₃+NO₂) concentrations as observed by RAMA air quality stations (dotted line) and

simulated by the CHIMERE model (full line, BIO-EP run) from 4 to 30 March 2006. As in Figure 3, the variability among observations is denoted by gray shading and main statistical indicators for the comparison are also given (bias, RMSE and correlation). All 16 measurement locations that provide both ozone and NO₂ measurements have been considered for this comparison.

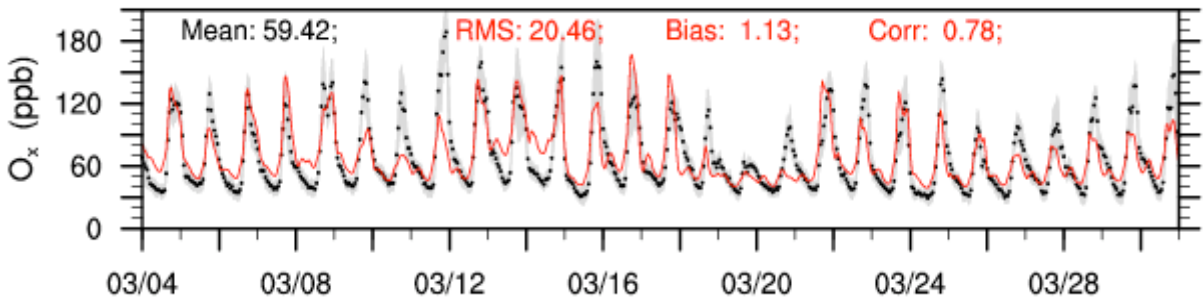
SI-Figure 3: Time series of O₃, NO₂, CO and O_x (=O₃+NO₂) concentrations as observed at the Lagunilla station of the RAMA monitoring network (dotted line) and simulated by the CHIMERE model (full line) from 4 to 30 March 2006. Statistical indicators for the comparison are indicated (bias, RMSE and correlation coefficient). The Lagunilla station is located 5km south of the T0 monitoring site, and is assumed here as representative of the conditions found at T0 site.

SI-Figure 4: Time series of O₃, NO₂, CO and O_x (=O₃+NO₂) concentrations as observed at the T1 site (dotted line) and simulated by the CHIMERE model (full line) from 10 to 30 March 2006. Statistical indicators for the comparison are indicated (bias, RMSE and correlation coefficient). Data for T1 is courtesy to L.G. Huey.

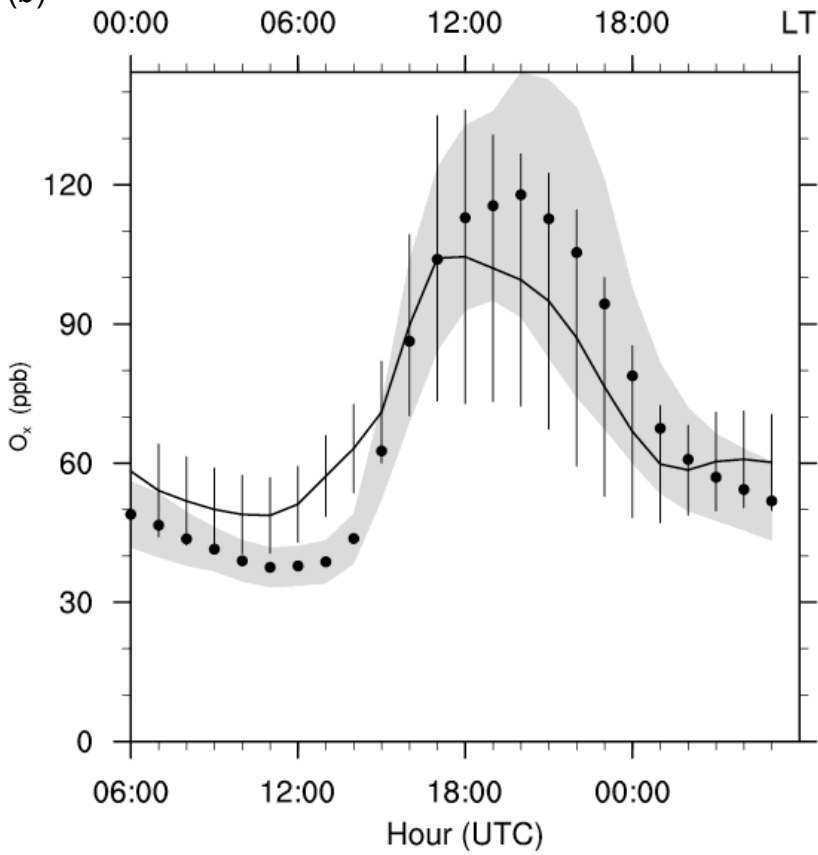
SI-Figure 5: Observed and predicted average diurnal profiles of oxygenated organic aerosol (OOA) at T0 for the available MILAGRO dataset. Similar to Figure 7, black dots and shaded area represent the observations associated with their variability, the red solid line and red vertical bars indicate the ANT-T model run. The blue line represents the aerosol fraction of the total oxygenated organic material that is present on the particle phase.

(a)

Mexico-City: average among RAMA stations

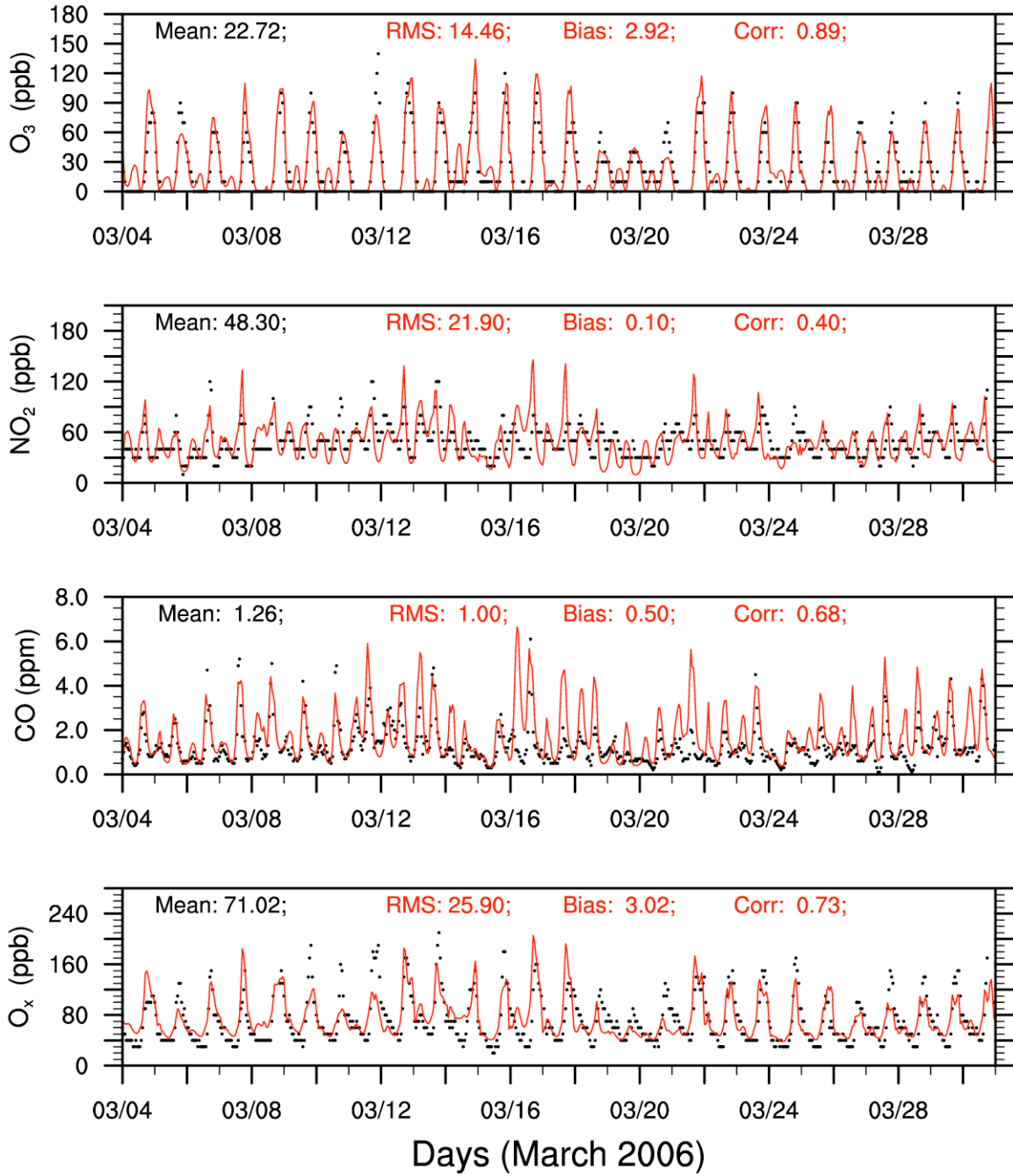


(b)



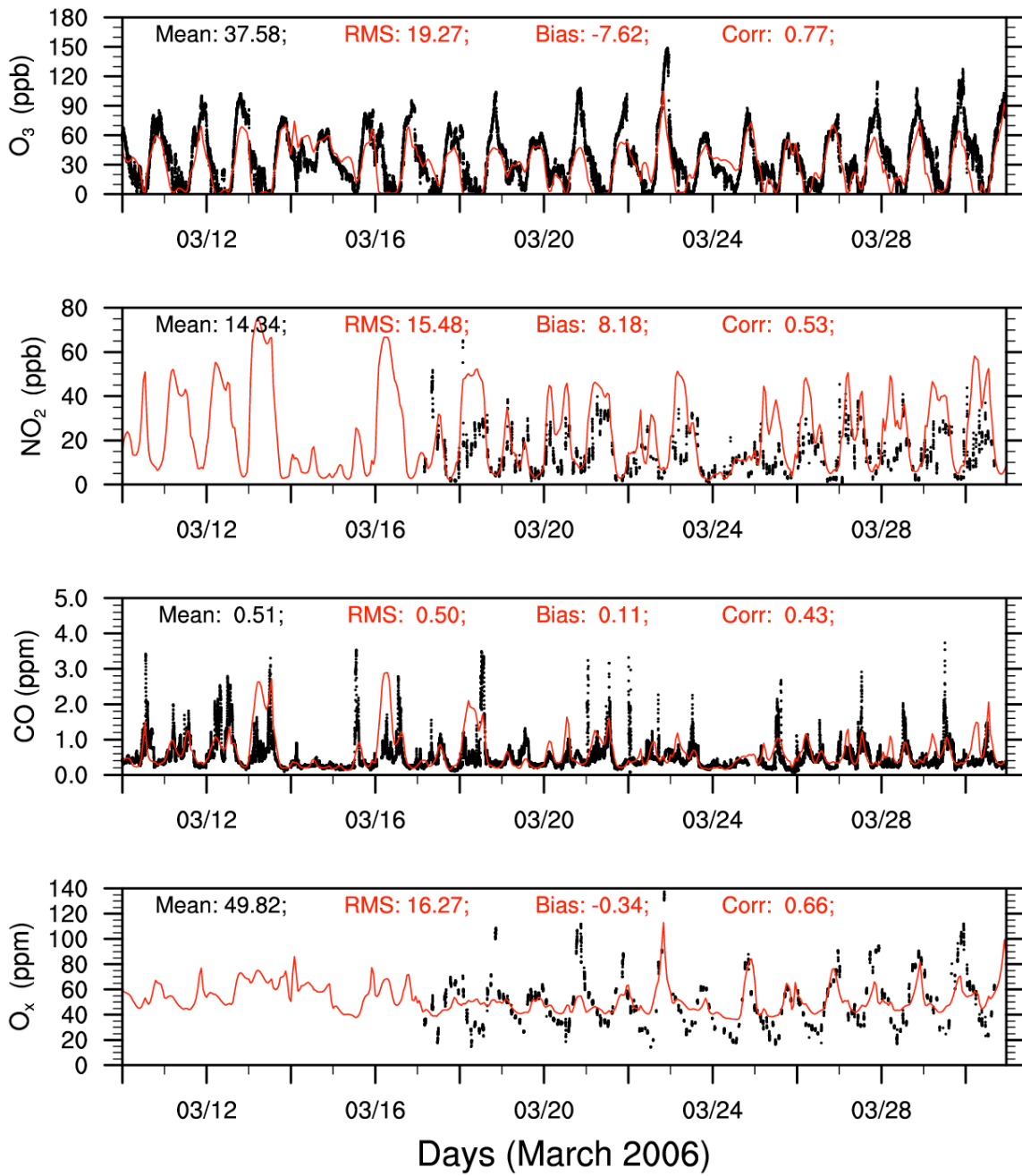
SI-Figure 2

Mexico-City LAGUNILLA: 19.44N / 99.14W

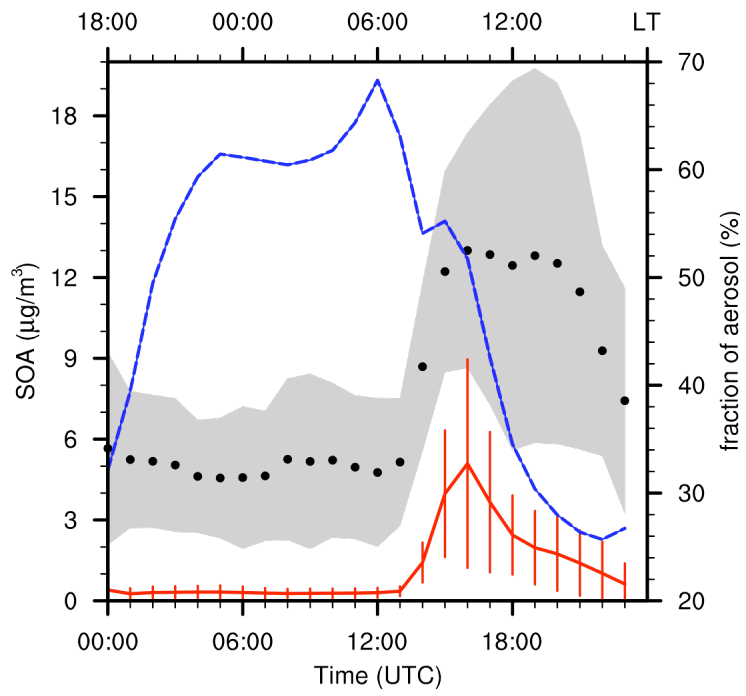


SI-Figure 3

a) Mexico-City T1: 19.703N,-98.982W



SI-Figure 4



SI-Figure 5