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Supplement of

Photochemical grid model implementation and application of VOC, NO_x, and O_3 source apportionment

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The ISAM instrument with CMAQv5.0.2 was released on Jun 10, 2014 on UNC Chapel Hill's Community Modeling & Analysis System (CMAS) website www.cmascenter.org

ISAM documentation about input requirements, specifications of users options, and setup of run case examples is available at http://www.airqualitymodeling.org/cmaqwiki/index.php?title=CMAQv5.0.2_Integrated_Source_Apportionment

Organization of Supporting Information

1) Additional methodology related to the photochemical grid model application

2) Additional Figures

Additional methodology related to the photochemical grid model application

The CMAQ model was applied from June 28 to July 5, 2007 for a domain covering the State of California (CA) using 12 km sized grid cells (79 columns and 106 rows) and 24 vertical layers extending to the surface (layer 1 height ~20 meters) to the model top of 50 mb. Meteorological inputs to CMAQ were generated using the Weather Research and Forecasting model (WRF), Advanced Research WRF core (ARW) model version 3.1 (Skamarock et al., 2008). The WRF domain uses the exact same grid projection (Lambert Conformal), grid origins, and datum as CMAQ. However, the WRF 12 km domain covers the continental U.S. so data used for the CMAQ simulation is a sub-set of the WRF simulation. Additionally, WRF used 34 vertical layers to represent the atmosphere to 50 mb so some layer collapsing was done when generating CMAQ inputs. Layers are matched one-to-one nearest the surface to best represent diurnal changes in the height of the boundary layer. Selected physics options, input analysis, grid structure, and evaluation are provided in detail elsewhere (U.S. Environmental Protection Agency, 2011).

The 12 km model domain was nested in a 36 km continental domain, and boundary inflow to the 36 km domain were based on spatially and temporally variant concentration data from a 2007 year-specific annual GEOS-Chem version 8-03-02 simulation (Yantosca, 2004). The GEOS-CHEM simulation had a grid resolution of 2.0 by 2.5 degrees using a latitude-longitude grid projection. The troposphere and stratosphere were vertically resolved with 47 vertical layers. GEOS-CHEM output was used to generate space and time (3-hourly) variant boundary conditions and initial conditions for CMAQ. Evaluation included comparison to model performance plots generated using a similar version of the model also applied for 2007 (Lam et al, 2010). Grid and chemical species translation of GEOS-CHEM to CMAQ was based on methods described in Henderson et al. (2014).

References

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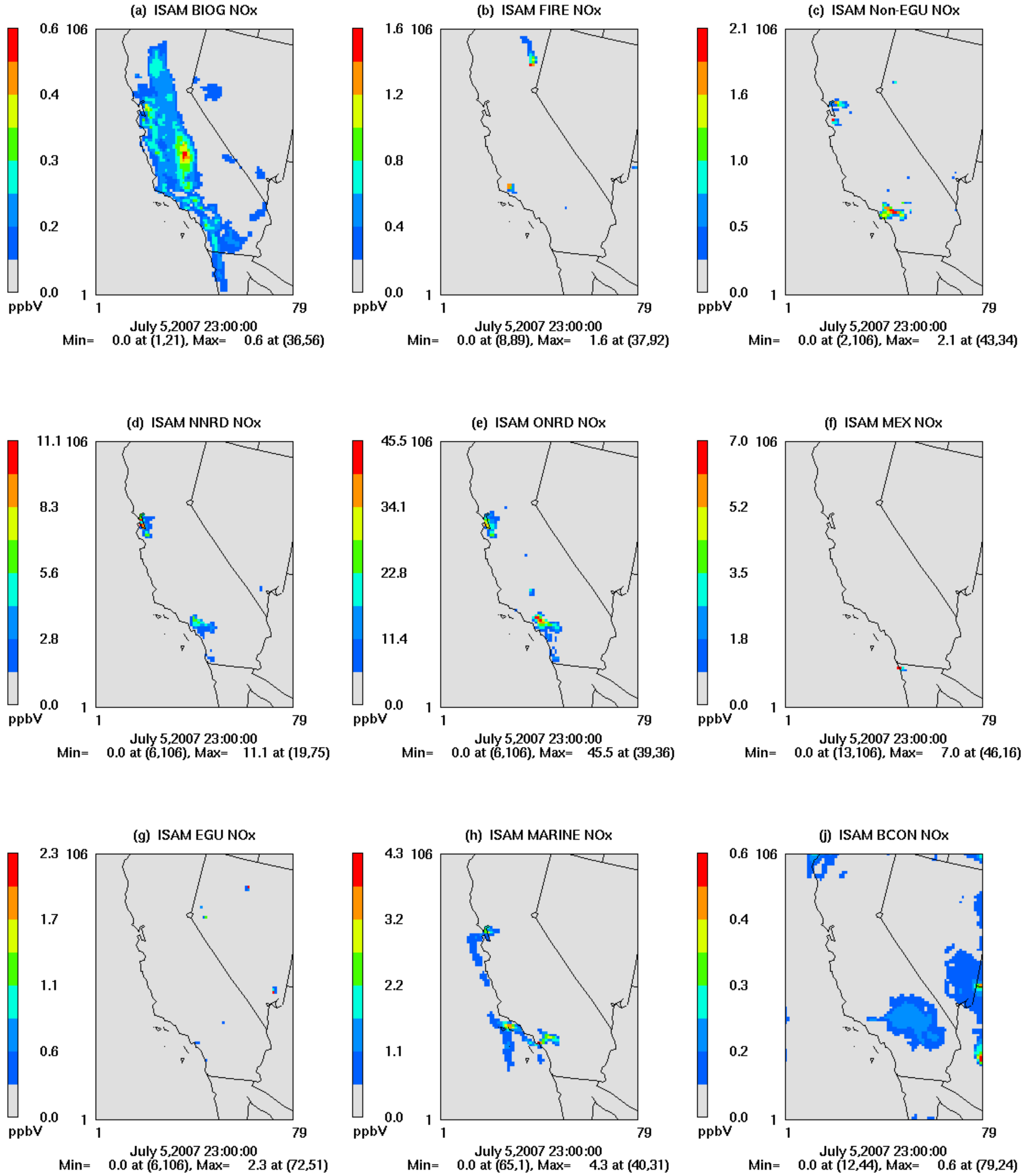
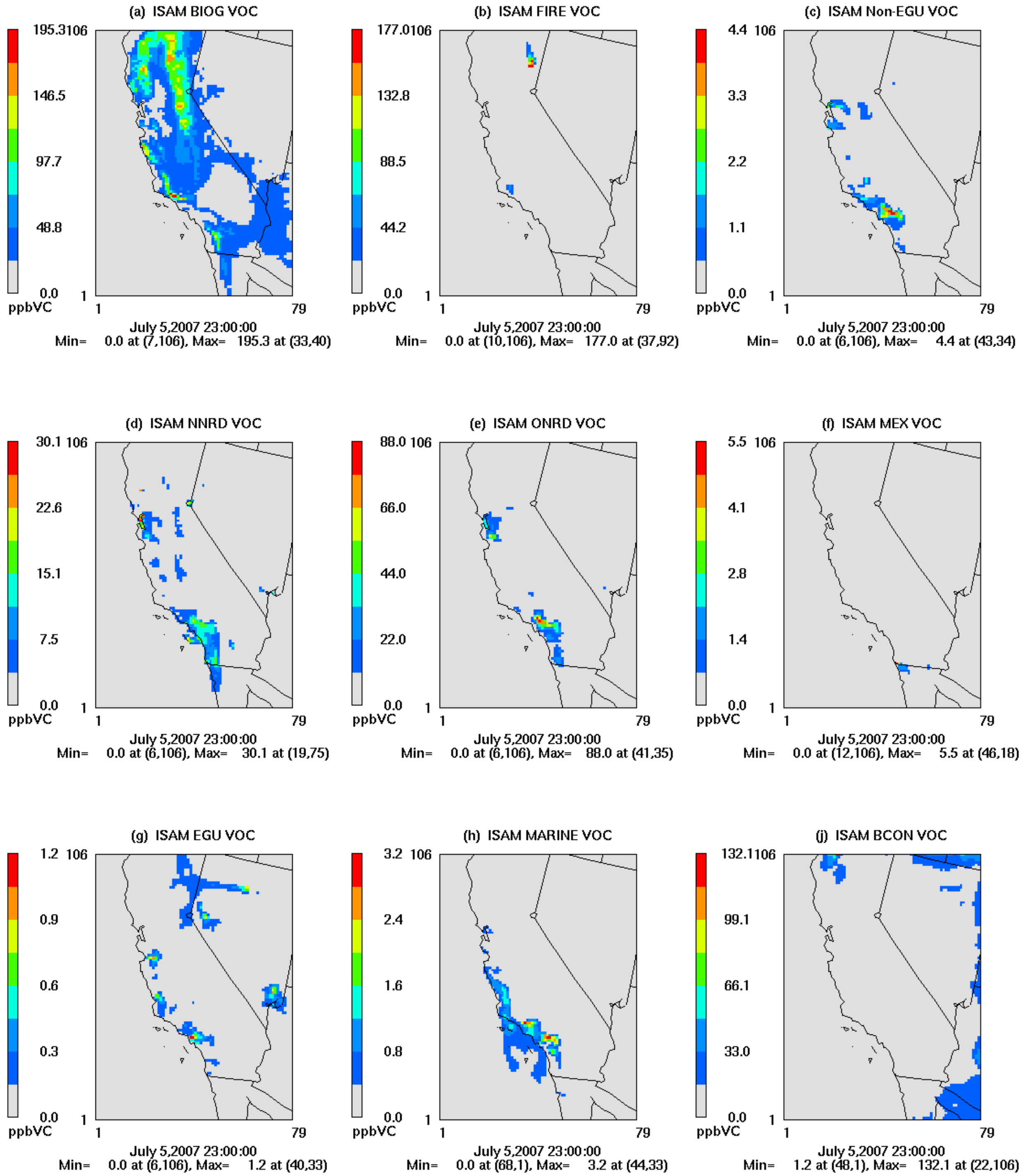
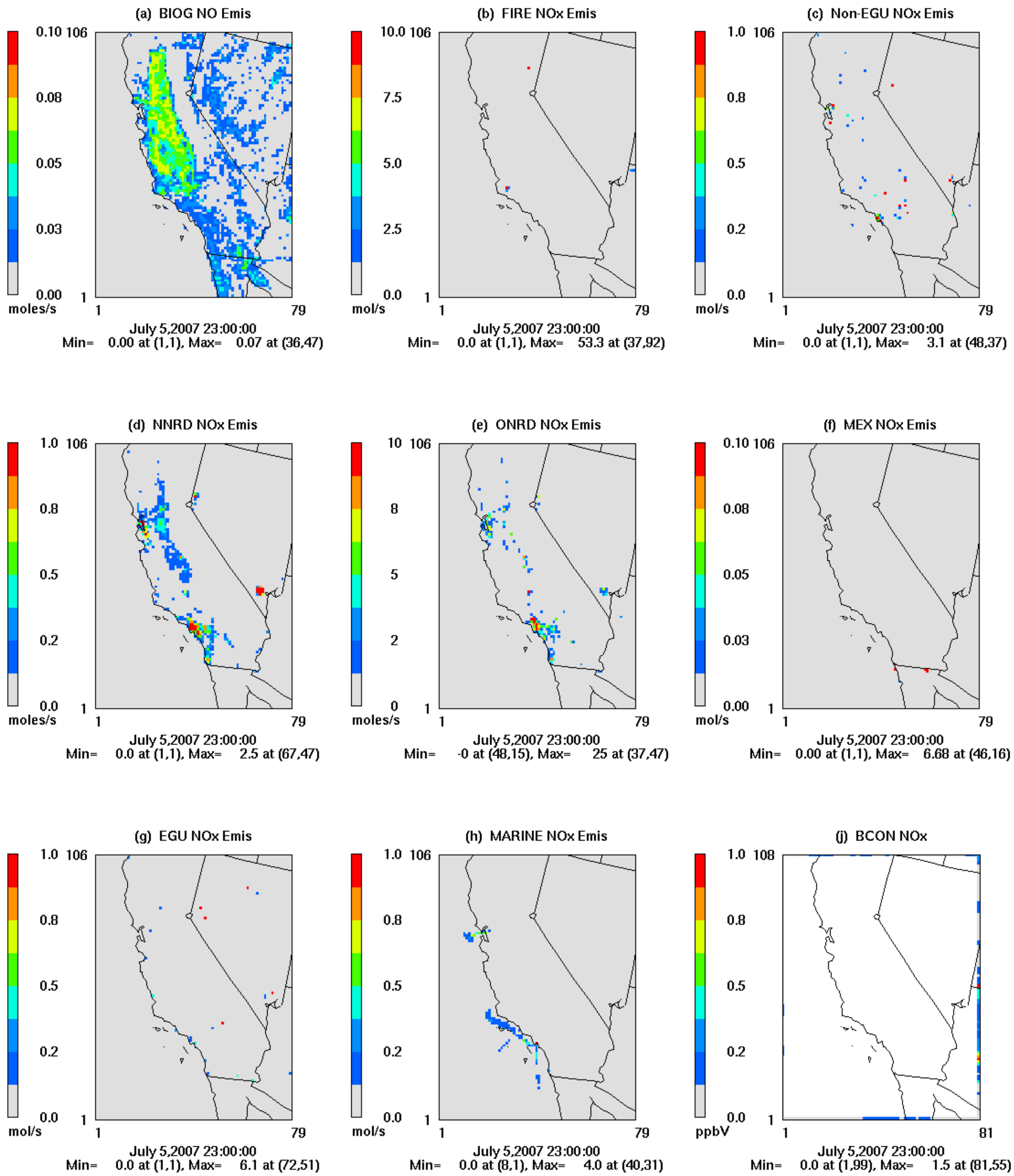


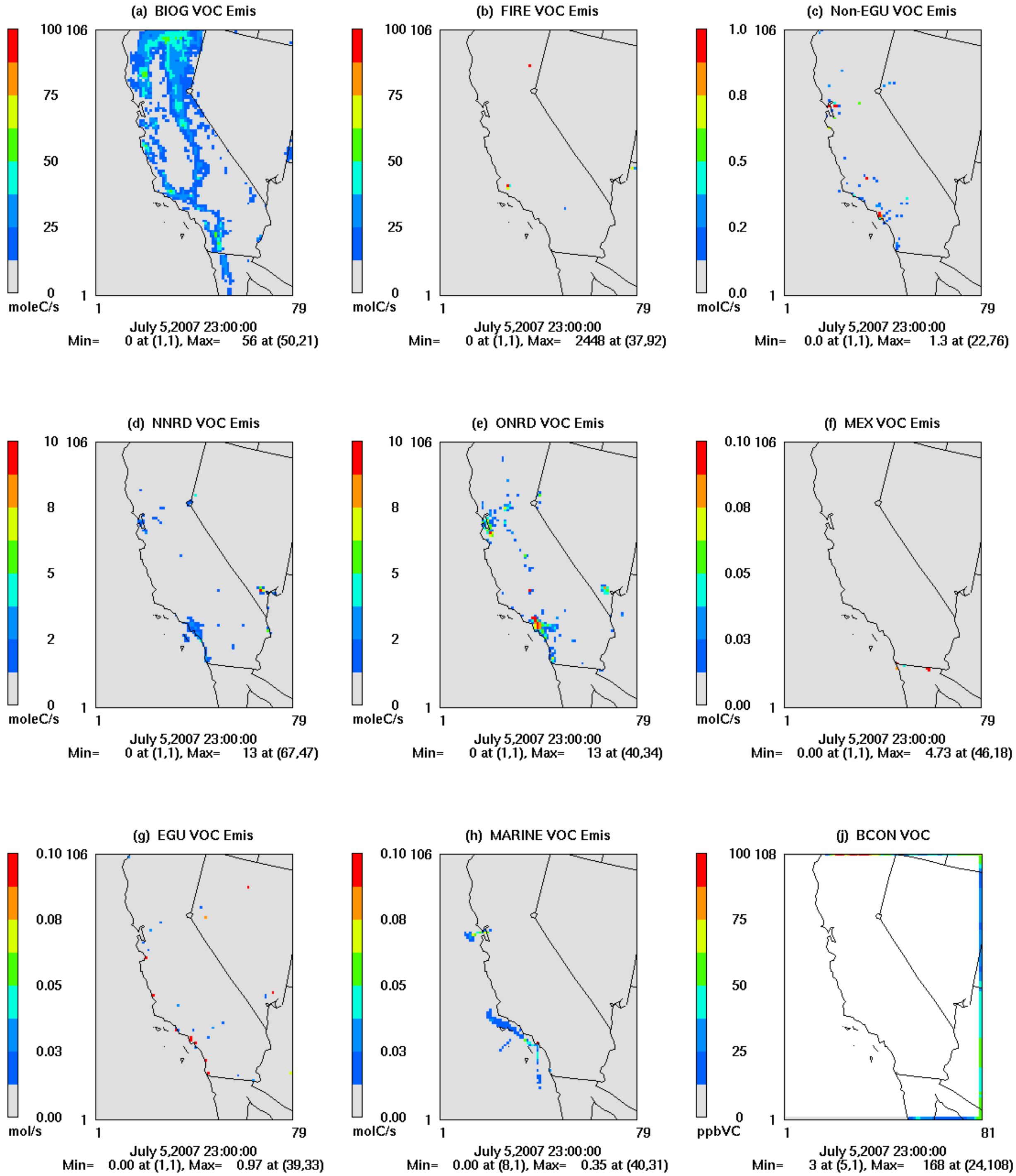
Supp. Figure 1. Spatial tiles of 9 source sectors contributing to ambient NOx, at 23UTC (16 PDT) July 5, 2007. (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generation units EGU, (h) marine MARINE, and (j) boundary conditions BCON. Note different scales across the tiles.



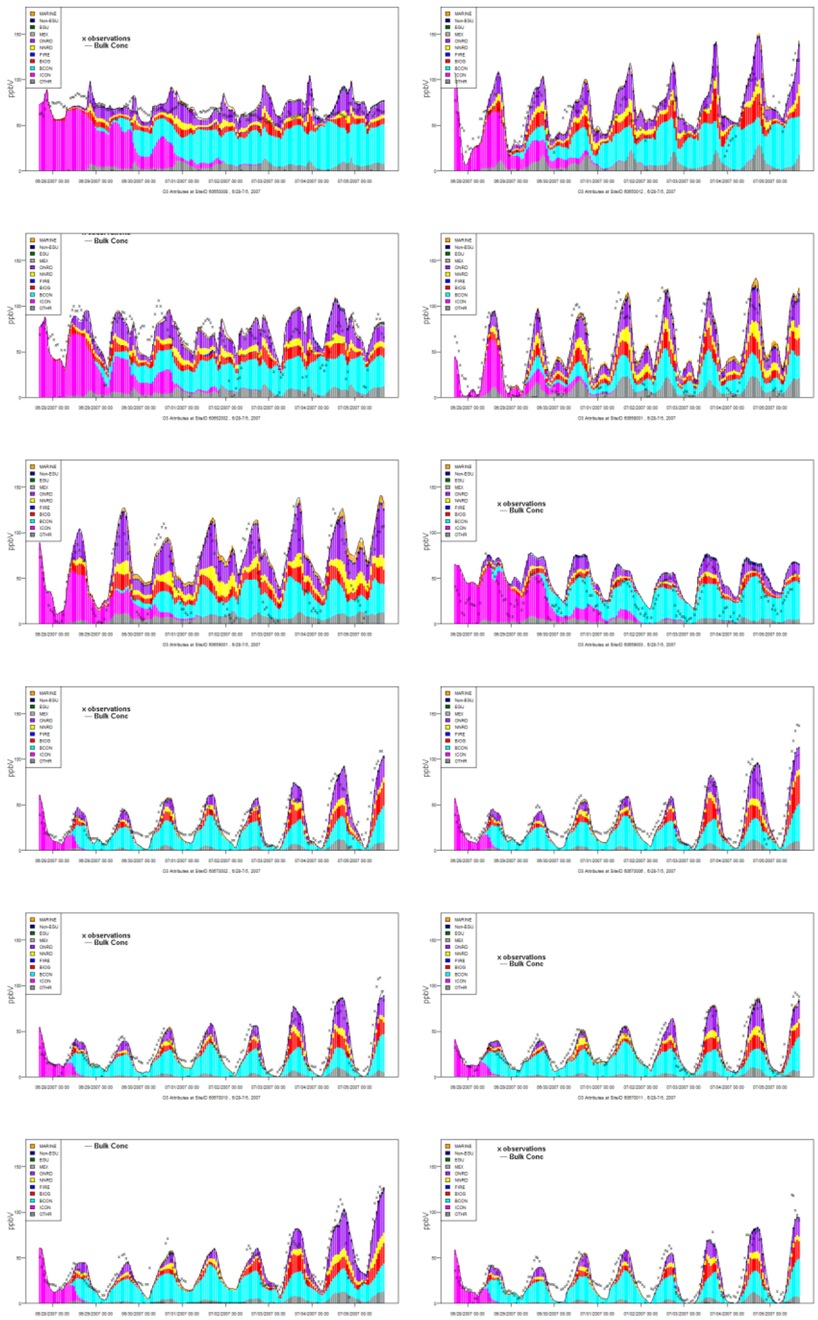
Supp Figure 2. Spatial tiles of 9 source sectors contributing to ambient VOC, at 23UTC (16 PDT) July 5, 2007. (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generation units EGU, (h) marine MARINE, and (j) boundary conditions BCON. Note different scales across the tiles.



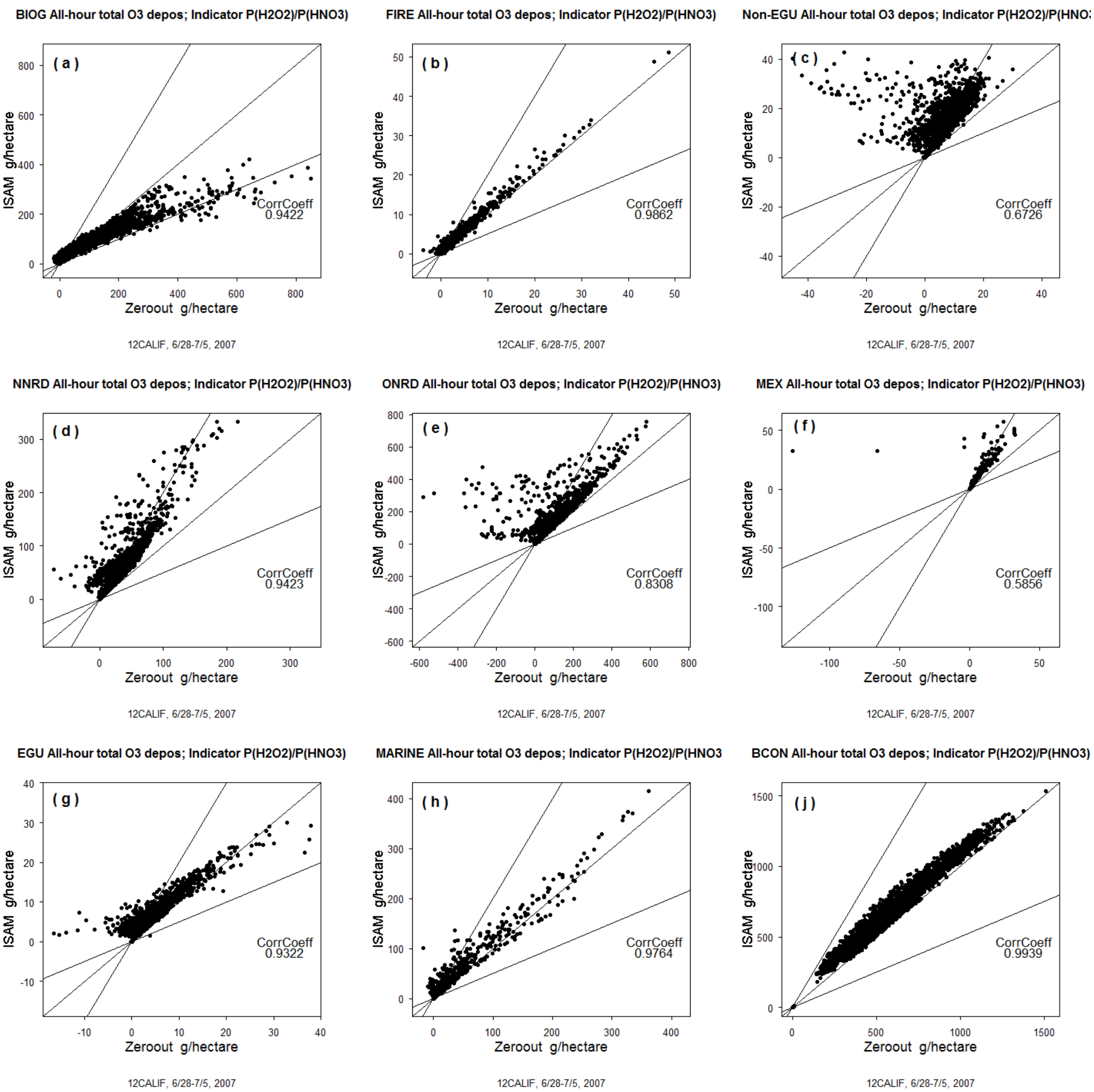
Supp Figure 3. Spatial tiles of NOx emissions and boundary condition sectors at 23UTC (16 PDT) July 5, 2007. (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generation units EGU, (h) marine MARINE, and (j) boundary conditions BCON. Note different scales across the tiles.



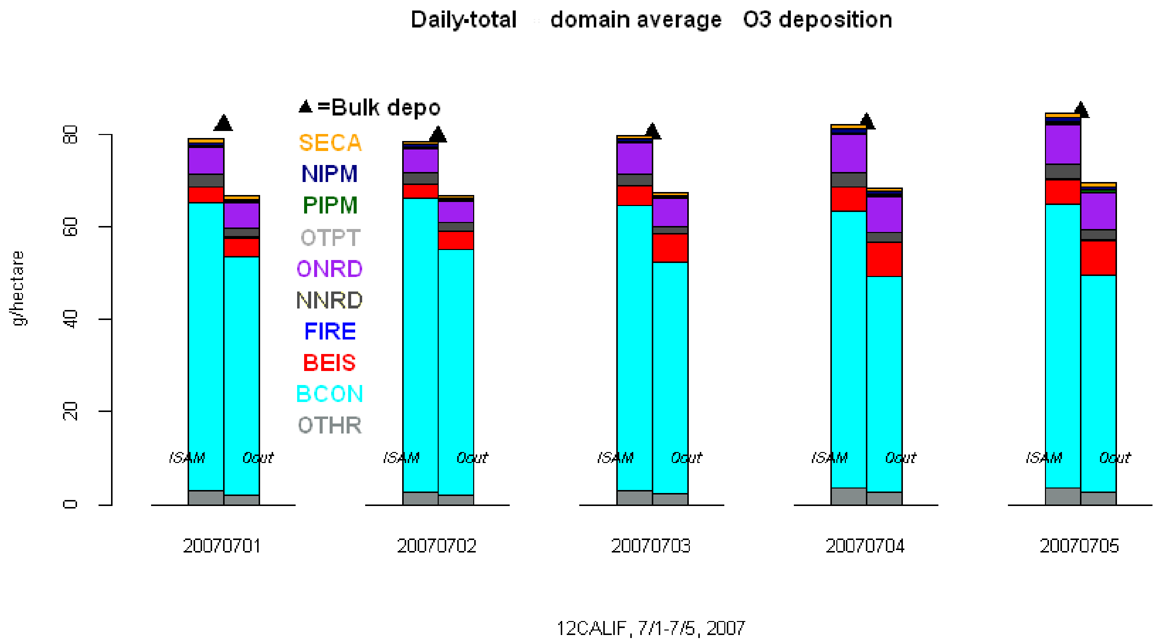
Supp Figure 4. Spatial tiles of VOC emissions and boundary condition sectors at 23UTC (16 PDT) July 5, 2007. (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generation units EGU, (h) marine MARINE, and (j) boundary conditions BCON. Note different scales across the tiles.



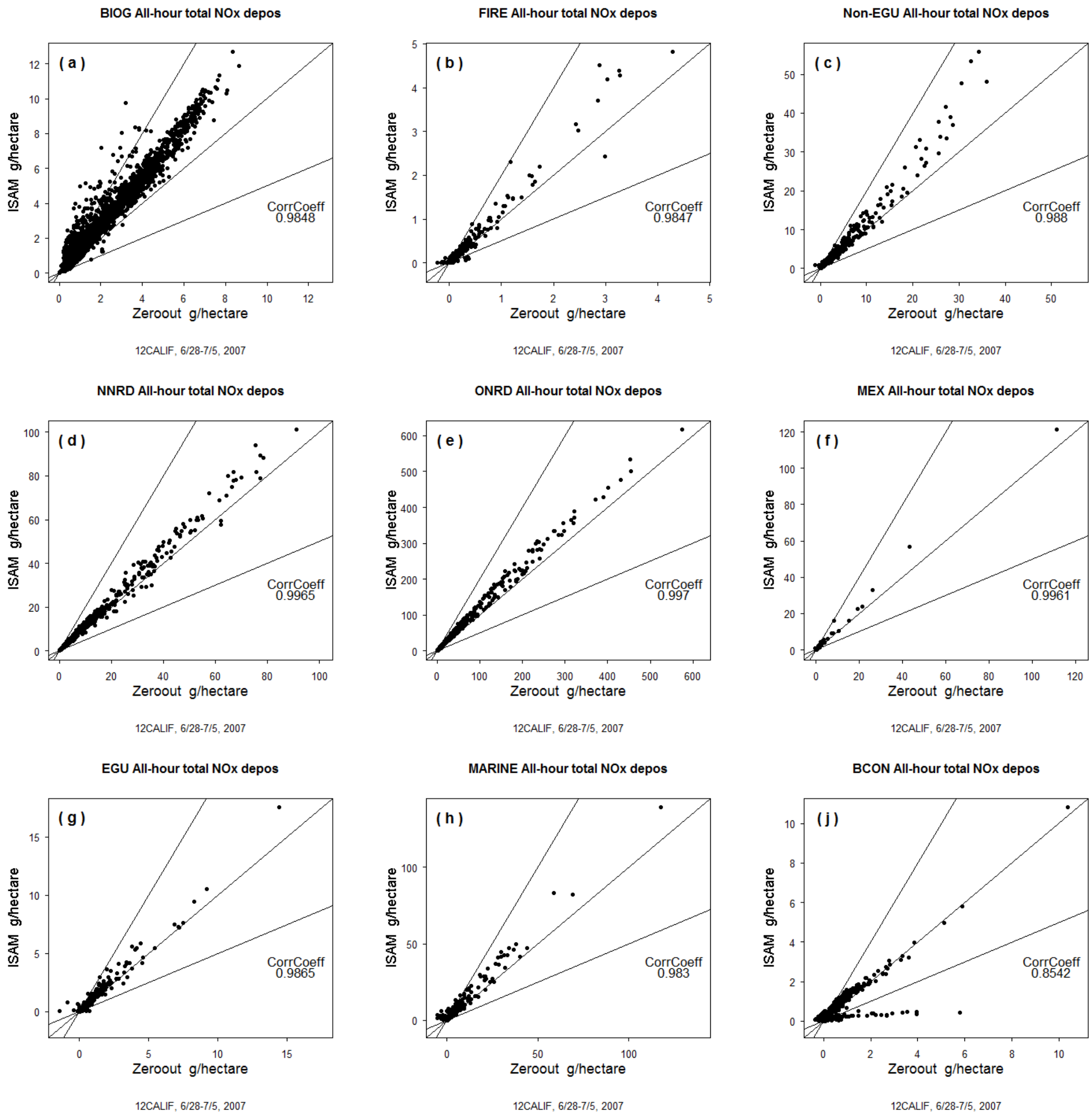
Supp Figure 5: Hourly time series of O3 observations (crosses) at sites of Californian Air Resources Board monitoring network; and the corresponding CMAQ-ISAM sector breakdowns (stacking colored bars). Locations are six distinct Riverside sites (top six panels) and six distinct Sacramento sites (bottom six panels). The colors represent sector sources: marine (MARINE orange), non-electricity generation units (Non-EGU deep blue), electricity generation units (EGU green), other point sources (MEX light grey), on-road mobile (ONRD purple), non-road mobile (NNRD yellow), wild fires (FIRE blue), biogenic (BIOG red), boundary conditions (BCON cyan), initial conditions (ICON magenta), and remaining unspecified emissions (OTHR grey). The solid black trace on top of the bars denotes the modeled bulk O3 concentration.



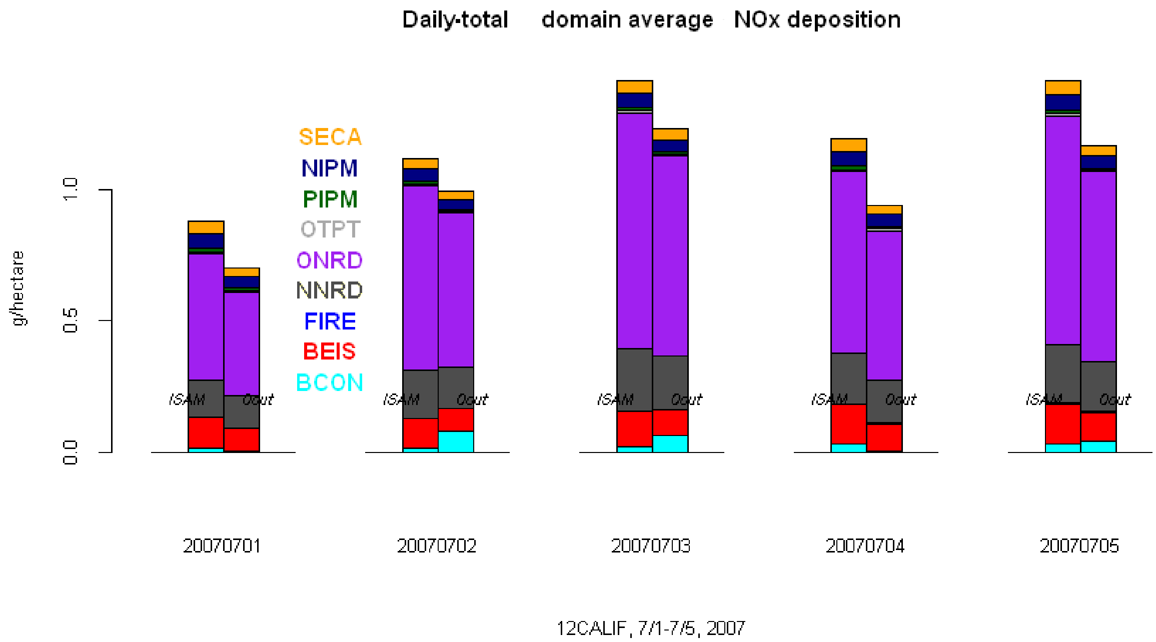
Supp Figure 6. ISAM/Both-out scatter plots of all-hour total O3 deposition for each sector. The sectors are: (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generating units EGU, (h) marine MARINE, and (j) boundary conditions BCON.



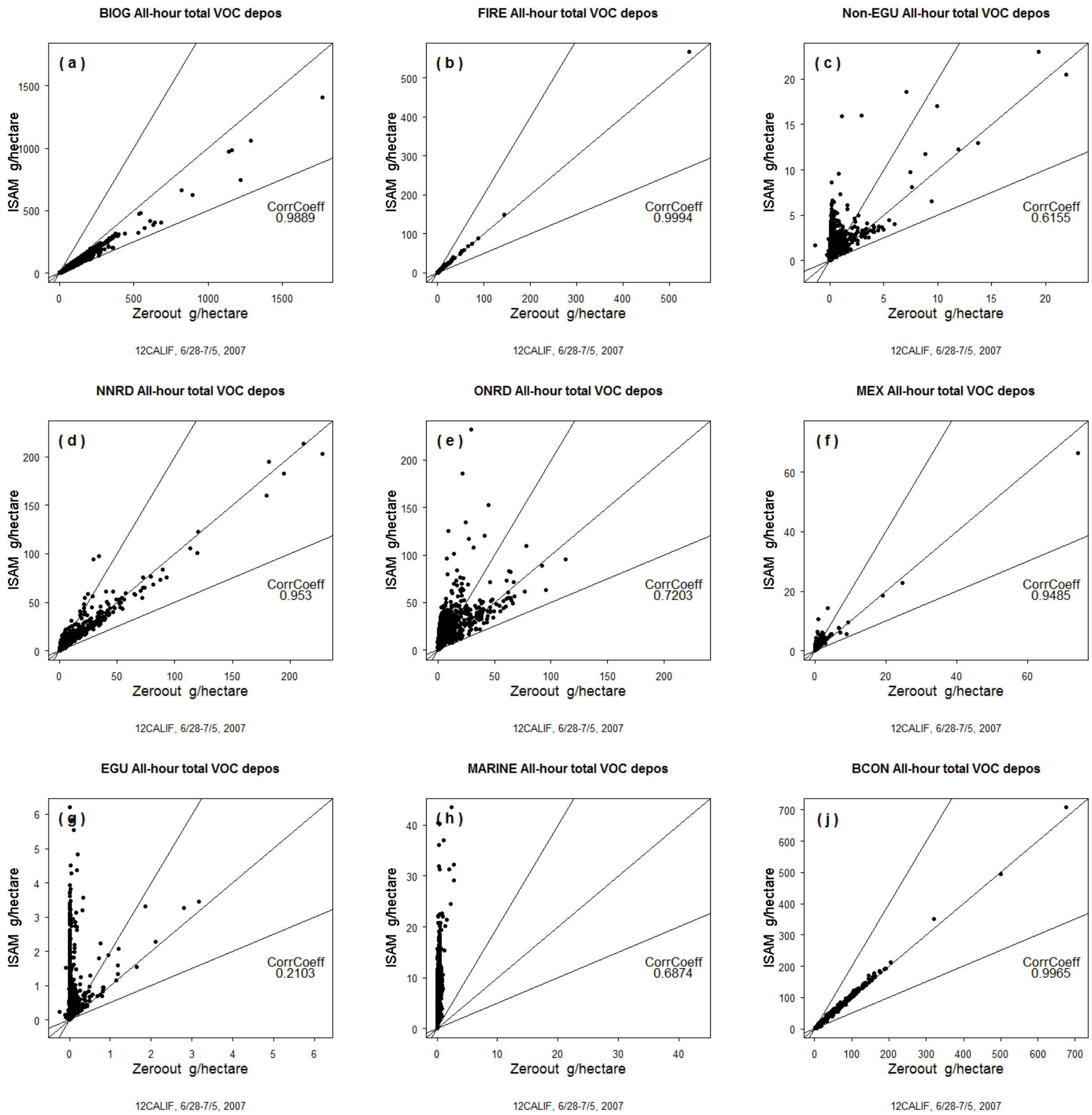
Supp Figure 7. Daily-total, domain-averaged O3 deposition (dry+wet), July 1-5, 2007. In the bar plot, each day consists of a pair of stacked columns (ISAM on the left; zero-out total on the right) and above them a black triangle designating bulk total deposition calculated from regular CMAQ. The colors represent sector sources: marine (MARINE orange), non-electricity generation units (NON-EGU deep blue), electricity generation units (EGU green), Mexican point sources (MEX light grey), on-road mobile (ONRD purple), non-road mobile (NNRD yellow), wild fires (FIRE blue), BIOG3 vegetations (BIOG red), boundary conditions (BCON cyan), and remaining unspecified emissions (OTHR grey).



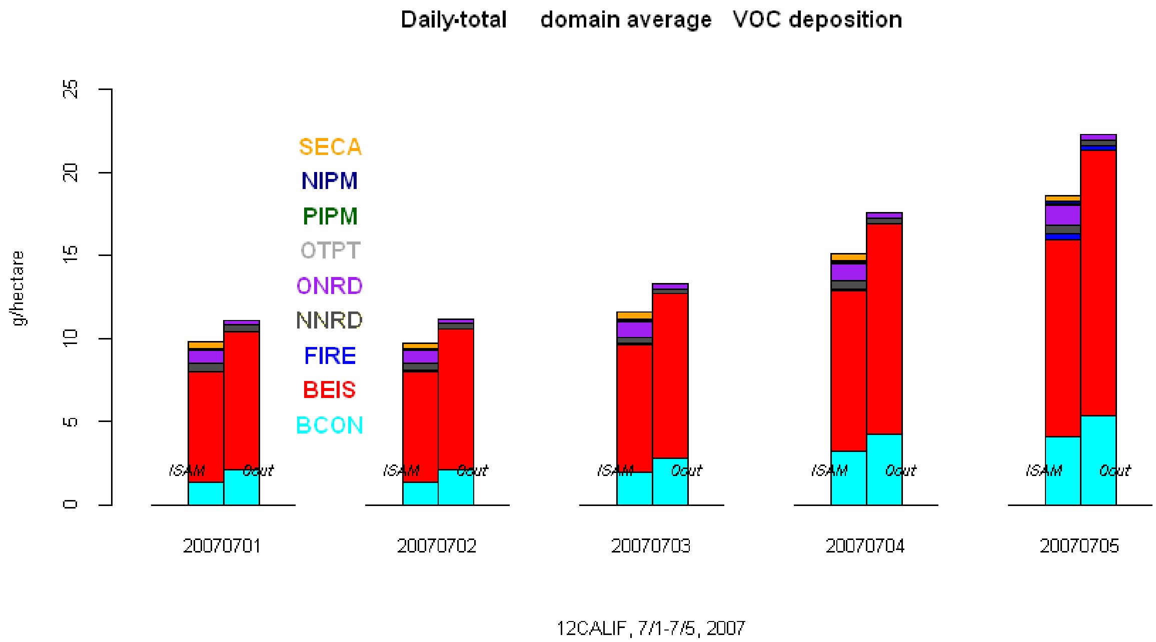
Supp Figure 8. ISAM/N-out scatter plots of all-hour total NOx (NO+NO_2) deposition for each sector. The sectors are: (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generating units EGU, (h) marine MARINE, and (j) boundary conditions BCON.



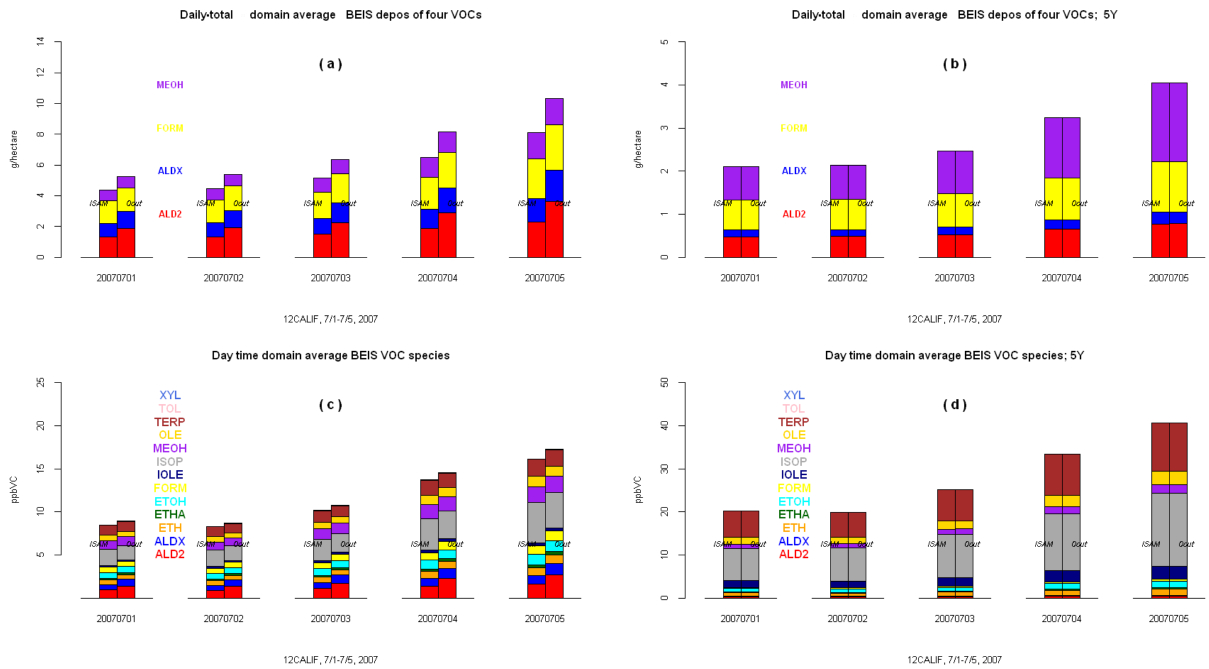
Supp Figure 9. Daily-total, domain-averaged NOx (NO+NO_2)deposition (dry+wet), July 1-5, 2007. As in Fig. 6, for each day left column designates ISAM total, and right one the zero-out. The colors represent sector sources: marine (MARINE orange), non-electricity generation units (NON-EGU deep blue), electricity generation units (EGU green), Mexican point sources (MEX light grey), on-road mobile (ONRD purple), non-road mobile (NNRD yellow), wild fires (FIRE blue), BIOG3 vegetations (BIOG red), and boundary conditions (BCON cyan).



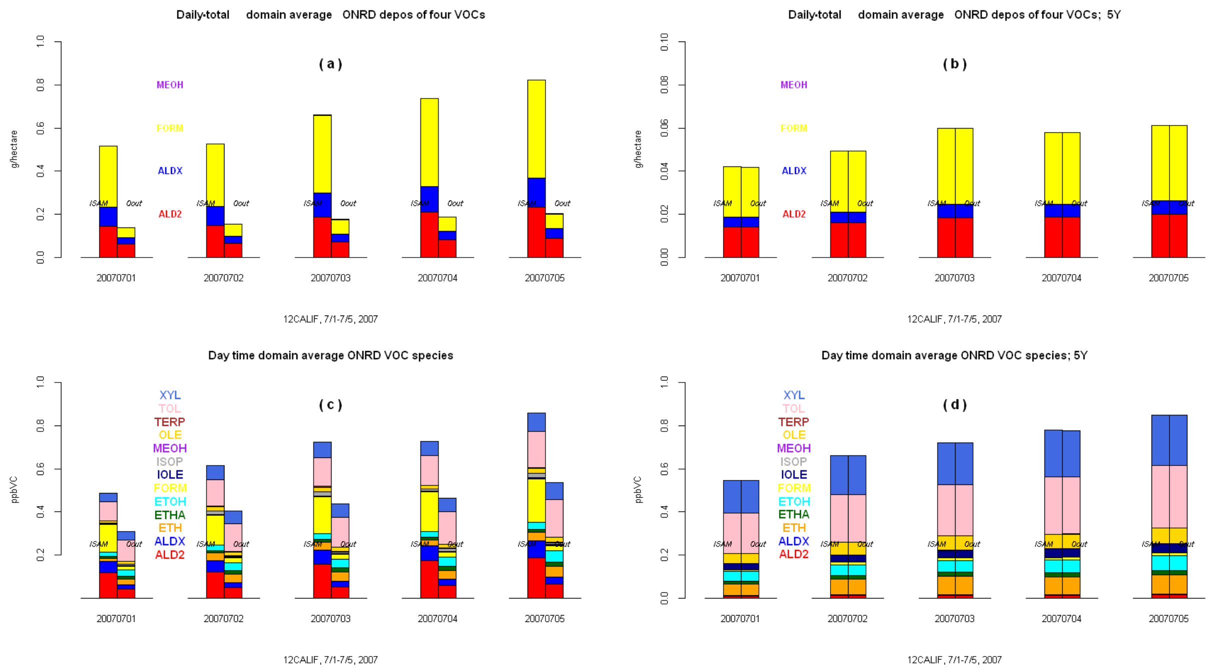
Supp Figure 10. ISAM/V-out scatter plots of all-hour total VOC deposition for each sector. The sectors are: (a) biogenic BIOG, (b) wild fires FIRE, (c) non-electricity generation units NON-EGU, (d) non-road mobile NNRD, (e) on-road mobile ONRD, (f) Mexican point sources MEX, (g) electricity generating units EGU, (h) marine MARINE, and (j) boundary conditions BCON.



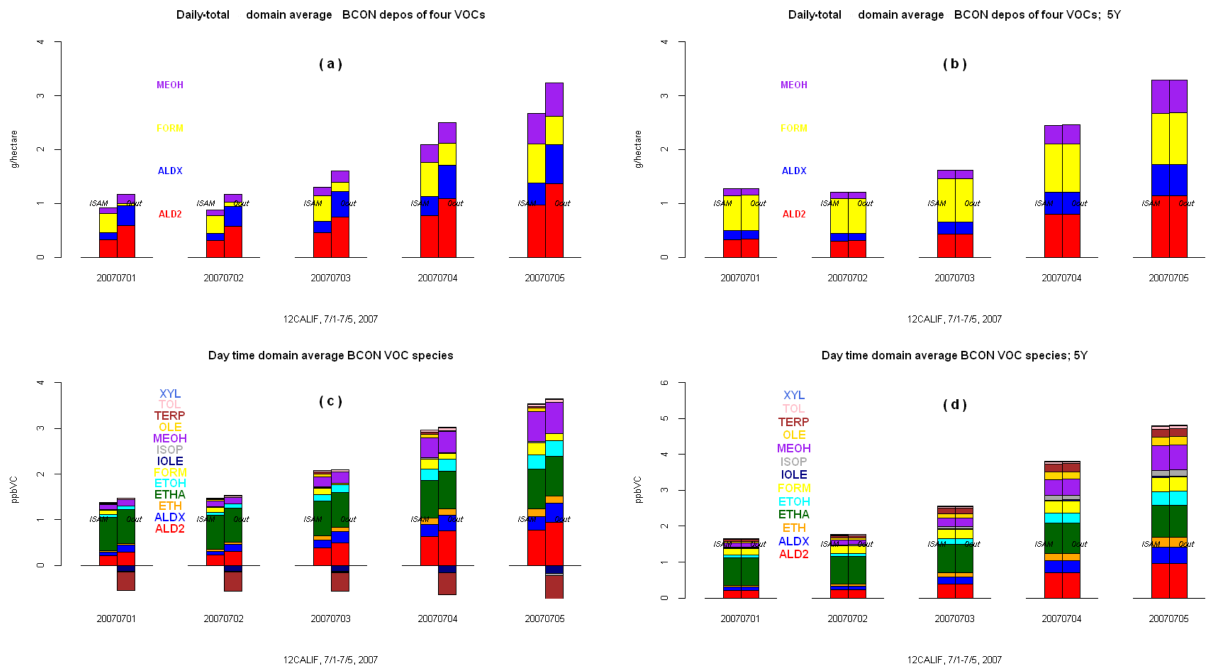
Supp Figure 11. Daily-total, domain-averaged VOC deposition (dry+wet), July 1-5, 2007. As in Fig. 6, for each day left column designates ISAM total, and right one the zero-out. The colors represent sector sources: marine (MARINE orange), non-electricity generation units (NON-EGU deep blue), electricity generation units (EGU green), Mexican point sources (MEX light grey), on-road mobile (ONRD purple), non-road mobile (NNRD yellow), wild fires (FIRE blue), BIOG3 vegetations (BIOG red), and boundary conditions (BCON cyan).



Supp Figure 12. Ambient and deposited VOCs in the biogenic sector during July 1-5, 2007. (a) daily domain total (wet + dry) deposition with full model processes; (b) daily domain total (wet + dry) deposition without gas-phase and aerosol processes; (c) daytime domain averaged ambient concentrations with full model processes; (d) daytime domain averaged ambient concentrations without gas-phase and aerosol processes. Species in ascending order: acetaldehyde(red), higher aldehydes(blue), ethene(orange), ethane(dark green), ethanol(cyan), formaldehyde(yellow), internal olefin(navy blue), isoprene(dark grey), methanol(purple), olefin(gold), monoterpenes(brown), toluene(pink), and xylene(royal blue). Note different scales across different toggling of processes (left vs right panels).



Supp Figure 13. Ambient and deposited VOCs in the onroad mobile sector during July 1-5, 2007. (a) daily domain total (wet + dry) deposition with full model processes; (b) daily domain total (wet + dry) deposition without gas-phase and aerosol processes; (c) daytime domain averaged ambient concentrations with full model processes; (d) daytime domain averaged ambient concentrations without gas-phase and aerosol processes. Species in ascending order: acetaldehyde(red), higher aldehydes(blue), ethene(orange), ethane(dark green), ethanol(cyan), formaldehyde(yellow), internal olefin(navy blue), isoprene(dark grey), methanol(purple), olefin(gold), monoterpenes(brown), toluene(pink), and xylene(royal blue). Note the increase in scale in deposition from partial (b) to full processes (a).



Supp Figure 14. Ambient and deposited VOCs from lateral boundary conditions during July 1-5, 2007. (a) daily domain total (wet + dry) deposition with full model processes; (b) daily domain total (wet + dry) deposition without gas-phase and aerosol processes; (c) daytime domain averaged ambient concentrations with full model processes; (d) daytime domain averaged ambient concentrations without gas-phase and aerosol processes. Species in ascending order: acetaldehyde(red), higher aldehydes(blue), ethene(orange), ethane(dark green), ethanol(cyan), formaldehyde(yellow), internal olefin(navy blue), isoprene(dark grey), methanol(purple), olefin(gold), monoterpenes(brown), toluene(pink), and xylene(royal blue). Note different scales in ambient concentrations ((c) and (d)).