EVALUATION OF CMAQ ESTIMATED GAS AND AEROSOL CARBON USING STN, IMPROVE, AND CALNEX FIELD MEASUREMENTS

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1. INTRODUCTION

The State of California currently has numerous counties designated as non-attainment for the PM2.5 National Ambient Air Quality Standard. Organic carbon is one notable component of PM2.5 in California. Air quality modeling is typically needed to support the development of emissions control strategies.

It is important that CMAQ and other photochemical models used for regulatory applications accurately characterize the atmospheric organic aerosol burden from precursor species to secondary organic aerosol formation so that emission control strategies elicit model response similar to the actual atmosphere. This enables accurate source attribution of atmospheric aerosol and development of effective control strategies to manage air quality.

2. APPROACH

Here we present an evaluation of both gas and aerosol carbon model estimates compared with observation data at two surface locations in California: Pasadena and Bakersfield. The Community Multiscale Air-Quality Model (CMAQ) version 5.0.1 (www.cmascenter.org) was applied to estimate air quality in California from May 5 to July, 2010, which coincides with the CalNex Study (Research at the Nexus of Air Quality and Climate Change; http://www.esrl.noaa.gov/csd/calnex/).

Ambient estimates of SOA based on measured chemical tracers and the fossil and modern composition of particulate carbon are presented and compared with model estimates to provide unique information about the nature of organic carbon at these locations in California. In addition, total VOC and speciated VOC measurements from the CalNex sites are compared with CMAQ estimates to provide a comprehensive overview of model performance of gas and aerosol carbon in California.

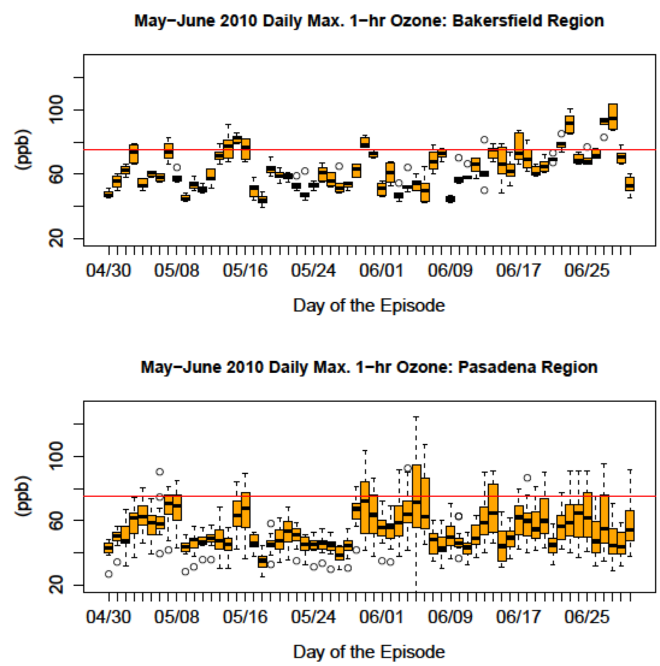

Fig. 1. Daily distribution of observed daily maximum 1-hr average ozone across routine monitors in the Bakersfield (top) and Pasadena (bottom) areas.

The CalNex field campaign period had a few days with elevated ozone near Bakersfield and Pasadena (Figure 1). PM2.5 measurements during this time period were fairly low near Bakersfield and moderate near the Pasadena site (Figure 2).

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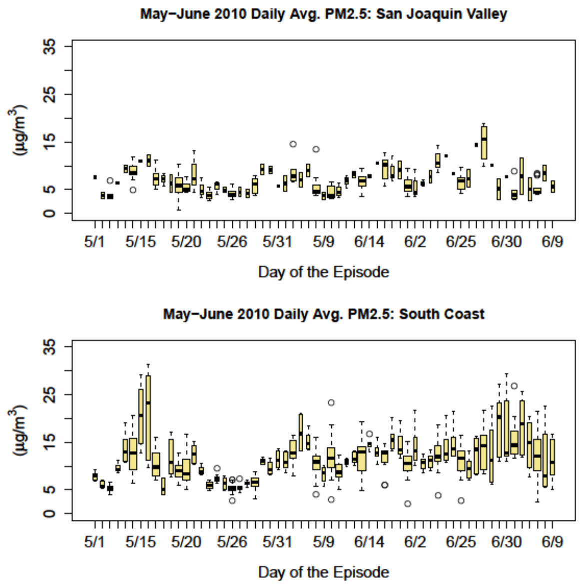

Fig. 2. Daily distribution of observed 24-hr average PM2.5 across routine monitors in the Bakersfield (top) and Pasadena (bottom) areas.

3. MODEL APPLICATION

The CMAQ model domain (Figure 3) covers California with 4 km sized grid cells and resolves the vertical atmosphere with 34 layers, both matching the grid structure employed with the Weather, Research and Forecasting (WRF) model. CMAQ was applied with SAPRC07T gas phase chemistry and AERO6 particle treatment. Secondary organic aerosol treatment is based on Carlton et al, 2010.

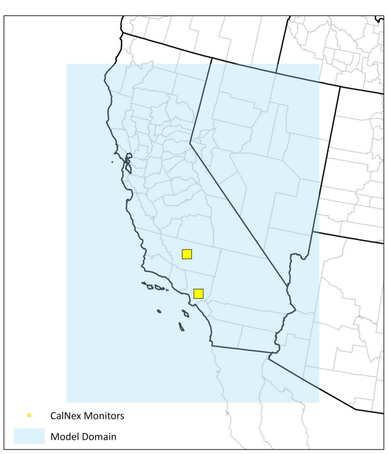

Fig. 3. Photochemical model domain.

Anthropogenic emissions are based on 2010 point source emissions where available and the 2011 National Emission Inventory for other sources. Biogenic emissions are based on BEIS version 3.14 using WRF estimated temperature and solar radiation as input (Carlton et al, 2011). CMAQ inorganic PM2.5 and precursor performance for this CalNex period is described in detail elsewhere (Kelly et al, 2014; Markovic et al, 2014).

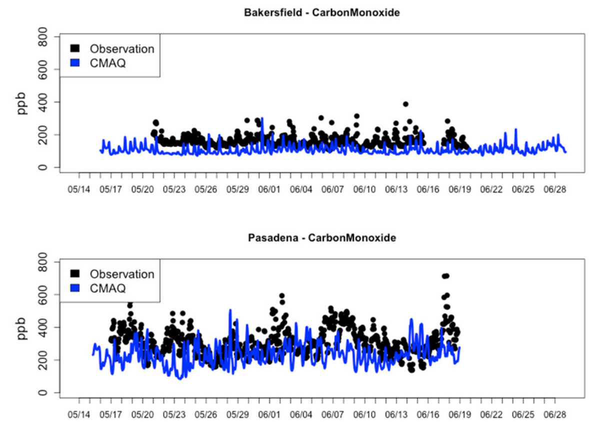

Fig. 4. Modeled and observed hourly carbon monoxide at both CalNex sites.

Boundary conditions come from a coarser CMAQ simulation covering the continental U.S. and that simulation used GEOS-CHEM for boundary inflow. Figure 4 shows carbon monoxide at both sites, which tends to be slightly underestimated and may be related to boundary inflow from the global model.

4. METEOROLOGY RESULTS

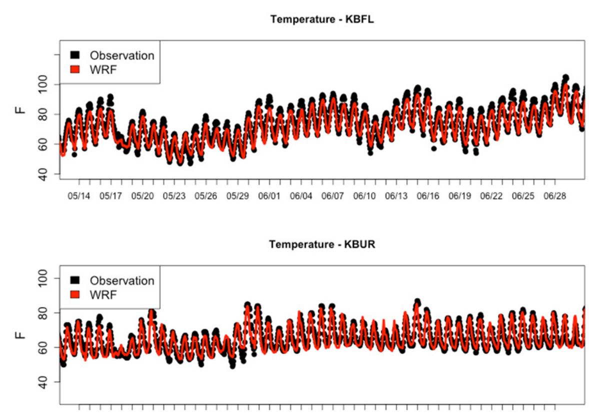

Fig. 5. Modeled and observed hourly temperature.

Figures 5 and 6 show hourly temperature and water mixing ratio at routine surface measurement stations near the CalNex monitor sites (KBFL near Bakersfield and KBUR near Pasadena). The WRF model captures day to day and diurnal patterns of both. Meteorological model application and performance results for this CalNex period are discussed in more detail elsewhere (Baker et al, 2013).

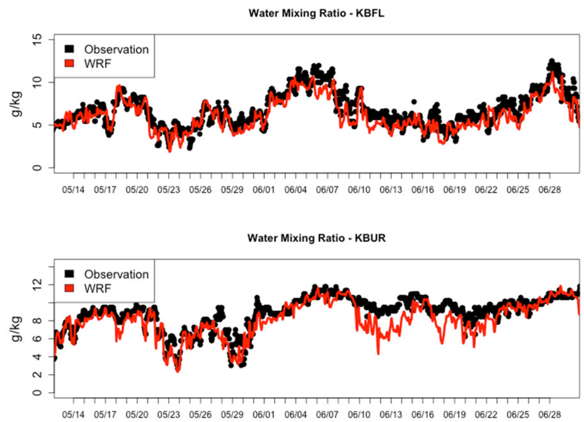

Fig. 6. Modeled and observed hourly temperature.

5. CARBON EVALUATION

5.1 PM2.5 Carbon

Measurements suggest daily average PM2.5 carbon at both Pasadena and Bakersfield is generally evenly mixed between modern and fossil origins (Figure 7).

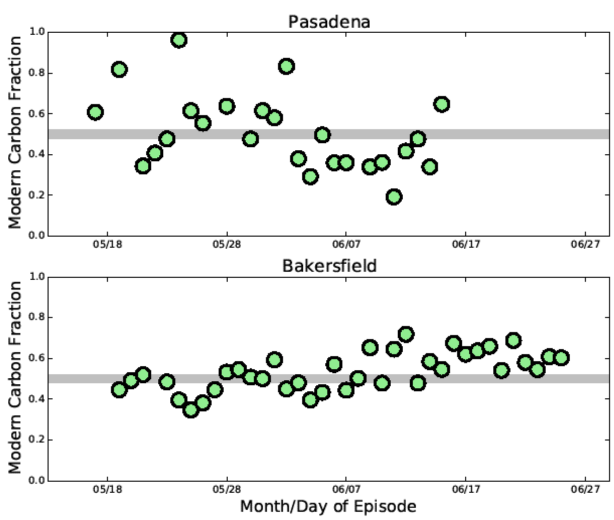

Fig. 7. Observed modern carbon fraction of daily average total PM2.5 carbon.

CMAQ model predicted PM2.5 carbon is compared with daily measurements taken at Bakersfield and Pasadena (Figure 8). The model tends to overestimate elemental carbon at Pasadena and organic carbon at Bakersfield.

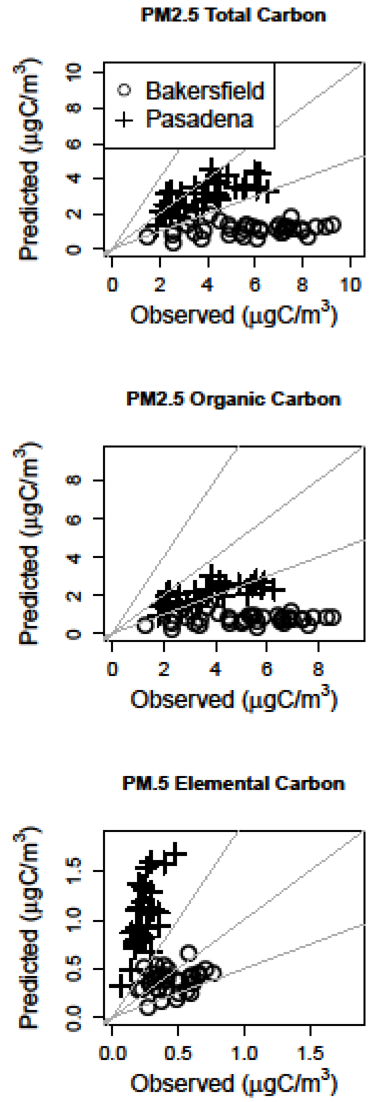

Fig 8. Modeled and observed daily average PM2.5 total carbon, organic carbon, and elemental carbon.

Daily average observations of PM2.5 secondary organic carbon tracer classes are compared with model estimates in Figure 9. These observations do not fully account for total observed PM2.5 secondary organic carbon. Anthropogenic tracers for toluenes and xylenes tend to be underestimated at both sites. Biogenic tracer groups are also underestimated at each site. The model estimated SOC from sesquiterpenes but that tracer was not measured. However, it is possible the observed tracer does not fully represent SOC from all different types of sesquiterpenes. A model sensitivity was performed where primarily emitted organic carbon emissions were increased by a factor of 2 to provide additional surface area for SOA formation and compensate for OC underestimates at these locations. The additional PM2.5 did result in some additional SOA formation but did not result in large increases in model predicted SOA.

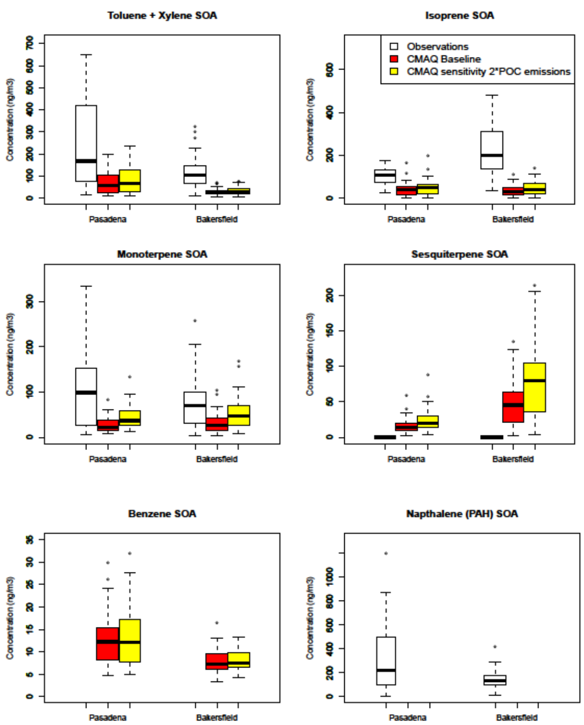

Fig. 9. Observed and modeled PM2.5 secondary organic carbon tracers.

5.2 VOC

This section provides a comparison of modeled and observed mid-morning 3-hr average VOC (Figure 10) and also a comparison of hourly average toluene and xylenes (Figure 11). Even though some SOC tracer groups are underestimated (e.g. toluenes and xylenes), the VOC percursors are fairly well characterized by the modeling system. This provides some confidence in the emissions estimated for sectors such as mobile sources that contribute most of the toluene, xylenes, and benzenes to these locations during this time period.

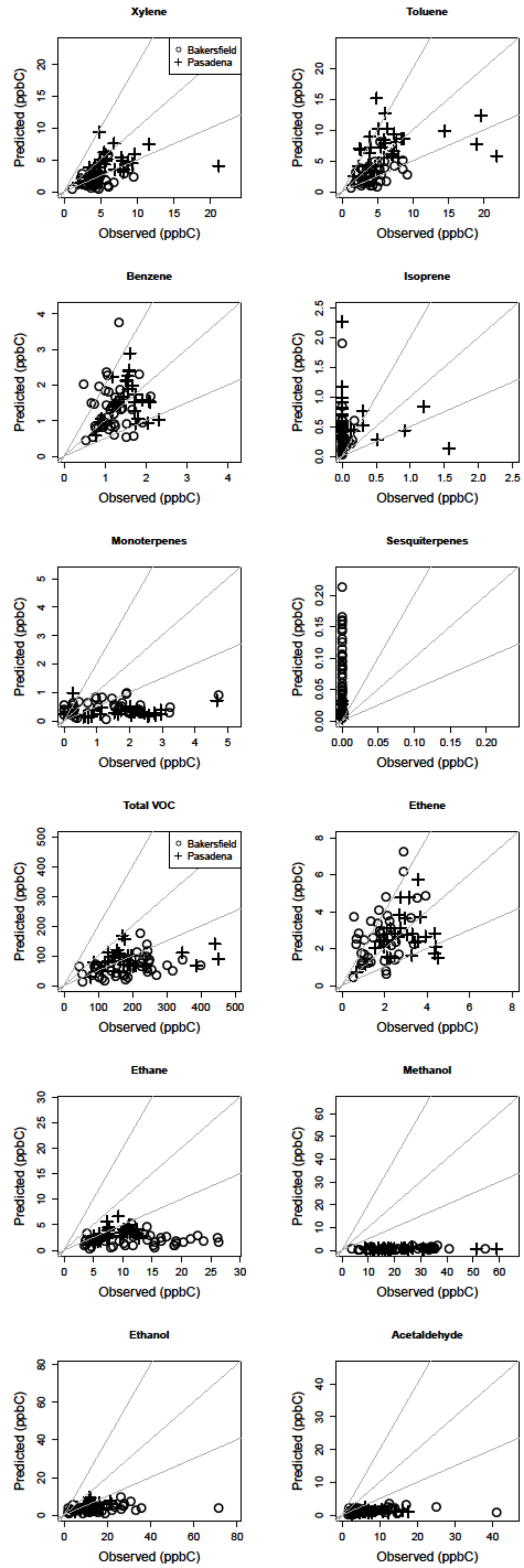

Fig 10. Observed and modeled mid-morning 3-hr average VOC species.

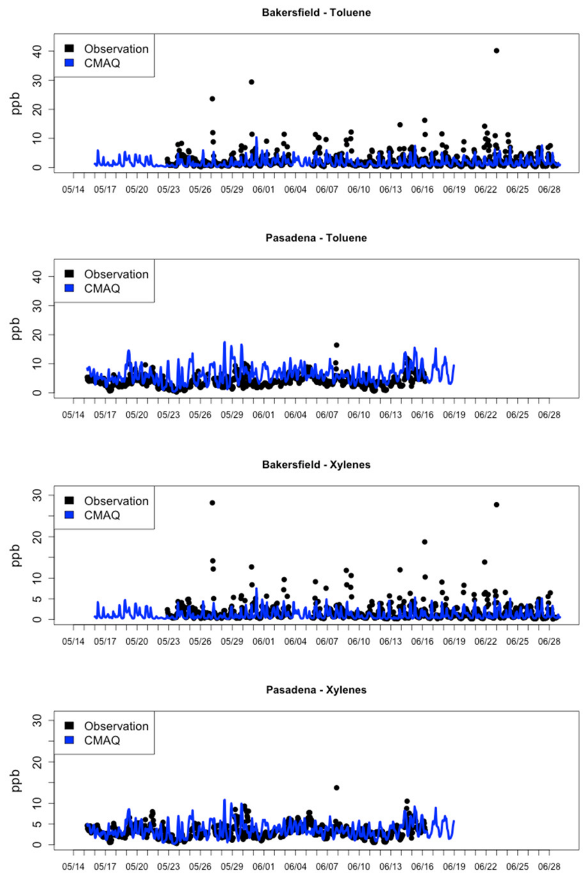

Fig 11. Observed and modeled hourly toluene and xylenes.

5.3 STN AND IMPROVE PM2.5 CARBON

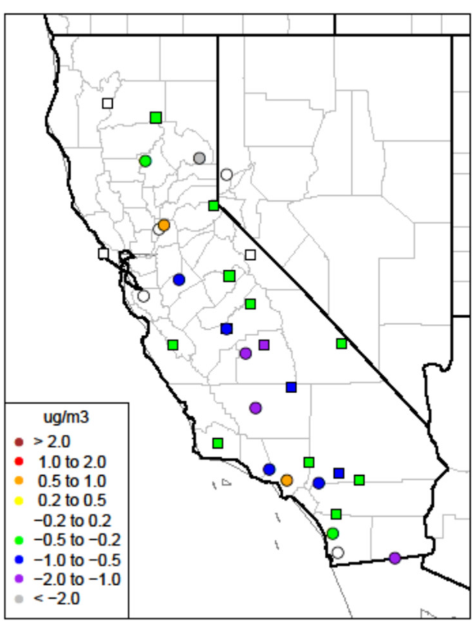

Fig 12. Episode average bias (model-observation) for PM2.5 organic carbon.

This section provides a comparison of modeled and observed episode average PM2.5 organic carbon (Figure 12). Warm colors indicate model overprediction and cool colors model underprediction. Model performance is discussed in more detail elsewhere (Baker et al., 2014).

6. REFERENCES

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7. Disclaimer

Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.