TOWARD A CHEMICAL CLIMATOLOGY OF OZONE CONTRIBUTIONS FROM LONG RANGE TRANSPORT IN THE PACIFIC NORTHWEST -- INCORPORATION OF OZONE TRACERS IN THE AIRPACT-4 AIR QUALITY FORECAST SYSTEM

Joseph K. Vaughan*, Serena H. Chung, Farren Herron-Thorpe, Brian K. Lamb, Rui Zhang, George H. Mount

Laboratory for Atmospheric Research, Department of Civil and Environmental Engineering, Washington State University, Pullman, WA, USA

1. INTRODUCTION

Air-quality modeling is an important tool for evaluating strategies for complying with the NAAQS. Two perennial issues of interest are the effects of long-range transport (LRT) and of stratospheric ozone intrusion (SOI) on air quality.

Under the EPA Exceptional Events Policy, for example, a nominal exceedance can be excluded from design value calculation if it can be credibly ascribed to long-range transport or stratospheric ozone intrusion.

Air-quality modeling is potentially an appropriate tool for attempting demonstration of LRT and SOI in making a case for Exceptional Event status for an exceedance. Also, ample evidence exists that local air pollution should sometimes be viewed in the context of a baseline pollution levels, and that these baseline levels are influenced by LRT and SOI (Wigder et al., 2013).

2. AIRPACT-4 FORECAST SYSTEM

2.1 Standard Operational System

AIRPACT-4 is an air quality forecast system operating nightly at the Laboratory for Atmospheric Research for the Pacific Northwest, and operates on a 4-km grid and covers the region including the states of Washington, Oregon and Idaho. The 4-km domain of 258 rows x 285 columns translates to a 1140 km (E-W) x 1032 km (N-S) domain of 4 km x 4 km grid cells. The 21 layers span from the surface to ~19 km with the top 3-4 layers representing the lower stratosphere. Typically the tropopause occurs at layers 18-19 (~12-14 km).

The system simulates transport and chemistry from local (Pacific Time) midnight (08 UTZ) forward for 48 hours. This system is a revised and higher-resolution version of the AIRPACT-3 system (Chen et al., 2008). AIRPACT-4 is a WRF-SMOKE-CMAQ system using the SAPRC99 chemical mechanism and the AE5 aerosol mechanism. Various system inputs are described next.

Forecast meteorology is obtained from 4-km WRF model runs at the University of Washington, Atmospheric Sciences Department's mesoscale forecasting project: http://www.atmos.washington.edu/mm5rt,

AIRPACT-4 Emissions are prepared for point, nonpoint, nonroad mobile, onroad mobile sources using recent information. For most point and nonpoint sources, the 2005 comprehensive inventories prepared to meet state, provincial, and national reporting requirements were used. The majority of mobile source emissions were prepared specifically for AIRPACT for the year 2009. The standard on-road mobile emissions were estimated using MOBILE6.2 in the USA, and MOBILE6.2C in Canada and adjusted according to the predicted hourly temperature. Emissions were processed through the Sparse Matrix Operating Kernel Emissions (SMOKE) for their chemical speciation, spatial and temporal allocation, and for the case of point sources, vertical allocation of elevated sources. Although SMOKE has the capability to calculate plume rise using hourly meteorological data, that calculation is completed using the inline approximation in CMAQ.

Initial conditions for each run are read from the previous day CMAQ results and chemical boundary conditions are obtained from global MOZART4 model runs that assimilate MOPITT/TERRA satellite CO (Herron-Thorpe et al., 2012).

2.2 Experimental Non-reactive Tracer System

To develop a chemical climatology for exploring the LRT and SOI contributions to the

**Corresponding author:* Joseph K. Vaughan, Laboratory for Atmospheric Research, Department of Civil and Environmental Engineering, Washington State University, Pullman, WA, 99164-2910; e-mail: jvaughan@wsu.edu

ozone background of the Pacific Northwest, we used a non-reactive tracer species version of the Community Multi-scale Model for Air Quality, CMAQv4.7.1. This build of the CMAQ chemical conversion and transport model turns off all the SAPRCC chemistry and also turned off deposition processes. Instead, a set of non-reactive gas tracer species were defined, numbering 21 to match the number of layers in the model domain and thus matching the number of layers of MOPITT-CO-assimilating MOZART boundary conditions (BCON) provided to CMAQ within AIRPACT-4, operationally. In the tracer version of the system, for this application, emissions are zeroed out. Each month is started off with zeroed initial conditions (ICON) and for the rest of the month the ICON come from the previous day CMAQ results.

To focus on long-range transport and stratospheric ozone intrusion, we are assigning the 21 layers of MOZART BCON for ozone on the western domain boundary to the 21 tracers. The eastern, northern and southern BCON are all zeroed for this application. And on the western boundary, all tracers for which the index (1-21) does not match the layer number are also zeroed. Thus, the only BCON in any layer that is non-zero is the tracer matching that layer number and it is given the ozone value for that layer from the MOZART BCON used in AIRPACT-4.

3. APPLICATION for May--August 2013

We ran the AIRPACT-4 non-reactive tracer system for the months of May, June, July and August 2013. The standard runs of AIRPACT-4 for these four months had completed and were available for comparison (with the exception of July 31, 2013, which failed for both the standard and the non-reactive tracer runs). Standard AIRPACT-4 results for ozone, PM2.5, and other gases and aerosols and PM2.5 are visualized for review at the project website: [http://lar.wsu.edu/airpact/gmap/ap4.html.](http://lar.wsu.edu/airpact/gmap/ap4.html)

4. RESULTS

The modeling results were analyzed for monthly statistics describing the contribution of a set of upper layers of the MOZART-sourced ozone western BCON to standard AIRPACT-4 ozone in the lowest, ground level, model layer. **All results are presented using an 8-hr ozone average value representing the afternoon to early evening, Noon through 7 PM (PT).** Results are presented for four ozone-season months, May through August 2013. The layer-16 tracer results were chosen for display after we observed that layer 16 generally showed the strongest transport of ozone to the surface layer.

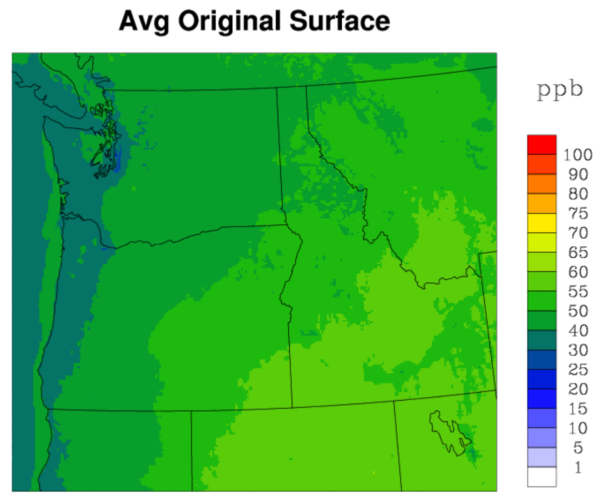

Figure 1. AIRPACT-4 surface O3, May 2013.

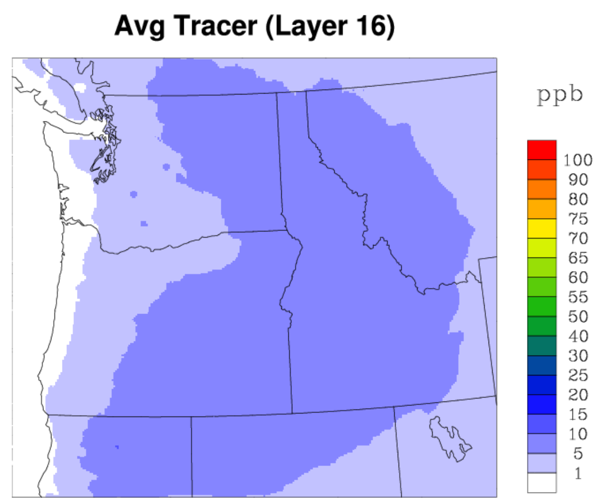

Figure 2. Surface layer-16 O3 tracer, May 2013.

Figures 1, 3, 5 and 7 show for the four months the average afternoon 8-hr average surface layer ozone from AIRPACT-4 standard simulations (forecasts). Figures 2, 4, 6, and 8 show for the four months the layer-16 tracer contribution to the surface layer. For May large areas show an average layer-16 tracer contribution of up to 10 ppb against AIRPACT-4 co-located results of 40-60 ppb. June appears similar to May. July shows average layer-16 tracer contribution of up to 15 ppb against AIRPACT-4 co-located results of up to 65 ppb. August shows lower layer-16 tracer results, over an overall smaller extent within the domain.

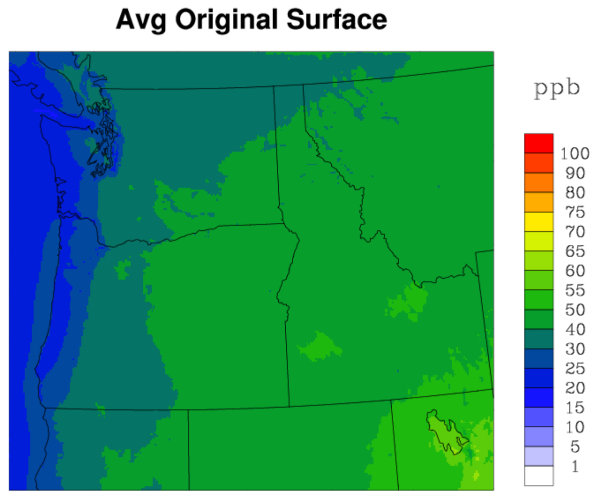

Figure 3. AIRPACT-4 surface O3,, June 2013.

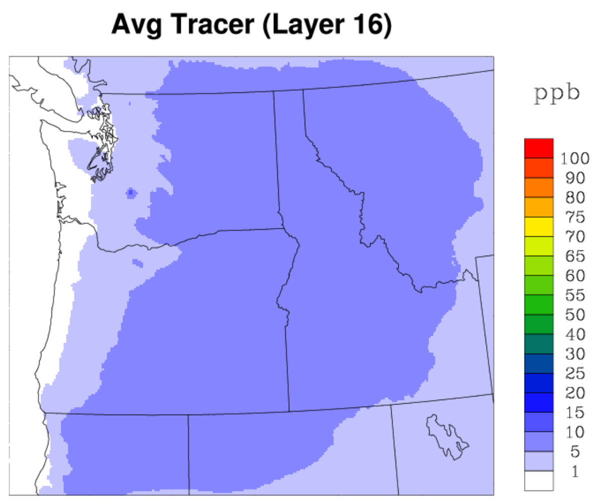

Figure 4. Surface layer-16 O3 tracer, June 2013.

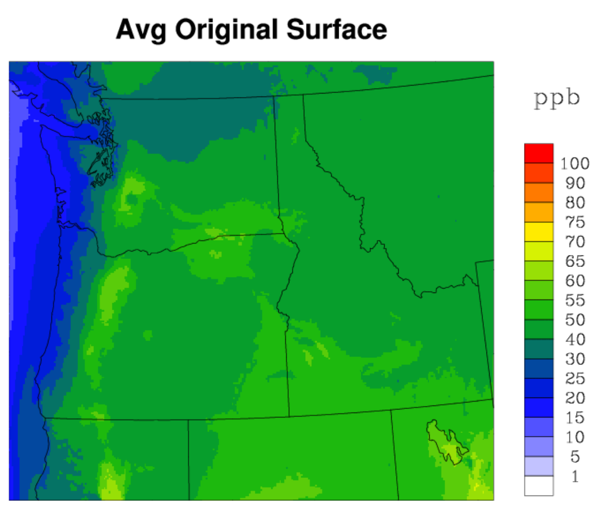

Figure 5. AIRPACT-4 surface O3, July 2013.

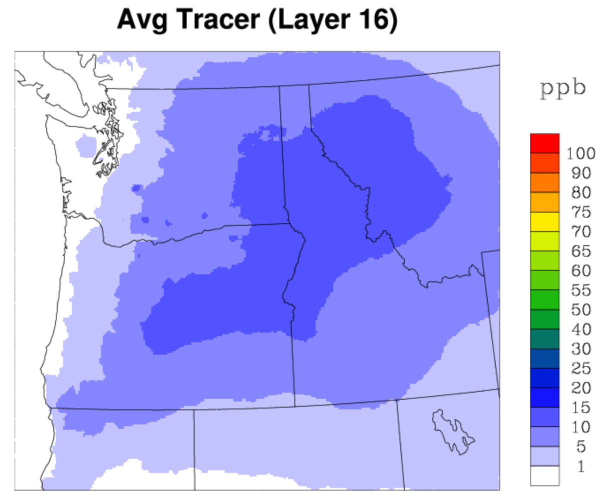

Figure 6. Surface layer-16 O3 tracer, July 2013.

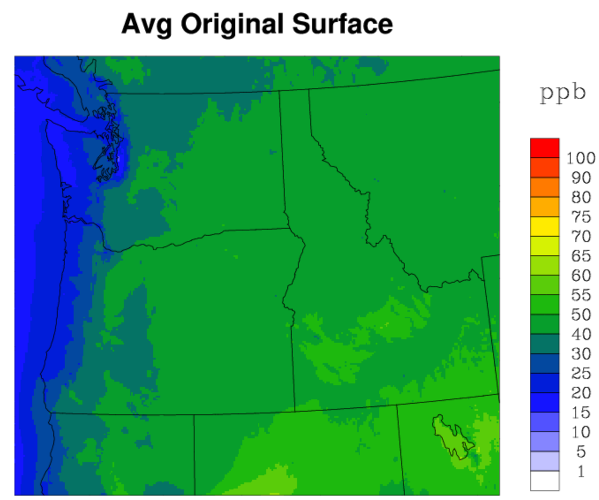

Figure 7. AIRPACT-4 surface O3, August 2013.

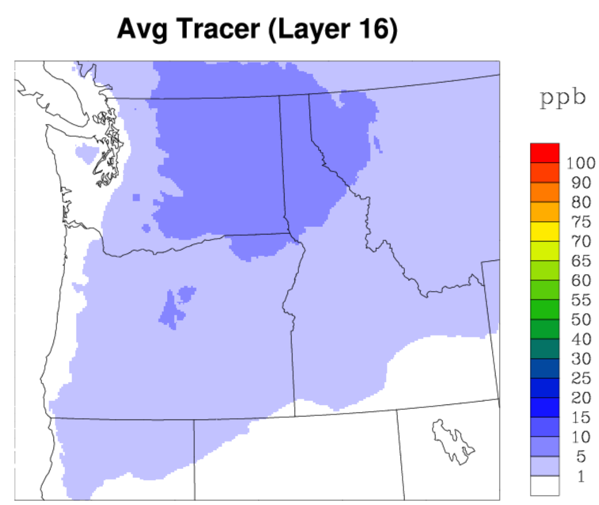

Figure 8. Surface layer-16 O3 tracer, August 2013.

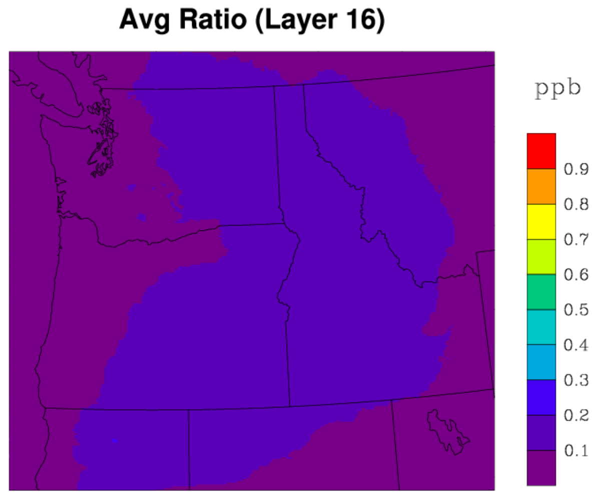

Figure 9. Ratio of layer-16 O3 tracer to AIRPACT-4 surface O3, May 2013.

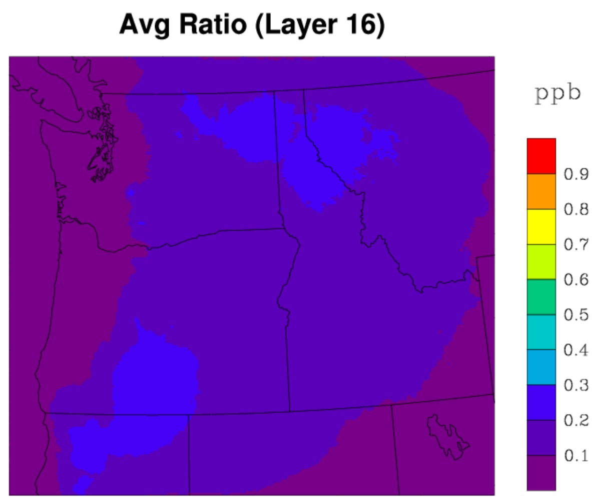

Figure 10. Ratio of layer-16 O3 tracer to AIRPACT-4 surface O3, June 2013.

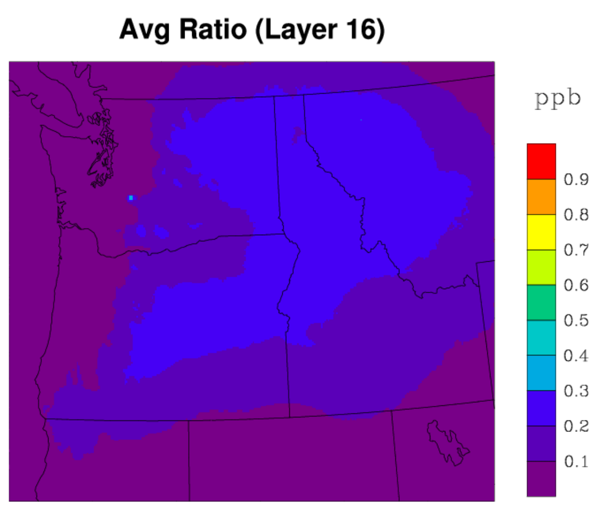

Figure 11. Ratio of layer-16 O3 tracer to AIRPACT-4 surface O3, July 2013.

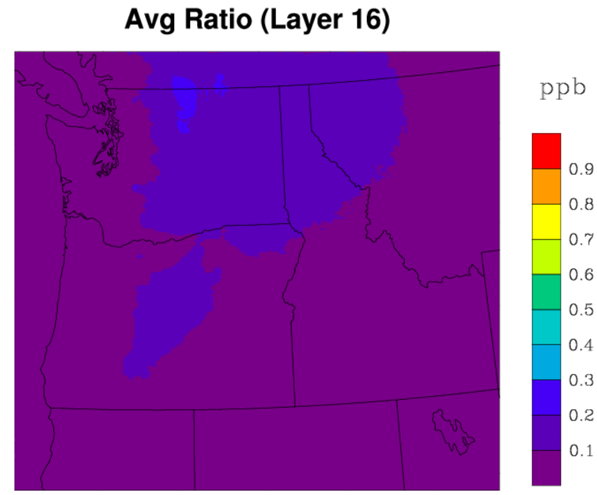

Figure 12. Ratio of layer-16 O3 tracer to AIRPACT-4 surface O3, August 2013.

Figures 9 - 12 show for the four months the average ratio of the layer-16 tracer surface layer contribution to the AIRPACT surface ozone For June and July extensive areas of the domain show ratio values of 0.2-0.3.

Figure 13 shows the July maximum layer-16 ozone contribution to the surface layer, and shows values as high as 40 ppb with extensive areas of the domain showing up to 30 ppb.

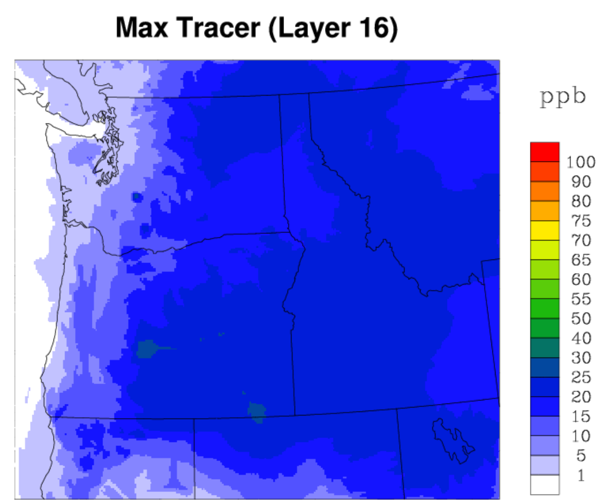

Figure 13. Ratio of layer-16 O3 tracer to AIRPACT-4 surface O3, August 2013.

5. Discussion

5.1 Long Range Transport

Results for addressing this phenomenon are still being generated and are not yet available for inclusion in this abstract. Long Range Transport across the western boundary of the AIRPACT-4 domain is expected to occur, particularly in spring, and may show when high ozone concentrations from mid-troposphere layers contributing to the surface ozone. Thus, analysis of these results involves examining the effect of transport from mid-tropospheric layers to the surface. These results are still being generated form the model runs and are not included in this abstract.

5.2 Stratospheric Ozone Intrusion

AIRPACT-4, driven using WRF meteorology and using CMAQ, in not perhaps ideally suited to modeling SOI. However, since the MOZART4 model results used as BCON do provide enhanced, dynamic ozone values on the boundary, something approximating SOI may be observable using the AIRPACT-4 system. The strength of the near-tropopause ozone transport to the surface seen in the statistics reviewed above suggests that analysis of specific episodes may further explicate the adequacy of AIRPACT-4 in capturing such SOI events. The important question of the temporal correspondence of apparent high contributions from aloft with episodes of high surface ozone is not well answered by these monthly statistics. That is another question to be pursued further.

Of course, in exploring the significance of the putative SOI, it may also be important to account for the variability in the ozone supplied on the boundary in addition to the strength of transport to the surface. We have not yet evaluated the month-to-month variability of the ozone BCON from MOZART-4. Nor have we fully accounted for other artifacts of our simplistic isolation of the western boundary inflow for analysis, such as the potential importance to SOI (or LRT) of ozone aloft on other boundaries. This first approximation approach is, however, thought to capture a mechanism of interest in the AIRPACT-4 modeling system.

6. References

Wigder, N. L., D. A. Jaffe, F. L. Herron-Thorpe, and J. K. Vaughan (2013), Influence of daily variations in baseline ozone on urban air quality in the United States Pacific Northwest, J. Geophys. Res. Atmos., 118, 3343–3354, doi:10.1029/2012JD018738.

Herron-Thorpe, Farren L., George H. Mount, Louisa K. Emmons, Brian K. Lamb, Serena H. Chung, and Joseph K. Vaughan (2012) Regional Air-Quality Forecasting for the Pacific Northwest Using MOPITT/TERRA Assimilated Carbon Monoxide MOZART-4 Forecasts as a Near Real-Time Boundary Condition, Atmospheric Chemistry and Physics, 12, 5603–5615. doi:10.5194/acp-12-5603-2012.

Meiyun Lin, Arlene M. Fiore, Owen R. Cooper, Larry W. Horowitz, Andrew O. Langford, Hiram Levy II, Bryan J. Johnson, Vaishali Naik, Samuel J. Oltmans, Christoph J. Senff. Journal: Journal of Geophysical Research. DOI: 10.1029/2012JD018151

Chen, J., J. Vaughan, J. Avise, S. O'Neill, and B. Lamb (2008) Enhancement and evaluation of the AIRPACT ozone and PM2.5 forecast system for the Pacific Northwest, J. Geophys. Res., 113, D14305, doi:10.1029/2007JD009554.

Byun, D. W., and K. L. Schere (2006), Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system, Appl. Mech. Rev., 55, 51–77.

Carolina Environment Programs (2005), Sparse Matrix Operator Kernel Emission (SMOKE) Modeling System. Univ. of Carolina, Carolina Environ. Programs, Research Triangle Park, N. C. (Available at http://www.smoke-model.org/version2.2/html)

Carter, W. P. L. (2000), Documentation of the SAPRC-99 Chemical Mechanism for VOC Reactivity Assessment, No. 92 – 329, 95 – 308, Final Report to California Air Resources Board, Calif. Air Resour. Board, Riverside Calif. (Available at http://helium.ucr.edu/ carter/reactdat.htm).