Western Meteorological, Emissions, and
Air Quality Modeling Workshop

Photochemical Model Performance Evaluations for Ozone in the Western States

Gail Tonnesen, EPA Region 8
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Acknowledgments: Slides 18-20 from Clark County DAQEM

Unique Attributes of Western Ozone

- High background/transported ozone levels.
- Elevated ozone at rural and high altitude sites.
- Winter, spring and summer ozone seasons.
- Large wildfire emissions.
- More frequent exceptional events?
- Less biogenic VOC in some arid regions.
- Widespread ozone modeling in NEPA analyses for energy development.

Model Performance Evaluation

- Calibration, Verification, Validation or **Evaluation**?
  - Oreskes et al., *Science*, 1994
  - Calibration can introduce compensating errors.
  - Impossible to Verify or Validate complex models.
  - Model can be used to investigate uncertainty and sensitivity to input data; used to challenge rather than confirm beliefs.
- Goal of MPE is to assess confidence in the model predictions. Do we have sufficient confidence in the mode to:
  - Guide the selection of type of control strategy.
  - Estimate the size of emissions reductions needed.

Model Performance Evaluation

- EPA has moved toward a more qualitative use of photochemical models:
  - No absolute criteria for acceptable performance.
  - Models are use in a relative sense with RRF.
  - Weight of evidence analysis is used to support model results.
  - Additional provisional emissions reductions are identified in the SIP in case the attainment demonstration is insufficient.

Model Performance Metrics

- EPA 1991 Guidance focused on metrics:
  - Unpaired Accuracy of the Peak < ±20%
  - Normalized Mean Bias < ±15%
  - Normalized Mean Gross Error <35%
- EPA 2007 Guidance emphasizes graphical analyses and diagnostic evaluation.

Types of MPE

- Operational MPE
  - Compare model concentrations with ambient data.
- Diagnostic MPE
  - Evaluation of component processes, including the sources and fate of radicals and NOx that catalyze O_3 production.
  - Evaluate ratios of species: VOC/NOx, O_3/NOy.
  - Use indicators for evaluating model O_3 sensitivity.
  - Evaluation of O_3 transport.
  - Sensitivity and uncertainty analysis.

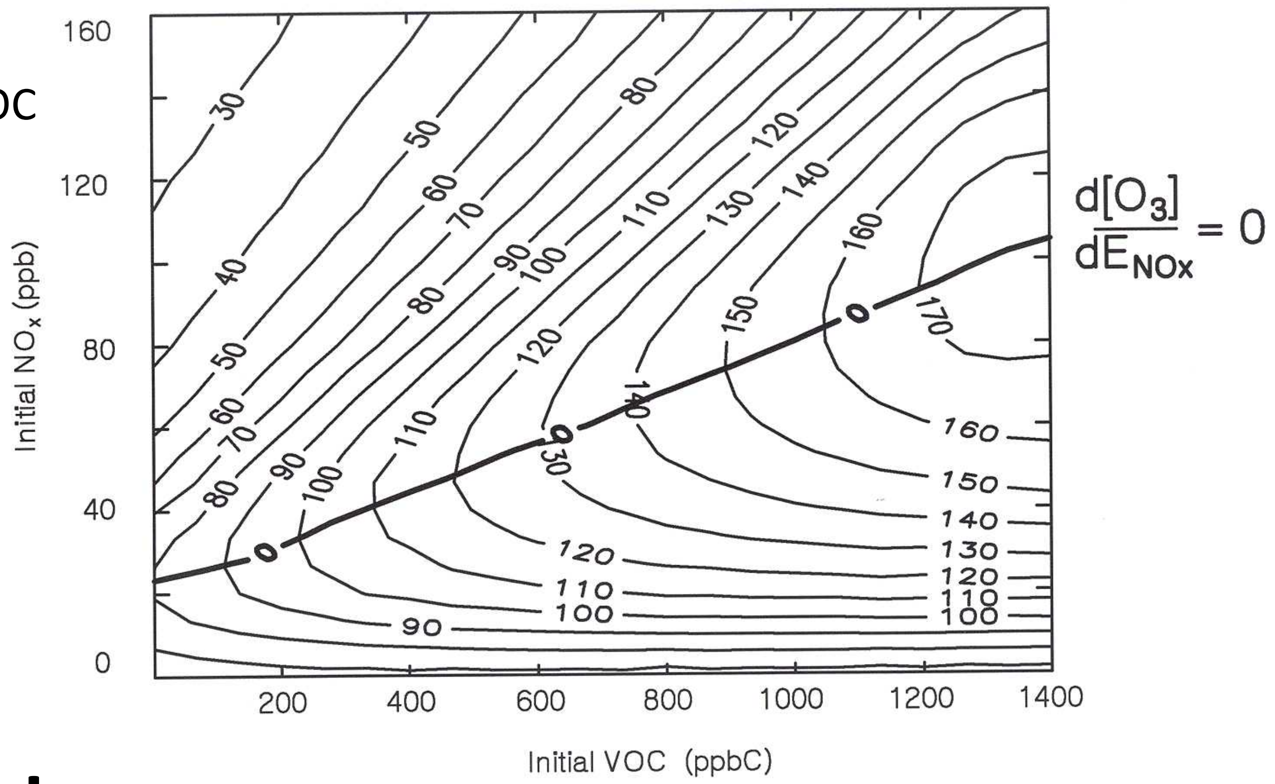
Above the O_3 ridgeline

Low VOC/NO_x ratios

O_3 is radical limited

O_3 is more sensitive to VOC

Ozone Isopleth Diagram



O3 Sensitivity to VOC and NOx

Below the O_3 ridgeline:

High VOC/NO_x ratios

O_3 is NO_x limited

O_3 is more sensitive to NO_x

Data Needs for Model Evaluation

- Monitoring of ozone and meteorology data.
- Monitoring of speciated VOC, HCHO, HONO and ozone to evaluate radical sources.
- Monitoring of NO, true NO_2, and NO_y
  - ➢ Most NO_x data is from chemiluminescence method that includes interference from NO_y
  - ➢ Need true NO_2 using photolytic or other research methods.

More Data Needs for MPE

- Tropospheric ozone profiles to understand transport and vertical mixing.
- CO to evaluate emissions from combustion sources.
- Indicator ratios to evaluate O_3 sensitivity to VOC & NO_x VOC/NO_x, HCHO/NO_2, O_3/NO_2
- Evaluation of ozone day of week effects
- Multiple sites to understand spatial variability.

Examples of Ozone MPEs

- CA and TX are atypical ozone western states:
  - Large urban areas & lower background O3 levels.
  - Higher O3 design values and long history of intensive studies:
  - 2000 Central California Ozone Study (CCOS), CALNEX 2010.
  - 2000 Texas Air Quality Study (TexAQS), TexAQS II (2005-2006)
- Inter-mountain western states:
  - Four corners Early Action Compact Ozone Modeling
  - 2006 Denver SIP Modeling
  - Clark County, Nevada SIP Modeling

CCOS 2000 MPEs

- Tesche et al., 2004, "Evaluation of the 16-20 September 2000 Ozone Episode for use in 1-hour SIP Development in the California Central Valley"
  - Comparison to precursors and indicator ratios
  - Analysis of ozonesondes and aircraft data.
  - 20 diagnostic model simulations.
  - Evaluation of meteorology and chemical processes.
  - Conclusion: likely that model VOC mass or VOC reactivity is too low.
- STI, 2008, "A Comparison of Ambient Measurements to Emissions Representations for Modeling to Support the CCOS "
- Blanchard, 2008, "Understanding Relationships Between Changes in Ambient Ozone and Precursor Concentrations and Changes in VOC and NOx Emissions from 1990 to 2004 in Central California"
- Even with comprehensive, multi-million dollar field study, it is difficult to model ozone. CALNEX 2010 Study addresses ozone and climate.

TexAQS, TexAQS II, TexAQS Radical and aerosol measurement project (TRAMP), HONO Intercomparison Study (HINT)

- Comprehensive field studies, including NOAA, BNL, University of Texas and others. Objectives included analysis of transient high ozone events:
- Measurement supported a comprehensive diagnostic model evaluation:
  - What are the main sources and sinks for radicals in the urban air of Houston?
  - What processes determine the radical budget in the urban air of Houston?
  - What are the impacts with regard to the formation of secondary species?
  - What are the anthropogenic vs. biogenic contributions in photochemical processes?
  - What kind of meteorological processes modulate the distribution of trace gases in the Houston area?
  - Better understanding of nighttime chemistry, in particular the formation of HONO and quantification of nighttime NOx removal processes
- Success in identifying causes and controls strategies for transient high O3, but challenges remain in attaining NAAQS.

Challenge of Ozone Modeling

- Previous experience in CA and TX follows a pattern:
  - Start with a multi-million dollar field study.
  - Perform numerous modeling studies with comprehensive diagnostic performance evaluation.
  - Repeat until you attain the NAAQS.
- Can we avoid this cycle in other western states?
  - CA and TX studies have advanced the science.
  - Continuing improvements in met and air quality models.
  - Continuing improvements in photochemical mechanisms.
  - However, challenges remain in both transport and chemistry.
  - The special measurements needed are still difficult and expensive.

Colorado 2006 SIP Modeling

- ENVIRON/Alpine Geophysics CAMx modeling focused on 3 episodes: June 17-19, July 13-15, July 27-29.
- Source apportionment showed about 50 ppb ozone from outside of the 12 km domain.

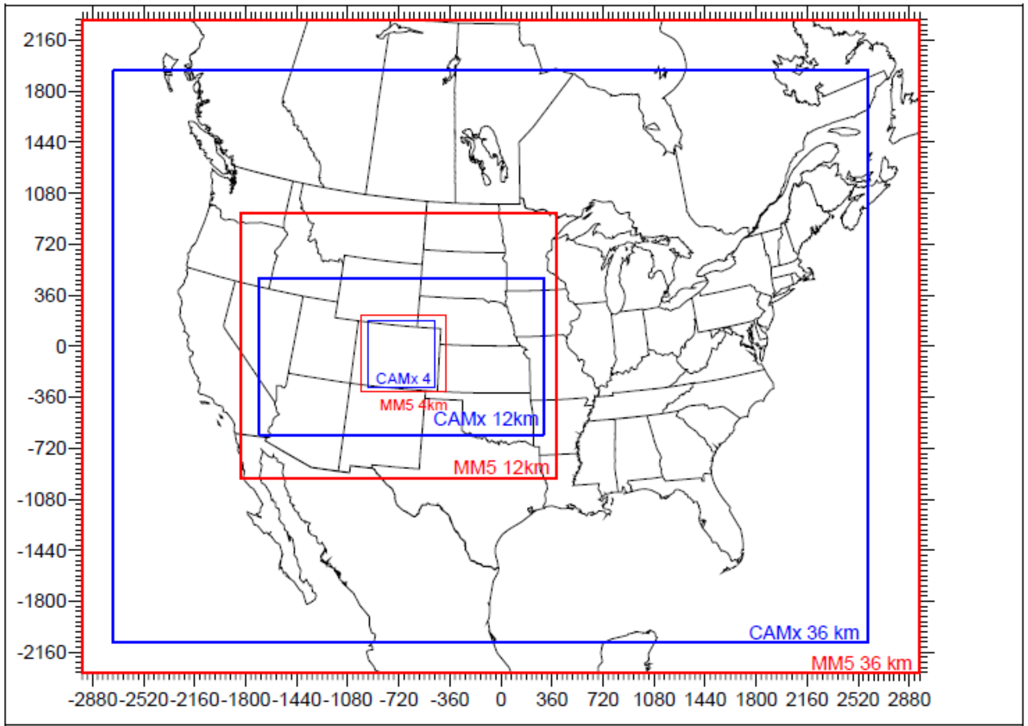


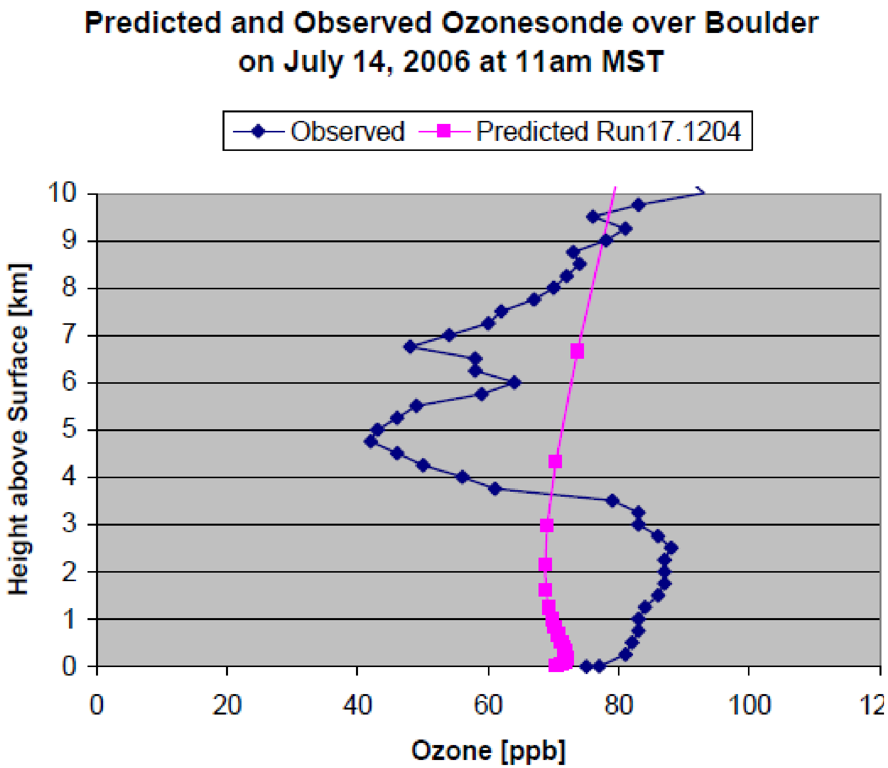
Figure 1-1a. Nested 36/12/4 km modeling domains for the Denver 8-hour ozone modeling study. Blue line domains are for CAMx/SMOKE domains that are nested in the MM5 red line domains.

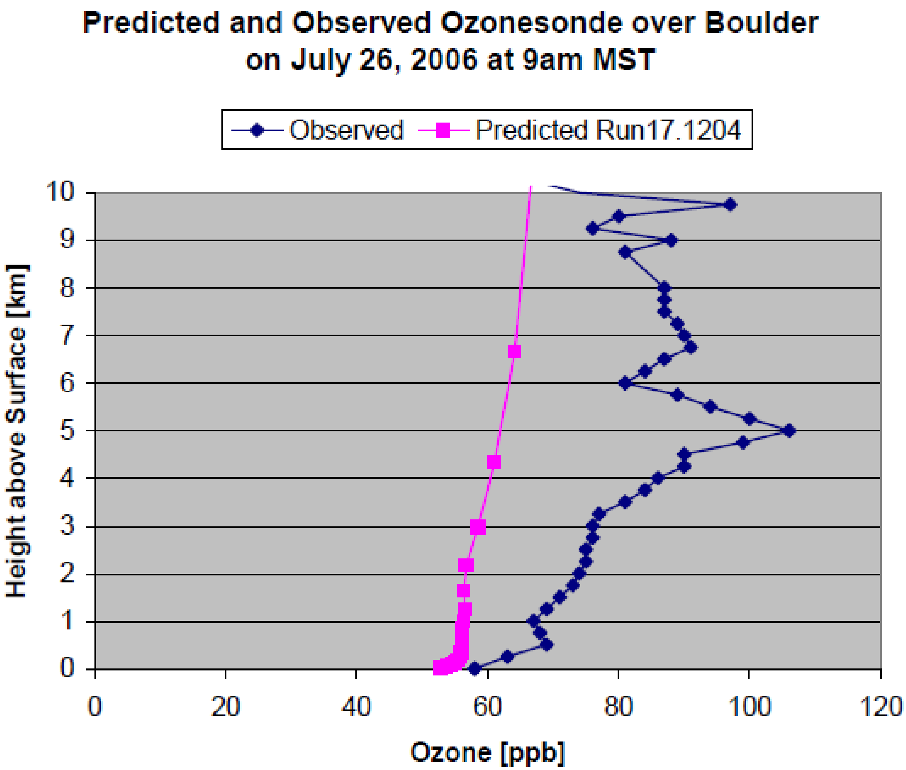
Colorado 2006 MPE

- Operational MPE and weight of evidence analysis for summer 2006 CAMx ozone modeling.
- Limited data available for diagnostic model evaluation:
  - VOC/NOx data at two Denver sites, but NOx data not available at Weld County sites with speciated VOC measurements.
  - Ozonesonde data at Boulder for six days.
- Model performed best for June 28-29 but had large negative bias and spatial errors for other ozone episodes.
- More monitoring data is needed to evaluate causes of model bias.

Boulder Ozonesonde data

Two of the weekly ozonesonde launches coincided with modeled ozone episodes – results inconclusive but failure of model to simulate high O3 aloft on June 26 might contribute to bias.





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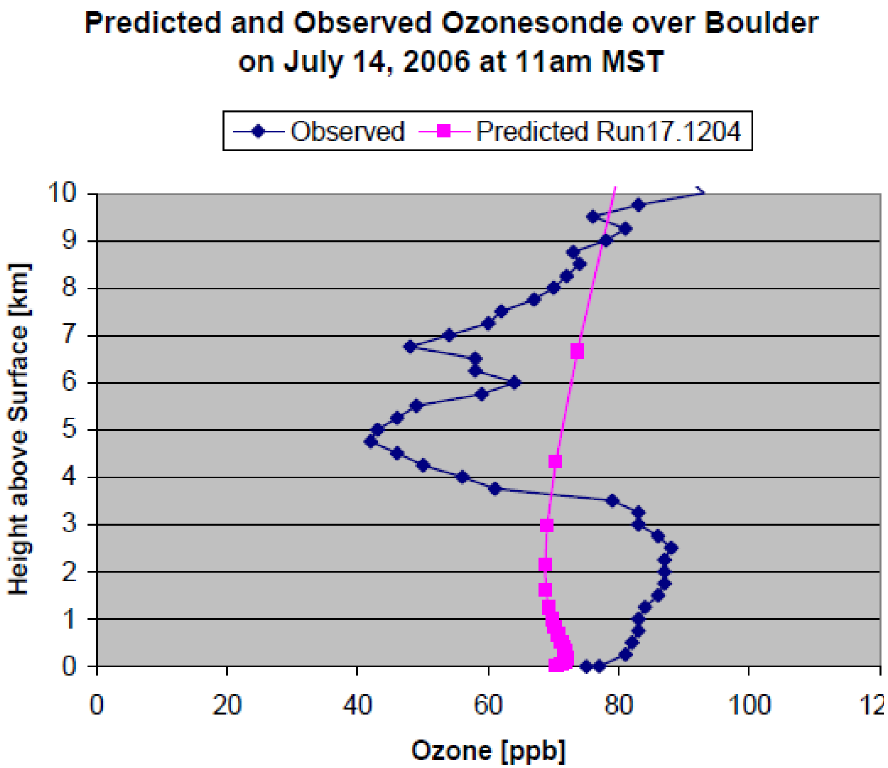
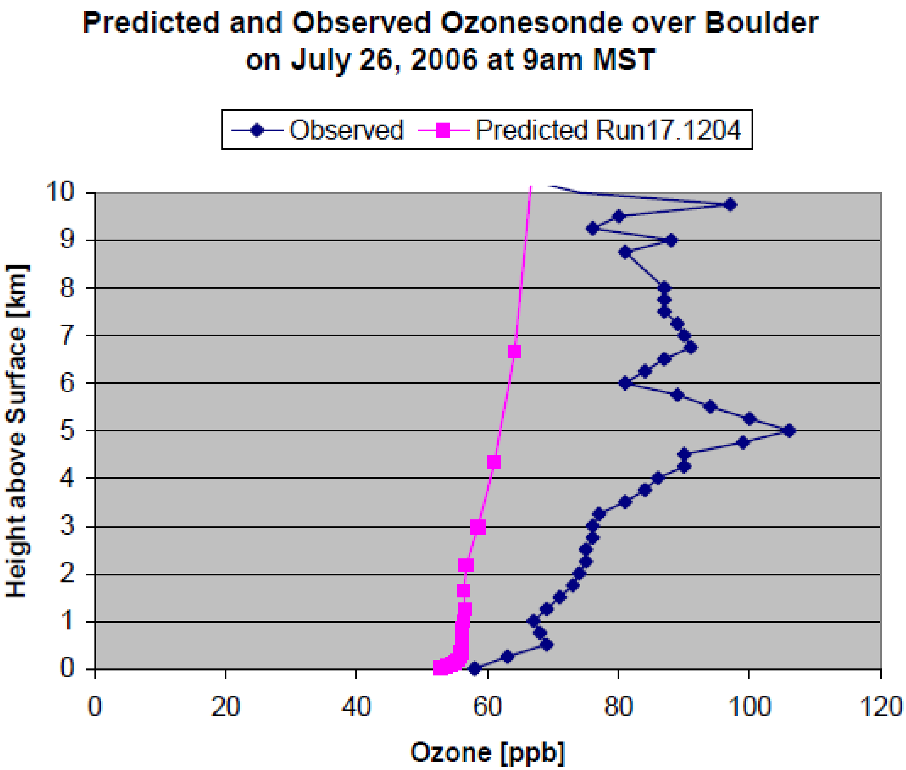
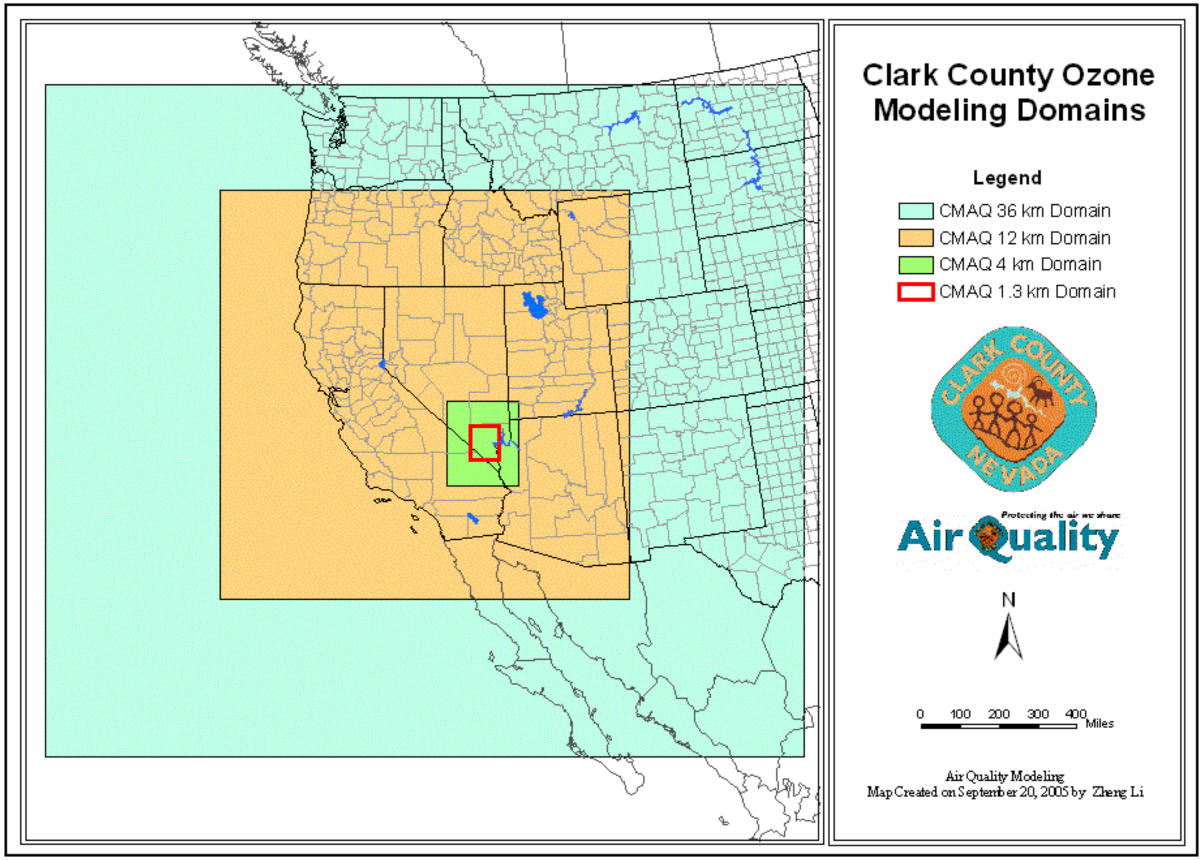




Clark County CMAQ Ozone Modeling



Four nested grids
36, 12, 4, 1.3 km

19 vertical layers

Lambert Conformal
Center: 37°, -118°
Parallels: 33°, 45°

Modeling Periods
May 19 – June 15, 2003
June 20 – July 23, 2003

Inputs:
CC SIP Inventories
PRO Inventories
2002 GEOS-CHEM BC
7 day spin-up
TOMS
MM5

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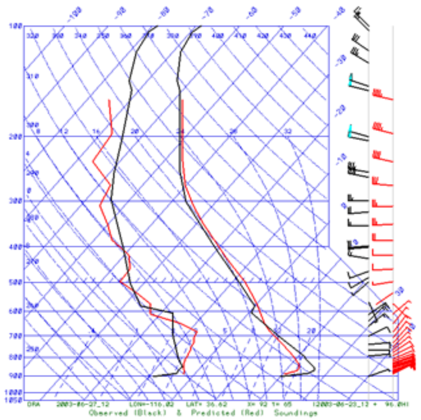
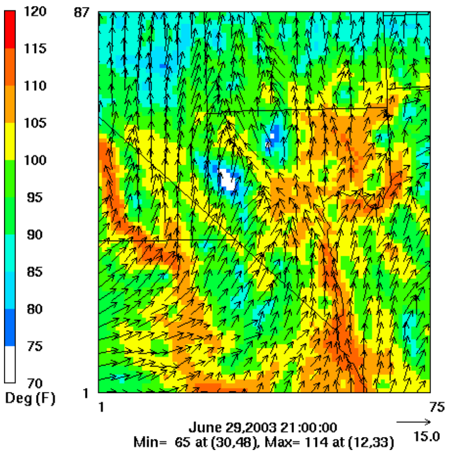
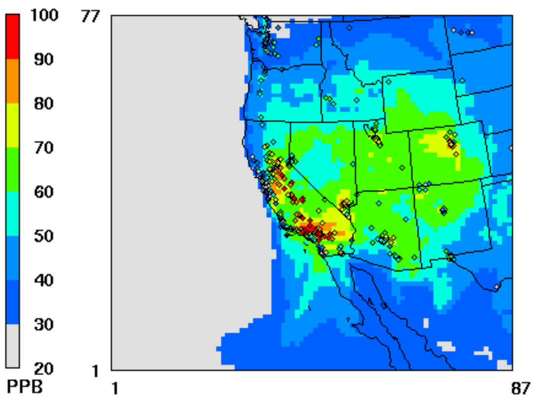
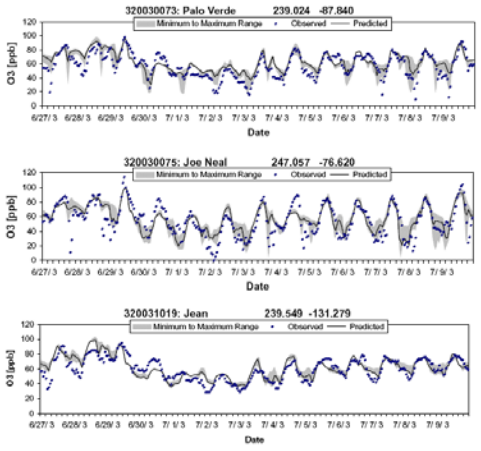
Model Performance Evaluations





Statistical and graphical analyses were performed. It was found that the modeling system (MM5/CMAQ) provides an adequate representation of key atmospheric processes associated with ozone formation and is suitable for use in examining ozone attainment issues in Clark County.





	Obs. Peak	Pred. Peak	Peak Accuracy	Bias (%)	Gross Error (%)
6/27/2003	91	96.9	6.5	1.5	11.8
6/28/2003	91	107.4	18.0	12.0	15.2
6/29/2003	114	103.1	-9.5	-1.7	10.4
6/30/2003	84	74.5	-11.3	-15.3	15.4
7/1/2003	70	77.2	10.2	-11.7	15.1
7/2/2003	68	84.4	24.1	-9.1	16.9
7/3/2003	87	88.6	1.8	2.5	8.6
7/4/2003	89	89.9	1.1	-5.5	9.5
7/5/2003	88	90.6	3.0	-7.7	9.2
7/6/2003	82	87.5	6.7	-1.0	8.9
7/7/2003	88	92.5	5.2	-2.6	6.8
7/8/2003	85	93.7	10.3	1.1	6.8
7/9/2003	104	100.6	-3.3	1.1	9.6
7/10/2003	95	89.8	-5.4	4.4	9.1
7/11/2003	73	82.3	12.7	-4.0	8.0
7/12/2003	81	83.2	2.8	-9.0	10.7
7/13/2003	83	78.4	-5.6	-9.2	10.1
7/14/2003	71	73.4	3.3	-2.5	4.2
7/15/2003	65	76.7	18.1	-2.0	5.7
7/16/2003	75	68.9	-8.2	-16.5	16.7
7/17/2003	96	76.5	-20.3	-15.9	16.6
7/18/2003	93	83.7	-10.0	-13.2	13.3
7/19/2003	83	69.8	-15.9	-26.9	27.0
7/20/2003	76	93.5	23.0	-7.8	15.1
7/21/2003	115	104.8	-8.9	-13.7	15.2
7/22/2003	90	64.2	-28.7	-35.7	35.7

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Summary of Study Findings

- Clark County is significantly impacted by ozone transport from California and other states in the western U.S. and there may be significant long-range ozone transport from areas outside the western U.S.
- Data analyses from the technical studies support the modeling results
- Wildfires can have a significant impact on ozone concentrations in Clark County and other areas within the Western Region
- Our study findings relating to ozone transport and wildfire impacts are consistent with studies done by WESTAR and EPA
- Our study results demonstrate there is a need for a regional approach to address wildfire impacts and regional transport of ozone

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Recommendations

- Additional ambient data needed for diagnostic model evaluations for intermountain states. Highest priorities are:
  - VOC/NOx and HCHO/NO2 data at multiple sites to evaluate ozone production and ozone sensitivity to VOC and NOx.
  - Continuous measurements of tropospheric O_3 profiles at a network of western sites to evaluate O_3 transport.
- Ozone is a regional pollutant in the west and coordinated regional/national efforts are needed to plan ambient monitoring studied for evaluation of long range transport.
- Need coordinated modeling and planning efforts for western states and coordination of WRAP WestJump &Three-State Data Warehouse.
- Recent or planned updates to photochemical mechanisms and models might significantly improve model performance.