Modeling Challenges for Ozone Exceptional Event Demonstrations

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Disclaimer: No positions expressed here represent official EPA policy

What I’ll Try to Cover

- Exceptional Events: Clean Air Act and Regulations
- Model Types
    - Photochemical Grid Model
    - Regression
    - Surrogate (with statistics)
    - Conceptual Model (qualitative)
- Modeling for wildfire ozone events
- Modeling for stratospheric ozone events
    - Complexities of lowered NAAQS
- Summary and Conclusions

Exceptional Events

- Exceptional events are air pollution events not readily controlled through traditional State Implementation Plan processes
- Clean Air Act Section 319 Definition
  - affects air quality;
  - is not reasonably controllable or preventable;
  - is an event caused by human activity that is unlikely to recur at a particular location or a natural event; and
  - is determined by the Administrator through the process established in the regulations . . . to be an exceptional event
- Clean Air Act Section 319 Demonstration Requirement:
  - Show that a clear causal relationship exists between the exceedances of a standard and the event to demonstrate that the event caused a specific concentration at a particular location

The “But-For” Demonstration

- To show that “the event caused a specific concentration at a particular location,” EPA’s regulation requires a demonstration show that there would have been no exceedance but for the exceptional event caused pollution
  - Implies some knowledge of what the ambient concentration would have been in the absence of the event
  - Implies some knowledge of the portion of the measurement attributable to the event
  - Could be either qualitative or quantitative
    - No explicit requirement to predict a specific concentration which would have been seen, nor to quantify the event attributable fraction
- But-For is where modeling can make the biggest contribution to exceptional event demonstrations

Ozone Exceptional Events

- Two types currently anticipated
  - Ozone enhancement due to wildfires emissions
  - Stratospheric Ozone Intrusions
- Underlying Challenge:
  - Wildfire smoke and stratospheric ozone downmixing are two major components of natural background ozone
- Exceptional Event Rule Preamble (72 FR 13569, March 22, 2007)

"Given the directive in section 319(b)(3)(B)(ii), that a clear causal connection must exist between the ''measured exceedances'' and the exceptional event, EPA believes that it would be unreasonable to exclude data affected by an exceptional event simply because of a trivial contribution of an event to air quality. Furthermore, we believe that it would be unreasonable to exclude more significant, but routine background air quality impacts, as this would disregard an important part of the public's exposure to air pollution upon which EPA's air quality standards are based."

Potential Modeling Efforts for Ozone Exceptional Events

- Model Types
  - Photochemical Grid Model
  - Regression
  - Surrogate
    - Statistical
  - Conceptual Model?
    - Qualitative vs. statistical

Photochemical modeling for Ozone and $PM_{2.5}$ Fire Exceptional Events?

- Expensive relative to what might be expected for Exceptional Event demonstrations
- Model uncertainty may be too large to accurately quantify concentration “but for” the fire
- Fire emissions are uncertain
  - Dispersion adds to the uncertainty
- However...
  - could provide useful evidence
  - academics manage to model despite expense
  - Might be justified for large events, especially if quantification needed

Regression Models

- Typically multivariate
  - 9 independent variables in Sacramento Demonstration,
  - 10-13 have been used elsewhere
- May have large residual errors
  - Inherent variability in ozone concentration can not always be predicted by meteorology

Sacramento O3 Regression Model

- Developed by STI for O3 forecasting based on 1997-2003 air quality and meteorological data
- For Exceptional Events “but for” test, fire impact estimated as difference between observed O3 and regression prediction

$$\text{1-hr Ozone} = \exp(13.72 - 0.03 \cdot \text{Clouds} - 0.04 \cdot \text{WindSpeed1} + 0.01 \cdot \text{WindSpeed2} + 0.0002 \cdot \text{WindDirection} - 0.01 \cdot \text{Pressure} - 0.02 \cdot \text{DewPoint} + 0.03 \cdot \text{AloftTemperature} - 0.009 \cdot \text{AloftWindSpeed} + 0.009 \cdot \text{TemperatureDifference})$$

Variable Abbreviations	Description
Clouds	Average hourly cloud cover from 6:00 a.m. PST to 6:00 p.m. PST where clear = 0, partly cloudy = 1, mostly cloudy = 2, and overcast = 3
WindSpeed1	Average wind speed from 6:00 a.m. PST to 12:00 p.m. PST in m/s
WindSpeed2	Surface wind speed at 00Z (4:00 p.m. PST on the previous day) in m/s
WindDirection	Surface wind direction at 00Z (4:00 p.m. PST on the previous day)
Pressure	Surface pressure at 12Z (4:00 a.m. PST) in mb
DewPoint	Surface dew point temperature at 12Z (4:00 a.m. PST) in °C
AloftTemperature	925-mb temperature at 00Z (4:00 p.m. PST on the previous day) in °C
AloftWindSpeed	925-mb wind speed at 12Z (4:00 a.m. PST) in m/s
TemperatureDifference	Temperature difference from 850 mb to the surface at 12Z (4:00 a.m. PST) in °C

Source: ARB’s Exceptional Event request Sacramento 1-hour Ozone, affected by Summer 2008; mainly from work by STI; available at http://www.epa.gov/ttn/analysis/exevents.htm

Sacramento O3 Fire Days vs. Surrogate Days

- Additional "but for" evidence: Compare fire-affected days to meteorologically similar "surrogate days"
- Similarity based on STI criteria used to predict high-O3 days: station temperatures, 500 mb height, inter-station pressure gradients; also examination of pressure charts, etc.
- Results consistent with regression model conclusions

1-hr O3, ppb Date	Folsom, CA Maximum observation	Regression model prediction	Surrogate day
6/23/2008	161	77	79
6/27/2008	129	76	84
7/10/2008	150	95	91

Source: ARB's Exceptional Event request Sacramento 1-hour Ozone, affected by Summer 2008; mainly from work by STI; available at http://www.epa.gov/ttn/analysis/exevents.htm

Multivariate Regression Residual Error

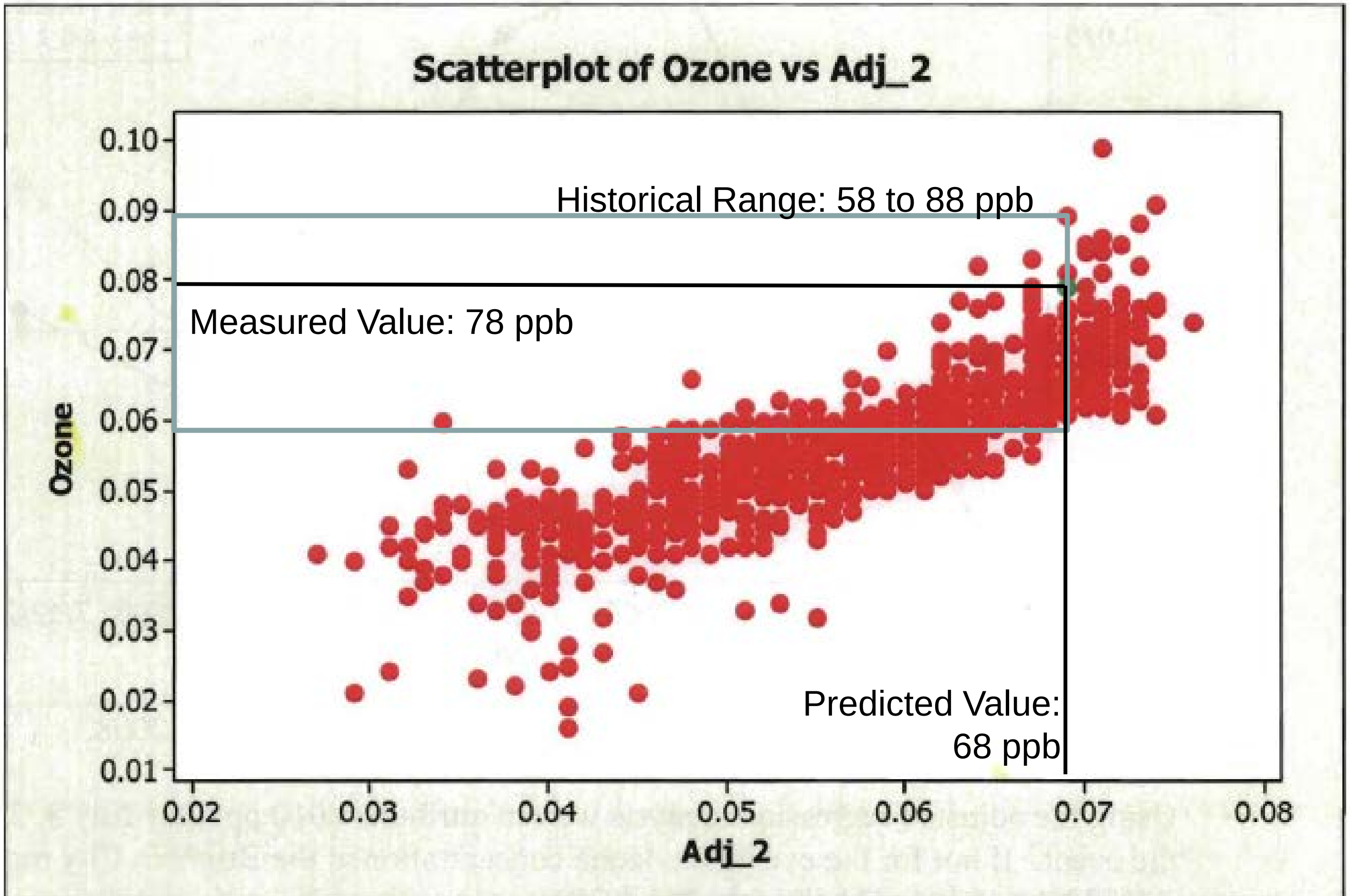


Figure 31. Scatter Plot Of Observed Versus Adjusted Predicted Ozone Values. The Green Dot Represents The July 8th 2008, Data Value.

Sacramento O3 Fire Days vs. Surrogate Days

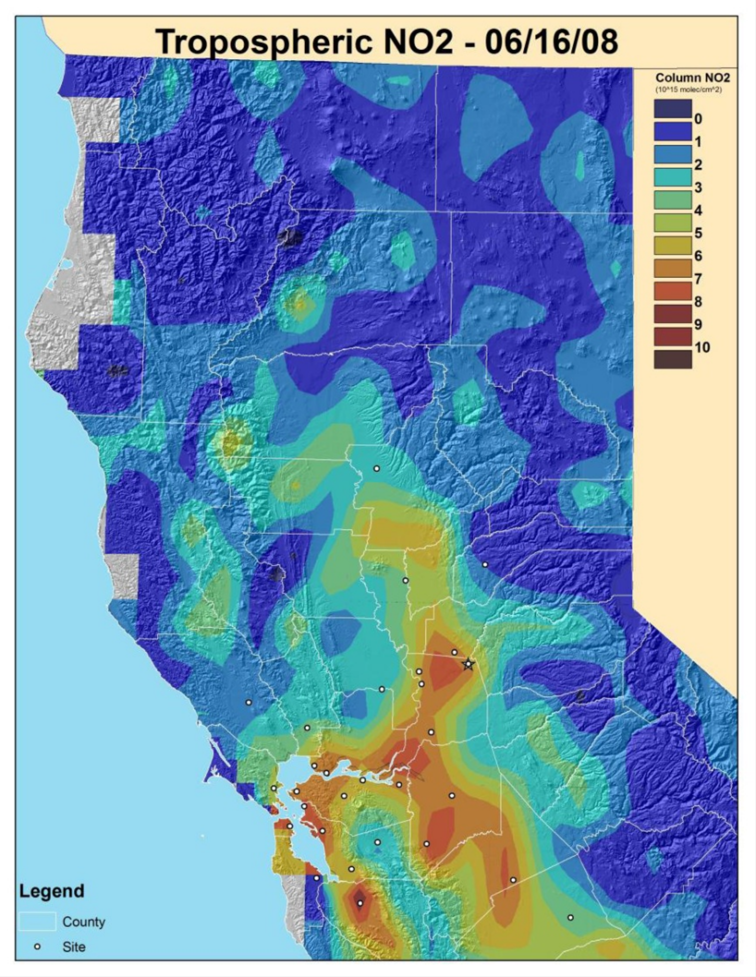
- STI criteria used to predict high-O3 days:

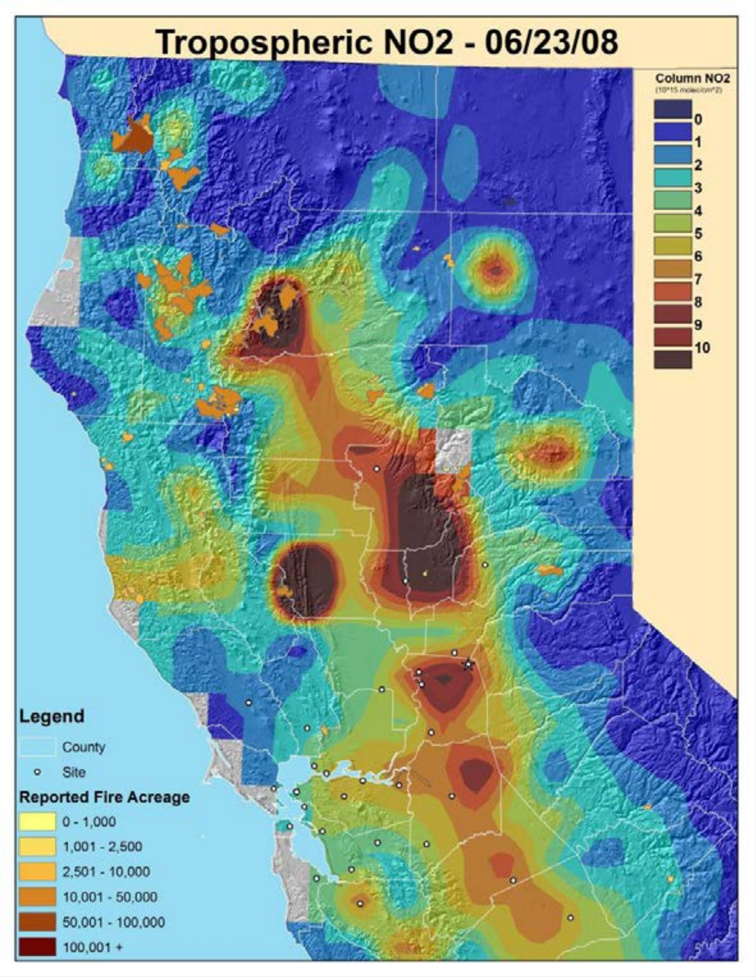
Meteorological Parameter	Criteria for 8-hour Ozone Above 0.095 ppm	Event Date (June 23, 2008)	Matching Surrogate Date (June 16, 2008)
12Z KOAK 925 mb Temp	≥25°C	21°C	19°C
12Z KSAC 500-mb Height	≥5850 m	5840 m	5830 m
KSAC High Temperature	≥93°F	86°F	84°F
9 to 11 a.m. PDT KSAC Wind Speed	<4 knots	2 knots	6 knots
9 to 11 a.m. PDT KSAC Wind Dir.	>150° and <270°	190°	211°
9 to 11 a.m. PDT KSUU Wind Speed	<15 knots	17 knots	19 knots
9 to 11 a.m. PDT KSFO Wind Speed	<10 knots	12 knots	10 knots
12 to 6 p.m. PDT KSAC Wind Speed	<6 knots	7 knots	7 knots
12Z KSFO – KSAC Gradient	<3.0 mb	3.3 mb	3.2 mb
00Z KSFO – KSAC Gradient	<4.0 mb	4.1 mb	4.0 mb
12Z KSAC – KRNO Gradient	<-2.0 mb	-2.3 mb	-1.9 mb
00Z KSAC – KRNO Gradient	<0.0 mb	0.5 mb	0.9 mb
Max. 8-hr Avg. Ozone Conc.		0.123 ppm	0.068 ppm
Max. 1-hr Ozone Conc.		0.161 ppm	0.079 ppm

Green indicates that a criterion for high ozone was not met. Note that, in general, all or nearly all criteria must be met for high ozone concentrations to occur.

OMI Tropospheric Column NO2 Concentrations on Surrogate Day and Fire Day

- O3 precursor, evidence for causal relationship and “but for”





Conceptual Model

- Conceptual model: generally, a narrative description of an episode
  - Describe the interaction of emissions, ozone chemistry, wind patterns
  - Discuss key factors and relative importance of:
    - The overall urban plume direction
    - Hour of peak ozone concentration and distance downwind
    - Typical wind flow patterns
    - Expected influence of major sources or emissions categories
    - Relationship between ozone concentrations to diurnal temperature and growth of mixing layer
    - Importance of ozone and precursors aloft
    - Multiple day carry-over of pollutants
- For EE demonstrations, could a “typical” ozone exceedance day conceptual model be developed, for comparison to that for the exceptional event day?
  - Can the “typical” day conceptual model include ranges of historical data
    - For example, “on all historical days with similar concentrations, winds were less than . . . “ for comparison to the Exceptional Event day

EPA Future Plans for Wildfire Ozone Exceptional Events

- EPA has some draft guidance documents out for stakeholder input
  - Overall Q & A document
  - High wind demonstration guidance document
  - Soliciting first round of comments by June 30
- EPA Regions 8 and 9 collaborating on wildfire exceptional event guidance
  - Emphasis on ozone impacts
  - Drafts later this year

Stratospheric Ozone Intrusions

- Historically difficult to assess
- With historic high NAAQS levels (120 ppb 1-hour average, 80 ppb 8-hour average) significant stratospheric impacts were very rare
- Lower NAAQS levels (75 ppb 8-hour average, or proposed 60 to 70 ppb 8-hour average), stratospheric impacts may be both more common, and harder to evaluate

Stratospheric Ozone Intrusions: Tools other than Models

- Unusual Monitor Trace
  - Ozone
  - RH
- Satellite Total Ozone Column
- Modeled Tropopause Height
- Ozone Soundings

Now <u>THAT'S</u> an Intrusion: Santa Rosa Intrusion, Nov. 19, 1972

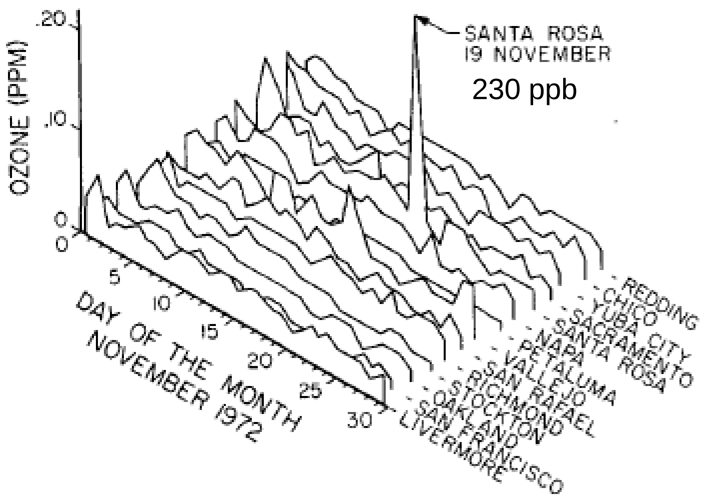


FIG. 1. Maximum hourly averaged oxidant concentration observed on each day of November 1972 at northern California monitoring stations surrounding the Santa Rosa area. (Data from California Air Resources Board, 1972.)

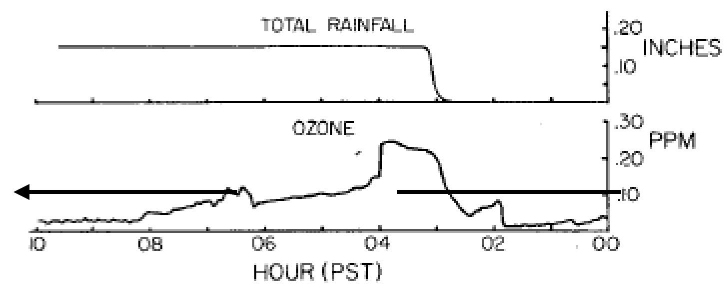
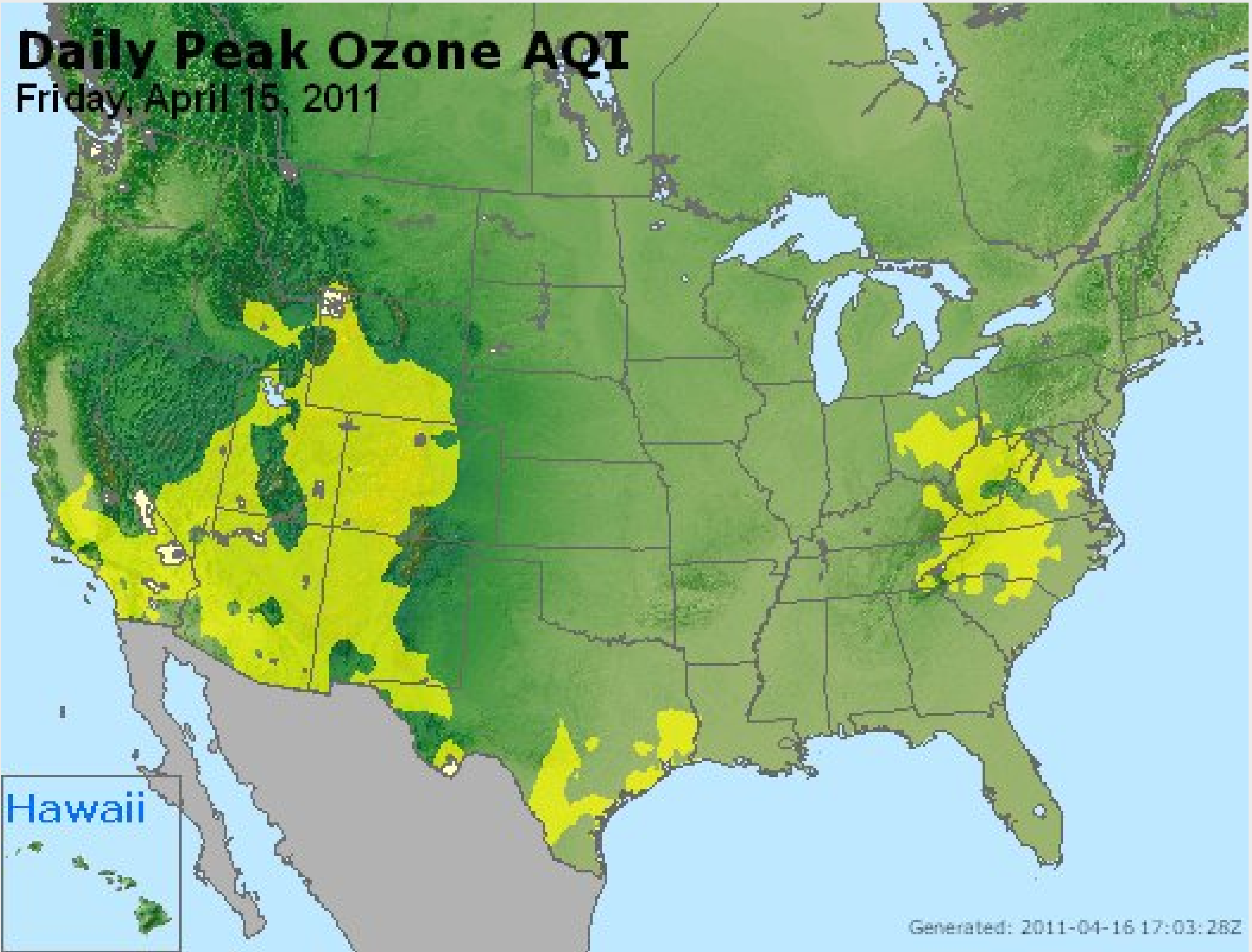


FIG. 14. Strip charts of the Santa Rosa oxidant recorder and the recording raingage at the Oakville 4SW Site for 19 November 1972. The oxidant recording is the same as that shown in Fig. 2. The location of the Oakville raingage is indicated in Fig. 13.

"The set of events that led to this episode, namely, a high-level intrusion of stratospheric air, tapping (sic) of the intruded layer in the lower troposphere by convective shower clouds, and transport of the layer's constituents by a precipitation-induced downdraft into a stagnant air mass at the ground, is most likely to occur in association with frontal passages."

Robert G. Lamb, *A Case Study of Stratospheric Ozone Affecting Ground-Level Oxidant Concentrations*, Journal of Applied Meteorology, Vol. 16, August 1977

Possible Stratospheric Ozone Intrusion Example: April 15, 2011

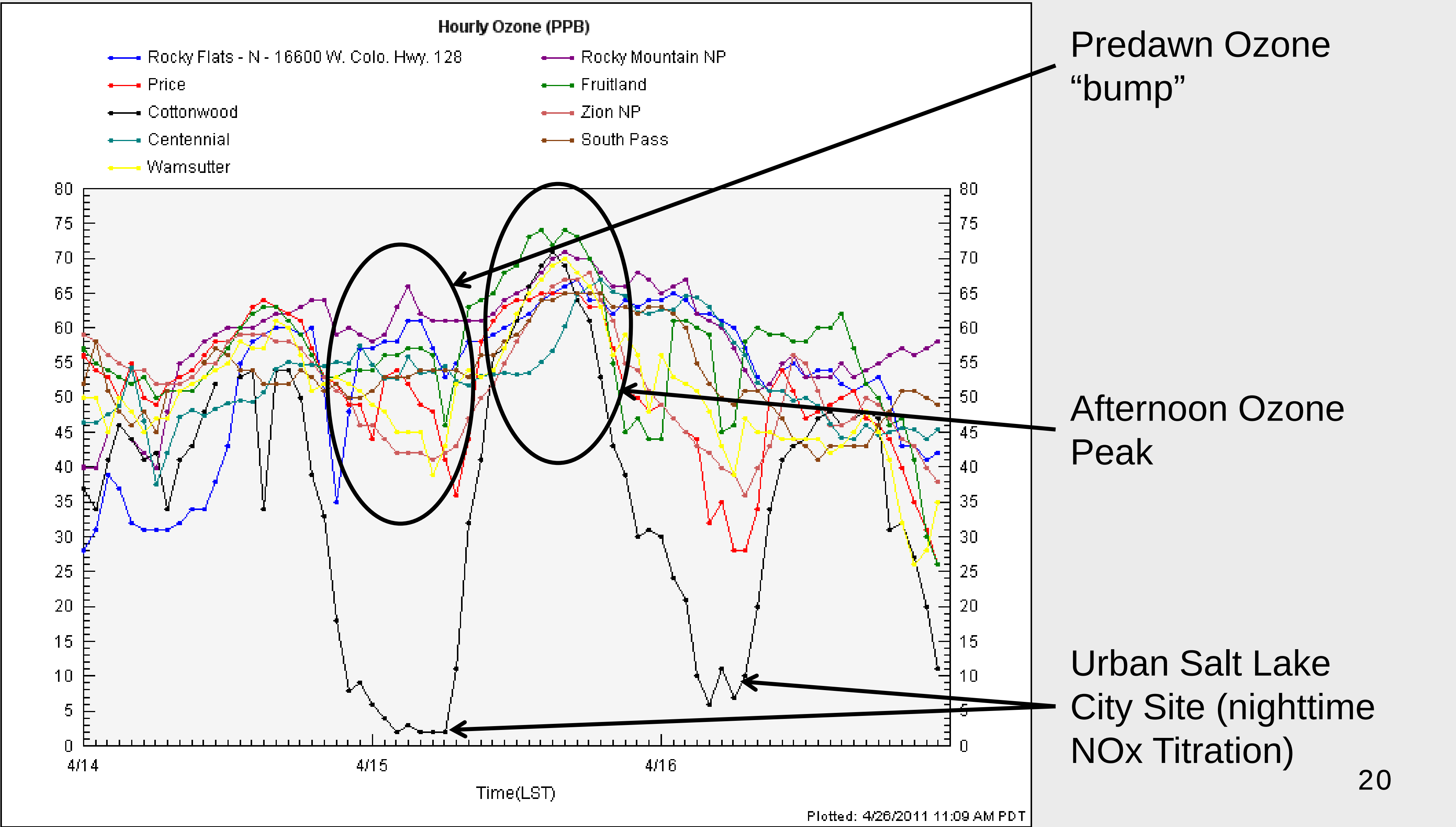


Yellow ≥ 61 ppb

Unusual Pattern:

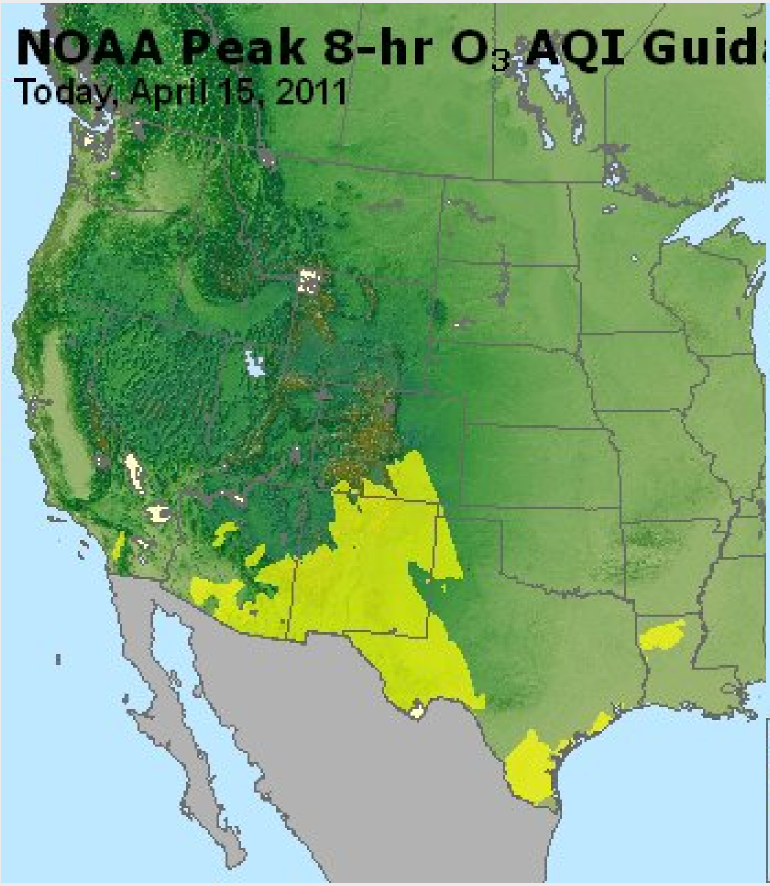
- Elevated O_3 over entire SW US
- No contrast between rural and urban areas
- No monitor above 75 ppb 8-hour average

Monitored Ozone Data, April 15, 2011

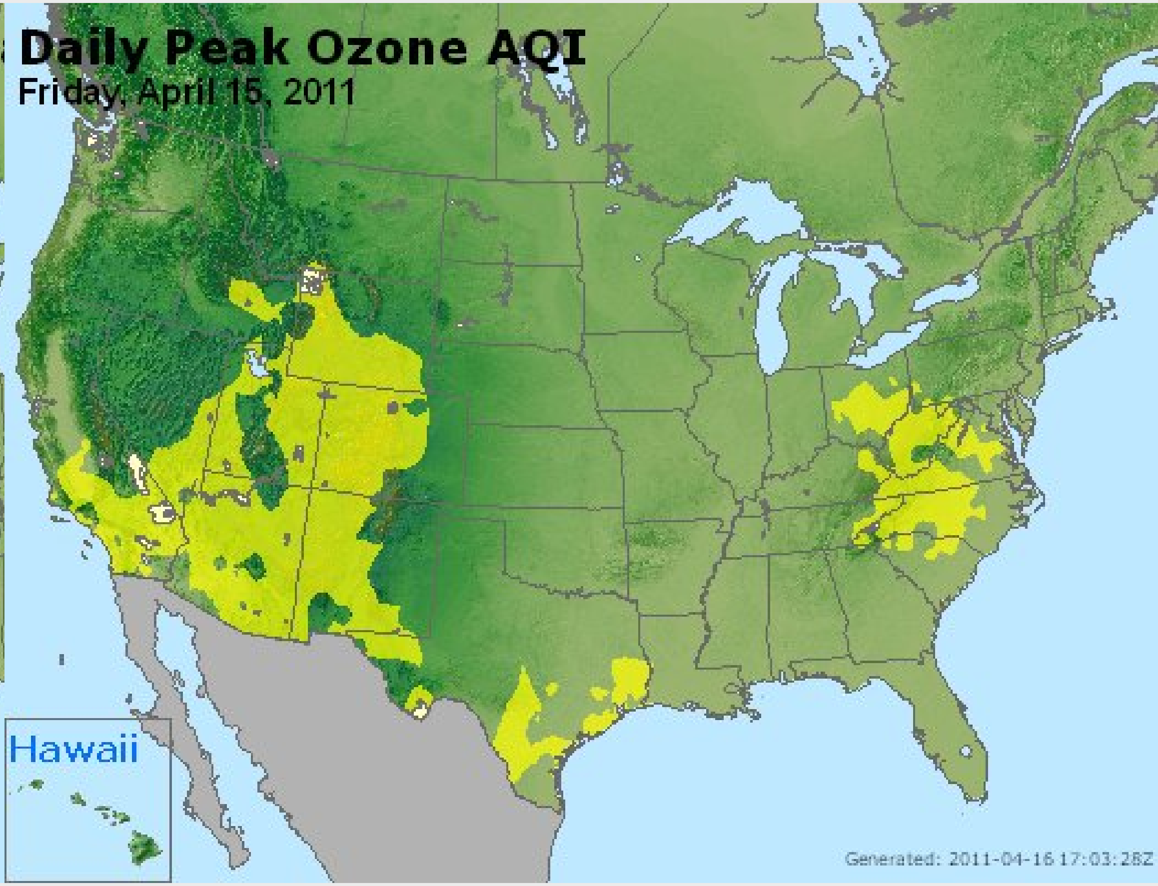


NOAA Forecast Run vs Obs.

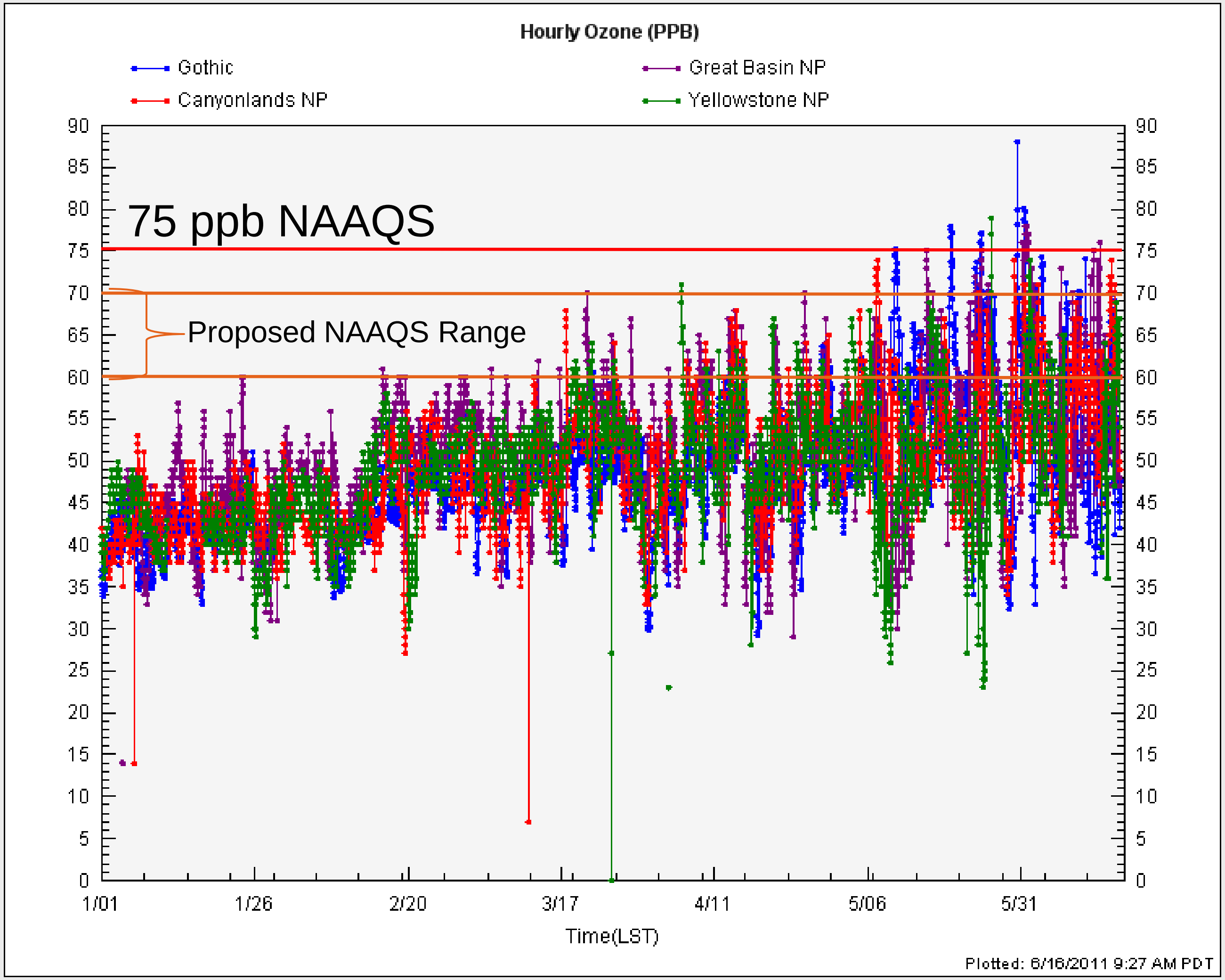
Modeled



Measured



Region 8 Rural Background



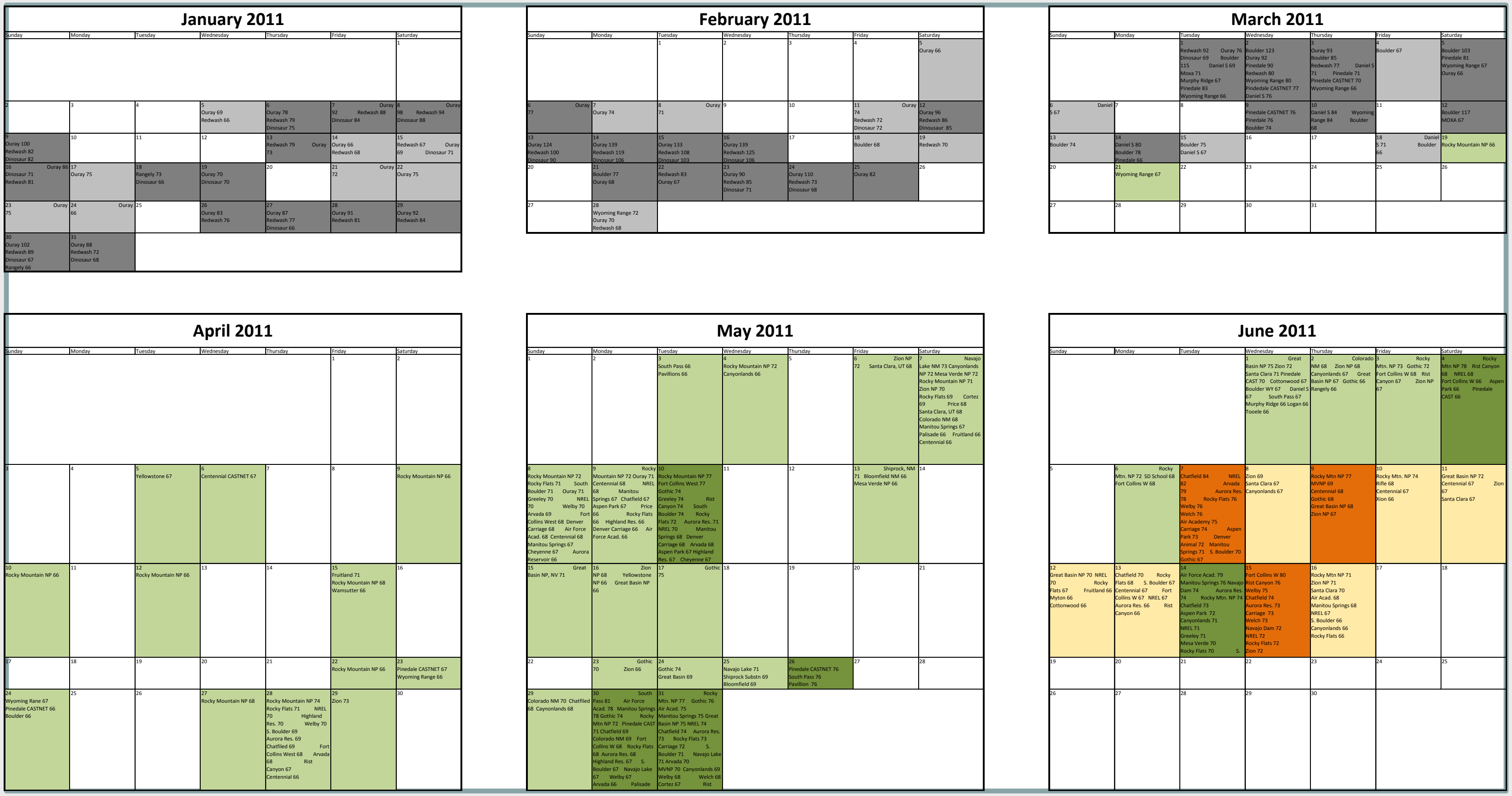
Great Basin NP
- 6,935 ft.
- Utah-Nevada Border

Canyonlands NP
- 5,662 ft
- SE Utah

Yellowstone NP
- 7,950 ft.
- NW Wyoming

Gothic CASTNET
- 9,600 ft.
- 10 m. N of Crested Butte, Colorado

Region 8/Rocky Mountains: 3 Ozone Seasons



Winter 66-75 ppb	Winter ≥ 76 ppb	Spring 66-75 ppb	Spring ≥ 76 ppb	Summer 66-75 ppb	Summer ≥ 76 ppb

Challenges for Modeling Spring Time Region 8 Ozone

- Lack of knowledge of through-troposphere boundary conditions
  - University of Alabama-Huntsville Lidar vertical profiles show more vertical ozone structure than models currently capture
- Lack of knowledge of stratosphere/troposphere exchange mechanisms and events
- Vertical transport physics within model
- Model layer limitations?
- Domain long range transport boundary conditions
- Others (audience knows better than I)

- But: Exceptional Events rule says we can’t exclude significant but routine natural contributions to elevated ozone
  - May mean we HAVE to model spring long range transport/stratospheric downmixing days for SIP development

Conclusions

- Moving from former 1-hour and 8-hour NAAQS levels to current and proposed 8-hour levels mean many more days will approach or exceed NAAQS levels
- Some days above NAAQS may be clearly non-conducive to local photochemical production
- Current models and input knowledge prevent existing models from replicating measured ozone on days without excessive local photochemistry
- With background levels near NAAQS, small increments from long range transport, stratospheric downmixing or wildfire smoke may push days over the NAAQS level
  - Current models challenged by all three scenarios
  - Exceptional Events Rule says routine incremental or significant contributions are not exceptional events
- Therefore, conflicts between a lowered NAAQS and elevated background cannot be dealt with exclusively by the Exceptional Events Rule