# Comparison of Photochemical Model Results With Ambient Air Quality Data

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# Introduction

- One of the uses for PAMS data is to compare photochemical model (e.g., Urban Airshed Model - UAM) output with ambient air quality data to assess model performance.
- Three broad types of ozone and precursor data useful for comparisons to model output include:
  - Surface air quality, including PAMS VOC, ozone, and $NO_x$ measurements
  - Aloft air quality and meteorology including PAMS upper-air meteorology and special studies data
  - Boundary conditions including PAMS VOC, ozone, and $NO_x$ measurements

# Photochemical Models (1 of 2)

- 3-D photochemical grid models are designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating physical and chemical processes that take place in the atmosphere. Example models include the urban airshed model and Models-3/Community Multi-scale Air Quality (CMAQ).
- These models use a mass balance in which relevant emissions, transport, chemical reaction, and removal processes are expressed in mathematical terms.
- Simulations are usually 24- to 72-hour periods during which episodic meteorological conditions persist.

# Photochemical Models (2 of 2)

- Steps in a typical photochemical model application include:
  - Select episodes (usually in which widespread exceedances of the ozone NAAQS occurred during typical meteorological conditions).
  - Select the modeling domain to encompass ozone monitors that reported exceedances and all major source regions.
  - Prepare model inputs using observed meteorological, emission, and air quality data for an episode.
  - Evaluate model performance.
  - Adjust model inputs and repeat the above steps.
- Once the photochemical model reproduces selected episodes satisfactorily, the model is used for analysis of spatially and/or temporally differentiated future emission control strategies and their effect on air quality in various parts of the modeling region.

# Evaluating Model Performance Using Surface Air Quality Data

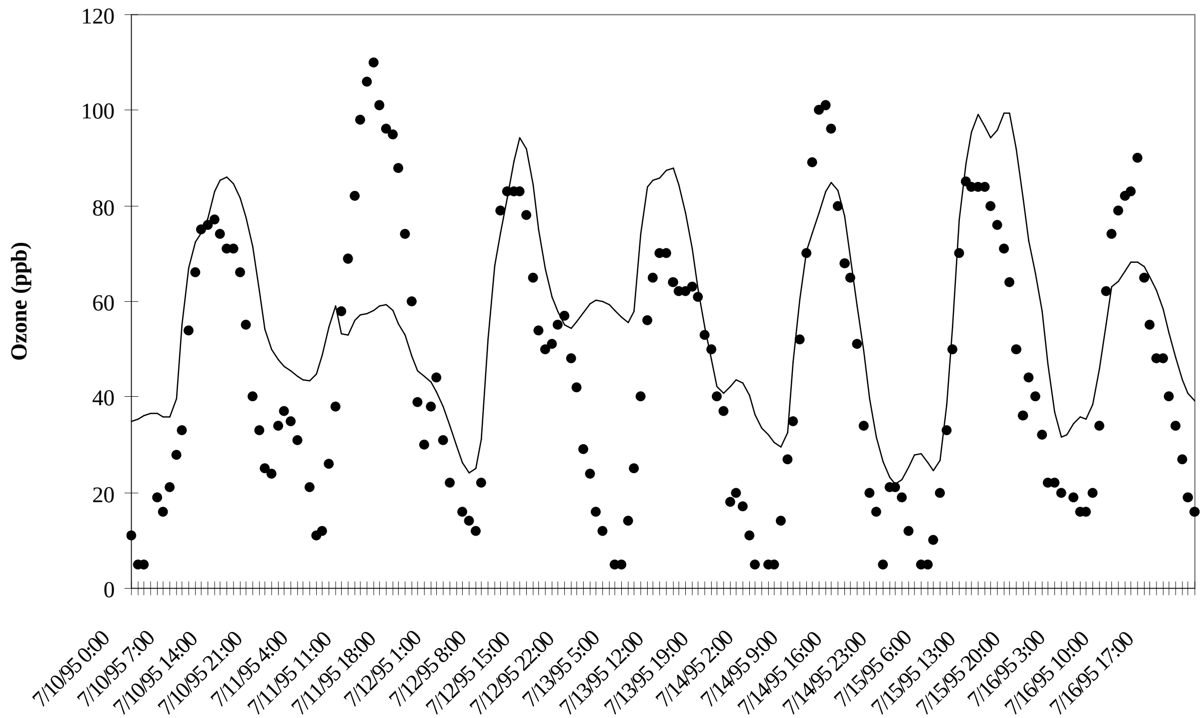
- Analytical tools with which to evaluate model performance using surface air quality data include graphical displays and statistics.
- Species of interest in these comparisons include ozone; NO, $NO_2$, $NO_x$, $NO_y$; VOC, and VOC/$NO_y$ or VOC/$NO_x$ ratios.
- Supplemental data useful for model evaluations include surface and upper-air meteorological data; emissions estimates; geophysical data; and data quality and completeness information.

# Example Graphical Displays

- Time-series plots
  - Compare observed and simulated pollutant hourly and 8-hr average concentrations for ozone, NO, $NO_2$ (or $NO_y$) and selected VOC for all monitoring sites within model domain.
  - Compare observed ozone concentrations with the minimum and maximum simulated concentrations within nine surrounding grid cells of a monitoring site for a 12 x 12 km area.
- Contour plots
  - Show simulated pollutant concentrations and observed concentrations for ozone, NO, $NO_2$ (or $NO_y$), and selected VOCs for each hour.
  - Of residuals (differences between hourly observed and predicted concentrations) for ozone.
- Scatter plots
  - Show observed versus predicted hourly concentrations.

# Example Comparisons (1 of 5)

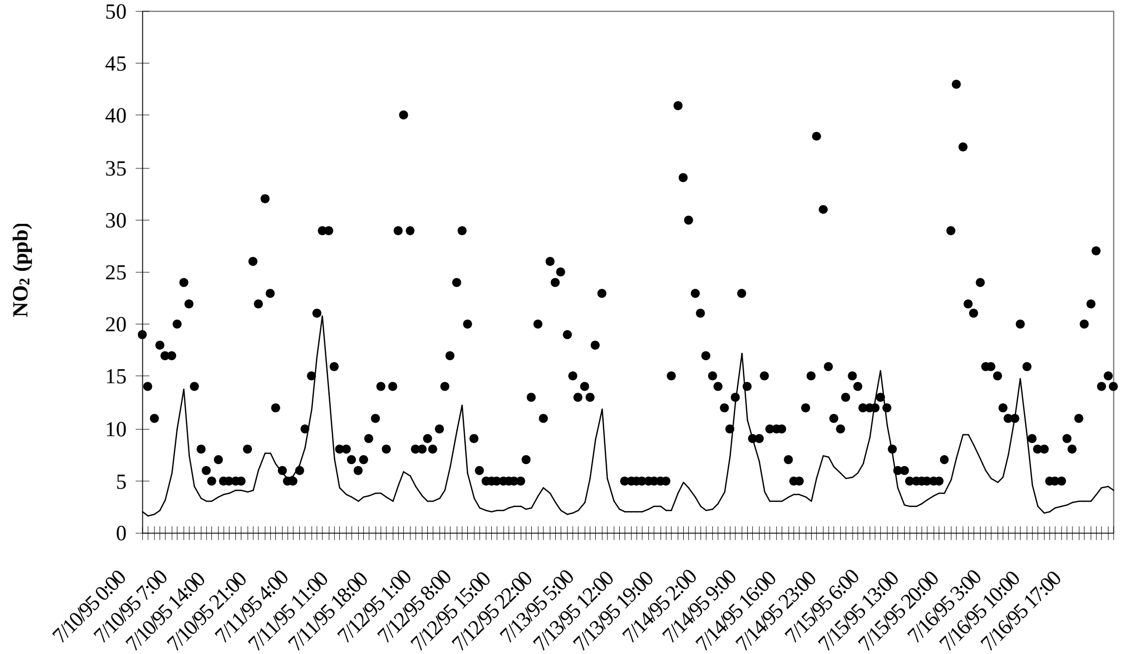
- Example time-series plot comparing observed (•) and predicted (—) hourly ozone concentrations at a site.
- In this example, the model fails to estimate the low ozone concentrations at night and significantly underestimates the peak ozone on some days.
- These types of plots can help explain biases in 8-hr versus 1-hr ozone concentration predictions.




MacDonald et al., 1998

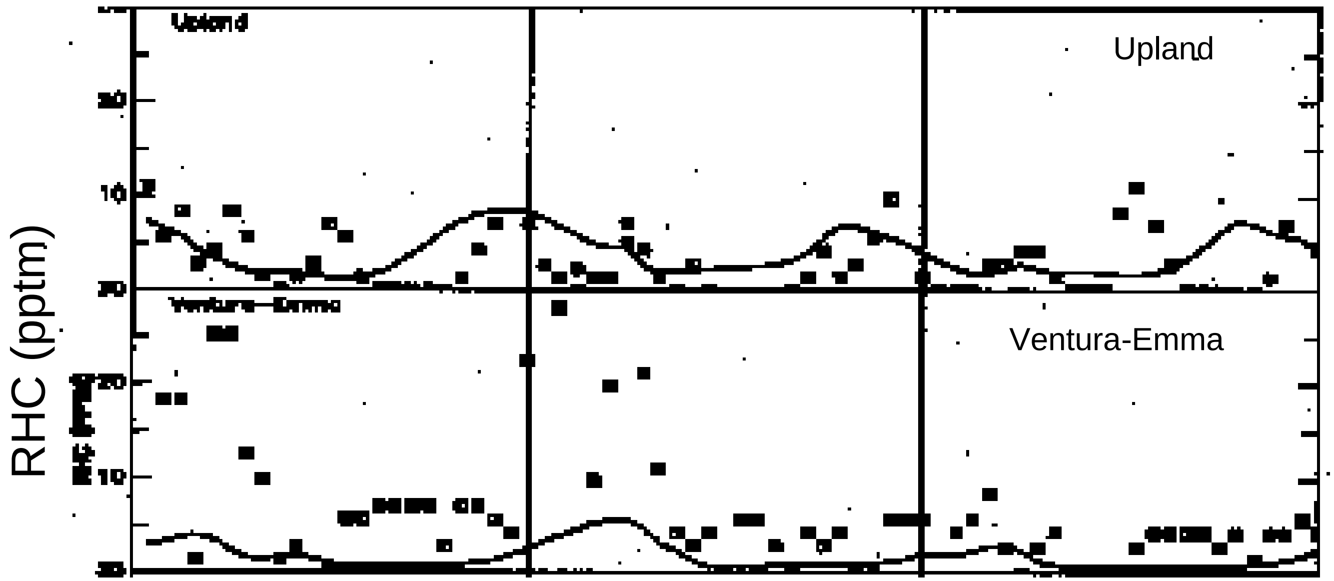
# Example Comparisons (2 of 5)

- Example time series plot comparing observed (•) and predicted (—) hourly $NO_2$ concentrations at a site.
- In this example, there are two distinct peaks of $NO_2$ observed on all days and the evening peak is always greater than the morning peak. The model underestimates the morning peak and completely misses the evening peak on all days.
- These plots should also be made with NO data.



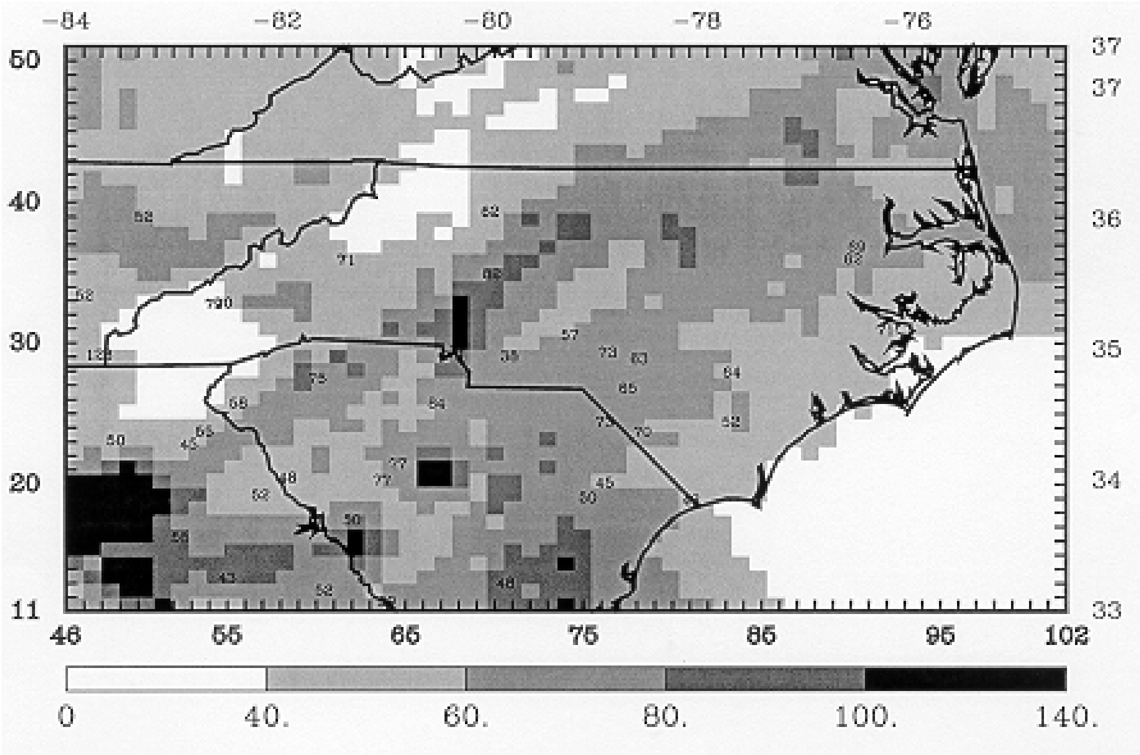

MacDonald et al., 1998

# Example Comparisons (3 of 5)




- Example time series plot comparing observed ( ■ ) and predicted (—) reactive hydrocarbon (RHC) concentrations (in pptm) at two sites in Southern California (Cassmassi et al., 1994). The solid line is the distance-weighted mean value (i.e., average of results from 4 grid cells). The model appears to frequently underpredict peak RHC concentrations.
- For RHC comparisons, the ambient data and model predictions need to be placed on the same basis (i.e., same species).

# Example Comparisons (4 of 5)

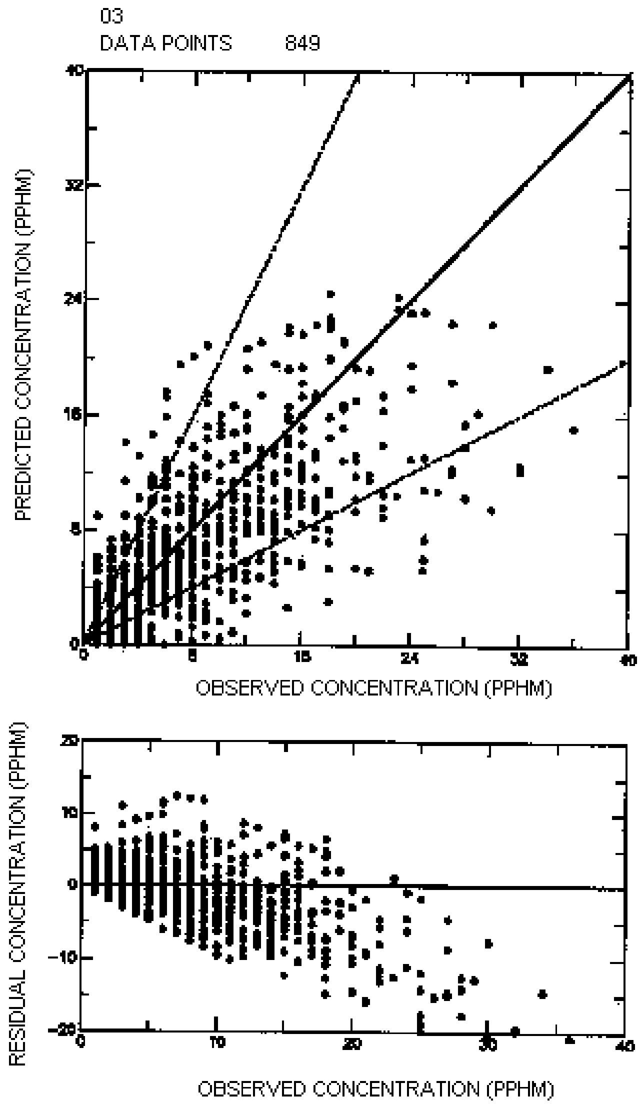


MacDonald et al., 1998

- Example spatial plot of predicted 8-hr ozone (ppb) from 1000 to 1600 EST on a summer 1995 day with observed values shown numerically for North Carolina. In this example, the spatial distribution of 8-hr ozone estimated by the model does not agree well with the observed distribution.
- Contour or spatial plots can also be made of differences between observed and predicted values. For example, the observed concentrations could be contoured and gridded, the difference between predicted and gridded observed values prepared, and the difference plotted.

# Example Comparisons (5 of 5)

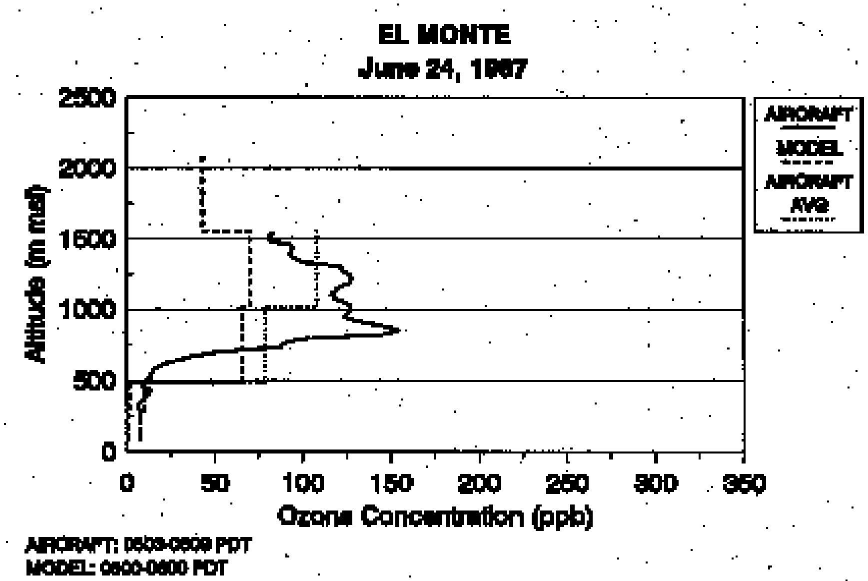
- This example shows a scatter plot of the predicted and observed ozone concentrations (top) and the residual ozone concentrations as a function of observed concentrations (bottom) for a selected day in Southern California (Cassmassi et al., 1994).
- In general, the model predictions were biased low (i.e., negative residuals) at higher observed ozone concentrations. This means the model underpredicts the peaks which are of interest because they are routinely compared to the level of the NAAQS.



# Comparing Model Results With Aloft Air Quality Data (1 of 2)

- Knowledge of pollutant concentrations aloft is important for understanding the evolution and sources of ozone concentrations measured at surface-based monitoring sites.

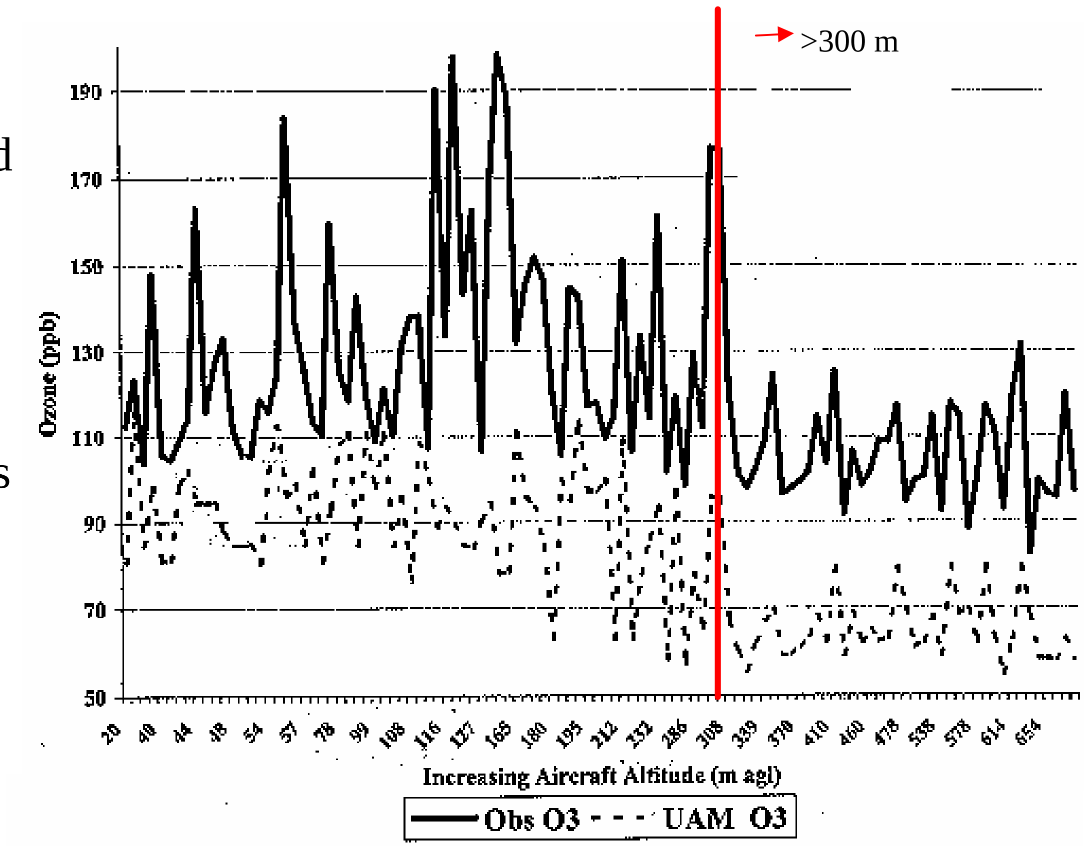
- The characteristics of aloft pollutant concentrations and the results of comparisons between simulated and measured concentrations (when available) can provide insights into ways to improve model representations of what is occurring in the atmosphere and ways to improve model performance evaluations.




Vertical profile of ozone concentrations measured by aircraft spiral compared to the urban airshed model averages for the afternoon of June 24, 1987 (El Monte, California). The 15-meter vertical average aircraft data, 5-layer model predictions, and model-layer averaged aircraft data are shown (Roberts et al., 1993b). In this example, the model predictions are lower than measured concentrations aloft.

# Comparing Model Results With Aloft Air Quality Data (2 of 2)

- In this example, aircraft-observed ozone concentrations were compared to urban airshed model (UAM) predictions for a July 1995 day in the Lake Michigan area.
- While the UAM underpredicts ozone concentrations aloft on this day, the model does simulate a decrease in ozone concentrations above about 300 meters as was observed.




Note that this data display is unique in that aircraft altitude is expressed on the x-axis in m agl and ozone concentration on the y-axis in ppb. The flight was from Ft. Wayne, IN, to Oshkosh, WI, over Lake Michigan on the afternoon of July 12, 1995. Data were sorted by altitude. (Adamski, 2000)

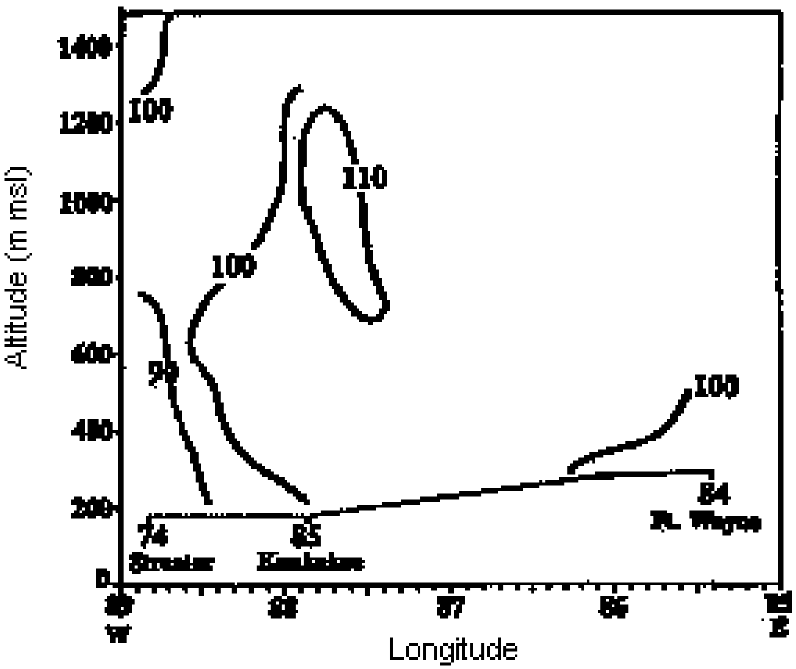
# Air Quality at Regional Boundaries (1 of 3)

Past studies have shown the following when investigating air quality at regional boundaries:

- Surface air quality data alone are not necessarily sufficient.
- Regional models often underpredict ozone at upwind boundaries.
- It is important to investigate precursor concentrations as well as ozone at the boundaries.
- The definition of a regional boundary affects the data analysis – how far upwind of the region does one consider the boundary?

# Air Quality at Regional Boundaries (2 of 3)

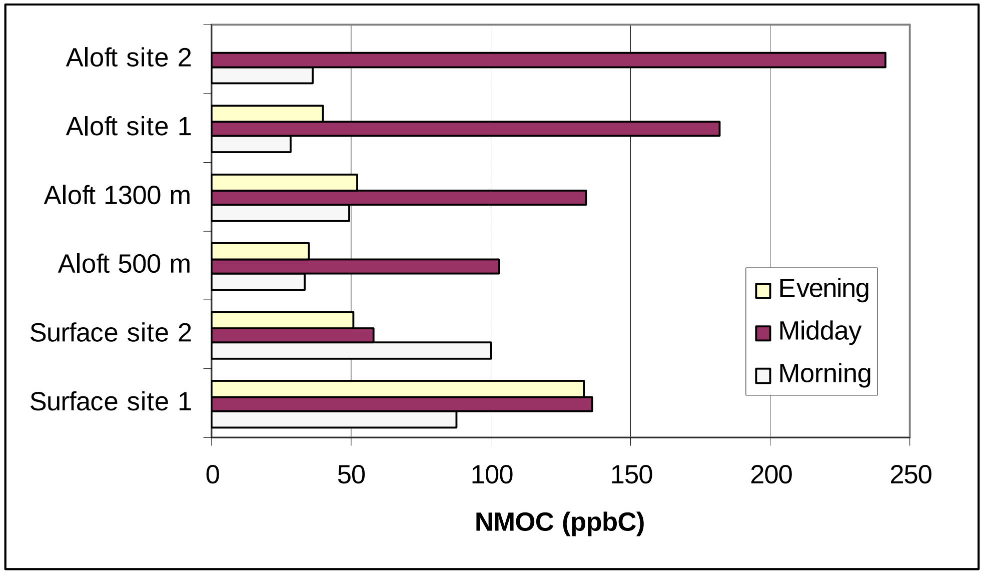
- When the data are available, aloft ozone and precursors at a regions boundary should be investigated. These data are important for understanding transport.
- In this example in the Lake Michigan area during the summer of 1991, aloft ozone concentrations were typically between 70 and 110 ppb all day; these concentrations are well above typical clean air background concentrations of about 40 ppb. Surface ozone concentrations at this boundary were typically lower than those measured aloft.




Surface and aloft ozone concentrations along the 1991 Lake Michigan Ozone Study southern boundary during the evening of July 18, 1991 (1745-1918 CDT). Ozone concentrations were hand contoured. (Roberts et al., 1994).

# Air Quality at Regional Boundaries (3 of 3)

- In this example in the Lake Michigan area during the summer of 1991, hydrocarbon and carbonyl compound data collected at the surface and aloft along the southern boundary of the study region are shown.
- Aloft NMOC concentrations were typically higher aloft than at the surface during the daytime at these sites.




Aloft and surface NMOC (NMHC + carbonyl compounds) concentrations along the 1991 Lake Michigan Ozone Study southern boundary in the morning, midday, and evening on July 18 (Roberts et al., 1994).

# Summary

- Comparisons of model output and ambient data should be performed with ozone and ozone precursors, including NO, $NO_y$, and speciated VOC.
- Investigation of surface and aloft ozone and ozone precursor concentrations should be performed at domain boundaries.

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Models-3/EMAQ home page: *http://www.epa.gov/asmdnerl/models3/*

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