

Overview of Model Evaluation Plans for CMAQ FY04 Release

Alice Gilliland*

Atmospheric Sciences Modeling Division
NOAA - Air Resources Laboratory
Research Triangle Park, NC

* On assignment to the National Exposure Research Laboratory, U.S. EPA.

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

Model Evaluation Team

Brian Eder (Team Lead)

Robin Dennis

Shawn Roselle

Robert Gilliam

Prakash Bhave

George Pouliot

Jenise Swall

Peter Finkelstein

John Irwin

Alfreida Torian

Steve Howard

Comprehensive evaluation approach to consider...

- How well does the model perform overall?
- What does the evaluation tell us about specific model processes and inputs (meteorology, emissions)?
- How will the model behave in regulatory emission control scenarios?
- How sensitive are the responses to different model specifications (e.g., chemical mechanisms, vertical grid structure)?
- What information can be fed back to model development?

Evaluation Plan Summary Outline

- Current Status:
 - Annual 2001 36km national simulation to be completed by April, 2004
 - CB4 chemical mechanism will be used (in collaboration with OAQPS)
 - MM5 version 3 meteorology completed, emissions underway
 - Additional simulations planned for winter and summer 2002

- Evaluation Plan for CMAQ Inputs:
 - Meteorology
 - Emissions

- CMAQ Evaluation:
 - Performance Evaluation (Eder presentation)
 - Diagnostic Evaluation (Dennis presentation)
 - Spatial and Temporal Analyses
 - Sensitivity Studies
 - Chemical mechanisms
 - Vertical Layer testing
 - Emission control strategies

Evaluation of CMAQ Inputs: Meteorology

Surface-Based

- 2-m Temperature
- 2-m Specific humidity
- 10 m wind (speed, direction)
- Hourly precipitation

Upper-Air

- Boundary layer wind profiles
- Boundary layer temperature profiles
- Specific humidity profiles

Evaluation will consider ...

- Full-domain summary
- Regional, local, and geographic-based summary
- Diurnal, synoptic, monthly and seasonal performance

Evaluation of CMAQ Inputs: Emissions

- Emission processing errors
 - gridding, chemical speciation, temporal allocation
 - diurnal and daily average emissions for key species
- Non-reactive particulate matter
 - Augment existing inventory by speciating primary PM_{2.5} emissions based on peer-reviewed literature (*elemental carbon, aluminum, barium, cadmium, calcium, chromium, copper, iron, lead, manganese, nickel, rubidium, silicon, sodium, strontium, tin, titanium, vanadium, zinc*)
 - Comparison with STN network observations
- Inverse modeling for seasonal NH₃ emissions

Performance Evaluation for CMAQ

- Compares model predictions at all observational network locations
- Summary statistics include R^2 , RMSE, Mean Bias, Normalized Mean Bias, and more...
- Comparisons made for O_3 , HNO_3 , SO_4 , NO_3 , NH_4 , EC, OC, ...
- Brian Eder's presentation summarizing performance evaluation for FY03 release will follow
- Summary comparison of model performance at all monitors can identify major problems to troubleshoot

Diagnostic Model Evaluation for CMAQ

- Comparison of model predictions to observations at intensive field sites (e.g., SOS, PM supersite campaigns) for July 2001
 - Chemical ratios and indicators considered: ozone production efficiency and response curve
 - Analyses designed to identify processes and/or inputs responsible for model predictions
 - High temporal resolution (hourly)
 - Low spatial density of data
 - 12 km CMAQ runs for this period
 - Special configuration of CMAQ
- Sensitivity analyses
 - Model responses to individual processes or inputs
 - Model against model comparisons for control strategy responses
- Box-model comparisons (photochemical, PM)
- Robin Dennis' presentation on diagnostic evaluation plans will follow

Spatial and Temporal Analysis for CMAQ

■ Spatial comparison

- Observational data spatially interpolated (e.g., kriging)
- Geographical areas identified where model performance better/worse
- Consider 1-hr and 8-hr max for O₃ and 24-hr average for aerosols, monthly assessment

■ Temporal comparison

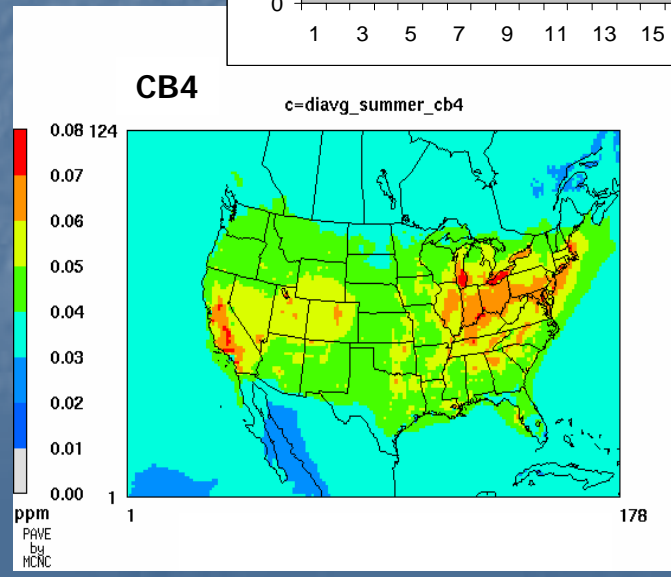
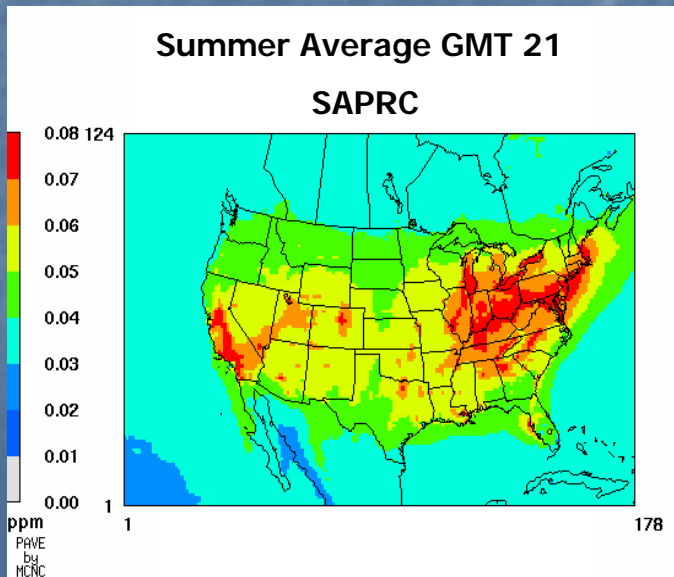
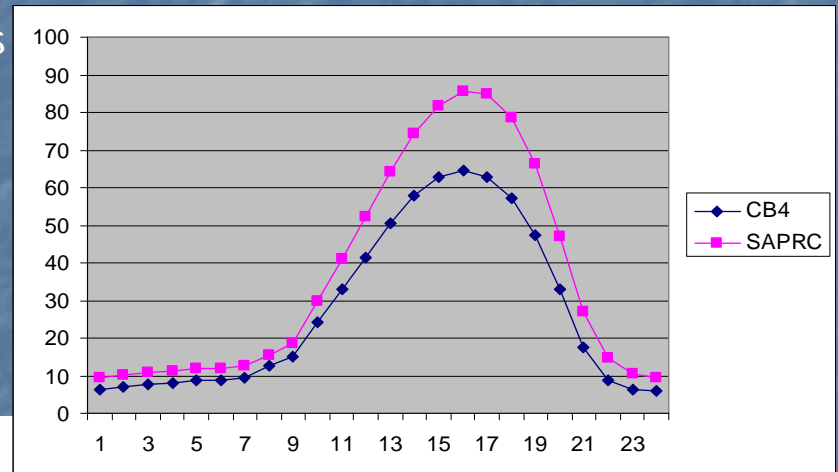
- Apply standard time-series analysis techniques such as the Kolmogorov-Zurbenko (KZ) filter
- Consider model performance at separate time-scales (seasonal/monthly, synoptic, and diurnal)
- Comparison against observations at individual locations, regions

CMAQ Evaluation: Sensitivity Tests

Comparison of Chemical Mechanisms

SAPRC vs CB4 during summer and winter cases

- Simulations performed with FY03 CMAQ
- Performance evaluation statistics
- Diurnal average differences
- Currently looking at summer O₃



CMAQ Evaluation: Sensitivity Tests

Vertical Layer Testing

- Comparison of model predictions with 14, 15, 18, 23, and 34 layers
- Simulations underway for Summer 1999 case
- Client needs require computational efficiency
 - Vertical layering an option
 - But, at what cost?
- Emission control tests included

CMAQ Evaluation: Sensitivity Tests Emission Control Strategies

- Tests using 2001 36km CMAQ domain
 - Clear Skies, Transport Rule reductions (collaboration with OAQPS)
 - 6 week simulations for different seasons
 - Chemical mechanism comparisons
- Domain-wide analyses
 - Major spatial changes
 - Relative reduction factors (RRFs)
- Diagnostic emission control strategy tests
 - Higher resolution CMAQ simulations needed
 - Identify model processes involved in response to strategy
 - Special model configurations to be used or new, development versions needed
- How will CMAQ respond to control strategies applications for States, RPOs, OAQPS?

Working schedule

- June 2004:
 - Performance evaluation for meteorology and CMAQ
 - Spatial and temporal CMAQ analyses
 - Sensitivity studies
 - chemical mechanism comparison
 - emission control strategy tests (RRFs)
 - vertical layer tests
 - nitrate prediction uncertainty characterization
- December 2004:
 - Supersite in-depth analyses
 - Sensitivity studies
 - nitrate replacement of sulfate testing
 - grid size effect on sulfate prediction (coordination with VISTA)
 - inverse modeling for NH_3
 - source apportionment tests for non-reactive $\text{PM}_{2.5}$ emissions

In Summary

- New evaluation plan constructed to support FY04 CMAQ Release for client needs and applications
- More comprehensive, fuller understanding of model performance
 - Performance evaluation, including meteorology
 - Diagnostic evaluation tests
 - Includes emission studies (source apportionment for primary PM_{2.5}, inverse modeling for NH₃)
 - Spatial and temporal analyses
- Sensitivity tests
 - Chemical mechanism sensitivity
 - Emission control strategy responses
 - Vertical layer specification
- Schedule based on June 2004 (CMAQ release) and follow-on tests December 2004