ENVIRON

Draft Report
Development of a Photochemical Modeling System for the BAAQMD to Support Ongoing Ozone Air Quality Analyses

BAAQMD MAC Meeting

September 15, 2004

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- **Original purpose:**
  - Modernize the District's modeling capabilities to align with CARB and CCOS
  - Use to develop a new photochemical modeling database to support the 2004 Bay Area SIP revision
- **Objectives of the study have shifted slightly, but the overall focus remains the same:**
  - Immediate and foremost goal:

    Provide a photochemical modeling system consistent with CARB to support on-going regulatory assessments in the SFBA and throughout northern/central California
  - Longer-range goal:

    Provide a modern tool base to build a modeling "climatology" of local/regional ozone and inter-basin transport

- **Original photochemical model protocol was developed in 2002:**
  - Provide conceptual model and episode typing for ozone events in the SFBA
  - Establish model selection
  - Plan application/evaluation methodologies
  - Provide peer and stakeholder review and acceptance of the proposed approach
- **This report provides an updated protocol to describe:**
  - Modeling systems
  - Supporting databases
  - Application methodology
  - Base case modeling results from two multi-day ozone episodes in the summers of 1999 and 2000

Key District Achievements

- Developed an air quality modeling capability for two characteristic but vastly different meteorological episodes
- Contributed significantly to CARB's compilation of the CCOS database
- Contributed significant and substantial improvements to CARB's ozone precursor emission inventories
- Fully engaged EPA, CARB, other districts, other agencies, environmental groups, and industry through the MAC
- Set the framework for a continuation of state-of-the-science photochemical modeling in the SFBA (8-hour ozone, PM2.5, toxics)

Summary and Highlights

Model Selection

- **Based upon consistency with District's preexisting modeling tools and those to be evaluated by the CARB for CCOS:**
  - Emissions Processing: Emissions Modeling System, 1995 version (EMS-95)
  - Meteorological Modeling: Regional Atmospheric Modeling System (RAMS) and PSU/NCAR Mesoscale Model (MM5)
  - Photochemical Modeling: Comprehensive Air quality Model with Extensions (CAMx)

Episode Selection

- **Carefully selected to maximize credibility and generality**
- **Selection Criteria:**
  - Ozone measurement > federal standard, representative of the region's "ozone design value" (regulatory measure of ozone levels in each air basin)
  - Representative of a class of episodes that occur frequently for greater generality of predicted changes in the design value (multiple episodes will further broaden generality)
  - Sufficient observations to determine the physical conditions that contribute to the ozone exceedances:
    - Provide data that satisfy model input needs
    - Evaluate model performance

Episode Selection

- **Regional transport:**
  - Beneficial to consider modeling episodes evaluated by CARB and other districts
- **Based upon the extensive review, and the criteria for data availability, we initially elected:**
  - July 31, 2000 (Type II)
  - June 15, 2000 (Type II) – later dropped from consideration
  - July 11 and 12, 1999 (Type I)
- **Type I: widespread ozone exceedances (east/south bay)**
  - Becoming less common
- **Type II: sharp isolated exceedances (Livermore)**
  - Becoming more common

RAMS Meteorological Modeling

- **Performed and documented by ATMET**
- **Overall, RAMS performance is consistent with past simulations of this type**
  - Errors of wind and temperature within the range expected
  - When temperatures are adequately simulated, RAMS tended to over predict wind speeds in the coastal sea breeze zones
- **Observations indicate that convergence zones are important in focusing ozone and the precursors**
  - Caused by the interaction of the on-shore sea breeze flow within the marine layer with the easterly large-scale flow forced by the subtropical high
  - Easterly flow can erode the marine layer, causing near-surface convergence zones in East Bay

RAMS Meteorological Modeling

- Convergence zones frequently do not extend to the ground

- **While error statistics were generally acceptable, there were various aspects needing significant improvements:**
  - Higher resolution than 1 km may be needed
  - Better information on irrigation patterns
  - Over-reliance on FDDA to "fix" model errors
    - Vast majority of observations at surface, but primary forcing mechanisms may not ever become apparent at the surface
    - Far too few observations aloft to adequately resolve the horizontal structure above the marine layer
  - TKE-based PBL modeling is better approach for these complex flow regimes

MM5 Meteorological Modeling

- **Performed by NOAA and BAAQMD for July/August 2000**
  - Among various MM5 simulations, overall the most accurate simulation was produced when using the Eta PBL, NOAH LSM, and observational FDDA
  - Simulated large-scale pattern was in fairly good agreement with analyses
  - Simulated low-level winds were in better agreement with observations in SFBA than in the central valley
  - Consistent performance issues were noted for winds, temperature, and humidity throughout the central valley
  - Good agreement was found between the observed and simulated boundary layer heights

MM5 Meteorological Modeling

- **Performed by CARB and BAAQMD for July 1999**
  - Used MRF PBL, 5-layer soil model, and various incarnations of FDDA
    - CARB: observational FDDA to the original unscreened meteorological dataset
    - BAAQMD tested FDDA, Eta PBL, and NOAH LSM
  - CARB run consistently performed better than any BAAQMD sensitivity test
    - MRF wind speed "phase-lag" problem clearly evident in central valley – Eta PBL fixes the problem
    - Wind direction performance was especially unacceptable on July 11-12 in the central valley
    - SFBA was too warm and the central valley was too cool
  - "Best" MM5 simulation is only moderately acceptable relative to performance benchmarks

MM5 Meteorological Modeling

- **Overall, the best MM5 simulation does not always lead to the best CAMx performance**
- **Remaining issues include:**
  - Good temperature performance leads to overly high SFBA winds, and vice-versa – MM5 deficiency?
  - There may be a need for more terrain-induced "drag" on the winds
  - The default MM5 surface roughness values as a function of land cover category are now known to be too low

Emissions Modeling

- **Performed and documented by Alpine and CARB**
- **Point and area sources:**
  - EMS-95 ° spatially, temporally, and chemically resolved TOG, NO_X, CO for CB-IV and SAPRC99
  - Day-specific emissions for July/August 2000
  - Ozone-season day emissions for July 1999
- **On-road mobile sources:**
  - ITN/DTIM/EMFAC ° spatially, temporally resolved TOG, NOx, CO (day specific)
  - EMS-95 ° chemical speciation to CB-IV and SAPRC99

Emissions Modeling

- **Biogenic sources:**
  - BEIGIS º spatially, temporally resolved BVOC (day specific)
  - BIOME/BEIS3/BELD3 º spatially, temporally resolved BNO
  - EMS-95 º chemical speciation to CB-IV and SAPRC99
- **Wildfires:**
  - Day-specific emissions were estimated for the July-August 2000 episode by the CARB
  - Standard season day fire emissions used for July 1999
- **Marine shipping:**
  - BAAQMD project team developed daily emission estimates based on SFBA ship movement

CAMx Applications

- **Developmental Simulations**
  - Since Fall 2002, ENVIRON and BAAQMD have conducted on the order of 50+ CAMx simulations
    - Test numerous emission and meteorological updates
    - Test model sensitivity to various options, treatments, and ancillary inputs
  - Discussed at the MAC meetings, documented on the project web site
  - Two consistent key performance issues:
    - 1) the emissions inventory was not sufficiently reactive
    - 2) flow fields in the SFBA were either too fast and/or insufficiently convergent in the east bay
  - Ozone under predictions of ~40 ppb incrementally improved to ~15-20 ppb after the numerous updates
  - Larger ozone shortfalls were simulated in the central valley

CAMx Applications

- **Performance Evaluation for VOC**
  - Performed by ENVIRON
  - Compared CCOS VOC measurements and CAMx predictions in the SFBA, Sacramento, and SJV
  - Large uncertainty concerning overall data quality in the CCOS VOC dataset, both for canister and GC-MS samples
  - Consistent model performance issues among the three basins
    - 1) Under prediction of total VOC (mainly PAR)
    - 2) Model lacks sufficient levels of higher aldehydes (ALD2), and often highly reactive OLE, TOL, XYL
  - Especially poor VOC performance at Parlier (Fresno)
  - Point to emission inventory as key source of problem, but cannot rule out other inputs, such as meteorological factors

CAMx Applications

- **Process Analysis**
  - Performed by Will Vizuete at UT
  - Study chemical phenomena in the eastern SFBA on July 31, 2000
  - Determined that the modeled atmosphere is NOx-rich and VOC-limited
    - VOC composition was predominantly low-reactive paraffins with a significant amount of biogenic isoprene
    - Under predicted levels of reactive VOC (by up to factors of 5) were inadequate to generate observed levels of ozone
    - Chemical NOx cycles, radical cycles, chemical production of ozone, and percentage of OH reacting with VOC were all at insufficient levels
  - The strongest possibility for low reactivity could be the lack of total VOC and/or the improper emissions speciation

CAMx Applications

- **Decoupled Direct Method (DDM)**
  - Performed by ENVIRON for July 1999 episode
  - Investigate sensitivity of ozone to IC/BC and emissions by source region
    - First glimpse into potential transport impacts
  - Key result – low model top (~5 km) and large ozone top BC (70 ppb) do not impact ozone in focus areas
  - Maximum SFBA BC sensitivity occurs in the east bay from northern boundary ozone and VOC
  - Sensitivity to emissions was much larger
    - Equivalent ozone sensitivity to anthro/biogenic VOC
    - SFBA sensitive to both NOx and VOC
    - Sacramento and northern SJV modestly sensitive to Bay Area NOx and VOC emissions (~10 ppb)

CAMx Applications

- **BAAQMD CAMx Simulations for July/August 2000**
  - MM5-CAMx couple using SAPRC99 produced reasonable predictions of ozone in SFBA
    - Under predictions continue for Sacramento and southern SJV
  - Locations of wind convergence zone related to simulated high ozone
    - MM5/5-layer LSM: central valley temperature too low, sea breeze accurate, convergence zone near Livermore (good SFBA ozone performance)
    - MM5/Noah LSM: central valley temperature accurate, sea breeze too strong, convergence zone too far east (poor SFBA ozone performance)
  - Some relatively subtle flow features can have a significant influence on the photochemical model performance

CAMx Applications

- **BAAQMD CAMx Simulations for July 1999**
  - Tests for two different MM5 runs used SAPRC99
    - SFBA: very little difference (statistically) resulted from the two meteorological realizations
    - Sacramento: larger differences among the two cases, but no clear winner in this region as well
    - SJV: both simulations very similar and show consistent under predictions – very little skill in this region
  - Test for two different chemical mechanisms used CARB MM5
    - Differences were minor on all days and for all three analysis regions (differs from J/A 2000)
  - SFBA ozone model performance is quite good using SAPRC99

Future Work

- Improve meteorological modeling
- Improve precursor emission estimates for future years
- Enhance modeling system utility and sensitivity assessments
- Assess impacts of future ozone strategies
- Assess alternative episodes