CMAQ Modeling for the CRPAQS 2000-2001 winter PM Episode: Part II

Jinyou Liang\(^1\) and Ajith Kaduwela\(^1,2\)

\(^1\)Planning and Technical Support Division
Air Resources Board
California Environmental Protection Agency

\(^2\)Department of Land, Air and Water Resources
University of California - Davis
Collaborators

- ARB:
  - Jinyou Liang
  - Qi Ying
  - Kathleen Fahey
  - Luis Woodhouse
  - Kemal Gürer
  - Paul Allen
  - Karen Magliano
  - Kasia Turkiewicz

- UCD:
  - Michael Kleeman
  - Anthony Wexler
  - Max Zhang

- CRPAQS Technical Committee

- EPA:
  - Prakash Bhave
  - Frank Binkowski

- STI:
  - Neil Wheeler

- Future:
  - Christian Seignure - AER
  - Yang Zhang - NCSU
  - Kim Prather - UCSD
  - Steven Reynolds, Envair
Overview

- Summary of previous presentation
- Progress since last September
- Corroborative Analysis
- Summary
- Future directions
185 x 185 horizontal grids, 4km x 4km size

Layer 1
11 km ASL
7 km
38 m
30 m

CMAQ Model Domain
Layer 15
Layer 2
Layer 1
Previous Presentation

• CMAQ PM model was updated for CRPAQS winter study
• 24 simulations were conducted at ARB to understand the processes responsible for the 12/25/00-01/07/01 episode.
• Simulated PM2.5, its components, and non-VOC precursors were compared with observations at surface and aloft.
Progress since last September

• 24 more runs using updated CMAQ
• VOC species evaluated with observations
• Corroborative analysis using an efficient PMF method
• FFT tool for time series analysis
Progress: Sensitivity Runs

• 24 more simulations were conducted
• Additional issues investigated
  – Chemistry: OH+NO₂+M, CH₄, NaCl, MGLY
  – Emissions: NH₃, NOₓ, AVOC, precursor reduction scenarios, Terpene
  – Meteorology: RH, LWC, observed winds & T
• Model results look better, but no dramatic changes from September PM results
MM5 vs. DWM

January 1, 2001 22:00:00
Min= 0 at (130, 23), Max= 5 at (130, 79)

January 1, 2001 22:00:00
Min= 0 at (128, 40), Max= 4 at (120, 48)
Progress: VOC Evaluation

• Emissions
  – Approximately 600 VOC species in the inventory

• Measurements
  – Photochemical Assessment Monitoring Stations (PAMS) species
    + extra: 57 organic compounds with significant concentrations
  – Stations: ANGI, BODB, BTI, FSF, SNFH, OLW, YOY

• Model
  – SAPRC99: 5 Alkanes, 2 Aromatics, 2 Olefins, 1 monoterpene
  – 2km average; 14km radius, best match
VOC Reactivity in San Joaquin Valley

02/08/2006

Planning and Technical Support Division

MIR-weighted VOC in San Joaquin Valley

VOC OH Reactivity in San Joaquin Valley
Model and observations at all CRPAQS sites

ALK1 ppb

FE=0.25
FB=0.12
R=0.81

Model and observations at all CRPAQS sites

ALK2 ppb

FE=1.19
FB=-1.19
R=0.45

Model and observations at all CRPAQS sites

ALK3 ppb

FE=0.49
FB=-0.47
R=0.73

Model and observations at all CRPAQS sites

ALK4 ppb

FE=0.29
FB=-0.26
R=0.6
Model and observations at all CRPAQS sites

- CMAQ vs. LE2: ME = 0.34, FB = 0.3, R = 0.62

- CMAQ vs. TERP: ME = 0.07, FB = 0.03, R = 0.98
Layer 1 PANd

Min = 8.9e-07 at (185,185), Max = 7.8e-04 at (124,20)

December 31, 2000 8:00:00
Current Case

• Domain-wide correlation plots
  – 4 km x 4km x 30m average vs. point
  – Gas (O₃, NO₂, NH₃, SO₂)
  – PM (PM₂.₅, NO₃, SO₄, OC)

• Time-history plots are shown for Angiola and Bakersfield (composite)
  – Gas (O₃, NO₂, NH₃, SO₂)
  – PM (PM₂.₅, NO₃, SO₄, OC)

• More graphics available at orthus.arb.ca.gov/SIP_Modeling/PM_Modeling/
Corroborative Analysis

• The NMFROC model
• A CMAQ case
• NMFROC diagnosis
• Improved results
• The efficiency of the NMFROC method
NMFROC Model: Functions

- $A \{v, s\} \rightarrow B \{v, p\} \times C \{p, s\}$; constraints
  - $A, B, C \{i, j\} \geq 0$;
  - $s > v > p$;
  - least squares error

- **Features**
  - Factorize large data matrix in a short time
  - Factors are as close to the interior of data set as possible
  - Input matrix must be non-negative, but no other assumption or inference
A CMAQ Case

Layer 1 ASO4Jf

Abnormally high PM sulfate in SJV
A CMAQ Case

• Symptom:
  – CMAQ sulfate was too high in Central Valley during CRPAQS 2000-2001 wintertime PM episode

• Possible causes
  – Emissions
  – Meteorology
  – \( \text{H}_2\text{O}_2 \) and/or \( \text{O}_3 \)
  – Catalytic pathway
  – Others

• What can NMFROC tell us about it?
NMFROC Diagnostics

• CMAQ inputs and outputs
  – Emissions of gas and PM species (34)
  – Key meteorological parameters (10)
  – Outputs of CMAQ species (32)
  – Two-week hourly data at three anchor sites

• Size of input matrix
  – $V = 76$, $S = 1008$
  – 76608 elements
NMFROC Diagnostics
Input matrix formation

• Problem 1
  – U, V, MOLI have negative values
  – Solution: coordinate shift

• Problem 2
  – Different units for emission, conc., and met.
  – Solution: similarity theory to remove the unit
NMFROC Results: Factors

• Emission factors
  – \((\text{NO}_x + \text{PNO}_3 + \text{PEC}, \text{MTBE} + \text{OLE2} + \text{SO}_2)\)

• \(\text{O}_3\) factors
  – Sunny \((\text{HNO}_3, \text{RGRND}, \text{PBL}, \text{ISOPRENE})\)
  – Rural \((\text{NH}_3, D_m, \sigma)\)
  – Cloud aloft \((\text{CFRAC}, \text{PBL}, \text{PAN})\)

• Fog and rain factors \((\text{QC}, \text{CFRAC}; \text{QR})\)

• Wet PM factor \((\text{AH}_2\text{O}, \text{ASO}_4)\)

• Plume factor \((\text{NO}, \text{SO}_2, \text{AORGPA})\)
Contributions (%) to CMAQ PM SO$_4$ in slide 6 at BAC site (P/O=1.28)
Layer 1 ASO4Jy

- Limit PM H$_2$O $\leq$ 0.1 g m$^{-3}$
- Turn catalytic pathway off
- PM SO$_4^{2-}$ reduced by ~10 folds (≈ slide 11)
Summary

• 48 winter simulations were conducted
• All PM components and precursors are evaluated against observations
• Corroborative analysis tools are employed
• More detailed look at input emissions, meteorological parameters, and observations
Future Directions

• Model improvements in (the) future
  – Boundary conditions from GEOS-CHEM
  – Alternate chemical mechanisms (e.g., CACM)
  – Internal+external mixing states, size bins

• Meteorology improvement and episode extension

• Quality assurance
  – Meteorological inputs
  – Emission inputs
  – Observed data
END of Presentation

• Question/Answer