An Operational Evaluation of the 2005 Release of Models-3 CMAQ

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CMAQ v4.5: Major Updates

1) Aerosols
   • Added sea salt (fine equilibrium; non-interactive coarse mode) -- aero4
   • Updated aerosol dry deposition algorithm
   • Updated ISORROPIA to v1.5 (25 Oct 2003) and fixed some discontinuities
   • Modified SO$_4$ used in ISORROPIA call
   • Corrected inconsistency in MINL2SG (aerodepv)
   • Corrected the EMSULF (H$_2$SO$_4$ emissions) unit conversion bug

2) Chemistry
   • Added CB4/chlorine chemistry and associated EBI solver
   • Added CB4/air toxics and SAPRC99/air toxics chemistry and associated EBI solvers

3) PBL modeling
   • Updated to use PURB (% urban) for setting minimum $K_z$

4) Clouds
   • Added new sub-grid cloud mixing algorithm/module (based on ACM)
Model Characteristics for Evaluation Simulation

- 2005 Release of CMAQ (v4.5)
- 12km × 12km Eastern U.S. domain
- 14 vertical layers
- CB-IV gas-phase chemistry, EBI solver and AE4 aerosol module
- ACM cloud module, EBI solver
- Mass continuity scheme
- MM5 meteorology (2001) processed with MCIP v3.0
Model Simulation - Emissions

- EPA’s 2001 NEI
- MOBILE6 of mobile emissions
- BEIS 3.13 for biogenic emissions
- Seasonality of NH$_3$ estimated by inverse modeling
  - Gilliland et al., available in Atmos. Env. special issue on model evaluation
- Emissions processed using SMOKE
Three Additional Evaluation Simulations

1. Annual simulation with 36km × 36km grid resolution using CMAQ v4.5 (parent domain for 12-km simulation)

2. Annual simulation with 36km × 36km grid resolution using CMAQ v4.4

3. 12km × 12km domain simulation using CMAQ v4.4 for winter and summer seasons only
Evaluation Report

• Comprehensive evaluation of CMAQ v4.5 at 12-km grid resolution was performed
  ▪ Seasonal analysis (winter (DJF), spring (MAM), summer (JJA) and fall (SON))
  ▪ Ozone, organic and inorganic aerosols, total PM$_{2.5}$ mass and precipitation chemistry
  ▪ 36-km versus 12-km performance comparison
  ▪ CMAQ v4.4 versus v4.5 performance comparison
• Model to Observation pairing accomplished using Site Compare (available with 2005 release)
• Statistics and plots generated using AMET (information available during poster session)
• A very small portion of the complete report is shown here
Observation Networks

- AQS (majority urban)
  - O$_3$
- IMPROVE (rural)
  - SO$_4$, NO$_3$, EC, OC and PM$_{2.5}$
- STN (urban)
  - SO$_4$, NO$_3$, NH$_4$, EC, OC and PM$_{2.5}$
- CASTNet (sub-urban and rural)
  - SO$_4$, NO$_3$, NH$_4$, HNO$_3$ and TNO$_3$
- NADP (rural)
  - Wet deposition SO$_4$, NO$_3$, NH$_4$; precipitation
8-hr Maximum Ozone
High bias at low concentrations (10 – 50 ppb)

CMAQ v4.5 (12km)

Good agreement during the day

Model not capturing overnight lows

Higher biases along the coast

Higher errors along the coast

NMB = 1.62%
NME = 17.4%
RMSE = 12 ppb
$O_3$ performance: v4.4 versus v4.5, 12km versus 36km

Similar $O_3$ bias and error at 12km for v4.4 and v4.5

Bias at 12km is improved versus 36km
Organic and Inorganic Aerosols

IMPROVE, STN and CASTNet
SO₄, NO₃ and NH₄, EC, OC, PM₂.₅, HNO₃
Under-predictions in SO$_4$, NO$_3$, EC and OC contribute to under-predictions in PM$_{2.5}$ in the spring and summer.

Over-predictions in SO$_4$ and NO$_3$ contribute to over-predictions in PM$_{2.5}$ in the fall.
Total PM$_{2.5}$ mass is over-predicted for much of the year (other than summer). Due to the over-prediction in NO$_3$, NH$_4$ and EC.

PM$_{2.5}$ performance during the summer is good, however, there appears to be compensating biases, with over-predictions in SO$_4$, NH$_4$ and EC and under-predictions in NO$_3$ and OC.
CASTNet (v4.5, 12km)

- SO$_4$ under-predicted in the winter
- NO$_3$ over-predicted in spring and fall
- NH$_4$ over-predicted in the fall, under-predicted in the summer
- HNO$_3$ and TNO$_3$ over-predicted for the latter half of the year
- NH$_3$ emissions adjustment may be needed in spring and fall
Under-predictions in winter and spring

Nearly unbiased in the summer

Over-predictions in the fall

SO$_4$ v4.5, 12km
Under-predictions in winter and spring, similar to 12km.

Summer SO$_4$
CMAQ v4.5 (36km)

Large under-predictions in summer at 36km, versus nearly unbiased at 12km.

Over-prediction in fall is larger at 12km.

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Large over-predictions of EC at urban STN sites.

EC is generally under-predicted at rural IMPROVE sites.

Issue in the urban areas?

EC v4.5, 12km
Over-prediction at STN sites not as large at 36km as 12km

36km EC performance at IMPROVE sites is similar to 12km performance

Over-prediction at STN sites not as large at 36km as 12km
CMAQ v4.4 versus v4.5
Soccer goal plot - Winter v4.4 versus v4.5

Better performance for IMPROVE NO₃ and PM₂.₅
Little change in performance of other species
• Better performance for SO$_4$ (all networks)
• CASTNet TNO$_3$ and NADP NH$_4$ improved
• IMPROVE EC and PM$_{2.5}$ performance decreases
• CASTNet NH$_4$ performance decreases
The bias of SO4 in the winter is slightly improved in v4.5. In the summer, the SO4 bias is much better in v4.5.
Nitrate

NO$_3$ bias and error in the winter is improved in v4.5

Winter NO$_3$
CMAQ v4.4 (12km)

Summer NO$_3$
CMAQ v4.4 (12km)

NO$_3$ bias in the summer is slightly worse in v4.5

Winter NO$_3$
CMAQ v4.5 (12km)

Summer NO$_3$
CMAQ v4.5 (12km)
Summer NH$_4$

NH$_4$ performance in the summer is mixed

Summer PM$_{2.5}$

PM$_{2.5}$ under-predictions at IMPROVE sites are larger in v4.5

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Precipitation Chemistry

NADP Wet Deposition SO$_4$, NO$_3$ and NH$_4$
NADP

- SO$_4$ performance is relatively good throughout the year
- NO$_3$ is under-predicted in the spring, summer and fall and over-predicted in the winter
- NH$_4$ is generally under-predicted throughout the year
- Precipitation performance is relatively good, although there are issues in the fall
Large under-predictions in the spring and summer

Wet Deposition NO₃

Winter NO₃
CMAQ v4.5 (12km)

Spring NO₃
CMAQ v4.5 (12km)

Summer NO₃
CMAQ v4.5 (12km)

Fall NO₃
CMAQ v4.5 (12km)
Differences in precipitation bias in the winter and spring are small.
Precipitation

Differences in precipitation bias in the summer and fall are relatively large.
Summary

- V4.5 O₃ bias and error similar to v4.4
- SO₄ bias and error is improved versus v4.4
- NO₃ bias is mixed between versions and grid resolutions
- EC bias and error is much higher at 12km than 36km
- Wet deposition SO₄ performance is relatively good
- Wet deposition NO₃ and NH₄ are generally under-predicted
- Precipitation bias and error values in the winter and spring are comparable at 36km and 12km
- Precipitation bias in the summer and fall is considerably different at 36km and 12km
Further Investigation

- $O_3$ overnight bias
  - $K_z$ minimum?
- EC and OC under-predictions at IMPROVE
- Large EC over-predictions at STN
  - Comparison issues
  - Urban emissions issue?
- $HNO_3$ over-prediction in spring through fall
- Wet deposition $NO_3$ under-prediction
  - Needs investigating
Lastly

- Complete evaluation report available through CMAS
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