CMAQ V5.0 Upgrade for ozone and Particulate Matter Predictions

http://www.emc.ncep.noaa.gov/mmb/aq

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February 17, 2017
CMAQ weaknesses Identified

• Overprediction of ozone in Eastern U.S. in Summer
  – Especially along coastal cities (NYC, DC, Cleveland)
    ➔ Update National Emission Inventory point sources to 2011 (project to 2016)
    ➔ Evaluate NOx emissions based on OMI satellite trends (Deferred)
    ➔ Evaluate Impact of NAM-X and reduced SW radiation under clouds
    ➔ Update CMAQ gas and aerosol chemistry/biogenic emissions to EPA V5.0.2

• Underprediction of particulate matter (PM) in Summer and near wild-fires
  ➔ Update 9 year old USFS BlueSky smoke emission system
  ➔ Introduce 24 h pre-analysis cycle to correct fire time mismatch with CMAQ initial time

• Underprediction of Ozone and PM when strong fires are present outside CMAQ domain
  ➔ Test NGAC full aerosol predictions for CMAQ lateral boundaries

• Overprediction of PM during winter-time stagnation episodes (cold, stable)
  ➔ Update emissions/chemistry as in bullet 1
Proposed CMAQ FY2017

Chemical Transport Model:

- **CMAQ5.0.2 for CONUS**
  - CB05 gas chemistry: increased from current 105 to 155 species: Improved heterogeneous, aqueous, and winter-time reactions
  - From current aero4 to aero6 chemistry: Improved SOA and coarse mode PM
  - LBC: Static from GEOS-CHEM + Dynamic LBC for dust derived from NGAC
  - Added a 24 h analysis PM field for initialization adjustment

For Wildfire Emission:

- Adopt Bluesky HYSPLIT/SMOKE emission strength and duration for the aforementioned 24h analysis and 48h forecast;
- New Bluesky version 3.5.1 from US Forest Service
- Upgrade Bias correction to include temporal trends (Kalman Filter Analog technique, ESRL)
- **NEW OUTPUT to MDL NDGD web site:** bias corrected hourly & daily 24 h avg M2.5
Emissions accompany CMAQ5.0.2

- **Point source**: Baselined from NEI2011v1 & updated by 2014 CEM & 2016 DoE Energy Outlook
  - Canada: Environment Canada 2006 Inventory made available as part of US EPA NEI2011;
  - Mexico: Inventory (MI) 2012 v2.2 for six Northern bordering states & 2.1 other states

- **Area Sources**
  - US EPA 2011 NEIs;
  - Canada 2006 Emission Inventories (in NEI2011 package);
  - Mexico 2012 EI for six Northern bordering states (in NEI2011 package);
  - US residential wood combustion and oil and gas sectors;
  - Snow/Ice effect on fugitive dust emissions;

- **Mobile Sources (on-road)**
  - NEI 2005 projected to 2011 using Cross-State Air Pollution Rule (CSAPR) projection for US sources and; Canada 2006 Emission Inventories; MI 2012;

- **Natural Sources**
  - Terrestrial biogenic emission: BEIS model v3.14;
  - Sea-salt emission: CMAQ online Sea-salt emission model based on 10m wind;
  - Fire emissions based on HMS fire detection and BlueSky V3.5.1 emission model

- **Windblown dust emission**: FENGSHA model
ARL ensures a robust and thorough quality check of emission files:

- Monthly emission quality assurance (QA) check and test results will be posted in ARL website so that the scope of check is shared with EMC and focus group.

- Annual emission delivery will happen in December and April. Testing should be conducted before both deliveries. Typically ARL mimics January 1st and June 1st 12 UTC cycle for the respective test. For leap years the December test should also include December 31st 12UTC cycle.

- Extend emergency contact list: Add Li Pan to the current ARL list: Pius Lee and Daniel Tong
New Updated BlueSky:

- The Fuel Characteristic Classification System version 2 (FCCS2) which includes a *more detailed description of the fuel loadings with additional plant type categories*.
- Explicit fuel load map for Alaska
- Improved fuel consumption model and fire emission production system (FEPS).

*Courtesy Ho-Chun Huang, EMC*
Analog Ensemble for PM$_{2.5}$ Bias Correction

- Analog metric is determined by (Monache et al. 2011)

$$\|F_t, A_{t'}\| = \frac{1}{\tilde{t}} \sqrt{\sum_{j=-\tilde{t}}^{\tilde{t}} \left( F_{i,t+j} - A_{i,t'+j} \right)^2}$$

where $F_t$ is current NWP forecast valid at future time $t$, $A_{t'}$ is analog at past time $t'$, $N_v$ is the number of variables, $\tilde{t}$ is half the number of additional computation time, $w_i$ weight, $\sigma_{f_i}$ standard deviation

Implementation in NAQFC
- Variables for Analog search: PM$_{2.5}$, $T_2$, WS/WD
- Ensemble members: 5
- Training period: one year

(Source: Djalalova et al., 2015)

Courtesy Jianping Huang, EMC
Resolution Changes
- CONUS (4 km) and Alaska (6 km) nests → 3 km
- Sync AK and CONUS On-Demand Fire Weather nests → 1.5 km

Select Model Changes
- Updated microphysics → Improved stratiform precip., better anvil reflectivity, lower peak dBZs, smaller areas of light/noisy reflectivity (rain treated as drizzle), improved nest QPF bias in warm season, Reduce incoming SW Rad under clouds; reduce warm season 2-m T warm bias
- More frequent calls to physics → Physics/dynamics more in sync (e.g. improved upper air, improved nest QPF)
- Improve effect of frozen soil on transpiration and soil evaporation → Improve cold season 2-m T/Td biases
- Adjustment to convection in 12 km NAM → Improve QPF
- Modify latent heat flux treatment → Improve visibility along CA coast

Data Assimilation:
- DA cycles for 3 km CONUS and AK nests → Much less ‘spin-up’ time
- Use of Lightning and Radar Reflectivity-derived temperature tendencies in initialization
  - Improved short-term forecasts of storms at 3 km
  - Improved 00-12 hr QPF
- New satellite radiances, satellite winds → Improved Initial Conditions

Courtesy Eric Rogers, EMC
CMAQ Version 5.0
Status as of 02/17/17

Leads: Jeff McQueen & Jianping Huang (EMC), Steven Earle(NCO)
Scope: Upgrade CMAQ to Cray with improved aerosol chemistry and emissions with 2011 base year estimates; Update BlueSky smoke emission system; Include 24 h pre-analysis run for smoke initialization; Use NGAC dust aerosol lateral boundary conditions; Update PM bias correction.
Expected benefits: AQM is improved and unified through improved chemistry, emissions and physics. Improved smoke emissions.
Dependencies: Transition code from ARL; BlueSky outputs from Hysplit

Issue: reproducibility issue between Cray machines.
Resolution: module versions differed (resolved, 2/15/17)
Risk: Not enough time remaining to test O-Conus updates;
Mitigation: do not upgrade O-Conus system: defer to FY18 (resolved)

<table>
<thead>
<tr>
<th>Milestones &amp; Deliverables</th>
<th>Date</th>
<th>Status</th>
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<tbody>
<tr>
<td>Freeze system code; deliver to NCO if applicable</td>
<td>12/15/16</td>
<td>Complete</td>
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<tr>
<td>Complete full retrospective/real time runs and evaluation</td>
<td>2/13/17</td>
<td>Complete</td>
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<tr>
<td>Conduct CCB and deliver final system code to NCO</td>
<td>2/17/17</td>
<td>On track</td>
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<tr>
<td>Issue Technical Information Notice</td>
<td>3/15/17</td>
<td>On track</td>
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<tr>
<td>Complete 30-day evaluation and IT testing</td>
<td>5/15/17</td>
<td>On track</td>
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<tr>
<td>Operational Implementation</td>
<td>5/30/17</td>
<td>On track</td>
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</table>

Staff: 0.8 Fed FTEs + 2 contractor FTEs; including Dev + ARL 0.8 Fed FTEs + 1.9 contractors FTEs
Funding Source: STI/NAQFC
Compute: Dev: 120 nodes (+40); Para: 40 nodes (+15); Ops: 20 nodes/cycle (+10)
Archive: Ops: 1TB/day (No change),
## Summary of work performed

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- Code delay
- Redo Script merging w/ops codes
- PM LBC/array bounds error
- Slowdown on Cray
- Cray reproducibility
- Grib2/wgrib2 library issues
- O-Conus scripts

**Q1FY17→ Q3FY17**

- Code delay
- Redo Script merging w/ops codes
- PM LBC/array bounds error
- Slowdown on Cray
- Cray reproducibility
- Grib2/wgrib2 library issues
- O-Conus scripts
Evaluations Performed

Ozone and PM

• EMC Real-Time: July 2016 → Present
• EMC NAM-X Retrospectives : July 2016
• EMC/ARL NOx emissions adjustments : Aug-Sept. 2016 retros

• NWS/STI & AQ Focus Group: Aug. Retros + RT runs
  – EMC maintains NRT comparison graphics and verification web sites
  – EMC provides daily ascii text predictions at monitor sites to following state forecasters :
    • AL, AZ, CA, CT, DE, GA, IA, MD, ME, NY, OH, PA, TN, VA
Upcoming NAM Q3FY17 Upgrade

Mean 2-M Temp vs. sfc obs (12h cycle) over the Western US for open NAM and parallel NAM forecasts from 201607190000 to 201608291200

WEST

Mean 2-M Temp vs. sfc obs (12h cycle) over the Eastern US for open NAM and parallel NAM forecasts from 201607190000 to 201608291200

EAST

2 m Temperature
July 2016 NRT CMAQ Prod vs V5.0.2

1 h avg Diurnal Ozone

- **CMAQ V5.0.2 NAM-X**: improvement in ozone over-prediction over the East

- **CMAQ V5.0.2 NAM-X**: Strongest underestimate over West

- Meteorological impact nearly as large as CMAQ/Emissions upgrade
Day 2  8h O3 Daily Max
August 12, 2016

CT/PA  DEP Noted numerous mixed exceedences with V5.0.2 Near Real-time parallels
Experiments to address missed exceedences

- **No NOx Adjustment for Mobile Emissions (green line) NAMX**
  - Cross State Air Pollution Rule (CSAPR) 2011 Mobile Emission
  - Should result in increased ozone product

- **Gridded NOx Mobile emission adjustment (red line) NAMX**
  - Adjustment factor also considers fine-scale features by taking into account the 12 x 12 km grid-by-grid satellite-observed NOx to NAQFC forecasted NOx ratio

- **V5.0.2 Para**: State wide NOx adjustment using NAM
August 2016
East vs West  Ozone

No-NOX: Slight improvement during day over East
Slightly better over West late August
August 2016
Sub-region Ozone **Diurnal** plot

**Midwest**

**Northeast**

**SE**

**SW**

No-NOX: slight improvement during day over NE/MW
Skill Score statistics
CONUS Ozone August 2016

NOX-Adj & Oper runs highest POD but also highest FAR
August 13, 2016 Day 1
NE Ozone exceedences

- Prod: Overprediction; NOx State Adj: Misses event
- NOX Grid Adj: Misses coastal CT exceedence
August 18, 2016 Day 1

- NAMx showed a great improvement over PROD;
- NAMx eliminated the four false alarms.

Courtesy Mike Geigart, CT DEP
August 30, 2016 Day 1
California

- All similar → less ozone over Ut/NV with parallel runs
Current issues of PM$_{2.5}$ predictions

- Significant seasonal bias
  - over-prediction in winter
  - under-prediction in summer

- Sources of the bias
  - Emissions ?
  - Met (PBLH) ?
  - CMAQ chemistry ?
  - LBCs?

Over-prediction in winter is improving and Under-prediction in summer is unchanged
Western Fires
August 21, 2015  1hr PM2.5 Max

Operational runs: Most sites impacted by fire smoke are severely under-predicted.
Experimental tests: Updated BlueSky and use of current day fire info
• Underpredict PM over Western U.S.
• Slight overprediction over Eastern U.S.
• *Bias Correction* strong improvement
July 29, 2016 Big Sur Fire forecast and comparison to PM measurements

Smoke Emissions
- Location
- Magnitude
- Ejection height
- Diurnal evolution
JULY 2016 PM Predictions
1 h avg PM : South West U.S. Fires

South West Coast

- Underprediction (except *Bias corr*) in general BUT:
- Overprediction of wild fire smoke events in morning
- No diurnal emissions profile used
**November 2016**

East vs West PM and Bias Corrected PM

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**EAST**

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<thead>
<tr>
<th>PM25MX THRESHOLD (UG-M3)</th>
<th>12 UTC CYCLE</th>
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<tbody>
<tr>
<td>OBSERVATION COUNTS</td>
<td>1153 919 756 525 282 179 69</td>
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**WEST**

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<thead>
<tr>
<th>PM25MX THRESHOLD (UG-M3)</th>
<th>12 UTC CYCLE</th>
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<tr>
<td>OBSERVATION COUNTS</td>
<td>811 563 474 369 257 173 80</td>
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</table>

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V5.0.2 – *KFAN BC* follows diurnal profile closely.
November 2016

Parallel Run PM BIAS by Region

Overprediction for NE and MW improved compared to Raw
November 15, 2016

South East U.S. Fires: Midwest impact

- Is smoke from fires moving too far downwind (Midwest)
- BC does good job for correcting in prod & para runs
November 15, 2016
1 h Daily Max PM : South East U.S. Fires

- BC underpredicts fire events, but still closer than other runs
Summary

- **V5.0.2 Ozone w/ NAM-X**
  - Improvement correcting over-prediction esp along coasts
    - Long Island Sound (CT DEP analysis)
      » 7 False Alarms compared to 17 from production for NYC area
    - Lake Erie/Michigan and Ohio Coastline
  - Much improved for Southwest and marginal or non-events
  - Missed exceedences in NE corrected after removing NOx adjustments

- **PM**
  - Large positive impact near forest fires:
    - Updated BlueSky and 24 h pre analysis run
    - Underprediction when external sources (Saharan dust, Canadian fires) are impacting CONUS
    - Emission timing and ejection height uncertainties
  - Continued overprediction in Winter from raw predictions

- **Updated NAM alone strongly improves ozone forecast**
  - Amount of incoming radiation under clouds critical
Future Emphasis

- Extend to 72 hours, update emissions to 2014 base
- Near real-time fire locations, strength, emissions
  - Canadian, Mexican & external source impacts
  - Top down (satellite) vs Bottom up (BlueSky) approaches
  - Improved temporal profiles and plume rise algorithms
- NGAC full aerosol boundaries
- Unification of AQ systems
  - HYSPLIT smoke/dust $\rightarrow$ NGAC Aerosol
  - CMAQ ozone & total PM
  - HRRR-smoke
- Extend Kalman Filter bias correction to ozone
- Improved Evaluations
  - Use of VIIRS/GOES-R/AERONET AOD, CALIPSO aerosols
  - Evaluate Operational models for field experiments (ESRL FireX 2018, FASMEE)
BACKUPS
Web pages
CMAQ V5.0.2

- Real-time parallel runs (July 2016-Present)

- No NOx adj/NAM-X/4x-day cycling (Aug. 7-Sept 10)

- Gridpoint NOx adj/NAM-X/1x-day cycling (Aug. 1-Sept 10)

- Verification statistics (prod,para, cmaqnox11, cmaqnox)
Impact of Experimental NAM on smoke

NAM PROD (left panel) and updated NAM Parallel (right panels)

20160717 06Z at FCST HR 36 and 48

Quite different between NAM Prod and NAM Para on
(a) Circulation pattern
(b) Stability -> plume rise -> emission release height
Winter Time PM

Southern CA, Jan. 17, 2017

Mid Atlantic, Jan. 21, 2017

• Improved out west, but overprediction sometimes worsened over East