Recent Enhancements to the Community Multiscale Air Quality Modeling System (CMAQ)

The CMAQ Team
Computational Exposure Division
National Exposure Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency

January 31, 2017
• **Purpose:** Provide Regions, States, and Tribes with summary of scientific updates included in new release of EPA’s Community Multiscale Air Quality (CMAQ) modeling system (v5.2)

• **Outline:**
  – **Background on CMAQ** (Rohit Mathur)
  – **Relevance of scale interactions**
  – **Process updates**
    • Meteorology–chemistry linkages (Jon Pleim)
      – PBL/LSM, clouds & precipitation, stratosphere-troposphere exchange
    • Chemistry (Ben Murphy)
    • Aerosols
  – **Evaluation** (Wyat Appel)
  – **Summary**
Evolution of Air Quality Models

To address increasingly complex applications and assessments

**Application Needs**

- Standards
- Assessments
- New Source Permitting
- NAPAP

**Model Development**

- PSD
- 1-hr O3
- NAAQS
- PM 2.5
- 8-hr O3
- 1-hr O3 SIP

**Evolution of Air Quality Models**

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**Application Needs**

- AQDM UNAMAP
- RADM-ROM
- Eulerian Grid Models
- Acid Deposition
- Ozone

**Model Development**

- MODELS3
- CMAQ
- For PM

**Evolution of Air Quality Models**

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**Application Needs**

- NATA
- Air Quality Forecasts
- - Hg
- - Toxics

**Model Development**

- NATA
- Air Quality Forecasts
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**Evolution of Air Quality Models**

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**Application Needs**

- Meteorology
- Air Quality Interactions
- Exposure
- Health

**Model Development**

- Multi-pollutant
- CMAQ
- Coupled
- WRF-CMAQ

**Evolution of Air Quality Models**

To address increasingly complex applications and assessments

**Application Needs**

- Background air pollution
- Met-AQ
- Interactions
- Exposure & Health
- Multimedia

**Model Development**

- Multi-pollutant
- Near-source to Global
- Reactive
- Multimedia:
  - Atmospheric-
  - Hydrologic

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**Application Needs**

- Multi-pollutant
- CMAQv5.2

**Model Development**

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The Community Multiscale Air Quality (CMAQ) Modeling System

- Comprehensive Eulerian Chemical Transport Model
  - Emission, advection, diffusion, chemistry, deposition
- Multi-scale: Hemispheric → Continental → Regional → Local
- Multi-pollutant & multi-phase:
  - Ozone Photochemistry
    - $\text{NO}_x + \text{VOC}$ (biogenic & anthropogenic) → $\text{O}_3$
  - Particulate Material (PM)
    - Inorganic chemistry & thermodynamics → Sulfate, Nitrate, Ammonium
    - Organic aerosol → primary, secondary
    - Geogenic aerosol → wind-blown and fugitive dust, sea salt
  - Acid deposition
    - Aqueous chemistry, Wet deposition
  - Air Toxics
    - Benzene, Formaldehyde, Hg, etc
- Coupled to the Weather Research & Forecast (WRF) Model
  1. “Off-line” – sequential operation
  2. “On-line” – 2-way coupled
Recent CMAQ Versions
Periodic public release of improved versions of the modeling system

- **CMAQv4.7** (Fall 2008) and **CMAQv4.7.1** (June 2010)
  - Supporting evaluation: Foley et al, Geoscientific Model Development, 2010

- **CMAQv5.0** (Feb. 2012)
  - Updates to gas-aqueous-aerosol chemistry and photolysis
  - Improved advective and turbulent transport
  - Major structural upgrades that improve flexibility and maintainability
  - 2-way coupling between WRF-CMAQ
  - Bi-directional exchange: NH$_3$ and Hg

- **CMAQv5.0.2** (May 2014)
  - Instrumented Models (*Direct Decoupled Method (DDM), Source Apportionment, Sulfur Tracking*)
  - Community Contributions (*Volatility Basis Set (VBS)*)

- **CMAQv5.1** (October 2015)
  - Revised gas chem and Photolysis
  - Aerosol updates: New pathways for SOA production
  - Improve computational performance
  - Supporting Evaluation: Appel et al., GMDD, 2016

- **CMAQv5.2** (β-version in November 2016; final version in June 2017)
  - New Organic aerosol treatment
  - New wind-blown dust model
  - CB6 chemical mechanism
  - Lightning – NOx and assimilation
  - Instrumented models compatible with process updates
  - Process options for hemispheric configuration
CMAQ Modeling System

"Numerical Laboratory" to synthesize our evolving understanding of processes (and interactions) regulating air pollution

- Meteorological Model (WRF)
- Meteorological-Chemical Interface Processor (MCIP) (AQPREP)
- CMAQ AQ Model - Chemical-Transport Computations
- SMOKE
  Anthropogenic and Biogenic Emissions processing
Current Multi-scale Modeling

- Hemispheric model needed to provide lateral boundary conditions (LBCs) for US Domain
  - Increasing importance of long range transport (LRT) contributions as NAAQS are reduced

- Fine scales:
  - Urban Environments
  - Linkage with human exposure & health studies
  - Residual non-attainment

Hemispheric model at 108 km provides LBCs for 12 km CONUS with nests to 4 km and 1 km.
Tightening NAAQS and greater emphasis on characterizing “background” air pollution requires *improved representation of scale interactions*
Trans-Atlantic Transport of Saharan Dust
Impact on surface-level PM$_{2.5}$ in the Gulf States

Space and time varying LBCs from hemispheric CMAQ helped capture impacts of long-range transport on episodic Saharan dust intrusion events.
Recent updates to Planetary Boundary Layer (PBL) and Land Surface Model (LSM)

- The Asymmetric Convective Model version 2 (ACM2) in WRF-CMAQ
  - Designed especially for AQ applications
  - Consistent PBL transport of meteorology and chemistry
  - Combined local and non-local closure scheme for convective conditions
  - Combines local scaling and boundary layer scaling for eddy diffusivities
  - Updates to ACM2 in WRFv3.7 and WRF v3.8
    - Different $K_m$ and $K_h$ ($Pr = K_m/K_h \neq 1$)
    - New eddy diffusivities for stable conditions

- PX Land Surface Model in WRF-CMAQ
  - Designed for consistent treatment of heat, moisture, and momentum fluxes in WRF and chemical fluxes (dry dep, bi-directional) in CMAQ
  - Updates to PX LSM:
    - Modified stomatal conductance function for PAR (F1) (WRFv3.8)
    - Reduced heat capacity of vegetation (WRFv3.7)

Together updates to PBL and LSM reduce biases in meteorology (particularly $T$ and $Q$) mostly at night
Updates also reduce over-prediction of ground level emitted species (e.g. NOx, CO, EC)
Effects of PBL and LSM Updates on O$_3$

Changes to PBL and LSM tend to reduce ozone during mid-day hours, resulting in reductions in the MD8hr O$_3$ bias.
Improvements in Clouds, Radiation, and Precipitation

WRF Lightning Assimilation in Kain-Fritsch
- Use lightning data from the National Lightning Detection Network (NLDN)
- Simple, computationally efficient approach: (builds off of Mansell et al. 2007)
  - Force deep convection where lightning is observed
  - Only allow shallow clouds where it is not

Heath et al., JAMES, DOI: 10.1002/2016MS000735, 2016

Predicting clouds and precipitation is challenging.
Example on the left shows both over- and underestimation of precipitation.
Lightning assimilation methodology improves clouds, precipitation, and O₃.
Improving Estimates of Lightning NO Generation

CMAQv5.1: monthly climatological data from the National Lightning Detection Network (NLDN) were associated with WRF’s gridded convective rainfall rate to distribute lightning strikes per grid cell.

CMAQv5.2: hourly raw NLDN data are now used to generate gridded hourly LNO, resulting overall in ~30% decrease in LNO.

Impact of using hourly NLDN Data:
Bias in hourly O₃ predictions decreased at 79% of the sites

Courtesy: Daiwen Kang
CMAQv5.2 Updates:
Impact of stratosphere-troposphere exchange on tropospheric $O_3$

- Modeled $O_3$ specified by enforcing the condition of proportionality to Potential Vorticity: $[O_3] = c \cdot PV$
- Used recent CMAQ multi-decadal simulations to develop a robust relationship that varies spatially and temporally: $O_3/PV = F(\text{spatial}) \times G(\text{temporal})$

Used observed $O_3$ data from 1990-2010 from 44 WOUDC sites

Comparison of Observed $O_3$ with Reference simulation and New PV scaling

Xing et al, ACP, 2016
CMAQ includes different mechanisms so that mechanism can be matched to application

<table>
<thead>
<tr>
<th>Mechanism family</th>
<th>Specific mechanisms in CMAQ</th>
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<tbody>
<tr>
<td>Carbon Bond</td>
<td>CB05tucl, CB05e51 (expanded nitrates), CB05e51h (with halogens), CB6r3</td>
</tr>
<tr>
<td>SAPRC</td>
<td>SAPRC07T (explicit toxics), SAPRC07tic (expanded isoprene)</td>
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<tr>
<td>RACM</td>
<td>RACM2</td>
</tr>
</tbody>
</table>

New in CMAQ v5.2 is CB6 (r3) mechanism:

- Updated reaction rates and yields \((matches \ current \ science \ recommendations)\)
- Updated nitrate yields in low temperatures \((winter \ simulations)\); 3 nitrates instead of 1 in CB05tucl
- More high-emitted, longer-lived species, including acetone, benzene, propane, carbonyls \((slower \ reacting, \ more \ transport)\)
- CMAQ extensions to CB6r3:
  - Customized to interface with SOA improvements
  - Can modify for emerging issues/pollutants \((respond \ faster \ to \ science \ updates \ and \ new \ research \ findings)\)
Issue: Halogen chemistry and deposition to water are key sinks for O₃ in marine environments; their accurate representation impacts predictions of both long-range transport and ambient levels in coastal areas.

CMAQv5.2 Updates: Improving representation of marine environments

Sarwar et al., ES&T, 2015
CMAQv5.2 Updates: Gas-phase chemistry for HAPs

- CB6r3 extended to predict concentrations of 41* Hazardous Air Pollutants (HAPs), used in 2014 National Air Toxics Assessment, to identify those air toxics which are of greatest potential concern in terms of contribution to population risk

Example: Use of CMAQ to quantify the VOCs that contribute the most to ambient formaldehyde in the Southeast from all VOCs (left) and breakdown from anthropogenic sources (right)

Example: Some of the important HAPs predicted by CMAQv5.2, including those which have been identified as national and regional cancer and noncancer hazard drivers.

<table>
<thead>
<tr>
<th>HAP name</th>
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<tbody>
<tr>
<td>formaldehyde - total and emitted</td>
<td>acetaldehyde - total and emitted</td>
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<tr>
<td>acrolein - total and emitted</td>
<td>1,3-butadiene</td>
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<tr>
<td>Benzene</td>
<td>Napthalene</td>
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<tr>
<td>Carbon tetrachloride</td>
<td>p-dichlorobenzene</td>
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<tr>
<td>Chloroprene</td>
<td>1,3-dichloropropene</td>
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<tr>
<td>Ethylene oxide</td>
<td>Chlorine</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>Chromium</td>
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<tr>
<td>Chromium 6 - fine and coarse modes</td>
<td>Arsenic - fine and coarse modes</td>
</tr>
<tr>
<td>Nickel - fine and coarse modes</td>
<td>Diesel PM elemental carbon - fine modes</td>
</tr>
<tr>
<td>Mercury - elemental and gas</td>
<td>Lead - elemental and gas</td>
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</tbody>
</table>

* users can now easily change model output to subset the 41 HAPs for their own applications
Secondary Organic Aerosols in CMAQv5.2

VOC Precursors + Oxidants → Condensable Organic Vapors → Secondary Organic Aerosol Particles

- **BIOGENIC EMISSIONS**
  - isoprene
  - sesquiterpenes
  - APIN monoterpenes
  - TERP monoterpenes
  - benzene
  - low-yield aromatics
  - high-yield aromatics

- **ANTHROPOGENIC EMISSIONS**
  - SV_ISO1
  - SV_ISO2
  - SV_BNZ1
  - SV_BNZ2
  - SV_TRP1
  - SV_TRP2
  - SV_SQT
  - SV_ALK1
  - SV_ALK2
  - SV_TOL1
  - SV_TOL2

- **AQUEOUS EMISSIONS**
  - + OH/NO
  - + OH/NO
  - + OH/NO

- **SECONDARY PROCESSES**
  - SV_ISO1 + OH
  - SV_ISO2 + OH
  - SV_BNZ1 + OH
  - SV_BNZ2 + OH
  - SV_TRP1 + OH
  - SV_TRP2 + OH
  - SV_SQT + OH
  - SV_ALK1 + OH
  - SV_ALK2 + OH
  - SV_TOL1 + OH
  - SV_TOL2 + OH

- **SECONDARY PRODUCTS**
  - AALK1
  - AALK2
  - AAXYL1
  - AAXYL2
  - AABNZ1
  - AABNZ2
  - AATRP1
  - AATRP2
  - ASQT
  - ATRP1
  - ATRP2
  - AISO1
  - AISO2
  - AAPAH1
  - AAPAH2
  - ATOL1
  - ATOL2
  - ATOL3
  - AORGC
  - AOLGB
  - AGLY
  - GLY
  - MGLY

- **SECONDARY PROCESSES**
  - + OH
  - + OH/NO
  - + OH/NO
  - + OH/NO

- **SECONDARY PRODUCTS**
  - + OH, +O₃, +NO₃, +O₃P
  - + OH, +O₃, +O₃P
  - + OH, +O₃, +O₃P

- **SECONDARY PRODUCTS**
  - + OH, +O₃P

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CMAQv5.2 Updates: Biogenic Secondary Organic Aerosol

Isoprene Epoxide (IEPOX) SOA

Strongly influenced by:
- urban/biomass-burning emissions
- isoprene emissions under low NO
- monoterpene emissions with low isoprene

Strongly influenced by:
- IEPOX SOA
- Other OA

Particulate Organic Nitrate Aerosols

(Percentage of total OA mass in green)

(Percentage of total OA mass in cyan)

Hu et al., 2015 ACP

Ng et al., accepted ACP
CMAQv5.2 Updates:
Organic aerosol co-benefits from SO$_x$ and NO$_x$ reductions

Better capture of Isoprene SOA dependence on aerosol sulfate

NO$_x$ reductions lead to substantial OA reductions via NO$_x$ participation in organic nitrate formation

(Pye et al., 2017 ACP, Mao et al., in review ACPD)

(Pye et al., 2015 ES&T)
CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

Organic aerosol in the atmosphere:
• is a significant contribution to mass throughout the world
• is becoming relatively more important for PM$_{2.5}$ predictions as PM sulfate and nitrate concentrations fall
• has been shown to evaporate with dilution from near-source to ambient conditions
• is primarily comprised of oxygenated compounds
  (Ng et al., *ACP*, 2010; Zhang et al., *Anal Bioanal Chem*, 2011)

Organic aerosol in CMAQv5.1:
• is dominated by primary, nonvolatile organic mass
• underestimates the response of OA to photooxidation in urban areas
  (Woody et al., *ACP*, 2016)
• overestimates OA observations in winter (due to high POA concentrations)
• underestimates OA observations in summer (due to low SOA concentrations)
Semi-volatile POA

- The research community and our own models tell us a significant fraction of POA should be volatilized.
- Distributed POA from inventory into separate species based on Volatility:

<table>
<thead>
<tr>
<th>Class</th>
<th>$C^*$ (μg m⁻³)</th>
</tr>
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<tbody>
<tr>
<td>ELVOC</td>
<td>$&lt; 10^{-3}$</td>
</tr>
<tr>
<td>LVOC</td>
<td>$10^{-3} \leq C^* &lt; 10^0$</td>
</tr>
<tr>
<td>SVOC</td>
<td>$10^0 \leq C^* &lt; 10^3$</td>
</tr>
<tr>
<td>IVOC</td>
<td>$10^3 \leq C^* &lt; 10^6$</td>
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</tbody>
</table>

Nonvolatile Configuration

Semivolatile Configuration

New Anthropogenic SOA model species

- Lump The uncertain processes into one NEW model surrogate: Potential SOA from Combustion Emissions (pcSOA)

CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

Nonvolatile POA is still available in CMAQv5.2 for backwards compatibility

(C$^*$ = 10⁻³ μg m⁻³)

(Hayes et al., ACP, 2013; Woody et al, ACP, 2016)
CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

OA Diurnal profiles for California 4-km simulation. May-June 2010.

Seasonal performance indicators for CONUS 2011 simulation
CMAQv5.2 Updates:
New physics-based windblown dust model

- Particles are mobilized when the aerodynamic drag and lift exceed gravitational and inter-particle cohesive forces
- Particles striking back to the surface result in vertical emission flux

<table>
<thead>
<tr>
<th>Update</th>
<th>Implications</th>
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<td>Threshold friction velocity</td>
<td>More realistic values of the threshold velocity smoothly distributed</td>
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<td>Roughness factor</td>
<td>Include the effect of roughness elements (both solid and vegetation)</td>
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<tr>
<td>Surface roughness</td>
<td>Develop a new relation for surface roughness based on data from several different studies</td>
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<td>Vegetation cover fraction</td>
<td>Spatially and temporally variable vegetation fraction based on satellite observations</td>
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</table>

Foroutan et al., JAMES, in review, 2017
CMAQv5.1 windblown dust model issue
Tendency to occasionally produce unrealistically high emissions

Extensive updates to the windblown dust module for CMAQv5.2 release
Foroutan et al., JAMES (in review)

EPA

Massive dust storm in Phoenix, AZ

CMAQv5.2 Updates:
Evaluation of windblown dust improvements

Time series of fine particulate soil for all IMPROVE sites (CONUS, 2011)

Difference in the soil error for entire year 2011 (CMAQv5.2 – CMAQv5.1)
CMAQv5.2 Instrumented Models

Decoupled Direct Method in Three Dimensions (DDM-3D)

- CMAQ-DDM-3D enables sensitivity calculations simultaneously with the standard concentrations and deposition calculations using the existing core model algorithms. Sensitivities are with respect to:
  - Emissions (gridded, point, biogenic, lightning, etc)
  - Boundary and/or Initial conditions
  - Reaction rates
  - Potential Vorticity
  - Region or Time of emission
- Second order sensitivity calculation (sensitivity of sensitivity) is also available.

Integrated Source Apportionment Method (ISAM)

- CMAQ-ISAM allows for source attribution calculations for both gaseous (O₃, VOC, and NOₓ) and particulate species (SO₄, NO₃, EC, OC, etc.) in a single model run.
- O₃ attribution is classified into VOC/NOₓ limited regimes.
- All reactive VOCs are explicitly tracked.
- Source attribution for user-defined combinations of emissions sectors and regions.
- Each simulation tracks IC/BC contributions as well as an other category to reconstruct the full bulk concentration.

A hypothetical relationship between emissions of SO₂ and sulfate concentrations. The green tangent line illustrates the sensitivity of sulfate concentration to emissions of SO₂.

An example of source-resolved particulate concentrations. This scenario demonstrates the effect of a wildfire plume impacting the receptor on May 6.
Updates in CMAQv5.2 reduce high bias in summer $O_3$ and low bias in summer $PM_{2.5}$ across much of the US. Changes in high bias in winter $PM_{2.5}$ are more spatially heterogeneous.

- Decrease in summertime $O_3$
  - Decreases summertime $O_3$ across much of the domain. Exception is over the Pacific. 
  - Improves bias
  - Increases $PM_{2.5}$ in summer
  - Decreases nitrate in winter

Lightning assimilation:
- Decreases summer $O_3$
  - Improves bias
- Mostly increases sulfate in eastern US in summer
- Increases nitrate in eastern US in winter
- Other changes in WRF3.8 have much smaller impact

V5.2 with CB05e51 chemical mechanism:
- Increases $PM_{2.5}$ in summer due to SOA updates
- Decreases $PM_{2.5}$ in winter due to addition of semivolatile POA
  - Improves bias in both seasons
- Impact on summer $O_3$ is mixed

V5.2 with CB6r3 chemical mechanism:
- Decreases summertime $O_3$ and $NO_2$
  - Improves bias
- Small decrease in summer SOA in the southeast

Update to Calculation of NO from Lightning:
- Decrease in summertime $O_3$
January 2011 Incremental Testing for PM$_{2.5}$
January 2011 Incremental Testing for PM$_{2.5}$

Improvements in bias due primarily to organic aerosol updates in v5.2 CB05e51.
Other model updates have less impact on mean bias.
January 2011 Improvement in PM$_{2.5}$ diurnal profile leads to decrease in bias at most locations
July 2011 Incremental Testing for PM$_{2.5}$

AQS Observations v5.1 Base

PM$_{2.5}$ Concentration – July 2011

PM$_{2.5}$ Bias

# of Sites: 655

Hour (LST)
July 2011 Incremental Testing for PM$_{2.5}$

Improvements in bias due primarily to organic aerosol updates in v5.2 CB05e51.
Switch to boundary conditions from Hemispheric CMAQ also decreases bias.
July 2011 Bias in modeled PM$_{2.5}$ decreases at most locations from v5.1 to v5.2
July 2011 Incremental Testing for O₃

O₃ Mixing Ratio – July 2011

O₃ Bias

AQS Observations v5.1 Base

# of Sites: 1300

# of Sites: 1300
July 2011 Incremental Testing for O₃

Consistent decrease in O₃ bias across all hours in v5.2 compared to v5.1.
July 2011
Bias in modeled O\textsubscript{3} decreases at most location from v5.1 to v5.2
• Model performance for v5.1 documented online:

• The release of v5.2 in June will correspond to updates in several evaluation tools:
  – New version of AMET (easier installation)
  – Updates to programs and scripts for post-processing CMAQ output to prepare for evaluation
  – New resources for users on CMAQ’s new website: www.epa.gov/cmaq
    (available June 2017)
Periodic scientific updates to the CMAQ model have led to the creation of:

- Dynamic and diverse user community
- More robust modeling system
- Diverse applications supporting
  - Regulatory analysis by EPA & States (State implementation plans and rulemaking, Clean Air Interstate Rule, Clean Air Mercury Rule, Renewable Fuels Standard Act-2)
  - Air quality forecasting & public health advisories (NOAA, internationally)
Vision for Next Generation Model

• The Next Generation model will be a 1-D AQ component coupled to meteorology models
  – Chemical tracers to be transported in meteorology model
  – Can couple to multiple Meteorology models

• Three configurations of flexible systems:
  – On-line global variable grid (e.g. MPAS, OLAM)
  – Online regional (WRF-AQ)
  – Offline regional (WRF-AQ with offline chem transport)

• One dimensional AQ component
  – Gas, aerosol, aqueous in modular box
  – Modules for biogenic emissions, dry dep/bidi, wind-blown dust, photolysis, etc

• Transport in met models for online systems (adv, diffusion)
  – Ensure mass conservation
  – Consistency with met parameters
  – Minimize numerical diffusion and dispersion

MPAS
Additional Information

• Download CMAQv5.2beta:  https://github.com/USEPA/CMAQ

• For additional information, contact Shawn Roselle (roselle.shawn@epa.gov)