The Community Multi-scale Air Quality (CMAQ) Modeling System:
Past, Recent Developments, and New Directions

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Why do we need atmospheric models?

- The **complexity of physical and chemical atmospheric processes**, combined with the **enormity of the atmosphere**, make results obtained from laboratory and field experiments difficult to interpret without a **clear conceptual model of the workings of the atmosphere**, e.g.:
  - Extrapolation of results to other geographic areas
  - Assessing atmospheric chemical state in response to emission perturbations

- Because an understanding of individual processes may not necessarily imply an understanding of the overall system, measurements alone cannot be used to
  - Explore the future state of the atmosphere
  - Formulate effective abatement strategies

- Close integration of state-of-the-science models and experimental measurements is needed to advance our understanding of various atmospheric pollution problems
Evolution of Air Quality Models

To address increasingly complex applications and assessments

Regulatory & Assessment Needs

<table>
<thead>
<tr>
<th>Year</th>
<th>Standard/Permitting</th>
<th>Model Development</th>
<th>Air Quality Change</th>
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<tbody>
<tr>
<td>1970</td>
<td>CAA</td>
<td>AQDM UNAMAP</td>
<td>Acid Deposition</td>
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<td>CAAA-PSD</td>
<td>RADM-ROM</td>
<td>Ozone</td>
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<td>CAAA</td>
<td>CMAQ</td>
<td>8-hr O3</td>
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<td>1994</td>
<td>NAPAP</td>
<td></td>
<td>SIP</td>
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<td>1997</td>
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<td>NATA &amp; Air Quality Forecasting</td>
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<td>SIPS Due - 8-hr O3 - PM - Hg - Toxics</td>
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<td>2004</td>
<td>NAAQS 8-hr O3</td>
<td>Neighbor Scale CMAQ</td>
<td>Multi-pollutant CMAQ</td>
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<td>2008</td>
<td>NAAQS PM 2.5</td>
<td>- CFD - Eta-CMAQ</td>
<td>Coupled WRF-CMAQ</td>
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<td>2010</td>
<td>NAAQS 8-hr O3</td>
<td>Multi-pollutant</td>
<td>Climate &amp; Air Quality Interactions</td>
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<td>2016+</td>
<td>NAAQS PM 2.5</td>
<td>Multi-scale (local to hemispheric) Interactions with Climate forcing and Air Quality changes</td>
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<tr>
<td></td>
<td></td>
<td>Reactive</td>
<td>Atmosphere-Biosphere Multi-scale (local to global)</td>
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Model Development & Application
Atmospheric Pollutants
Space and Time-scales

Adapted from Seinfeld and Pandis
CMAQ Formulation: Equations

- The theoretical basis for model formulation is the **conservation of mass** for atmospheric trace species transport, chemistry, and deposition.

- General form of chemical species equation:

  \[
  \frac{\partial c_i}{\partial t} = \left( \frac{\partial c_i}{\partial t} \right)_{adv} + \left( \frac{\partial c_i}{\partial t} \right)_{diff} + \left( \frac{\partial c_i}{\partial t} \right)_{cloud} + \left( \frac{\partial c_i}{\partial t} \right)_{dry} + \left( \frac{\partial c_i}{\partial t} \right)_{aero} + R_{gi} + E_i
  \]

  - \( \left( \frac{\partial c_i}{\partial t} \right)_{adv} \) Rate of change of \( c_i \) due to advection.
  - \( \left( \frac{\partial c_i}{\partial t} \right)_{diff} \) Rate of change of \( c_i \) due to turbulent diffusion.
  - \( \left( \frac{\partial c_i}{\partial t} \right)_{cloud} \) Rate of change of \( c_i \) due to cloud processes (scavenging, evaporation, aqueous chemistry, wet deposition).
  - \( \left( \frac{\partial c_i}{\partial t} \right)_{dry} \) Rate of change of \( c_i \) due to dry deposition.
  - \( \left( \frac{\partial c_i}{\partial t} \right)_{aero} \) Rate of change of \( c_i \) due to aerosol processes (interphase transfer between gas and aerosol, aerosol dynamics).
CMAQ Formulation
Modular, Generalized, and Extensible

Generalized Coordinate Formulation

\[
\frac{\partial \phi_i^*}{\partial t} + \nabla \cdot \left[ \phi_i^* \nabla \phi_i^* \right] + \frac{\partial (\phi_i^* \hat{\phi}_3)}{\partial x^3} + \nabla \cdot \left[ \rho \sqrt{\gamma} \hat{F}_{q_i} \right] + \frac{\partial (\rho \sqrt{\gamma} \hat{F}_{q_i}^3)}{\partial x^3} = \sqrt{\gamma} R_{\phi_i}(\bar{\phi}_1, \ldots, \bar{\phi}_N) + \sqrt{\gamma} S_{\phi_i} + \left[ \frac{\partial (\phi_i^*)}{\partial t} \right]_{\text{cld}} + \left[ \frac{\partial (\phi_i^*)}{\partial t} \right]_{\text{aero}}
\]

where, \( \phi_i^* = \sqrt{\gamma} \bar{\phi}_i = (J_{\xi} / m^2) \bar{\phi}_i \)

\( \sqrt{\gamma} \) encapsulates coordinate transformation from physical to computational space

Solution Method: Fractional Steps

Office of Research and Development
National Exposure Research Laboratory
CMAQ Modeling System

Meteorological Model (WRF)

Meteorological-Chemical Interface Processor (MCIP) (AQPREP)

CMAQ AQ Model-
Chemical-Transport Computations

SMOKE

Anthropogenic and Biogenic Emissions processing
The Community Multiscale Air Quality (CMAQ) model:

- **Eulerian** grid chemical transport model
- **Multi-scale**: Hemispheric $\rightarrow$ Continental $\rightarrow$ Regional $\rightarrow$ Local
- **Multi-pollutant (and multi-phase)**:
  - **Ozone Photochemistry**
    - $\text{NO}_x + \text{VOC} (\text{biogenic} & \text{anthropogenic}) \rightarrow \text{O}_3$
  - **Particulate Material (PM)**
    - Inorganic chemistry & thermodynamics $\rightarrow$ Sulfate, Nitrate, Ammonium
    - Organic aerosol $\rightarrow$ primary, secondary
  - **Acid deposition**
    - Aqueous chemistry, Wet deposition
  - **Air Toxics**
    - Benzene, Formaldehyde, Hg, etc
- **Community Model**
  - First version publicly released in \(~2000\)
  - CMAQv5.1 released in December 2015
Typical Regional-Scale CMAQ Applications

Regional-scale air quality modeling studies (time-scales ranging from hours to years)

Simulating the **effectiveness** of emission **control strategies**
- Clean Air Interstate Rule
- Clean Air Mercury Rule
- Renewable Fuels Standard Act-2
- State Implementation Plans
CMAQ Applications: Atmospheric N Depositions

Nutrient loading to sensitive Ecosystems

CMAQ is able to capture main spatial pattern and magnitude of wet deposition.
Defining Dry Deposition Monitoring Needs
Modeled spatial trends vs. CASTNET location

Current coverage is not representative, budget based on obs will be misleading

Need for greater spatial coverage
Examining U.S. Air Quality in Context of the Changing Global Atmosphere: Emerging Need

Tracer Transport: 12/22/05-1/20/06 Layer 22 (2.6-3.2km)
Tracers emission: 200 moles/s over 5x5 grid cells at the surface

Tracer Footprint: Maximum values
Air Pollution-Radiation-Meteorology Interactions

New Delhi, January 2015
AQI at U.S. Embassy: ~180-250

Beijing, December 2011; PM$_{2.5}$ ~ 260 μg/m$^3$

N. Minnesota fire smoke over Chicago, 2011

Phoenix, 2014: Dust Storm
Flexible design of model coupling allows:
• data exchange through memory resident buffer-files
• flexibility in frequency of coupling
• identical on-line and off-line computational paradigms with minimal code changes
• both WRF and CMAQ models to evolve independently;

Maintains integrity of WRF and CMAQ

Aerosol Optics & Feedbacks:
• Volume weighted refractive indices for each wavelength based on:
  - Composition and size distribution
  - $\text{SO}_4^{2-}$, $\text{NO}_3^-$, $\text{NH}_4^+$, $\text{Na}^+$, $\text{Cl}^-$, EC, POA, anthropogenic and biogenic SOA, other primary, water
• Both RRTMG and CAM Shortwave radiation schemes in WRF
• Effects of aerosol scattering and absorption on photolysis
• Effects of O$_3$ on long-wave radiation
Surface PM$_{2.5}$

Aerosol Optical Depth

Surface SW Reduction

Increase in BL pollution (PM$_{2.5}$)

PBL Reduction

July 14, 2006 21Z
Case Study: California Wildfires

Widespread wildfires resulted in significant PM pollution during mid/late June 2008 in California and surrounding states.

Incorporation of feedbacks **improves performance of both meteorology and air quality** at locations impacted by smoke plumes.

- **Feedback effects can be important in conditions of high aerosol loading**

<table>
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<tr>
<th></th>
<th>O₃ (ppb)</th>
<th>PM₂.₅(µg/m³)</th>
<th>SWR (W/m²)</th>
<th>T (K)</th>
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<tr>
<td></td>
<td>NF</td>
<td>WF</td>
<td>NF</td>
<td>WF</td>
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<tr>
<td>ME</td>
<td>15.2</td>
<td><strong>14.6</strong></td>
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<td><strong>28.6</strong></td>
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<tr>
<td>R</td>
<td>0.69</td>
<td>0.69</td>
<td>0.45</td>
<td><strong>0.47</strong></td>
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</tbody>
</table>
Contrasting changes in emissions are altering air quality on hemispheric to local scales

- In Asia: larger populations are being exposed to higher PM$_{2.5}$ concentrations
- Europe/N. America: Control measures have reduced population exposure to PM$_{2.5}$
Comparisons of Trends in NO₂ Column: 2003-2010

SCIAMACHY

WRF-CMAQ

Both observations & model show reductions in NO₂ in urban areas and regionally

- Illustrating the impact and effectiveness of control strategies and technological advances in reducing NOₓ emissions

Model estimated NO₂ column as well as trend are lower than retrievals

- What level of quantitative agreement should be expected?
Simulated and observed Trends: 1990-2010

**Annual PM$_{2.5}$**

- **Summer trends at the median concentration and high ranges show decreases across majority of sites**
- **Increasing trend at many locations during Spring**

**50th Percentile O$_3$**

- **Summer trends at the median concentration and high ranges show decreases across majority of sites**
- **Increasing trend at many locations during Spring**
Decreasing trends in PM$_{2.5}$, and AOD evident across the eastern U.S. in observations and model calculations

Trends in clear-sky SW radiation show “brightening” in regions where aerosols have reduced, but are underestimated.

Gan et al., 2015 (ACP)
Simulated and Observed Trends: *Clear-sky SWR at TOA (upwelling): 2000-2010*

Cloud & the Earth’s Radiant Energy System

- Better agreement between modeled and observed trends when aerosol feedback effects are considered.
- Lack of any trend and lower R in the “no-feedback” simulation, suggest trends in clear-sky radiation are influenced by trends in aerosol burden.
Surface-cooling partially offsets GHG-related T increase
— Is mitigating PM pollution a climate disbenefit?
— A cooler climate a health benefit?

Reduced ventilation leads to a more stable atmosphere
— Exacerbates air pollution
— A health disbenefit?
Impact of DRE on Air Quality

Seasonal mean (dots); Maximum daily mean (bars)

DRE impacts on cooling and ventilation impact AQ:
- Emission Control Dividend
- Emissions Growth Penalty

Xing et al., 2015 (JGR)
— **Health impacts from enhancement in PM$_{2.5}$ are 3-6 times larger than those reduced due to cooling**

— **ADRE related health effects have reduced by ~45-65% due to control measures in N. America and Europe**

— **Aerosol pollution control have direct benefits on health and indirect benefits on health through changes in local climate**

— **Control measures in N. America & Europe have reduced excess mortality due to ADRE – “Dividend”**

— **“Penalty” in regions witnessing increasing air pollution**

Xing et al., 2016 (ES&T)
Integrated Environmental Exposure Assessment: 
Example: Multi-Media Scenarios of Nitrogen Management in the Face of Changes in Climate & Land Use

Integration through the Nitrogen Cascade

- Nitrogen is a priority problem for Water
  - Leading cause of freshwater impairment (e.g., toxic algal blooms)
  - Major contributor to acidification of fresh waters
  - Main cause of coastal (estuarine) impairment
  - A cause of drinking water contamination

- Nitrogen air emissions impact human health (O₃ & PM₂.₅) and aquatic and terrestrial ecosystems (O₃, deposition)

- Nitrogen flow in the environment is multi-media in character
  - Media connected by the nitrogen cascade

Regional stressors such as climate and land use changes can result in too little or too much nitrogen in the biosphere, prompting unsustainable levels of economic growth and societal behaviors that can degrade air, land and water quality.

Need for an integrated modeling approach: The “one-biosphere” model
Especially for Nitrogen: Air, Land and Water are Interconnected
A One-Environment Capability Can Illuminate Win-Win Cases

- **Agriculture Management**
  - Greenhouse Gas ($N_2O$) – Climate

- **Combustion**
  - NOx, VOC

- **Climate**

- **Meteorology**

- **Hydrology**

- **Air Quality**
  - $O_3$, PM$_{2.5}$ – Health; Visibility – Aesthetics

- **Water Quality**
  - Recreation – Aesthetics; Groundwater Nitrate – Health; Biodiversity

- **Hypoxia**
  - Ecosystem Health; Economic Health

- **Ecosystem Health**

- **Economic Health**

- **Recreation**
  - Aesthetics

- **Groundwater Nitrate**
  - Health

- **Biodiversity**

- **Hydrodynamics**

- **Greenhouse Gas**
  - Climate

- **Air Quality**
  - N, P Load

- **Water Quality**
  - N, P Load

- **Hypoxia**
  - N, P Load

- **Recreation**
  - Aesthetics

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  - N, P Load

- **Recreation**
  - Aesthetics

- **Groundwater Nitrate**
  - Health

- **Biodiversity**

- **Hydrodynamics**
Periodic scientific updates to the CMAQ model have led to the creation of:

- dynamic and diverse user community
- more robust modeling system
Summary

- CMAQ has evolved considerably (processes, species, space & time scales, user & development community) over the past decade to address the increasingly complex applications needed to understand and characterize emerging environmental issues.

- Many emerging & scientifically challenging environmental problems are at the intersection of traditional disciplinary boundaries.
  - Multiple *inter-dependent impacts* from stressors and potential *unintended consequences* of actions often arise from complex interactions and feedbacks in these systems.
  - Requiring *integration and connection of modeling systems*.

- Acknowledgements
  - Numerous scientists in the Computational Exposure Division, U.S. EPA have contributed to the development, evaluation, and evolution of the CMAQ modeling system.

- Model code and documentation available at:
  - [http://www.cmascenter.org/](http://www.cmascenter.org/)
References

- Summary of the Clean Air Act, https://www.epa.gov/laws-regulations/summary-clean-air-act
- State Implementation Plans and Modeling: https://www3.epa.gov/airquality/urbanair/sipstatus/overview.html
Extra Slides
Model Evaluation Framework

- **Operational Evaluation:** *Are we getting the right answers?*
- **Dynamic Evaluation:** *Are we capturing the observed changes in air quality?*
- **Diagnostic Evaluation:** *Are we getting the right answers for the right (or wrong) reasons?*
- **Probabilistic Evaluation:** *What confidence do we have in the model predictions?*

→ *Can we identify needed improvements for modeled processes or inputs?*

CMAQ

Growing number of model evaluation studies

Simón et al., Atmos. Env. 2012
Emerging need: Improvements in Fine-scale simulations

Representing spatial gradients
➢ Bay breeze impacts on inland monitors

O₃ at 3pm LT

Office of Research and Development
National Exposure Research Laboratory
Improvements in Fine scale simulations
Comparison with aircraft measurements
DISCOVER-AQ; July 2, 2011

Average Diurnal Cycle of Obs/Mod Correlations ($R^2$) Across Space for 69 AQS O3 Monitors
Sensitivity Analysis: Direct Decoupled Method

CMAQ-DDM-3D: an efficient and accurate approach for calculating first- and second-order sensitivity of atmospheric pollutant concentrations and accumulated deposition amounts to changes in photochemical model parameters (emissions, chemical reaction rates, initial/boundary conditions, etc.)

Sensitivity of species $i$ to model parameter $j$:

$$\frac{\partial S_{i,j}}{\partial t} = -\nabla (u S_{i,j}) + \nabla (K \nabla S_{i,j}) + J S_{i,j} + E'_i$$

January PM$_{2.5}$

PM$_{2.5}$: LBC Contribution

Courtesy: Sergey Napelenok
Reduced form model based on Taylor series: The response from fractional changes in the amounts of $\Delta \varepsilon_j$ and $\Delta \varepsilon_k$ to two model parameters $j$ and $k$ can be described as:

$$C_{\varepsilon_j,\varepsilon_k} \approx C_0 + \Delta \varepsilon_j S_j^{(1)} + \Delta \varepsilon_k S_k^{(1)} + \frac{\Delta \varepsilon_j}{2} S_{j,j}^{(2)} + \frac{\Delta \varepsilon_k}{2} S_{k,k}^{(2)} + \Delta \varepsilon_j \Delta \varepsilon_k S_{j,k}^{(2)}$$

Ensemble time series of CMAQ daily max 8-hr average ozone predictions at a monitoring site in downtown Atlanta for July 2002.

Courtesy: Kristen Foley
Background

• *The impact of human-induced perturbations on the chemical state of the atmosphere has received significant attention for several decades:*
  – Acid deposition, elevated tropospheric ozone, particulate matter, visibility, direct/indirect radiative effects of aerosols, greenhouse gases

• *Scientific efforts to understand these have involved a combination of:*

  ➢ **Laboratory Experiments**
    – Provide basic data on physical/chemical processes
    – Provide parameters used by models

  ➢ **Field Experiments**
    – Study limited number of atmospheric processes under conditions in which a few processes are dominant
    – Snapshot of conditions at particular time & location

  ➢ **Modeling Experiments**
    – Tools to integrate and synthesize our evolving knowledge of various atmospheric processes