2009 AMAD Peer Review: Session 1
Model Development and Diagnostic Testing

Modeling Atmospheric Particulate Matter: Description and Evaluation of the CMAQ Aerosol Module

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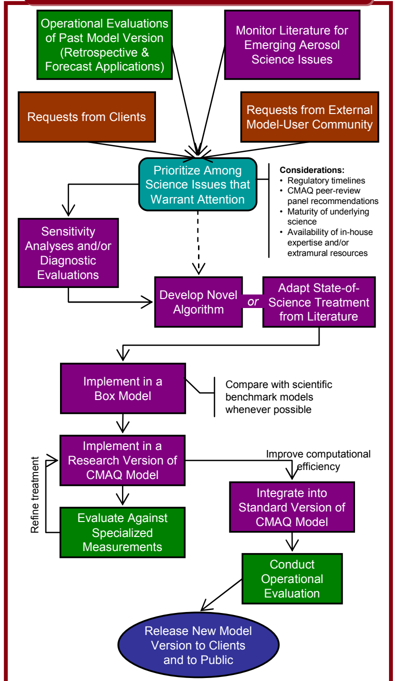
Environmental Issue

Atmospheric particulate matter has been linked to acute and chronic health effects, visibility degradation, acid and nutrient deposition, and climate change. Accurate predictions of the PM mass composition and size distribution are necessary for NAAQS attainment demonstrations and for assessing the potential impacts of future air quality regulations and climate change on human health and environmental outcomes.

Research Objectives

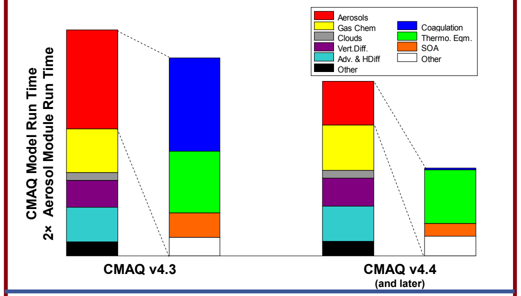
Improve predictions of PM mass concentrations and chemical composition by advancing the scientific algorithms, computational efficiency, and numerical stability of the CMAQ aerosol module.

Approach

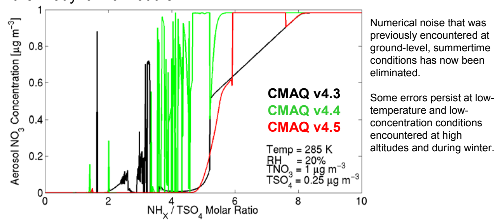


Results and Discussion

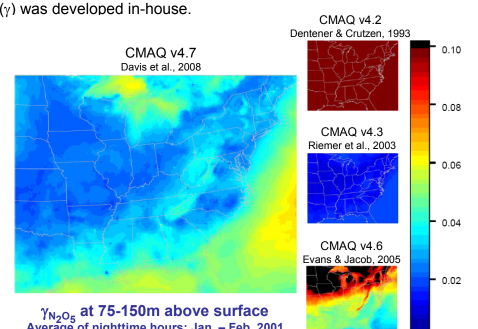
Computational Efficiency. In preparation for CAIR simulations, aerosol calculations were sped up by factor of 2.3 by improving the computations of coagulation coefficients and SOA partitioning.



Numerical Stability. Since 2003, we have worked with the developer of ISORROPIA to address numerical issues in the inorganic thermodynamic module.



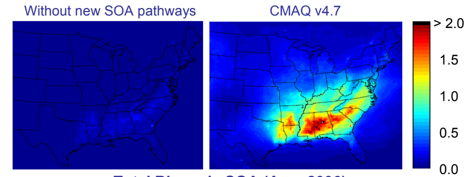
Wintertime Nitrate. Ambient $PM_{2.5}$ concentrations during winter are driven by primary emissions and secondary nitrate. Since 2002, AMAD efforts focused on reducing model overpredictions of total nitrate (gas-phase HNO_3 + particulate NO_3^-). Recently, a new parameterization of the heterogeneous reaction probability of N_2O_5 (γ) was developed in-house.



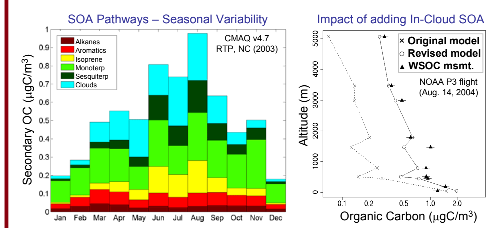
$\gamma_{N_2O_5}$ at 75-150m above surface
Average of nighttime hours: Jan. – Feb. 2001

Summertime Organics.

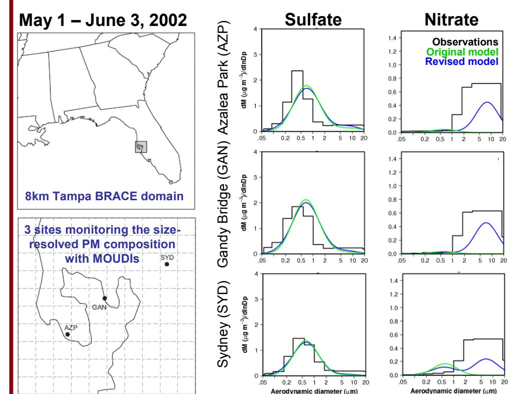
- Diagnostic evaluations using an instrumented version of CMAQ v4.4 indicated that biogenic SOA was largely responsible for underpredictions of summertime OC (see Poster 2.3).
- A vastly improved SOA module was incorporated into CMAQ v4.7 that treats several new SOA precursors (benzene, isoprene, and sesquiterpenes) and pathways (in-cloud oxidation, polymerization, acid-catalysis, and NO_X-dependent yields).



Total Biogenic SOA (Aug. 2006)



Coarse PM Chemistry. Dynamic interactions between inorganic gases and the coarse PM mode were tested first in a research model and later implemented in CMAQ v4.7. CMAQ simulations of coarse-mode PM composition are far more accurate now than before.



Conclusions

- Scientific quality, computational efficiency, and numerical stability of the CMAQ aerosol module have been enhanced greatly over the past 5 years.
- Scientific basis and model performance have been improved for total nitrate, biogenic SOA, and coarse PM composition.
- Computational burden of the aerosol calculations has been reduced by more than a factor of two.
- Numerical stability of thermodynamic module has been improved substantially.

Future Directions

- Recent operational evaluations revealed large model overpredictions for unspeciated $PM_{2.5}$ material, thereby prompting model investigations of the trace-elemental composition of $PM_{2.5}$, non-carbon organic material, and sampling artifacts associated with gravimetric $PM_{2.5}$ measurements.
- Anticipating the promulgation of a coarse PM standard, efforts are underway to simulate emissions of natural windblown dust and the interactions between crustal ions and inorganic gases.
- Improve representation of the optical and radiative properties of PM, for linkage with the two-way coupled WRF-CMAQ model.
- Simulate episodic events when $PM_{2.5}$ concentrations in urban areas exceed the new 24-h standard (35 $\mu g/m^3$).
- Parameterize the volatility distribution of organic material and the effects of atmospheric oxidation processes on that distribution.

Impact

- Aerosol module has been used for regulatory and forecasting applications (e.g., EPA-CAIR, NOAA-NCEP) because it is scientifically credible, computationally efficient, and numerically stable.
- Due to recent scientific enhancements, confidence has been increased in the utility of CMAQ predictions of PM for future regulatory applications (e.g., RFS2).
- Outside of EPA, the CMAQ user community has more than tripled in size over the past 3 years.

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