Improving Atmospheric Deposition Processes in CMAQ for Ecosystem Applications

Jesse Bash, Prakash Bhave, Jonathan Pleim, Robin Dennis, Christopher Nolte, Ellen Cooter

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Linking Air Quality and Ecosystem Health

Environmental Issue

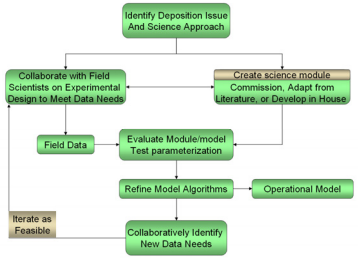
- Excess nitrogen deposition (from NO_x and NH_3 emissions) to ecosystems can lead to nutrient imbalances and eutrophication.
- Providing an accurate nitrogen deposition estimate is important to biogeochemical cycling calculations with ecosystem models to simulate ecosystem degradation and recovery
- Providing accurate dry deposition estimates has the highest priority for water and soil chemistry modeling due to the lack of monitoring data
- Nitrate that condenses on coarse sea-salt particles deposits more rapidly than HNO_3 to coastal waters which are highly sensitive to nitrogen exposure.
- Evasive losses of ammonia from fertilized agriculture operations, the second largest sources of atmospheric ammonia, are poorly quantified and make a large contribution to downwind deposition.

Research Objectives

- Address nitrogen dry deposition issues that are most important to reducing uncertainty, filling gaps in pathways, incorporating new science process insights, and establishing model credibility
- Improve the modeled transport and chemical mechanisms to better understand the exposure of ecosystems to excessive nutrients and toxins.
- Collaborate with measurement groups on experimental designs of field campaigns to maximize the utility of the data for the development of mechanistic models.
- Use the refined models to estimate ecosystem exposure where monitoring data are unavailable.

Modeling Approach

- Review current literature and model sensitivity to identify current deposition/ ecosystem exposure issues.
- Collaborate with measurement community on the experimental design to ensure the measurement of the critical variables that are needed for robust model evaluation and development.
- Implement and refine model algorithms using newly collected field data.



Results and Discussion

1. Coarse-particle Nitrate:

- Commissioned the development of CMAQ-UCD, a sectional aerosol module with fully-dynamic mass transfer of inorganic species between the gas phase and each particle size bin
- Evaluated CMAQ-UCD model results against size-resolved particle composition measurements taken during the intensive Tampa BRACE field campaign

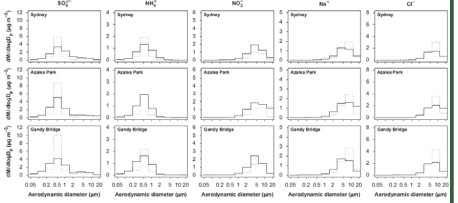
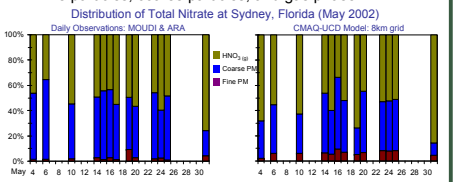
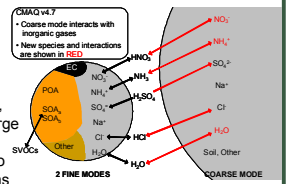


Fig. 3. Observed (solid) and model-predicted (dotted) size distributions of inorganic aerosol components at three Tampa-area sites averaged over 15 sampling days (14 at Sydney) during May 2002. Nolte et al. (*Atmos. Environ.*, 2008)

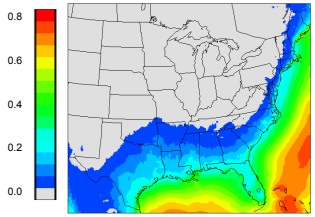
- Assessed the model's partitioning of total nitrate between fine particles, coarse particles, and gas phase



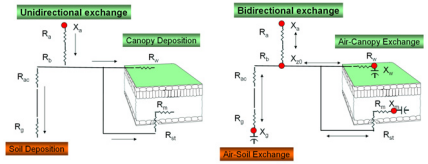
- Implemented dynamic mass transfer treatment in the operational version of CMAQ
- Using CMAQ v4.7, we found that a large fraction of the TNO_3 deposition to coastal ecosystems occurs in the form of coarse-mode nitrate.



Fractional Contribution of Coarse PM to Total Nitrate Deposition (2002)



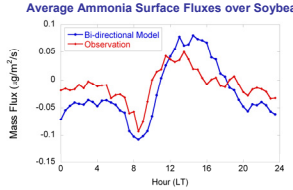
2. Bidirectional exchange



- A prototypes of the NH_3 and Hg bi-directional models were developed from algorithms and conceptual models published in the literature.
- Model sensitivities assessed to aid in field campaign experimental design
- Data collected in collaboration with U.S. EPA NRMRL and NOAA/ARL scientists provided measurements of variables necessary to refine bi-directional NH_3 exchange algorithms.

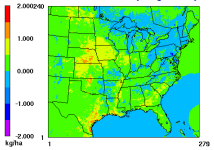
	Resistance to deposition
⊣⊢	Capacitance for re-emission
R_a	Atmospheric resistance
R_b	Laminar boundary layer resistance
R_{ac}	In-canopy atmospheric resistance
R_g	Ground resistance
R_{uc}	Cuticular resistance
R_{st}	Stomatal resistance
R_m	Mesophyll resistance
X_a	Atmospheric concentration
X_{a2}	Air compensation point at $z = z_0$
X_g	Soil compensation point
X_m	Mesophyll compensation point
X_w	Cuticular compensation point

Average Ammonia Surface Fluxes over Soybeans

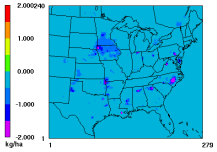


- CMAQ dry deposition algorithms have been modified to parameterize air-surface exchange of NH_3 and Hg.
- CMAQ v4.7 simulations estimate NH_3 emission sources from fertilized fields, particularly in the Midwest U.S. and the Gulf States
- Model deposition (designated with negative values) increased in areas of the Northeast U.S. and Mid-Atlantic States with large livestock emission sources

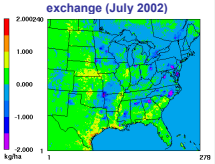
Bidirectional minus Unidirectional CMAQ (July 2002)



CMAQ with unidirectional exchange (July 2002)



CMAQ with bidirectional exchange (July 2002)



Conclusions

- New algorithms advanced the science of CMAQ and make a difference in its predictions.
- An open dialogue with measurement groups and inclusion of modelers in the experimental designs were critical to ensure usable data for model parameterization and evaluation.
- Development of the bidirectional ammonia exchange and coarse-nitrate algorithms improved the oxidized and reduced nitrogen budgets as well as the partitioning of nitrate between gas and size-segregated aerosol phases.
- Bidirectional model results showed the need to develop an ammonia surface flux model and helped prioritize specific measurement needs for future field experiments.

Future Directions

- Evaluate the newly developed modules with routine monitoring and intensively-collected field data.
- Refine a compartmentalized model with 2007 – 2008 data, collected in collaboration with EPA/NRMRL and NOAA/ARL, to predict the NH_3 flux and in-canopy exchang processes between soil, vegetation and atmosphere.
- Develop techniques based on a simplified soil biochemistry model to derive soil concentrations of NH_4^+ and H^+ from fertilizer application data to be used in the ammonia surface flux model.
- Sectors of the NH_3 emission inventory which are currently adjusted by inverse models need modifications to account for the new bidirectional flux algorithm.
- Leverage mercury field campaigns to measure the variables needed to refine and evaluate the bidirectional mercury model (see poster 5.4).

Impact

- Model developments make the nitrogen budgets of CMAQ more credible for ecosystem assessments.
- Nitrogen deposition to estuary/coastal-ocean surfaces is enhanced, increasing the impact of atmospheric nitrogen on estuaries like Chesapeake Bay and Tampa Bay.
- Bidirectional algorithm increases the range of influence of NH_3, affecting strategies to reduce $PM_{2.5}$ exposure and watershed loading.
- Opened the door to inter-laboratory collaboration to better use EPA resources
- CMAQ-UCD model was used for Tampa Bay Total Maximum Daily Load (TMDL)

Contributors/Collaborators

Jeff Arnold (EPA/NCEA)*; James Kelly (CARB)*; John T. Walker (EPA/NRMRL); Matthew Jones (DOE/ORISE); Uma Shankar (UNC); Anthony Wexler (UC Davis); K. Max Zhang (Cornell Univ.); Winston Luke, Tilden Meyers, and LaToya Myles (NOAA/ARL); Robert Mason (Univ. of Connecticut)
* Formerly of NERL/Atmospheric Modeling and Analysis Div.