Investigation of atmospheric nitrate and ammonium and their impact on air quality in GMI

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1. Introduction

➢ **GOALS**:

• Introduce a new capability to GMI to simulate atmospheric aerosol components nitrate and ammonium.

• Examine the impact of multiphase chemical mechanism and new aerosol components on air quality and climate change.

➢ **APPROACH:**

- Implement new tracers (ammonia NH3g, ammonium NH4a, nitrate NO3a) in GMI, set up NH3g emissions, and determine parameters for scavenging and chemical processes.
- Implement a thermodynamic equilibrium model (RPMARES) from GEOS-CHEM for a SO4-NO3a-NH4a-H2O system to partition semi-volatile species, such as HNO3, between gas (i.e. HNO3g) and aerosol phases (NO3a).
- Implement HNO3 heterogeneous reactions on dust and sea salt particles.
- Analyze one year simulation results (year 2006) after one year spin up. Evaluate model aerosol results with the ground station observations from CASTNET and EMEP.
- Understand the change of chemistry fields with and without inclusion of NO3a and NH4a, i.e. CoupleNO3 versus CoupleNoNO3.

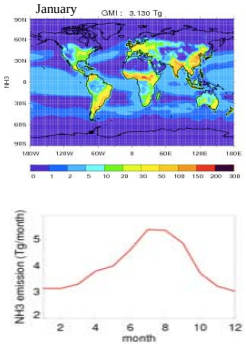
2. GMI and its new capability

• GMI is a global 3D CTM with a coupled gas-aerosol chemistry scheme for troposphere and stratosphere.

• Previous GMI aerosol components include sulfate, BC, OC, dust, and sea salt.

• In this work, we expand GMI by adding aerosols NH4a and NO3a.

NH3g emission



Annual NH3g emissions in 2001: 47.9 Tg

GEIA inventory of Bouwman et al. [1997]: Domesticated animals, Fertilizers, Human bodies, Industry, Fossil Fuel, Ocean, Crop, Soils, Wild animals.

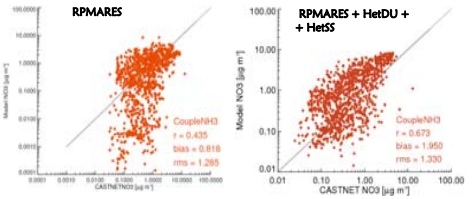
Seasonal variation:
Exponential dependences on T [Aneja et al., [2000] for domesticated animals and soils and linearly to the number of daylight hours for crop and fertilizers [Park et al., 2004]

GFED2, Van der Werf et al. [2006]: Biomass burning
Yevich and Logan [2003]: Biofuel

Emission factor = 1.3 g NH3 per kg DM [Andreae and Merlet, 2001]

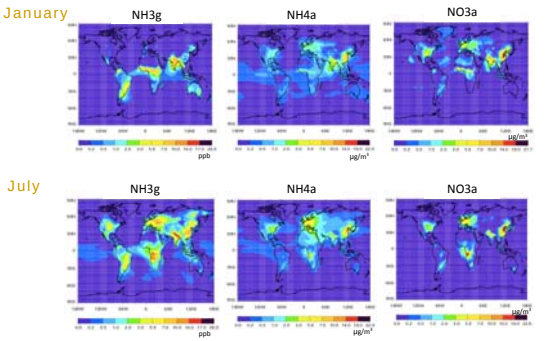
3. Results for NH4a and NO3a simulations

NO3a model-observation comparisons with different approaches



Model-observation NO3a over CASTNET stations in US for two model approaches: 1. using a thermodynamic equilibrium model (RPMARES) for multiphase chemistry; 2. similar to 1 but adding HNO3 heterogeneous reaction on dust and sea salt (RPMARES+HetDU+HetSS).

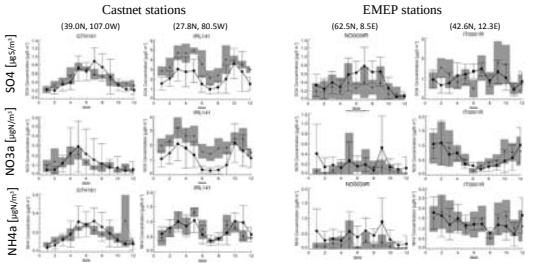
Surface NH3g, NH4a, and NO3a distributions



1. All three tracers concentrated over land regions and follow their emission patterns in both seasons.
2. In January, both NH4a and NO3a spread more widely over Northern Hemisphere (NH) mid-latitudes compared to NH3.
3. Both NH3 and NH4a were higher in July, but seasonal change of NO3 varied in regions.

Compare with station measurements

Over single station

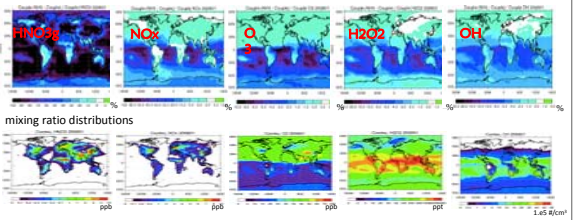


GMI captured measured aerosol values and seasonal change better over Castnet stations (North America, NA) than over EMEP stations (Europe, EU).

4. Impact of NH4a and NO3a on surface chemistry field

January

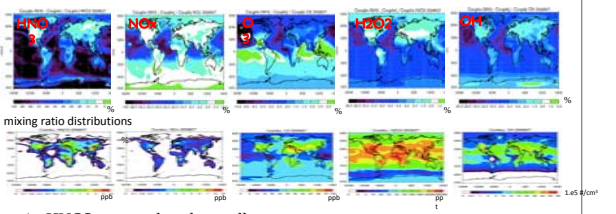
Change (%) = (CoupleNO3 – CoupleNoNO3) / CoupleNoNO3



1. HNO3g decreased globally in CoupleNO3 since part of HNO3g in CoupleNoNO3 went into nitrate aerosol.
2. Decreased HNO3g drove global NOx and OH reduction through deceasing its photodissociation.
3. Further analysis is needed to understand the response of H2O2 and O3 to the changes of OH and NOx.
4. The largest percentage change of NOx, OH, H2O2, and O3 occurred over Southern tropical and subtropical oceans in January.
5. The average global change of O3 was less than 2%; its largest percentage change occurred over low O3 regions.

July

Change (%) = (CoupleNO3 – CoupleNoNO3) / CoupleNoNO3



1. HNO3g was reduced as well.
2. The NOx, OH, H2O2, and O3 were also decreased except in regions with extremely low NOx and O3.
3. The largest percentage change of NOx, OH, H2O2, and O3 occurred over NH oceans in July.

5. Summary

1. GMI has a new capability of simulating aerosol ammonium and nitrate.
2. Nitrate simulation needs including not only multiple chemistry reactions in a SO4-NO3a-NH4a-H2O system, but also the heterogeneous reactions of HNO3 on dust and sea salt.
3. All three tracers (NH3g, NH4a, and NO3a) concentrate over land regions at surface. Concentrations of NH3g and NH4a are generally larger in summer than in winter.
4. Nitrate simulation has a little impact on sulfate simulation, but it results in non-negligible regional changes of some gas tracers including NOx, HOx, and O3.