New capabilities in GMI : Gas-aerosol coupling and nitrate aerosol

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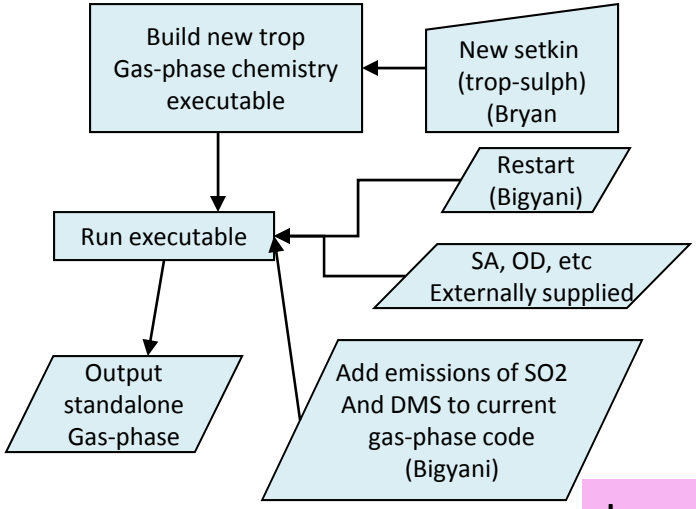
GMI workshop, Oct. 9, 2010

Acknowledge: Bryan Duncan, Duncan Fairlie, Rokjin Park,

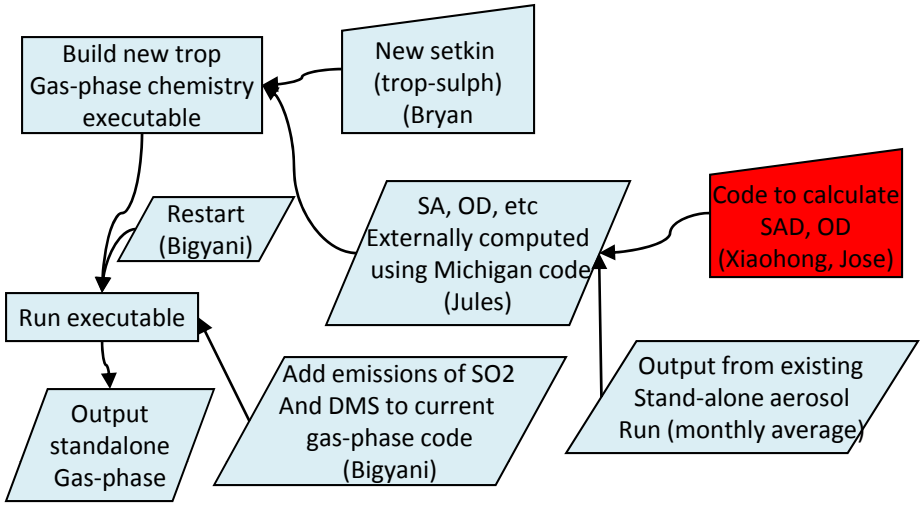
Pete Colarco, and Susan Strahan

Step 1. We test that indeed the tropospheric gas-phase chemistry code works with the new added species and reactions .

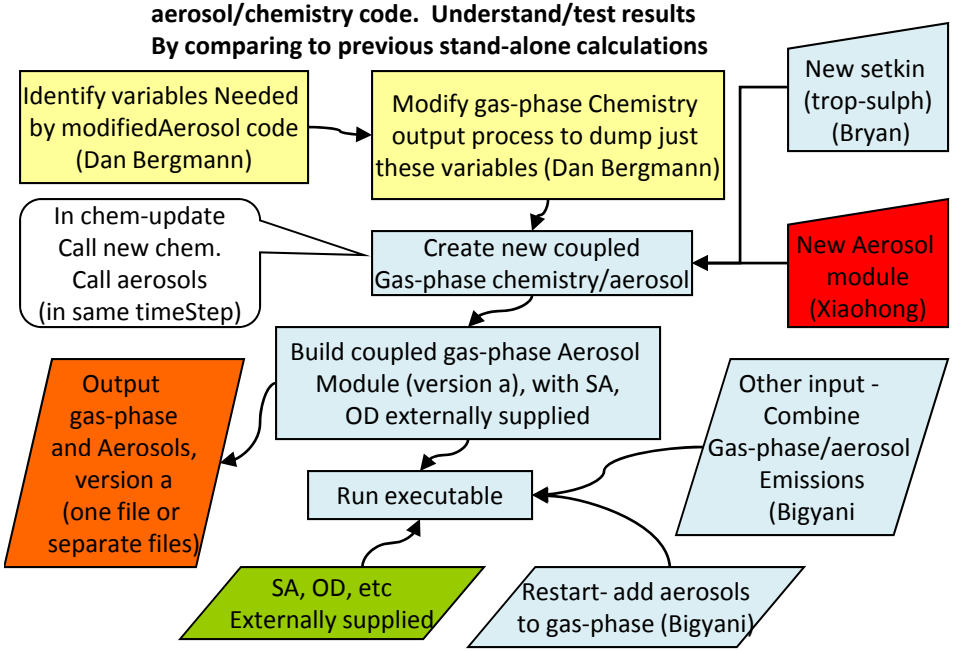


Jose Rodriguez

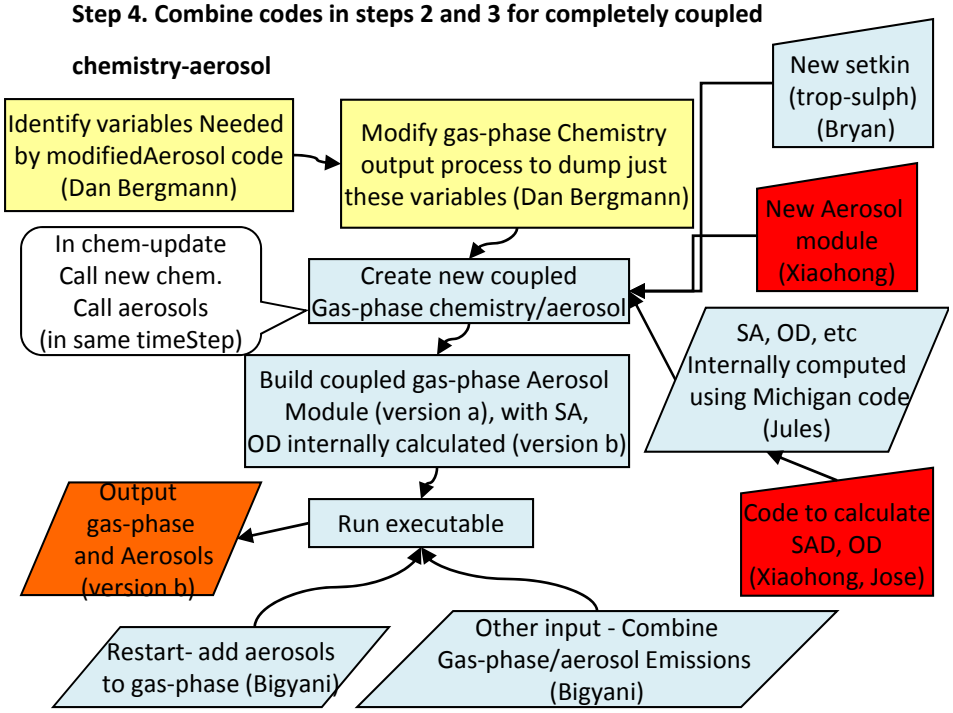
Step 3 (parallel to 2): Jules utilizes output from existing stand-alone aerosol runs and Michigan Code to calculate SAD, OD. Run gas-phase code, test with other simulations (should be similar, but not the same).



2. Xiaohong/Dan Bergmann deliver version a of modified aerosol/chemistry code. Understand/test results By comparing to previous stand-alone calculations



Step 4. Combine codes in steps 2 and 3 for completely coupled chemistry-aerosol



Gas – aerosol coupling

GMI runs to evaluate the work of gas-aerosol coupling

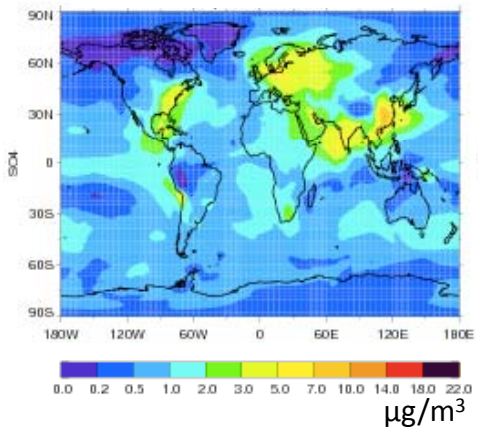
GMI-COUPLE	Modify GMI model framework and dataflow to handle new species and reactions. Merge sulfate gas phase chemistry into Combo chemistry package. Consider dynamic feedback of H2O2 etc in aqueous phase reaction. Use online aerosol fields for photolysis and tropospheric heterogeneous reaction calculation.
GMI-GOCART	Using archived GMI Couple monthly mean oxidant fields for sulfur chemistry. Provide reference aerosol fields.
GMI-COMBO	Using archived GMI Couple monthly mean aerosol fields for photolysis and tropospheric heterogeneous reaction. Provide reference gas tracer fields.

Gas – aerosol coupling

January 2001

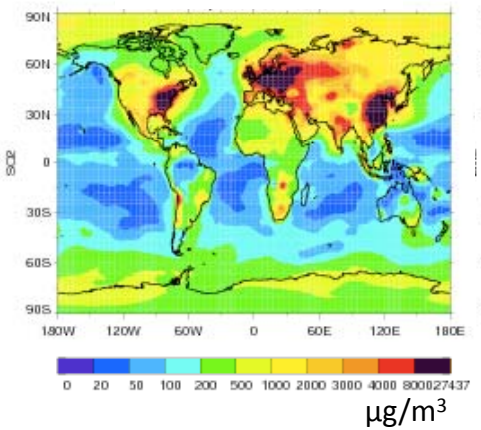
Aerosol surface distributions from Couple

SO4



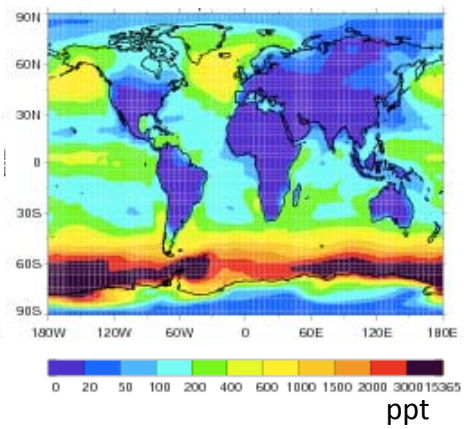
µg/m^3

SO2



µg/m^3

DMS



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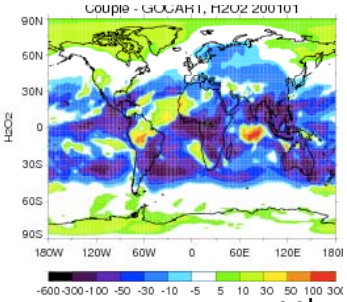
Changes in gas tracers

H2O2



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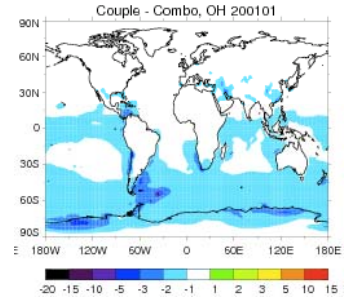
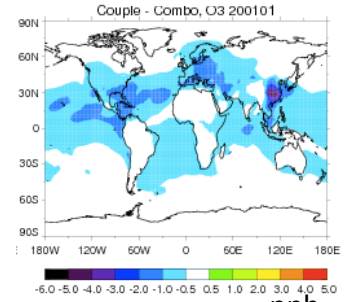
OH



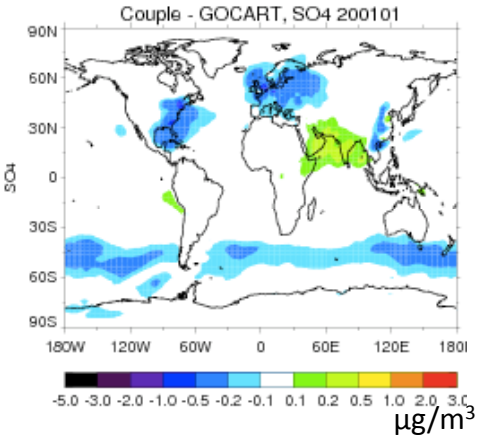
1.e5 #/cm^3

O3

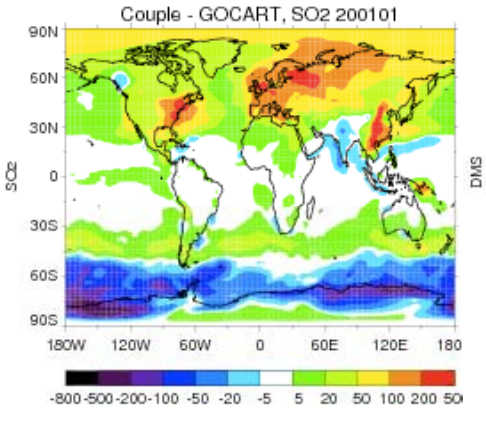


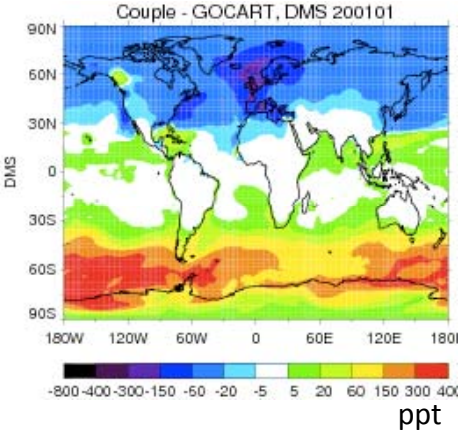
ppb

Aerosol change due to coupling (Couple – GOCART)



µg/m^3





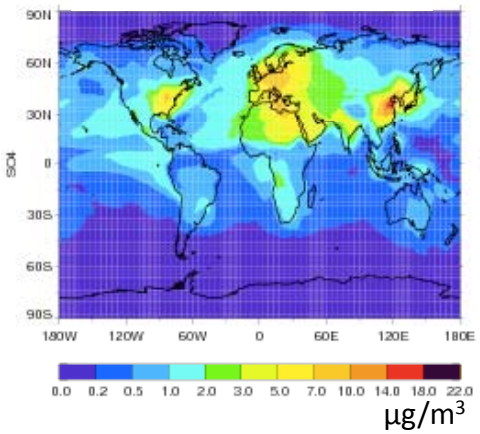
ppt

Gas – aerosol coupling

July 2001

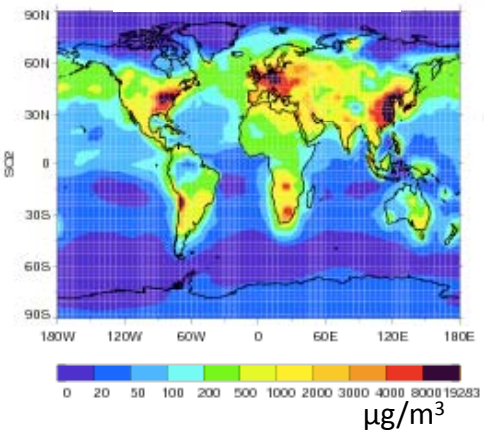
Aerosol distributions from Couple

SO4



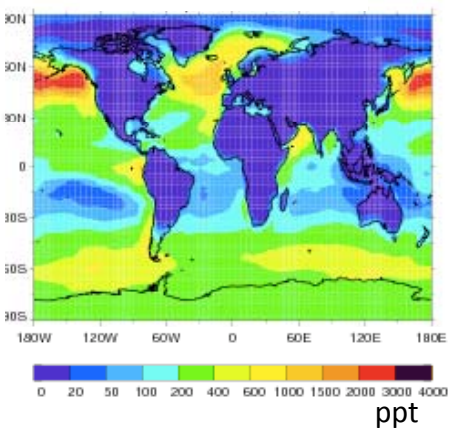
µg/m^3

SO2



µg/m^3

DMS



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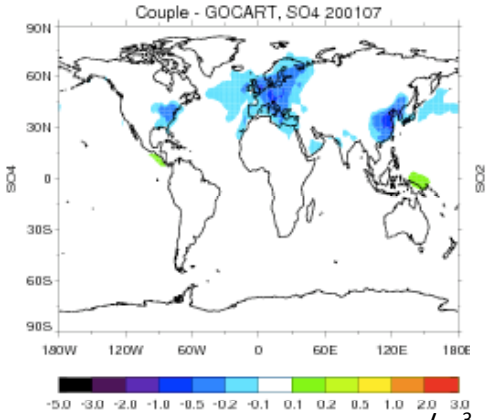
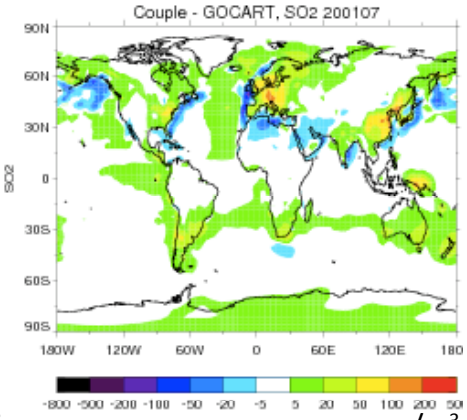
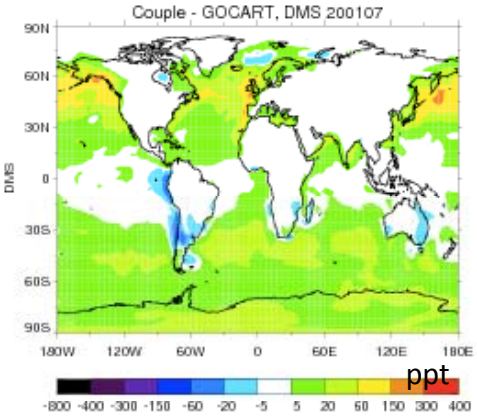


µg/m^3



µg/m^3



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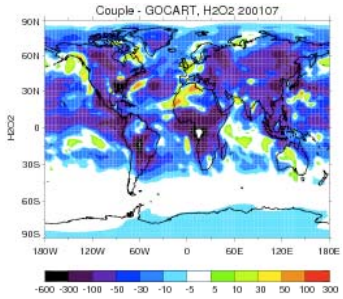
Changes in gas tracers

H2O2



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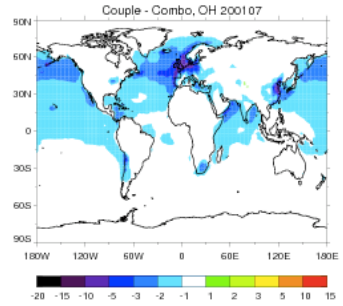
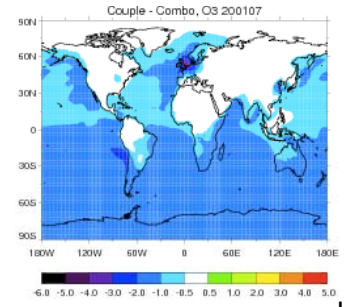
OH



1.e5 #/cm^3

O3



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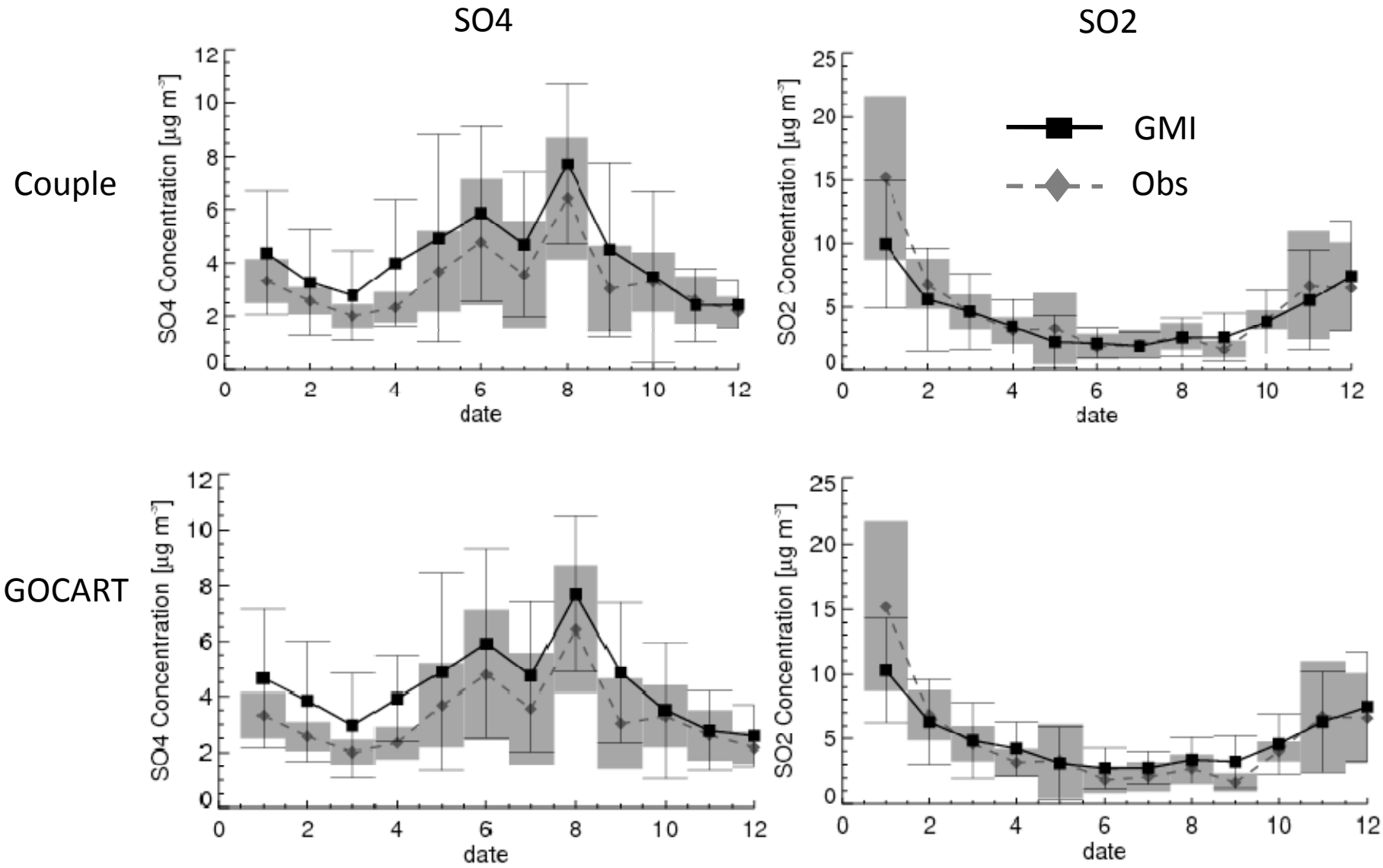
Gas – aerosol coupling

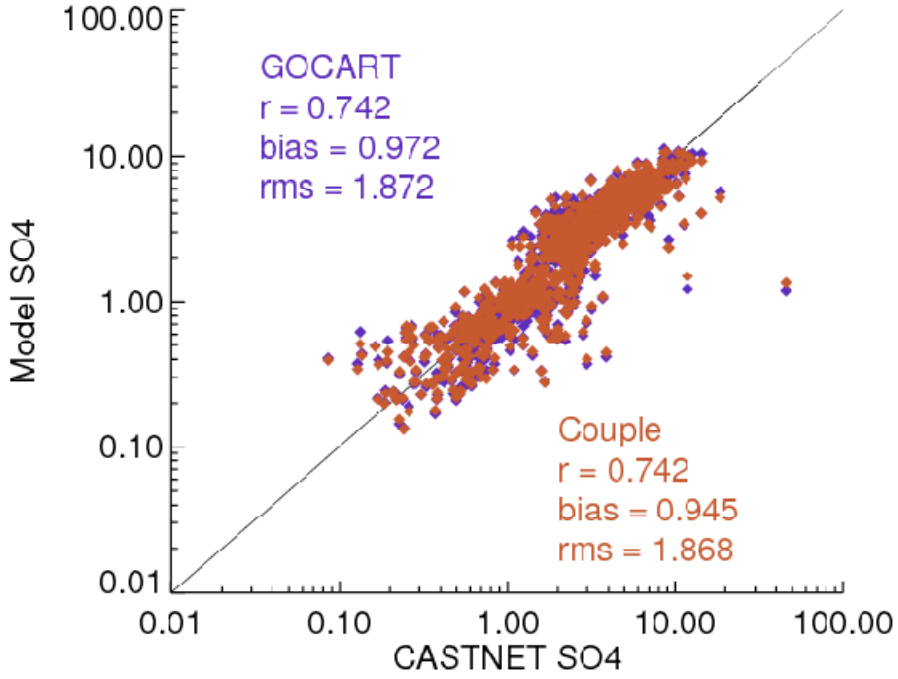
Compare with CastNet station ABT147 (41.8N, 72.0W)



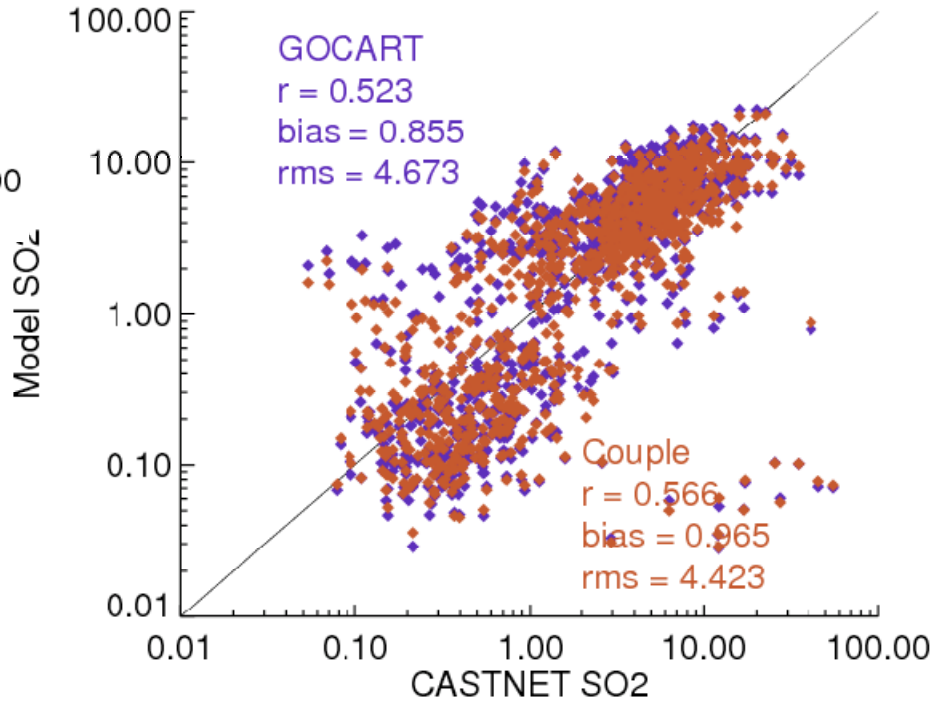
Gas – aerosol coupling

Overall compare with CastNet

SO4



SO2



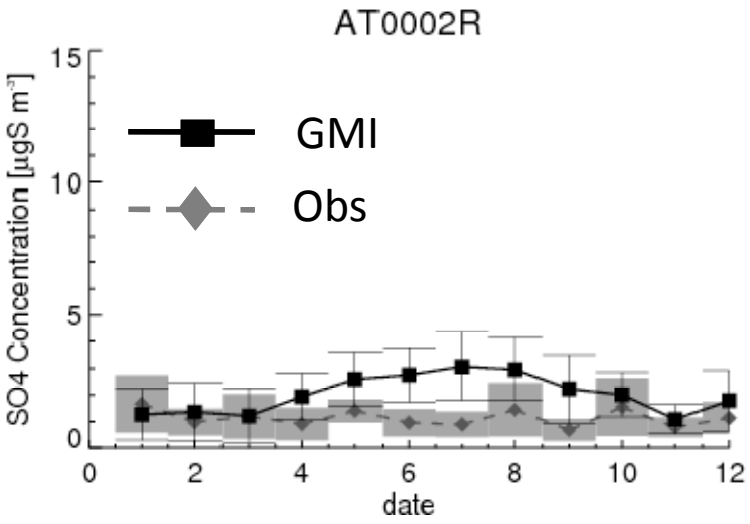
Gas – aerosol coupling

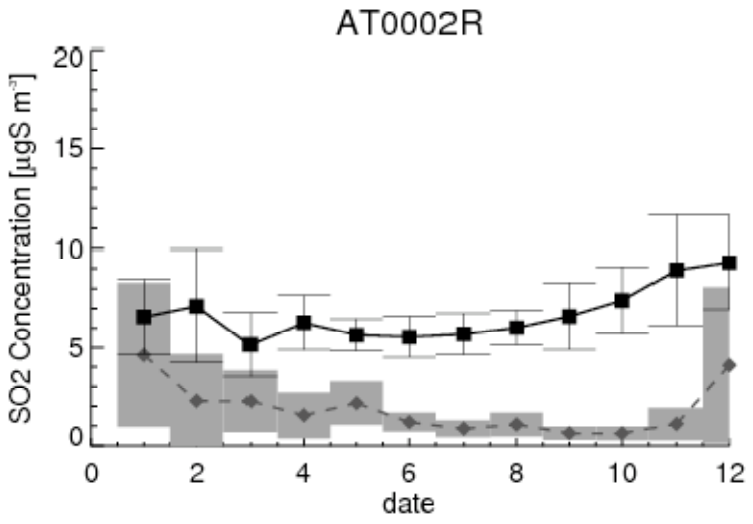
Compare with EMEP station ATOO02R (47.5N, 16.5E)

SO4

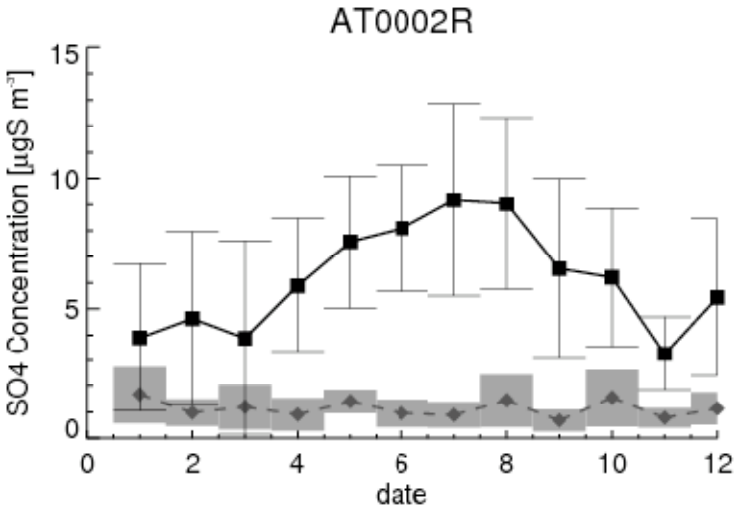
SO2

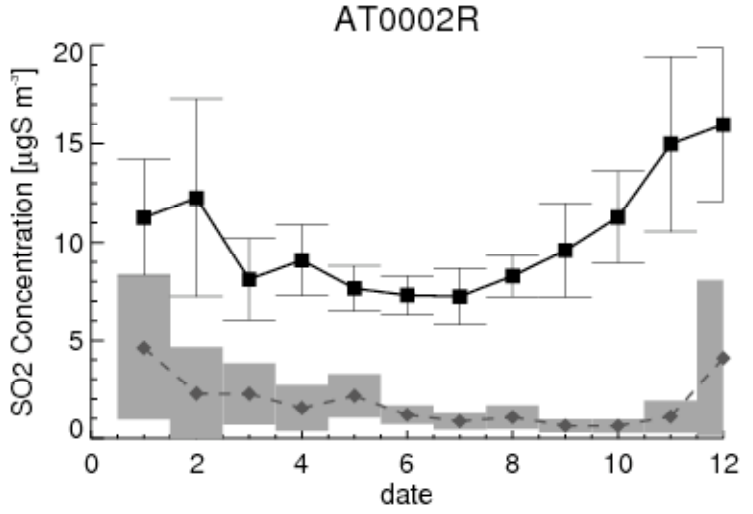
Couple





GOCART

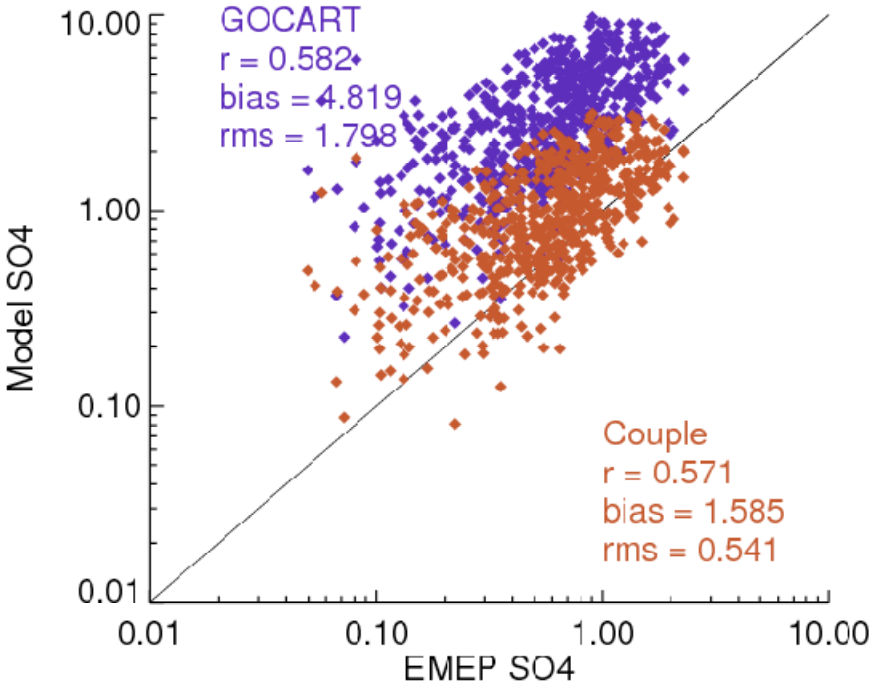




Gas – aerosol coupling

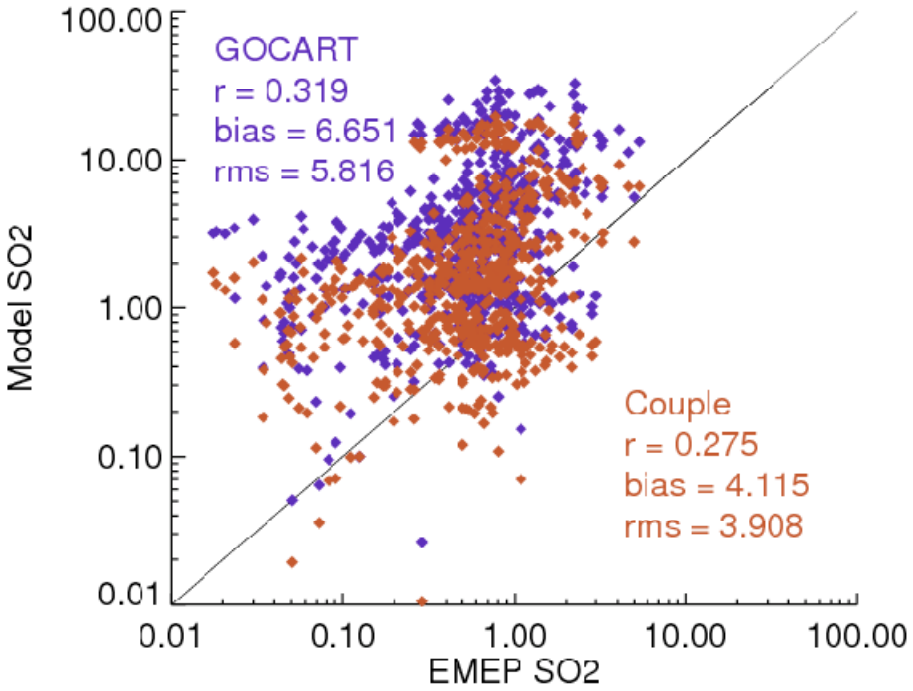
Overall compare with EMEP

SO4



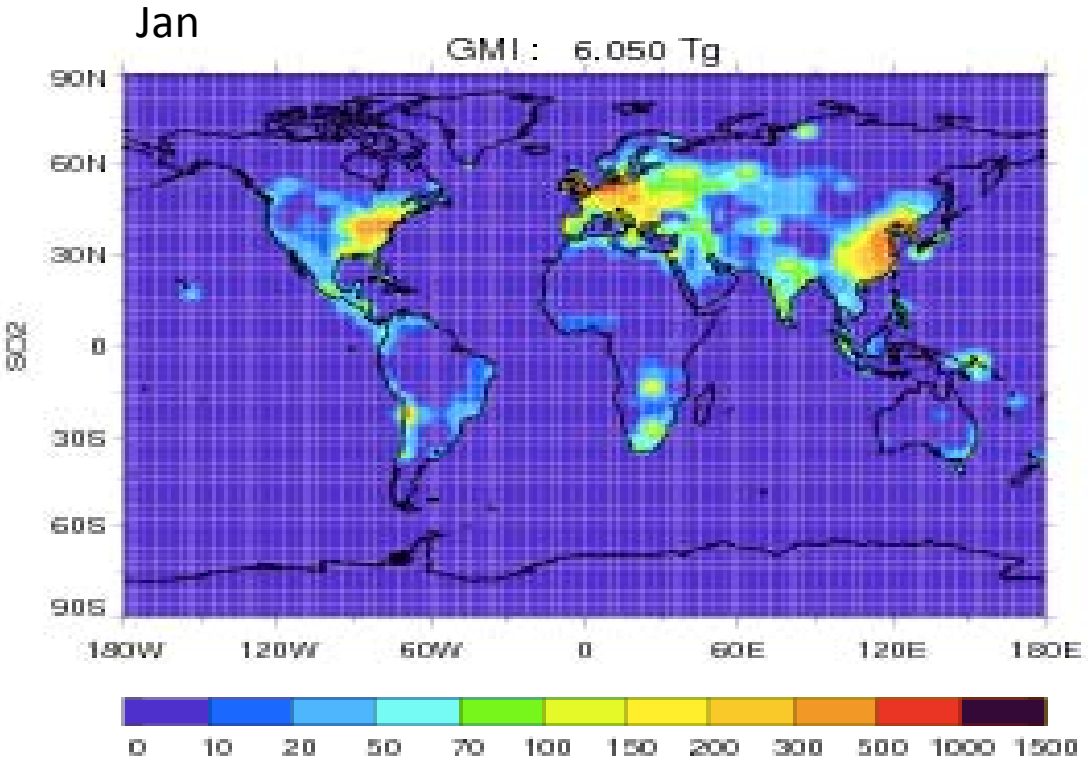
Why so2 and so4 both decreased with Couple approach?

SO2



Gas – aerosol coupling

SO2 Emission



Anthropogenic emission comes from David Streets Over Europe, he adopts EDGAR v3.2

Annual total sulfate emission (Tg/year)

GMI	Aerocom		
	mean	minimum	maximum
72.6	58.2	40.9	77.4

Summary for

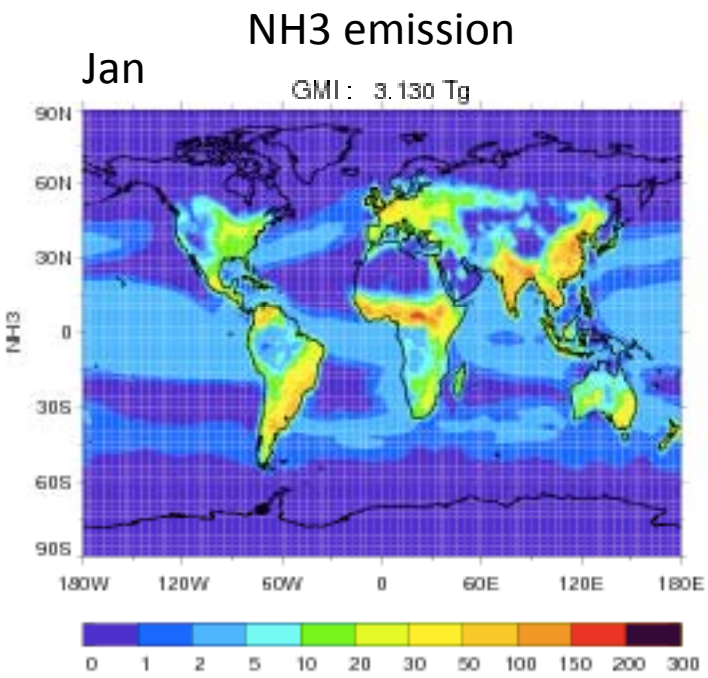
- GMI has an option for gas-aerosol coupling finally.
- Dynamic feedbacks between gas and aerosol fields in the coupling approach reduce oxidant fields and slowdown chemical reactions.
- Coupling approach results in a better model-observation comparison for aerosol simulation, particular over Europe area.
- Need to investigate SO2 emissions over Europe area.

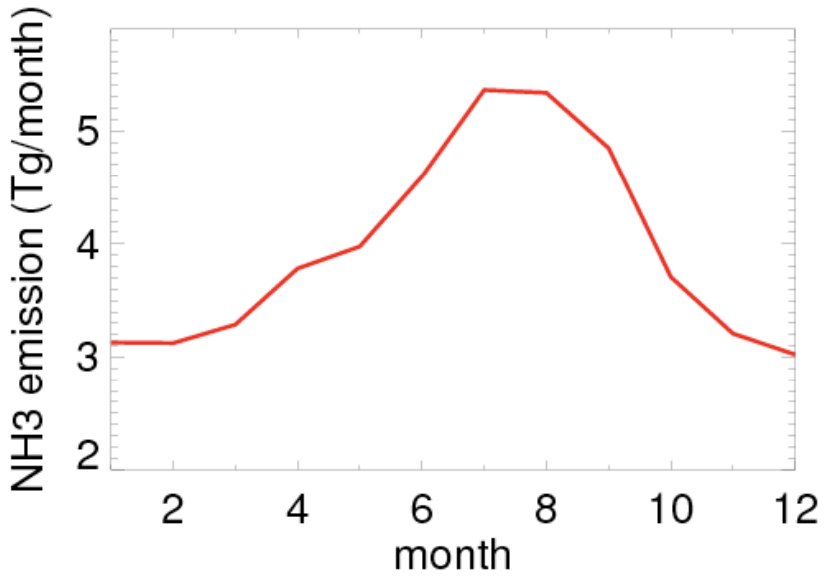
New aerosol components

GMI runs analyzed here

GMI-COUPLE	Modify GMI model framework and dataflow to handle new species and reactions. Merge sulfate gas phase chemistry into Combo chemistry package. Consider dynamic feedback of H2O2 etc in aqueous phase reaction. Use online aerosol fields for photolysis and tropospheric heterogeneous reaction calculation.
GMI-COUPLENH3	Based on COUPLE. Add NH3, NH4a, and NO3a. Prepare emission fields. Determine various parameters for scavenging and chemical processes. Implement GEOS-CHEM EQM to partition tracer between gas and aerosol.

New aerosol components





Annual NH_3 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

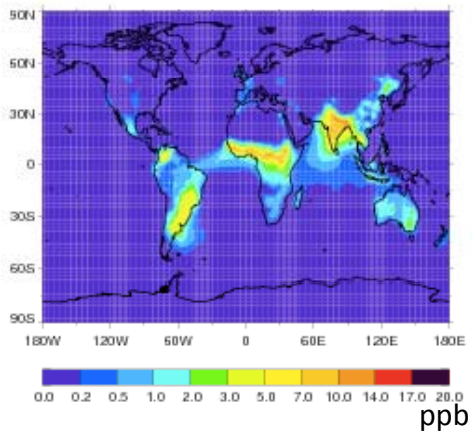
Emission factor = 1.3 g NH3 per kg DM [Andreae and Merlet, 2001]

New aerosol components

Surface nitrate simulation (run case: CoupleNH3)

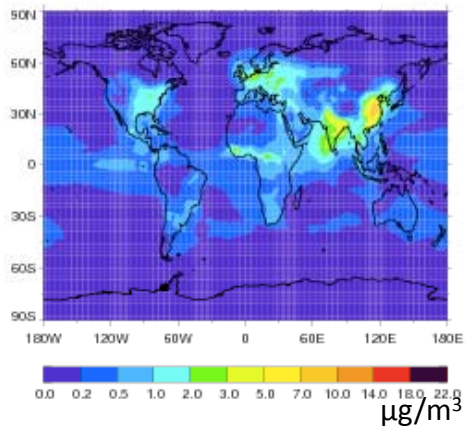
January

NH3



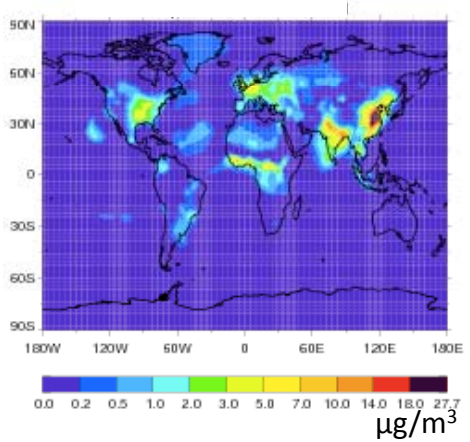
ppb

NH4a



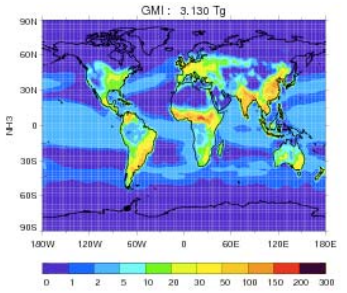
µg/m^3

NO3a



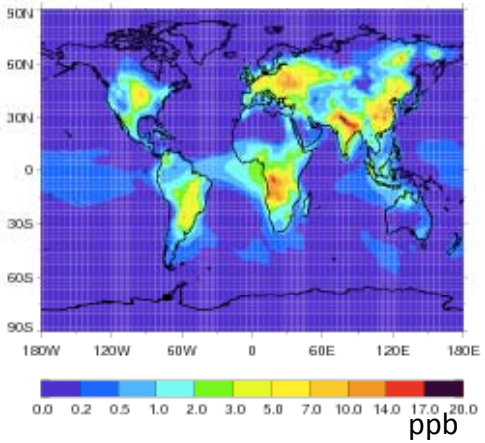
µg/m^3

NH3 emi: 3.13 Tg



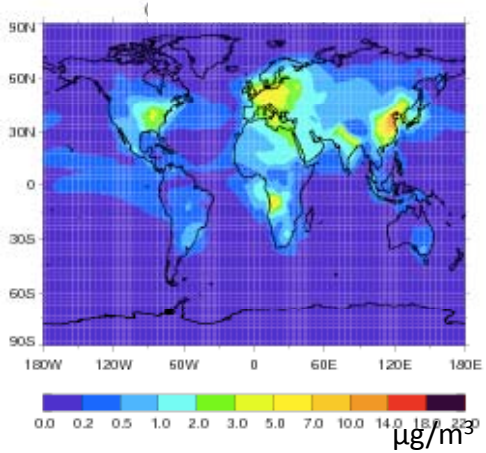
July

NH3



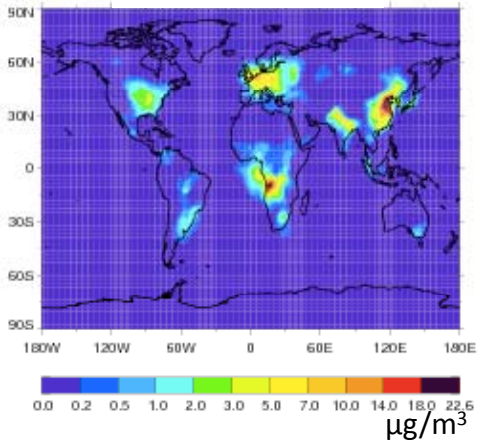
ppb

NH4a



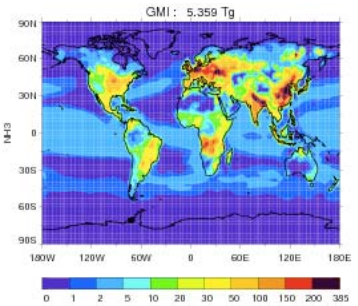
µg/m^3

NO3a



µg/m^3

NH3 emi: 5.36 Tg

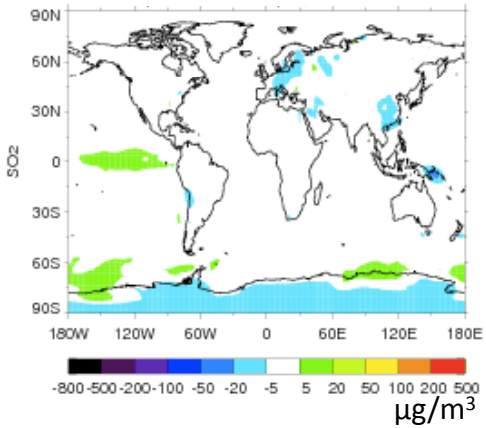


New aerosol components

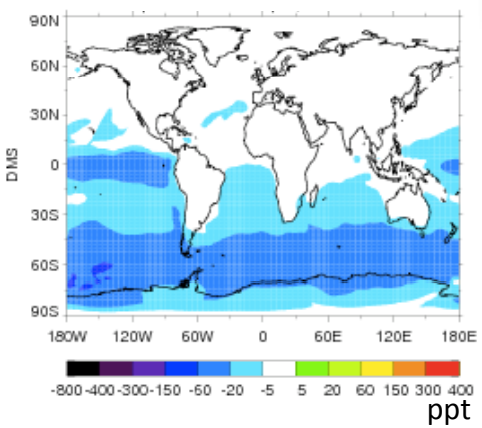
January 2001

Impact of nitrate aerosol on other gas and aerosol fields (CoupleNH3 – Couple)

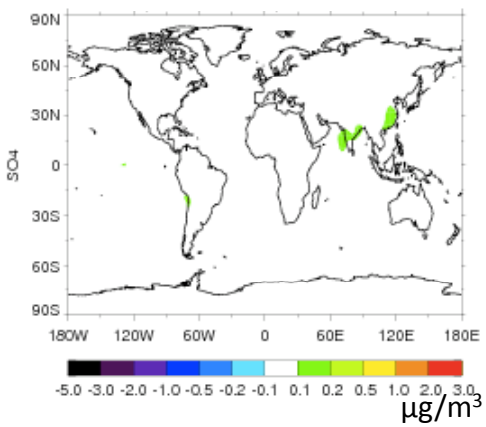
SO2



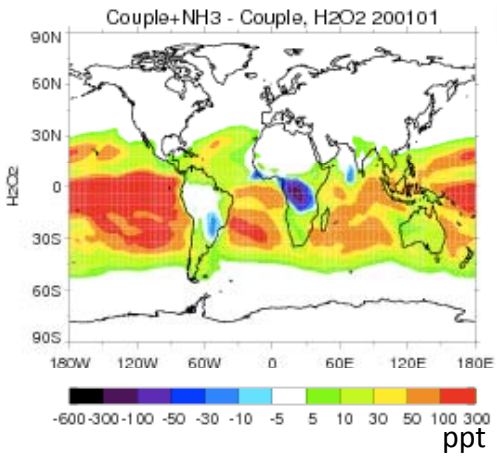
DMS



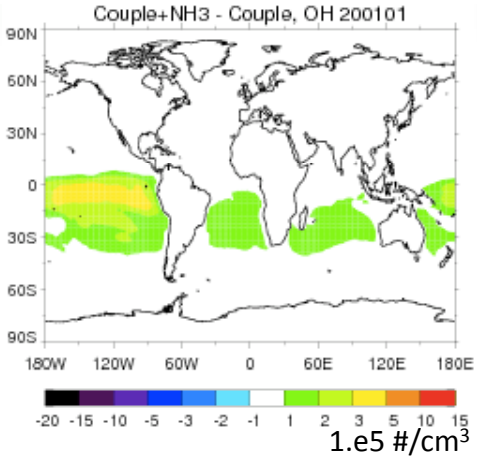
SO4



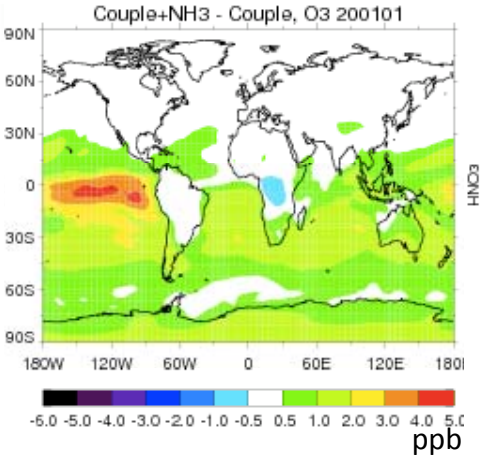
H2O2



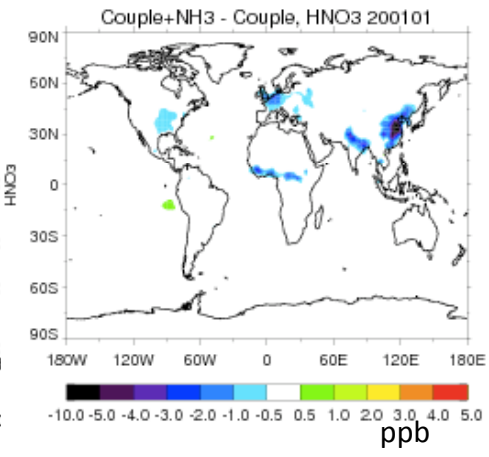
OH



O3



HNO3

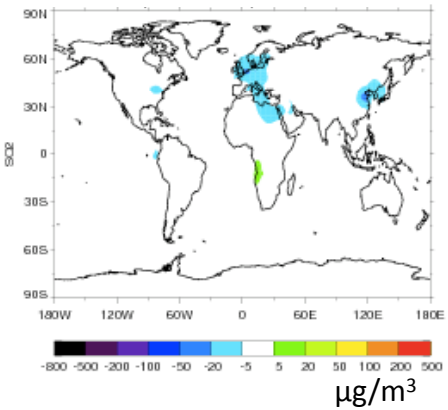


New aerosol components

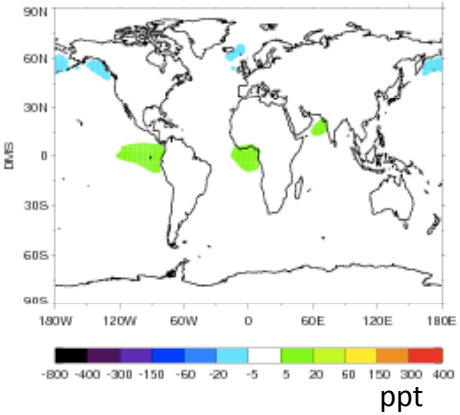
July 2001

Impact of nitrate aerosol on other gas and aerosol fields (CoupleNH3 – Couple)

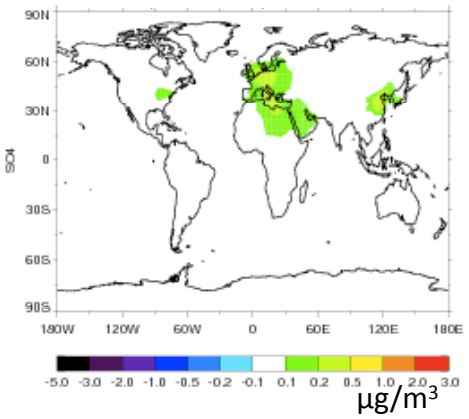
SO2



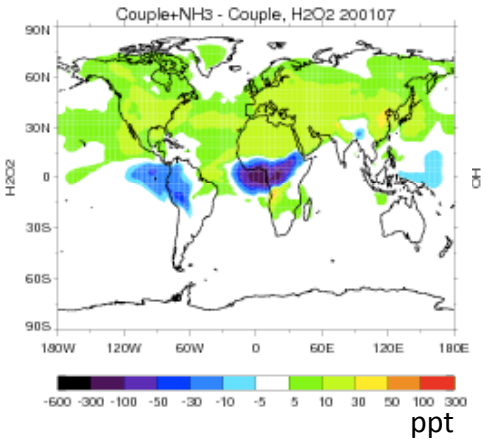
DMS



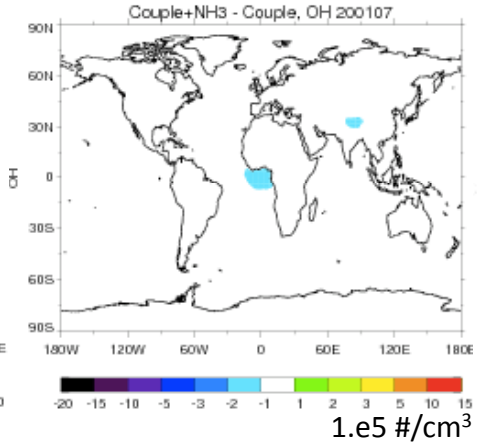
SO4



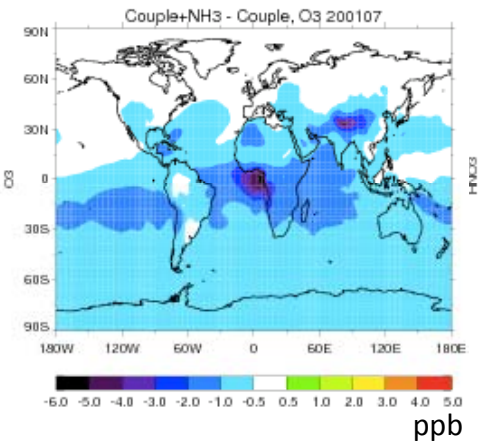
H2O2



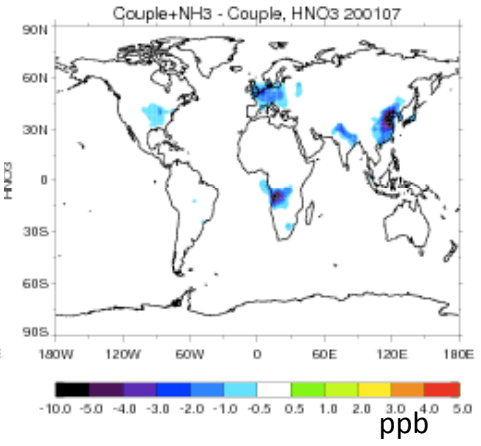
OH



O3

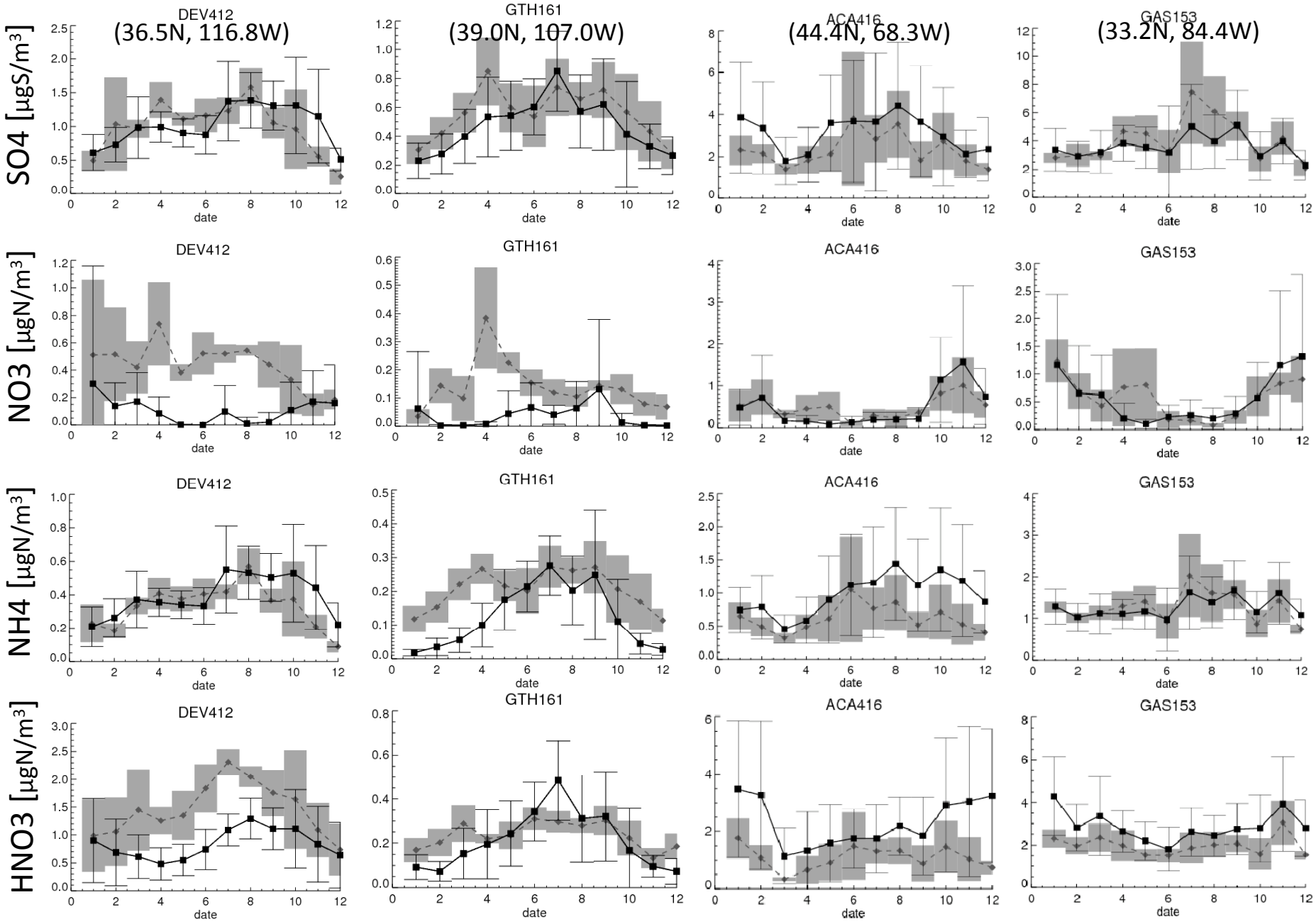


HNO3



New aerosol components

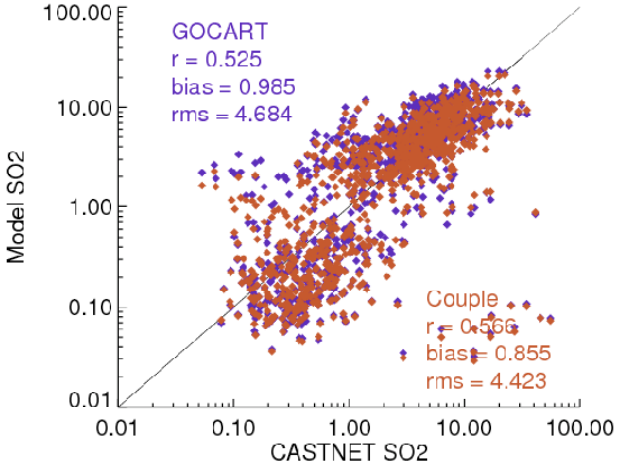
Compare Couple with CastNet observation



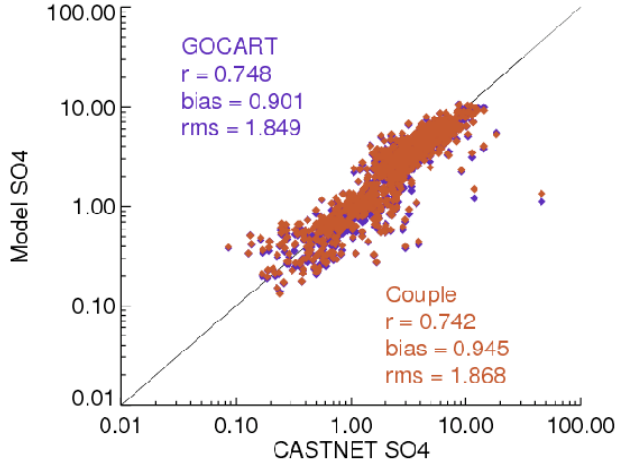
New aerosol components

Overall comparisonwith CastNet

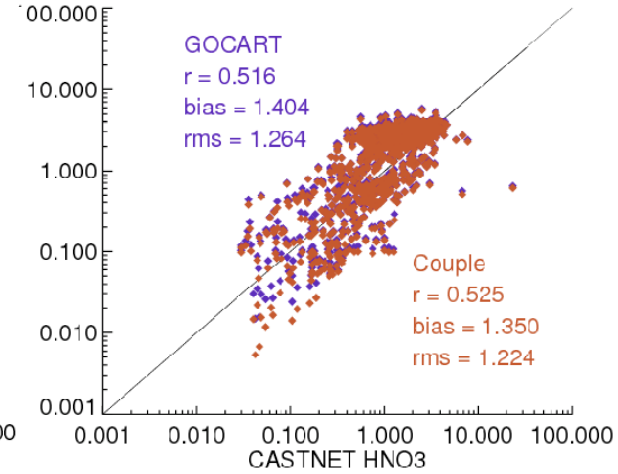
SO2



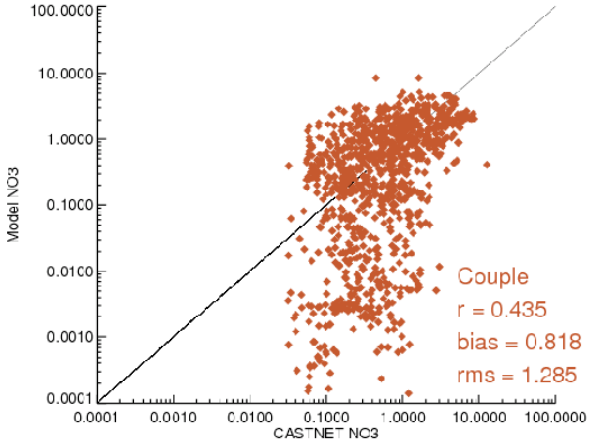
SO4



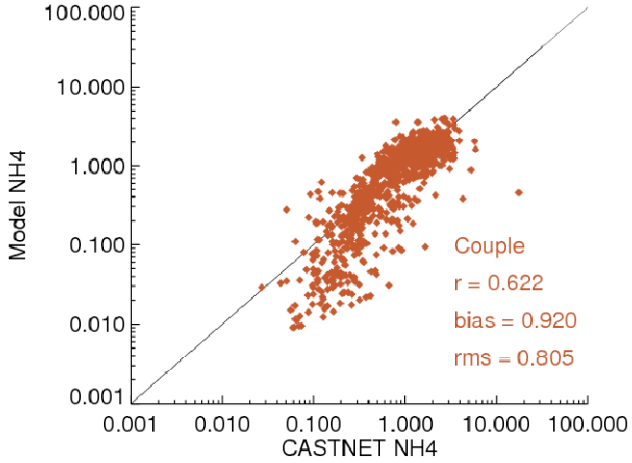
HNO3



NO3a

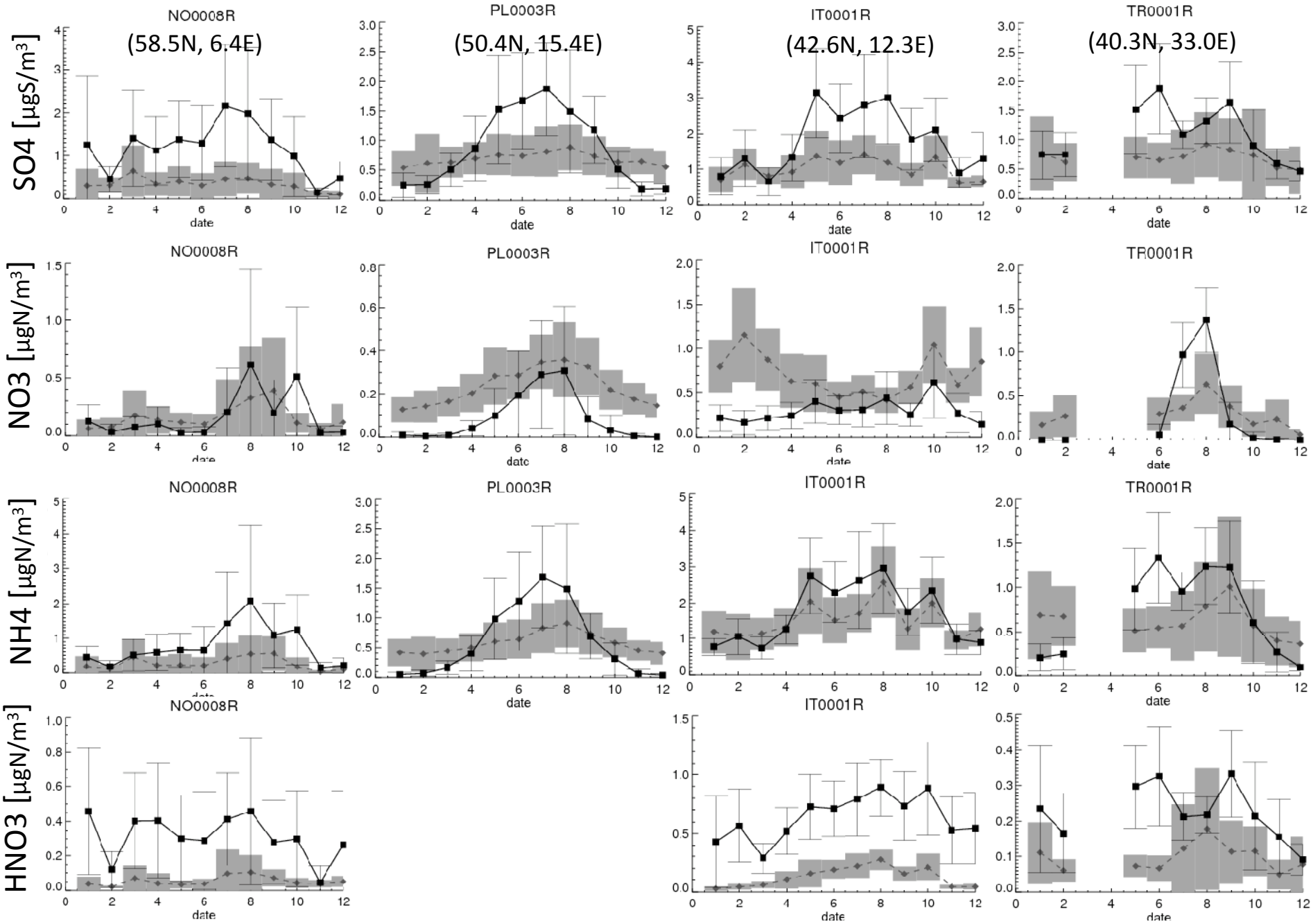


NH4a



New aerosol components

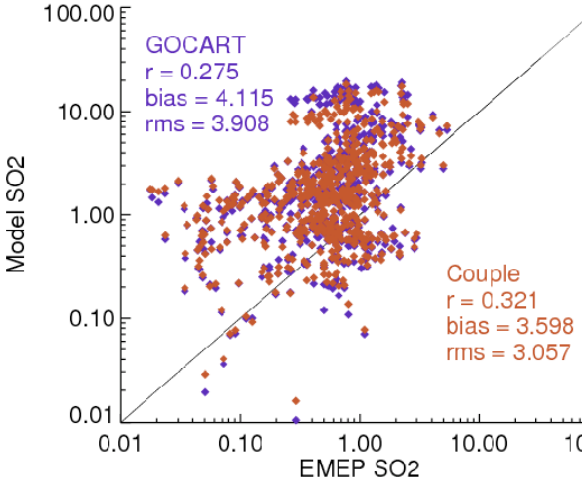
Compare Couple with EMEP observation



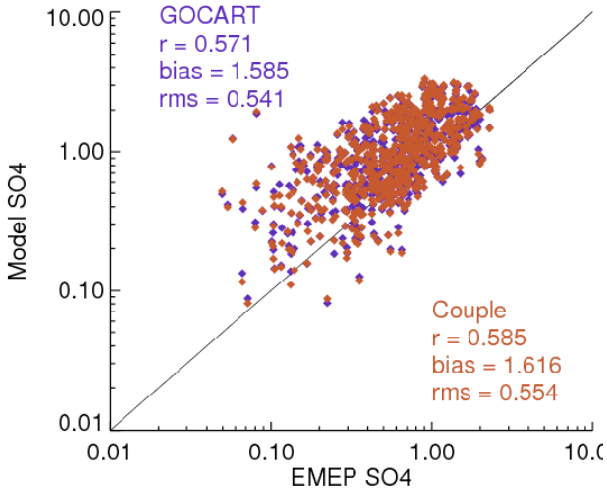
New aerosol components

Overall comparison with EMEP

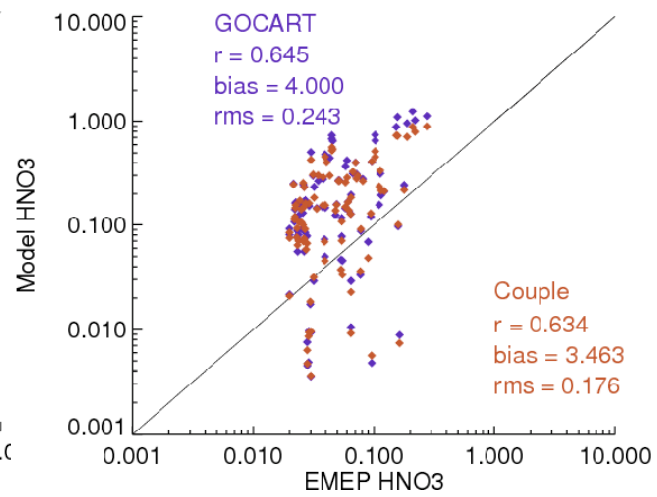
SO2



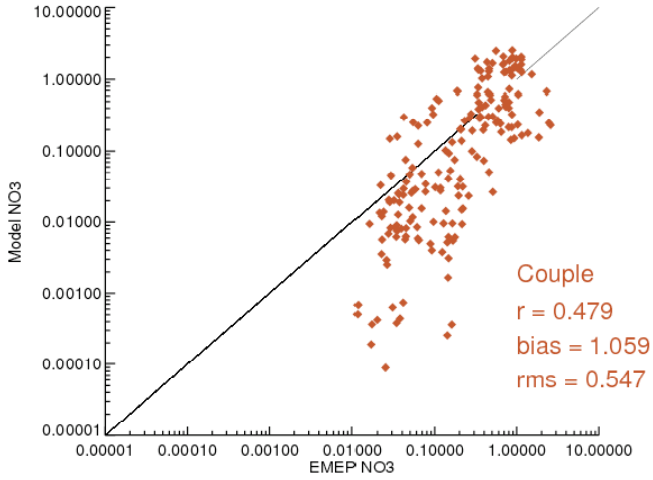
SO4



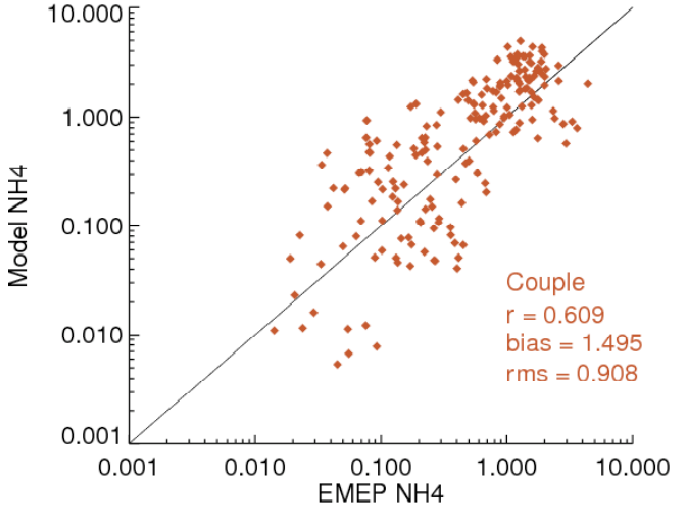
HNO3



NO3a



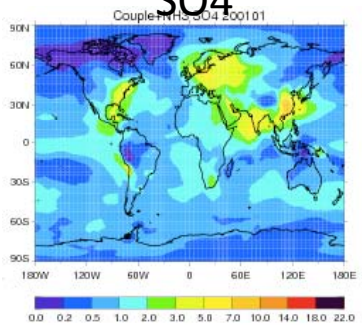
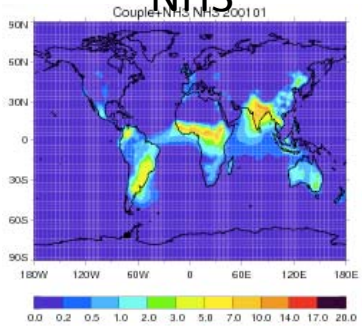
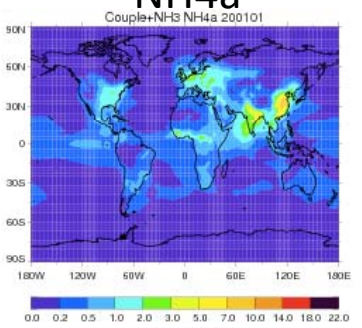
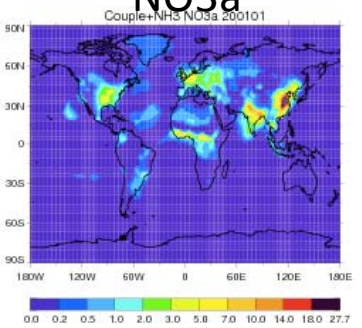
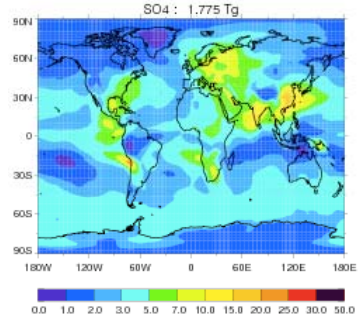
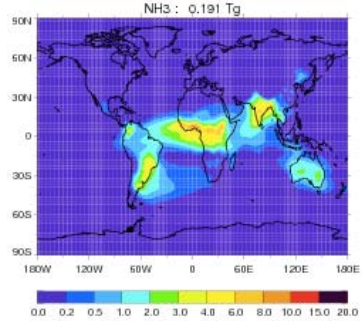
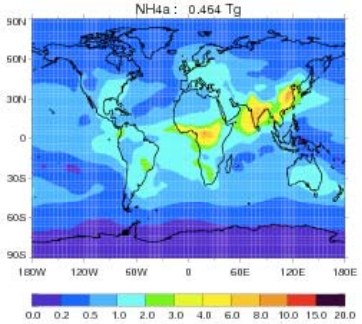
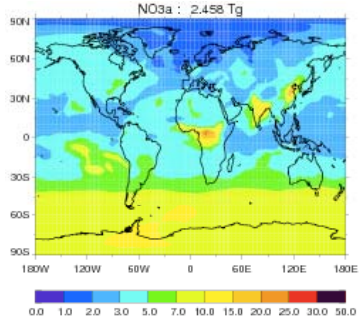
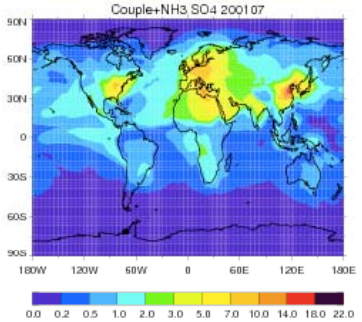
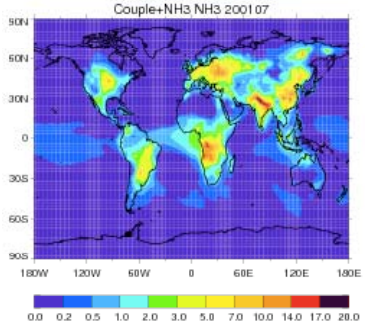
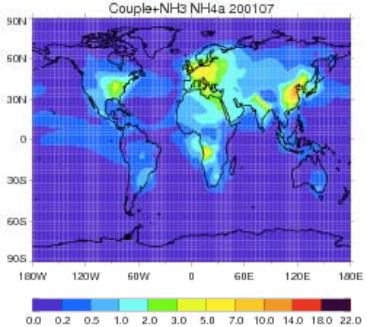
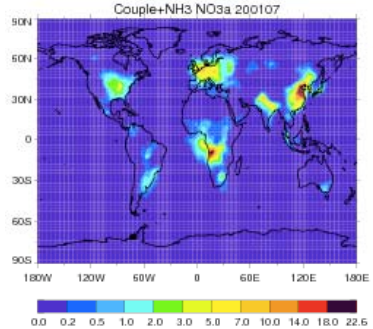
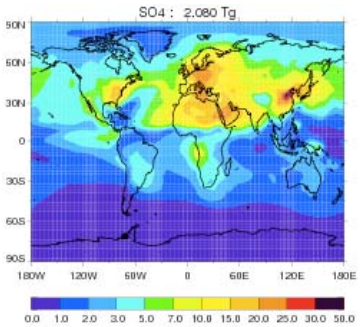
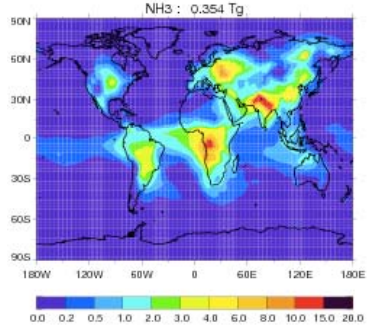
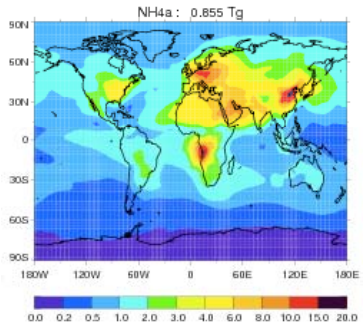
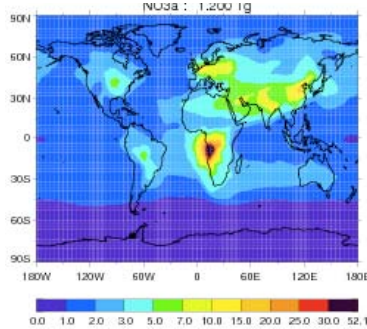
NH4a



Summary

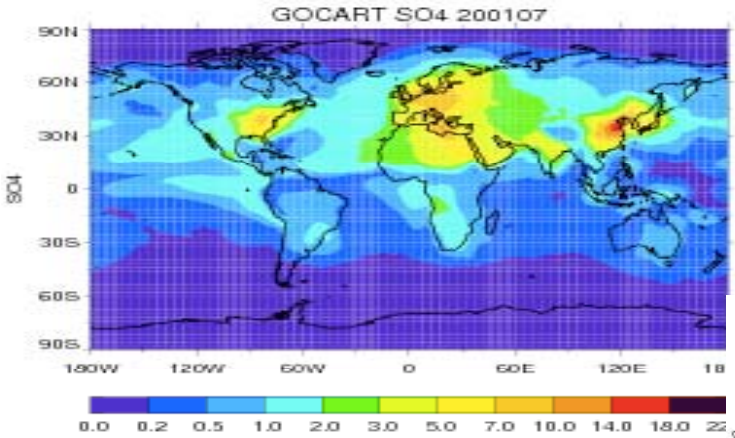
- GMI has a new capability for the simulation of aerosol ammonium and nitrate.
- All three tracers (NH3, NH4a, and NO3a) concentrate over land regions at surface. Concentrations of NH3 and NH4a are generally larger in summer than winter.
- Model gives a better nitrate distribution in eastern US than in western by comparing with CaseNet measurement. Model overestimates all tracers over Europe by comparing with EMEP measurement.
- Nitrate simulation has a little impact on sulfate simulation, but it results in changes in some gas tracers particularly HNO3 and O3.

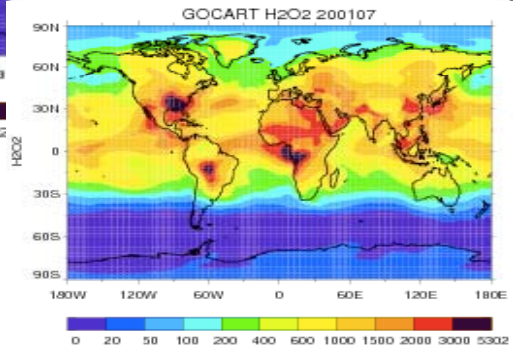
New aerosol components

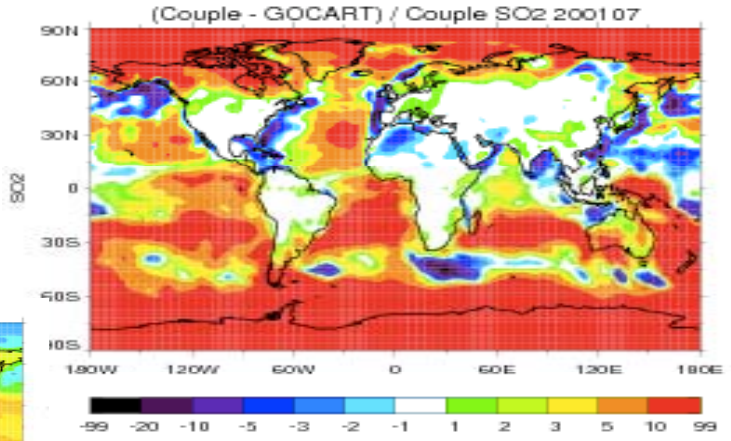
	SO4	NH3	NH4a	NO3a
January surface				
January column				
July surface				
July column				

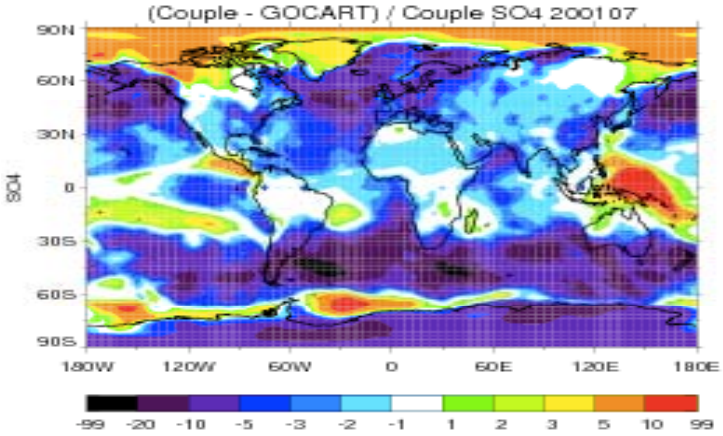
Gas – aerosol coupling

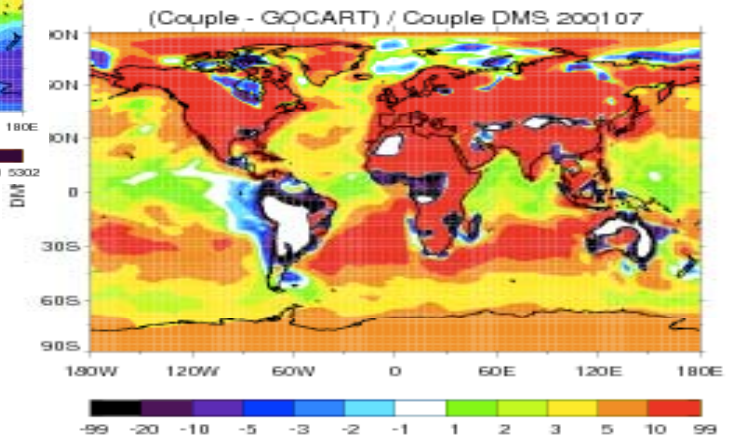
t at surface:

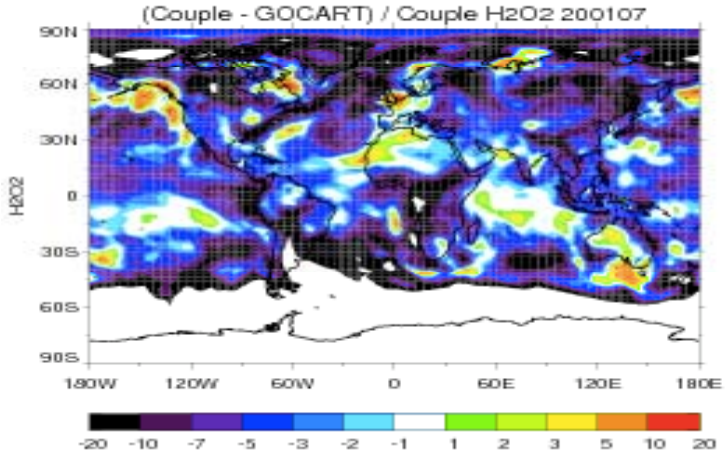


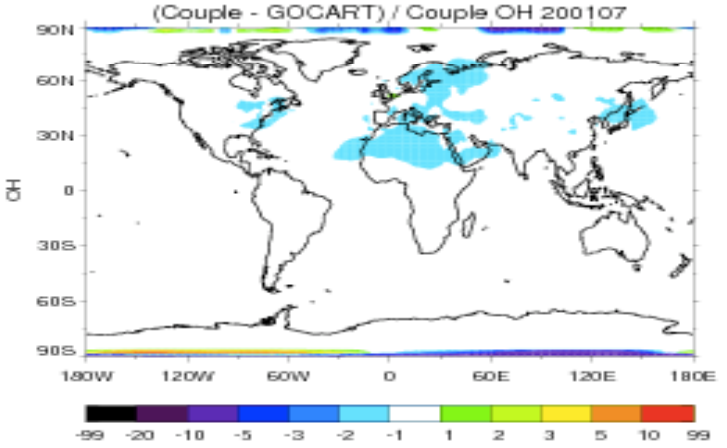




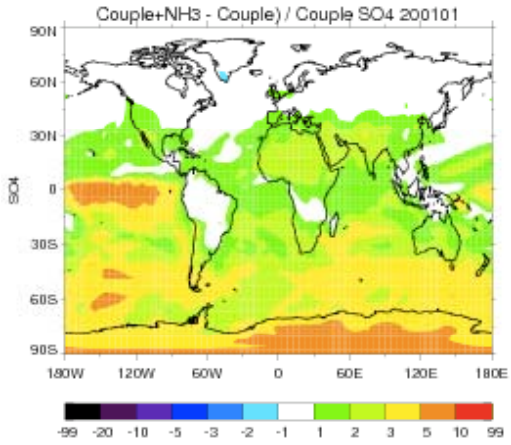


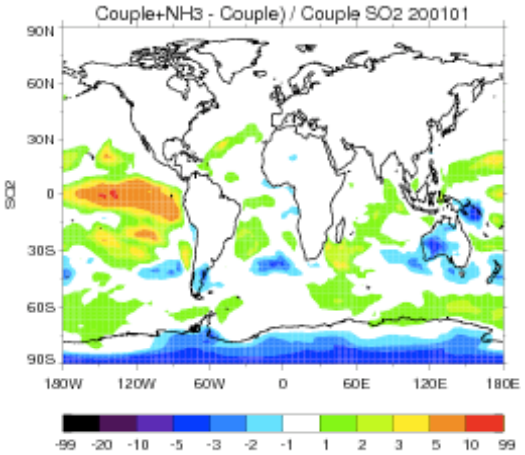


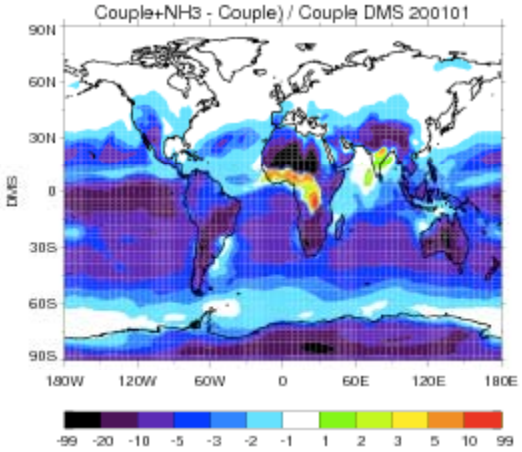


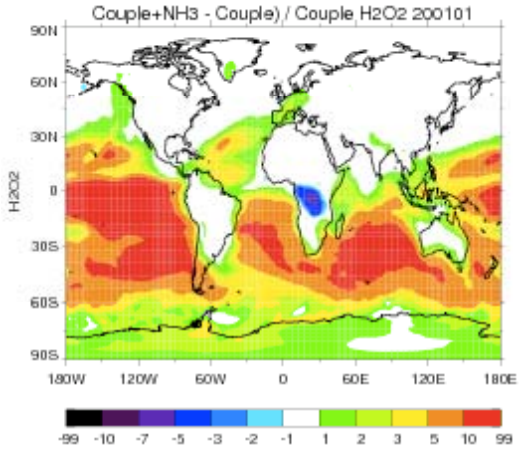


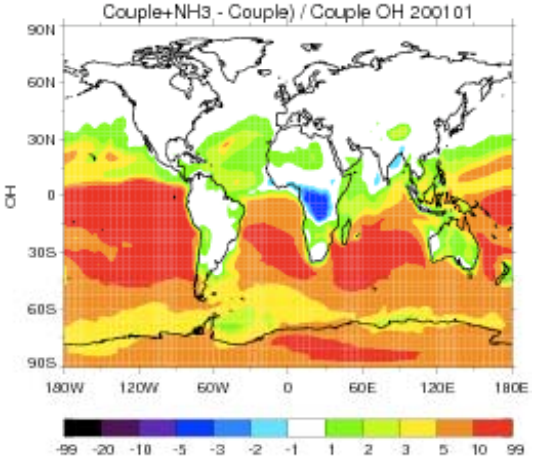
New aerosol components

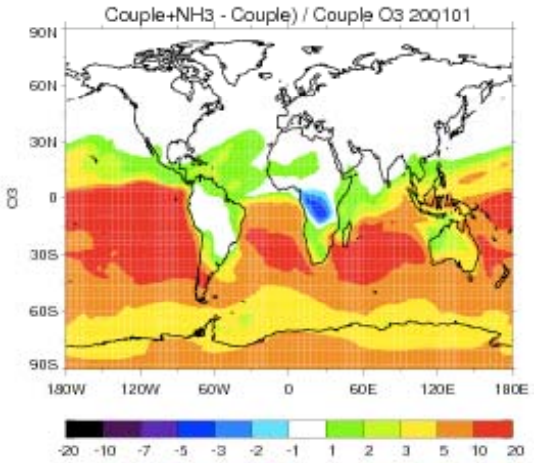


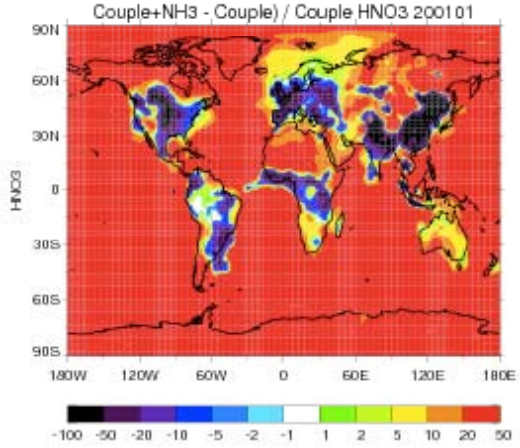


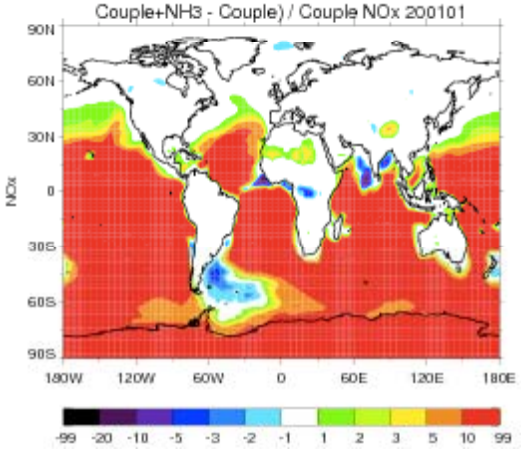












New aerosol components