

*First results from
ISORROPIA-lite/TM5-MP simulations*

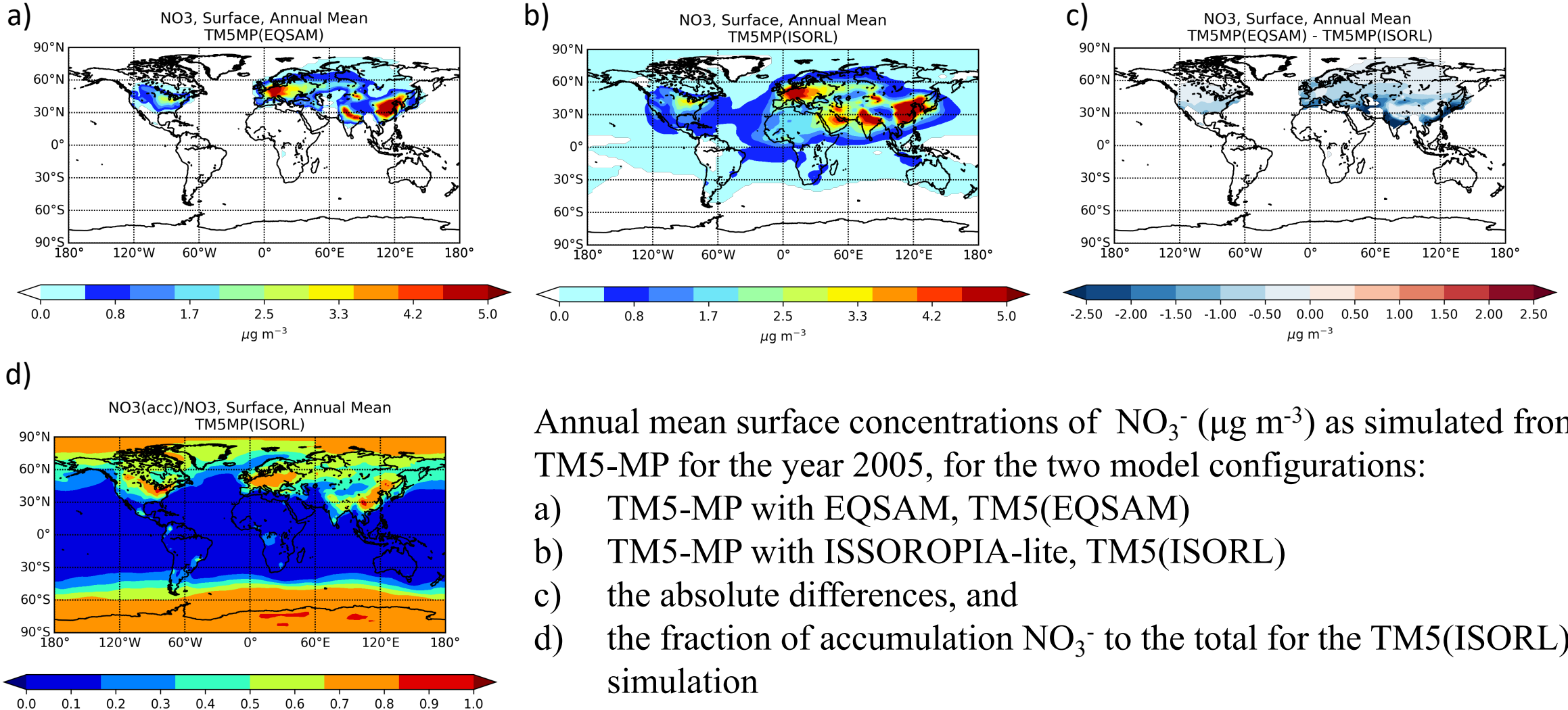
Stelios Myriokefalitakis

steliosm@noa.gr

Outline

- Results from TM5-MP simulations using the new ISORROPIA-lite module (i.e., the lite version of ISORROPIA module) for the year 2005 are here presented and compared to the previous model configuration (i.e., using the EQSAM).
- For new the ISORROPIA-lite configuration, extra species are accounted in the model, i.e., for
 - the coarse nitrate aerosol
 - the coarse ammonium aerosol
 - and for the accumulation and coarse insoluble modes of calcium from dust (as calculated based on mineralogy (calcite) maps. The rest of the mineral dust composition is based on Karydis *et al.*, 2016.
 - For sea spray aerosols, respectively, we assume a mass composition of 55% Cl⁻, 30.6% Na⁺, 7.7% SO₄⁼, 3.7% Mg²⁺, 1.2% Ca²⁺, and 1.1% K⁺ (Seinfeld and Pandis, 2006).
- For the ISORROPIA-lite configuration, the thermodynamic module is called for both the accumulation and the coarse modes, in contrast to the single call when the EQSAM is used (bulk approach).
- The new ISORROPIA-lite configuration accounts also for kinetic limitations for the gas/aerosol partitioning. Thus, the amount of gases kinetically able to condense onto the aerosols within a timestep, is calculated assuming a diffusion-limited condensation. Then, ISORROPIA-lite re-distributes the masses between the gas and the aerosol phases.
- A first comparison (scatterplot) for the two model configurations with NO₃⁻ observations (Alexandra Tsimpidi pers. com., 2021) is also presented.

Surface Nitrate Concentrations

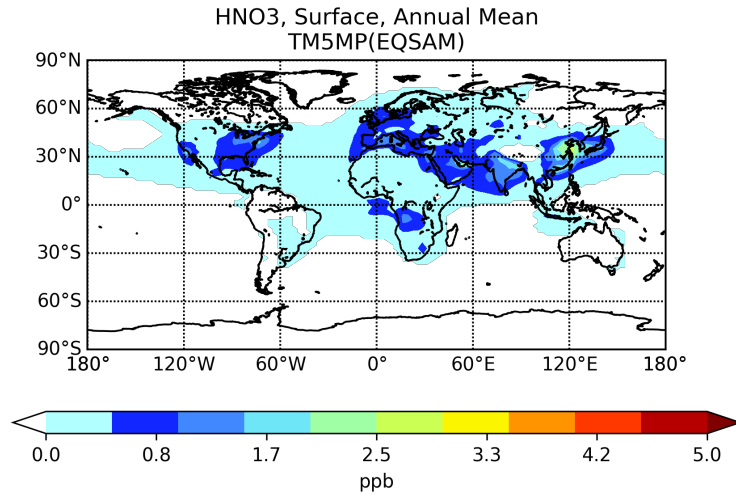


Annual mean surface concentrations of NO_3^- ($\mu\text{g m}^{-3}$) as simulated from TM5-MP for the year 2005, for the two model configurations:

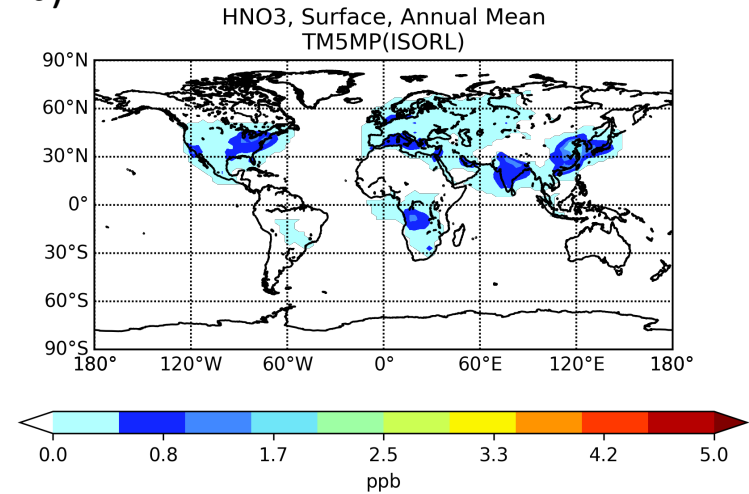
- a) TM5-MP with EQSAM, TM5(EQSAM)
- b) TM5-MP with ISSOROPIA-lite, TM5(ISORL)
- c) the absolute differences, and
- d) the fraction of accumulation NO_3^- to the total for the TM5(ISORL) simulation

Surface Nitric Acid Concentrations

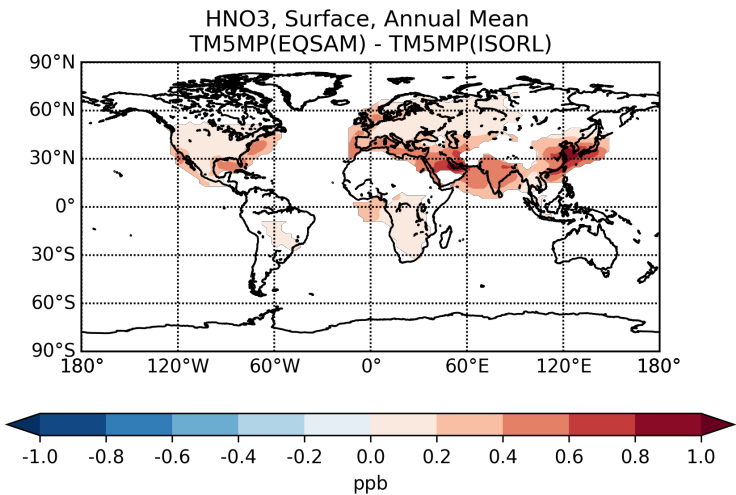
a)



b)



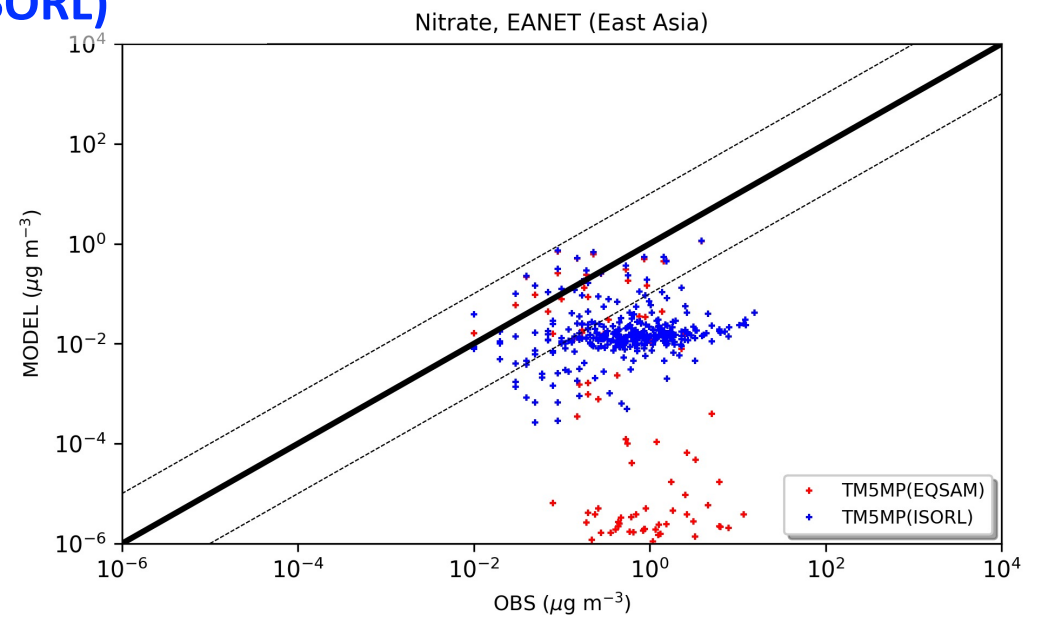
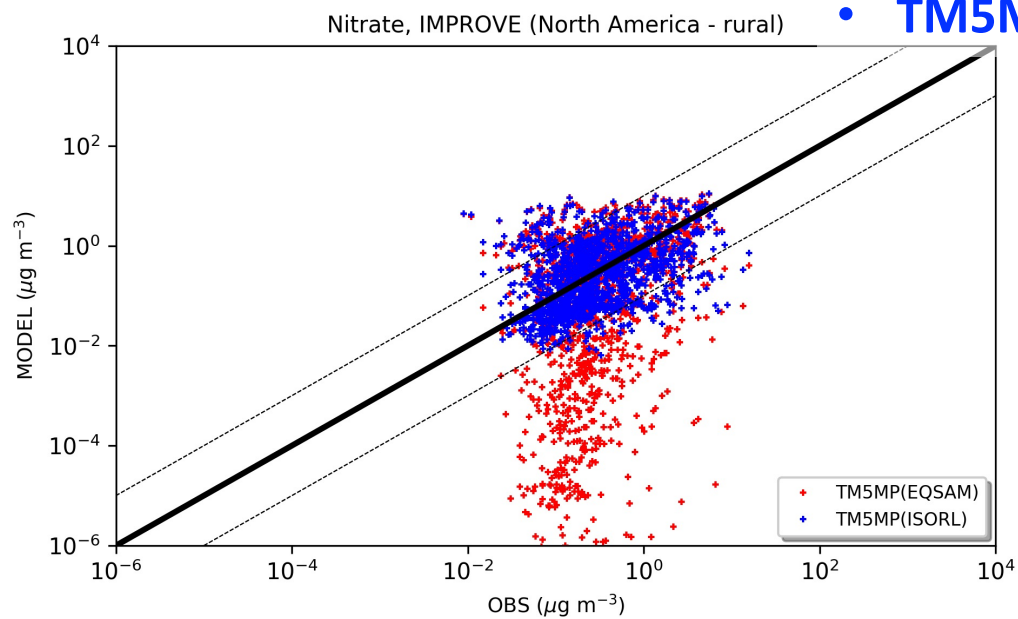
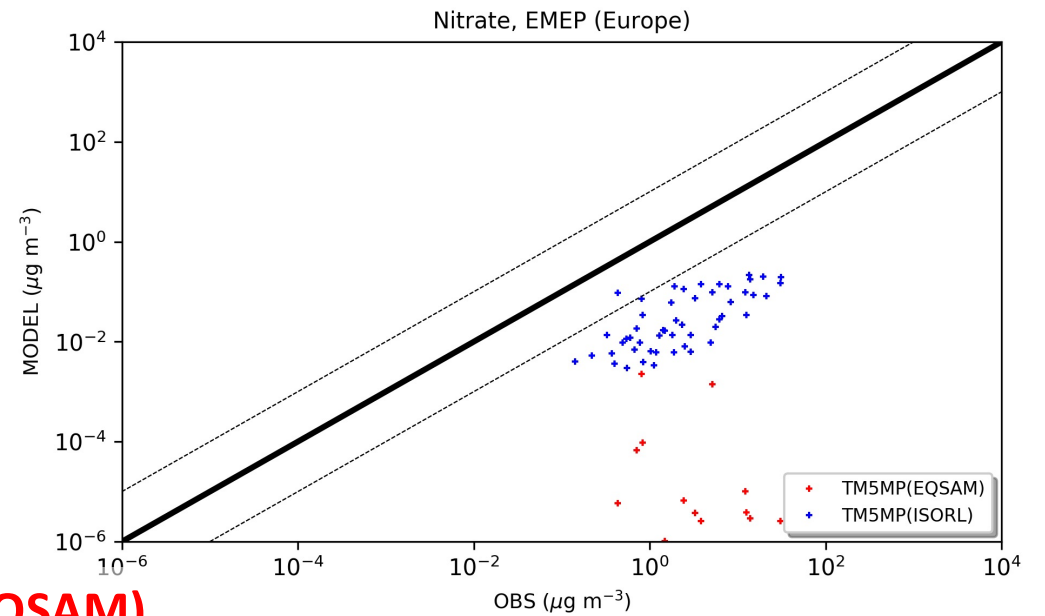
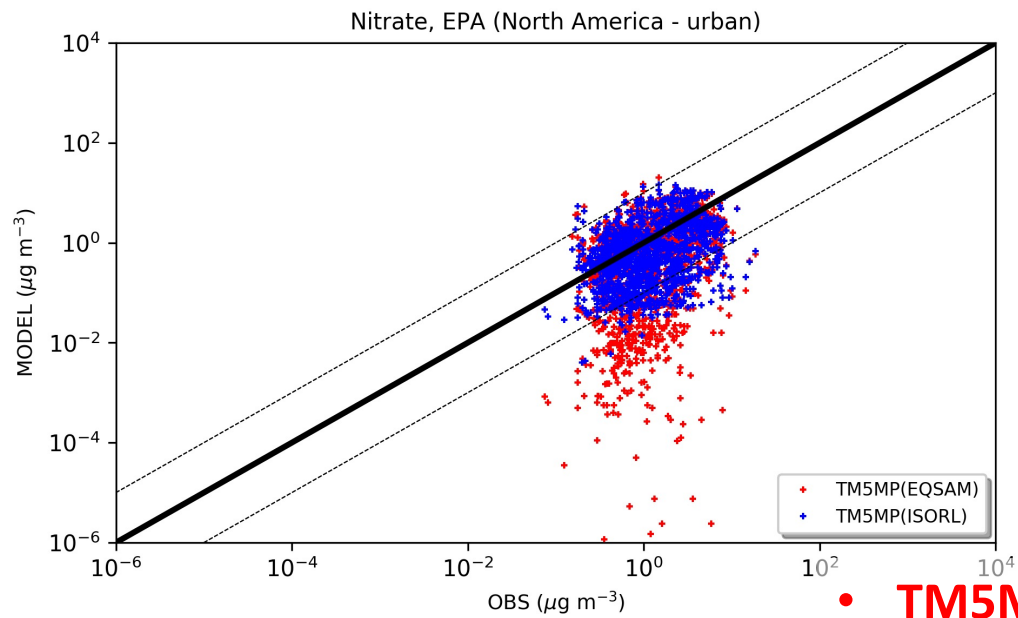
c)



Annual mean surface HNO₃ concentrations (ppb) as simulated from TM5-MP for the year 2005, for two model configurations:

- a) TM5-MP with EQSAM, TM5(EQSAM)
- b) TM5-MP with ISSOROPIA-lite, TM5(ISORL) and
- c) the absolute differences

Comparison with Observations (2005)*

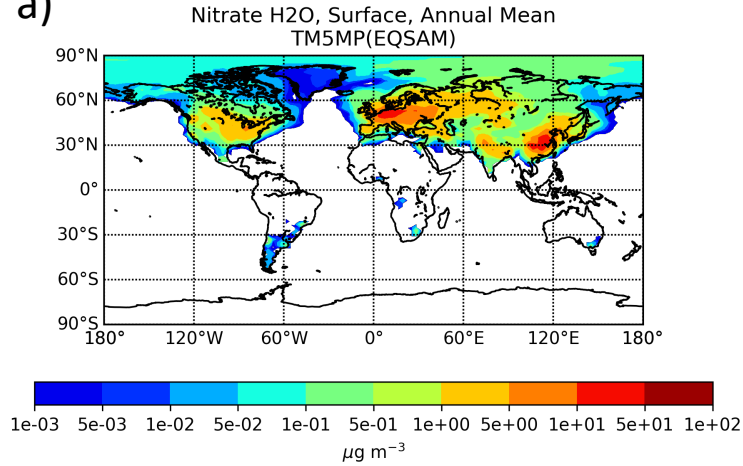


- TM5MP(EQSAM)
- TM5MP(ISORL)

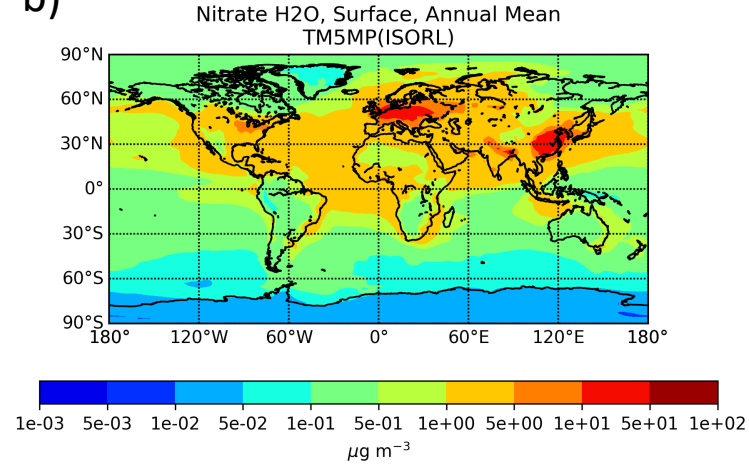
*Observations compiled by Alexandra Tsimpidi
(a.tsimpidi@fz-juelich.de)

Aerosol water from deliquesced nitrates

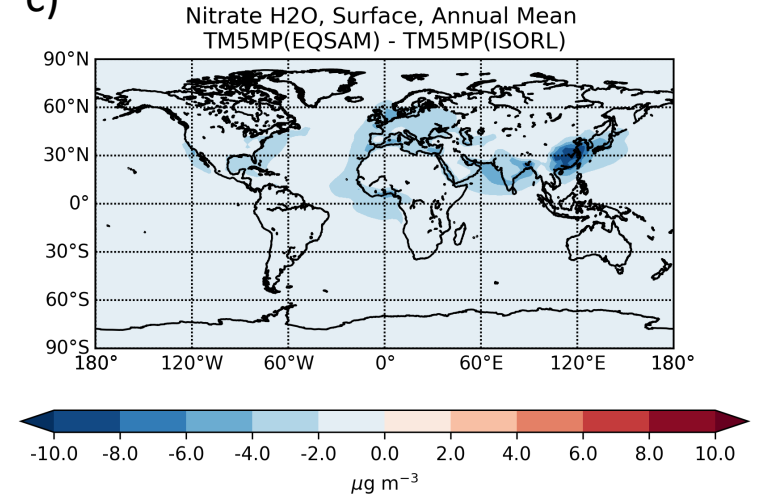
a)



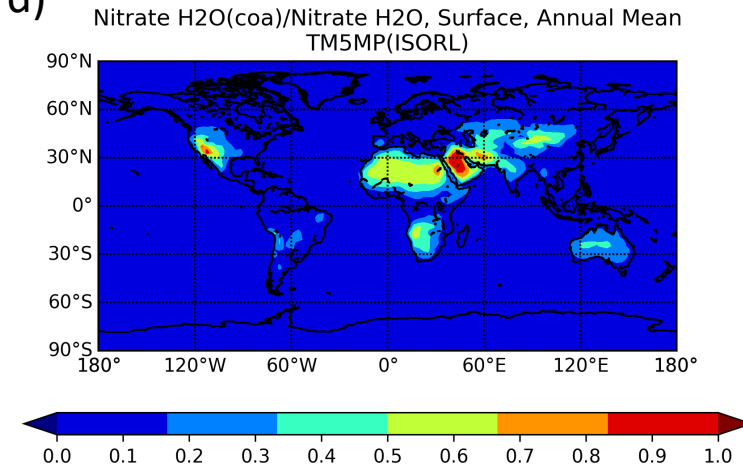
b)



c)



d)



Annual mean surface concentrations of aerosol water from deliquesced nitrates ($\mu\text{g m}^{-3}$) as simulated from TM5-MP for the year 2005, for the two model configurations:

a) TM5-MP with ISSOROPIA-lite, TM5(ISORL)

b) TM5-MP with EQSAM, TM5(EQSAM)

c) the absolute differences

d) the contribution of coarse aerosol water to the total.

Summary

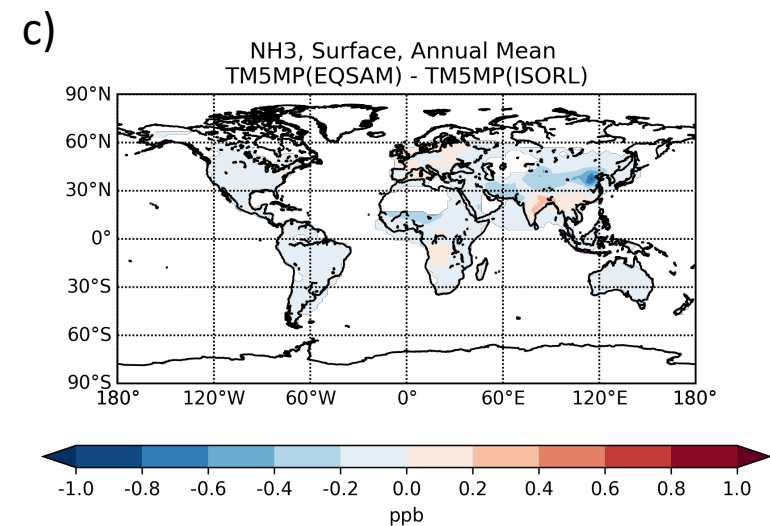
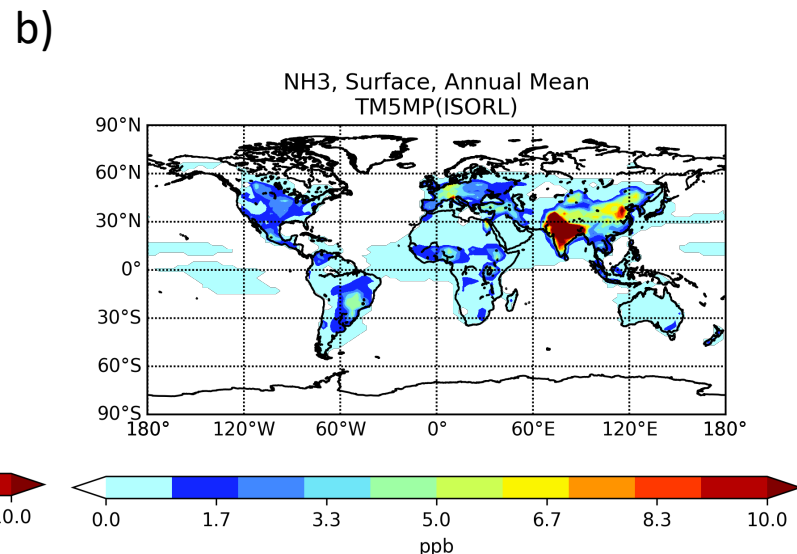
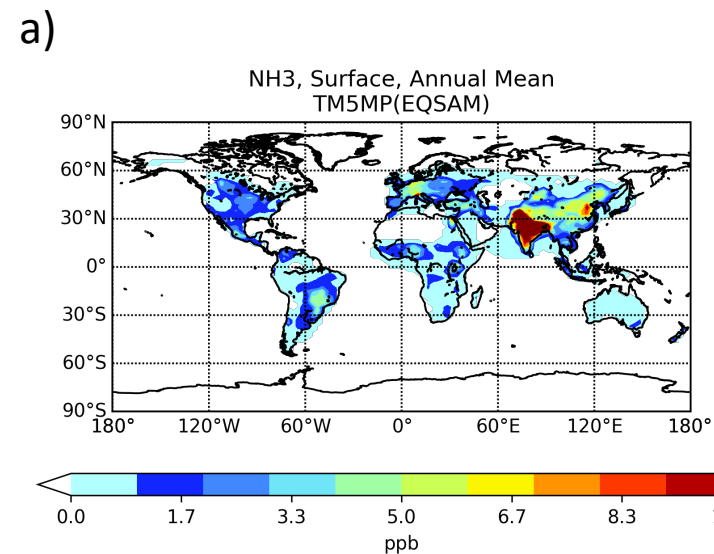
- The simulations were here performed on the ARIS-GRNET HPC using 180 cores.
- The model runs at a $3^\circ \times 2^\circ$ horizontal resolution (lon x lat) and 34 layers in the vertical, driven by meteorological fields for the year 2005 from the ECMWF ERA-Interim reanalysis, with an update frequency of 3 hours.
- Compared to the EQSAM configuration (x1), the coupling of ISORROPIA-lite (x2) does not significantly impact the overall performance of the TM5-MP standalone version (roughly *2.1 Vs 2.6 SYPD* for the ISORROPIA-lite and EQSAM configurations, respectively).
- ISORROPIA-lite configuration tends to simulate higher NO_3^- concentrations compared to the previous (EQSAM) one, especially over coastal and dust regions due to the contribution of coarse mode NO_3^- aerosols.
- HNO_3 concentrations are simulated lower in ISORROPIA-lite configuration, affecting thus the NO_3^{T} partitioning fraction (i.e., towards the particulate phase) and thus its atmospheric deposition rates.
- The model evaluation indicates that the new model configuration with ISORROPIA-lite improves the nitrate simulated concentrations compared to the previous EQSAM configuration.
- The aerosol water from deliquesced nitrates is increased in the ISORROPIA-lite configuration, with the contribution of the coarse aerosol water being calculated as rather important.



Thank you for your attention

Extra slides

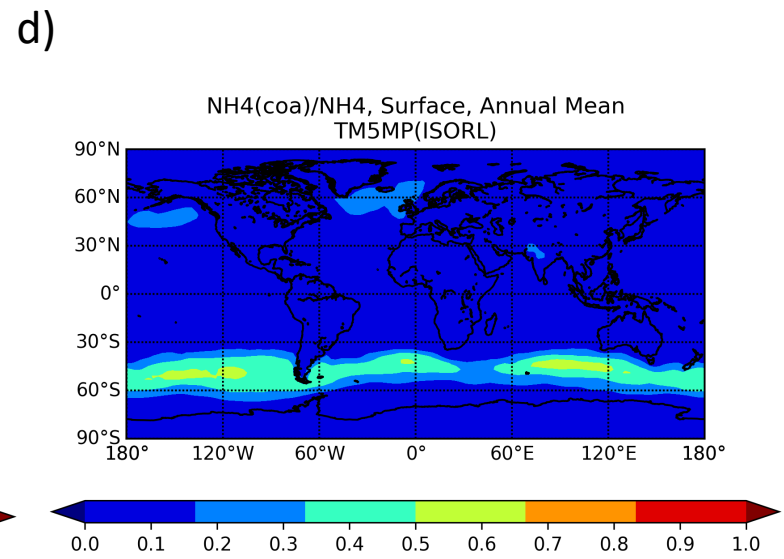
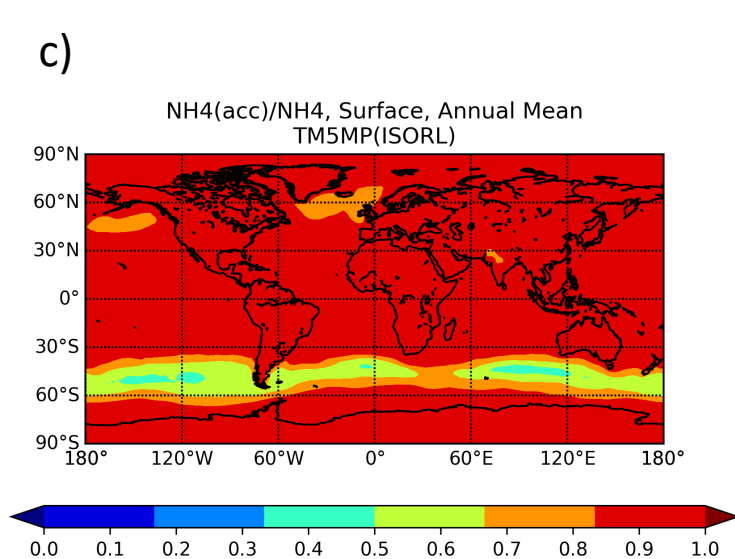
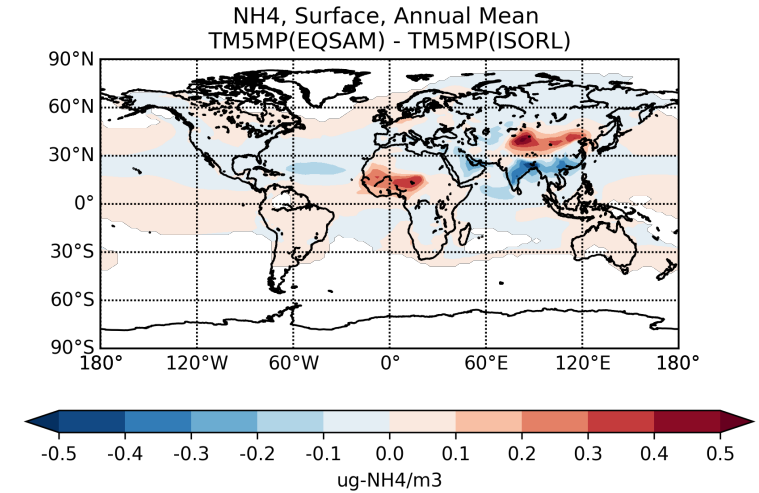
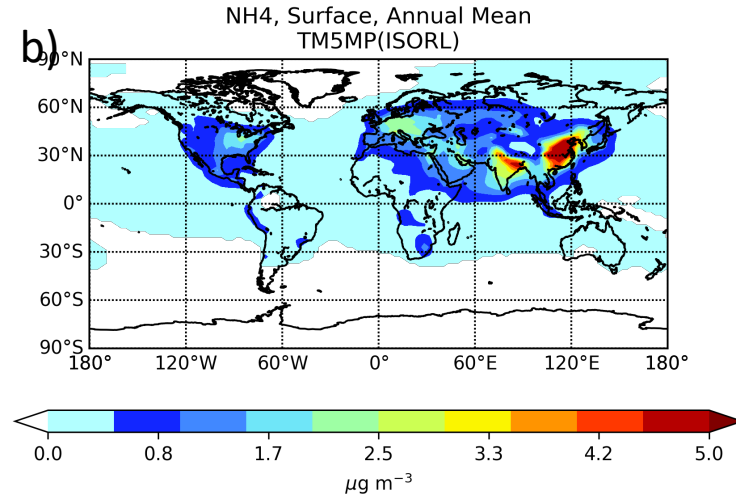
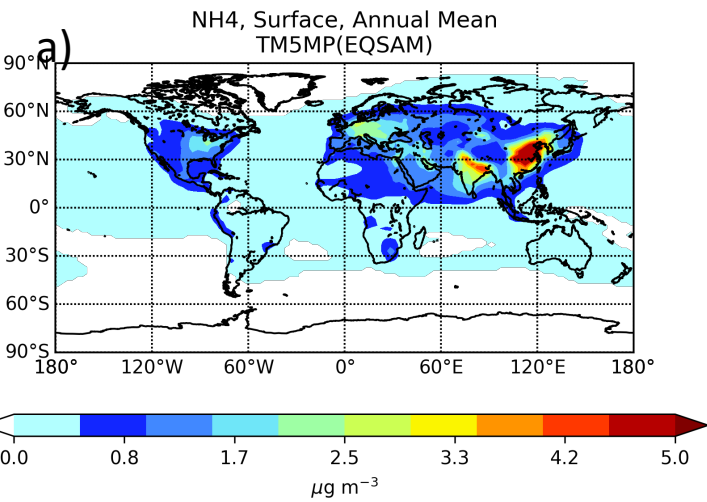
Ammonia



Annual mean surface concentrations of NH₃ (ppb) as simulated from TM5-MP for the year 2005, for the two model configurations:

- a) TM5-MP with ISSOROPIA-lite, TM5(ISOR)
- b) TM5-MP with EQSAM, TM5(EQSAM) and
- c) the absolute differences.

Ammonium



Annual mean surface concentrations of NH₄⁺ ($\mu\text{g m}^{-3}$) as simulated from TM5-MP for the year 2005, for the two model configurations:

- TM5-MP with ISSOROPIA-lite, TM5(ISORL)
- TM5-MP with EQSAM, TM5(EQSAM)
- the absolute differences
- the contribution of acc. mode to total, and
- the contribution of coa. mode to total.