Nitrate simulation: Unique feature, Current status, challenge, Remaining issues, Evaluation, and future work

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What is the unique feature in nitrate simulation?

- HNO3: involved in O3 chemistry and a semi-volatile species
- NH3: a weak base
- Nitrate aerosol size: fine and coarse size particles
- Nitrate aerosol type: inorganic and organic

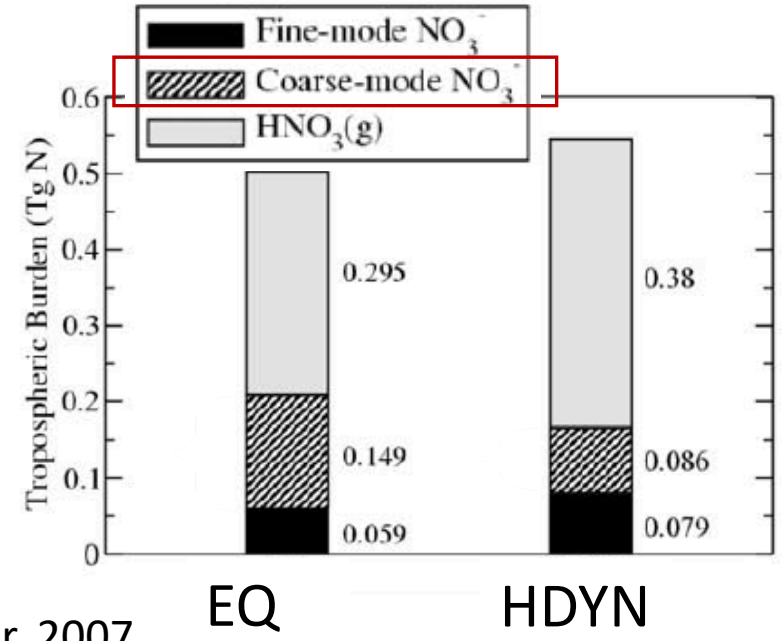
Current status

- AeroCom III nitrate experiment: 8 models
- More global models include nitrate aerosol simulation
- Diversity of nitrate simulation is larger than sulfate simulation among the models

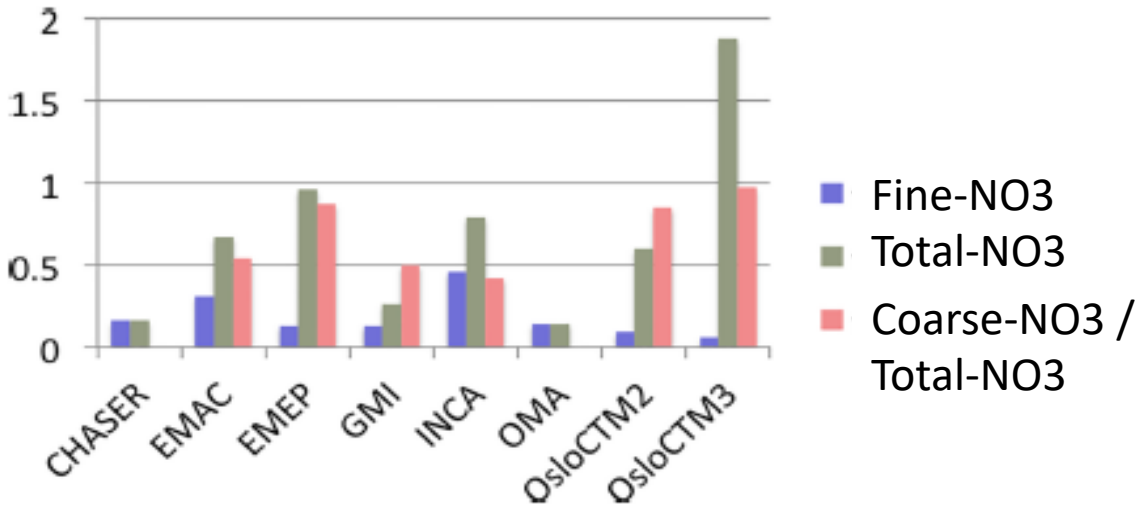
Challenge for inorganic nitrate simulation:

1. A large diversity in HNO3: A full O3 gas phase chemistry.
2. HNO3: **A semi-volatile species**. Need thermodynamic equilibrium module (TEQM) solving the SO4-NO3-NH4-H2O system. How to account for **sea salt, dust**, and organic acid contribution, how to account for aerosol in low RH (stable-state or metastable), and how to optimize chemical calculation, etc.
3. Nitrate aerosol: **fine and coarse size particles**

➔ TEQM or dynamic mass transfer equation.



Feng and Penner, 2007



Bian et al. 2017

Challenge for inorganic nitrate simulation:

NH3: a weak base ➔ pH dependent efficient Henry's law coefficient

Table 5. Effective Henry's law constant used in the models.

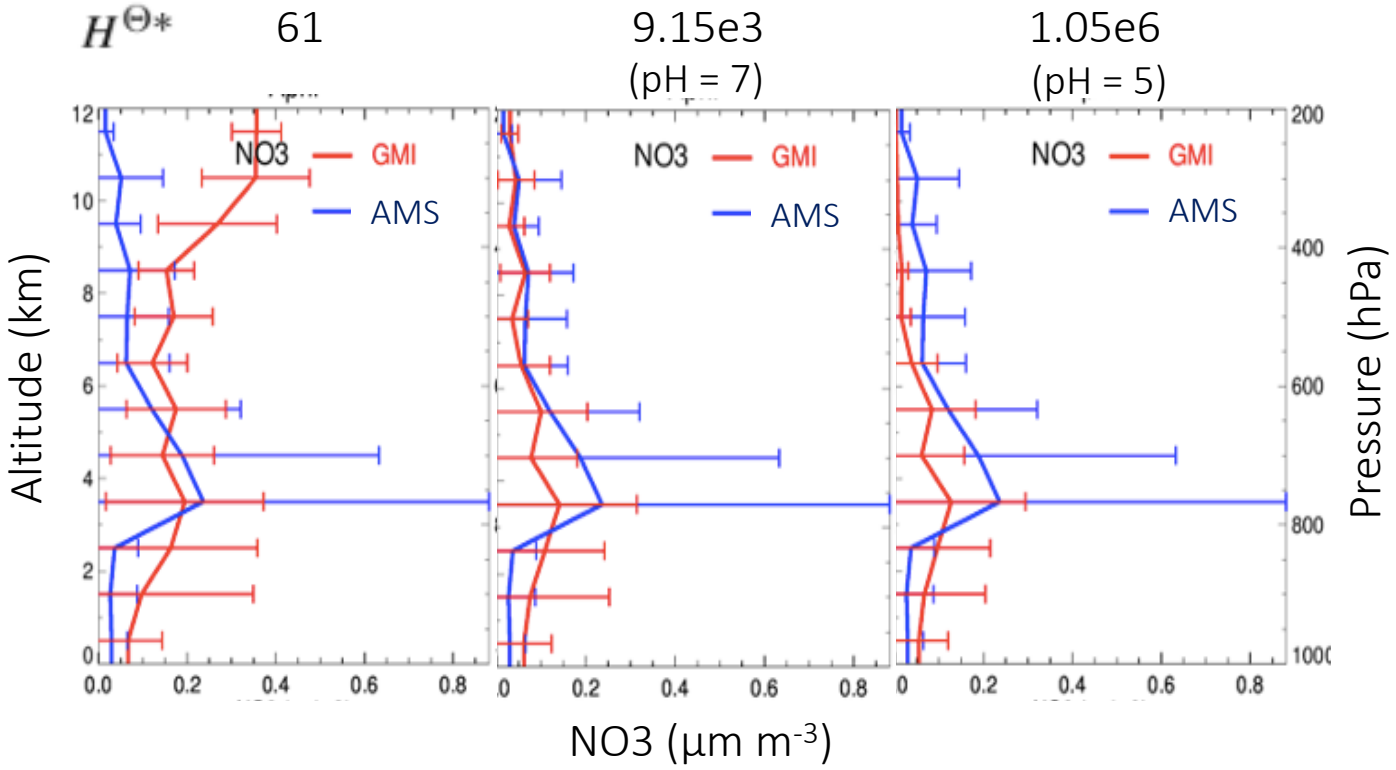
AeroCom model	$H^{\Theta*}$ (M atm^{-1})	$-\Delta H_{sol}/R$ (K)
CHASER	3×10^5	3400
EMAC[a]	–	–
EMEP[b]	–	–
GISS-MATRIX	1×10^2	3415
GISS-OMA	1×10^2	3415
GMI	1.05×10^6	4200
INCA	7.4×10^1	3400
OsloCTM2	3.3×10^6	0
OsloCTM3	3.3×10^6	0

[a]EMAC: explicitly calculate wet scavenging with aqueous phase reaction

[b]EMEP: adopt a simple empirical scavenging ratio of 1.4e6 for in-cloud and 0.5e6 for below-cloud for NH3.

Bian et al. 2017

ARCTAS April

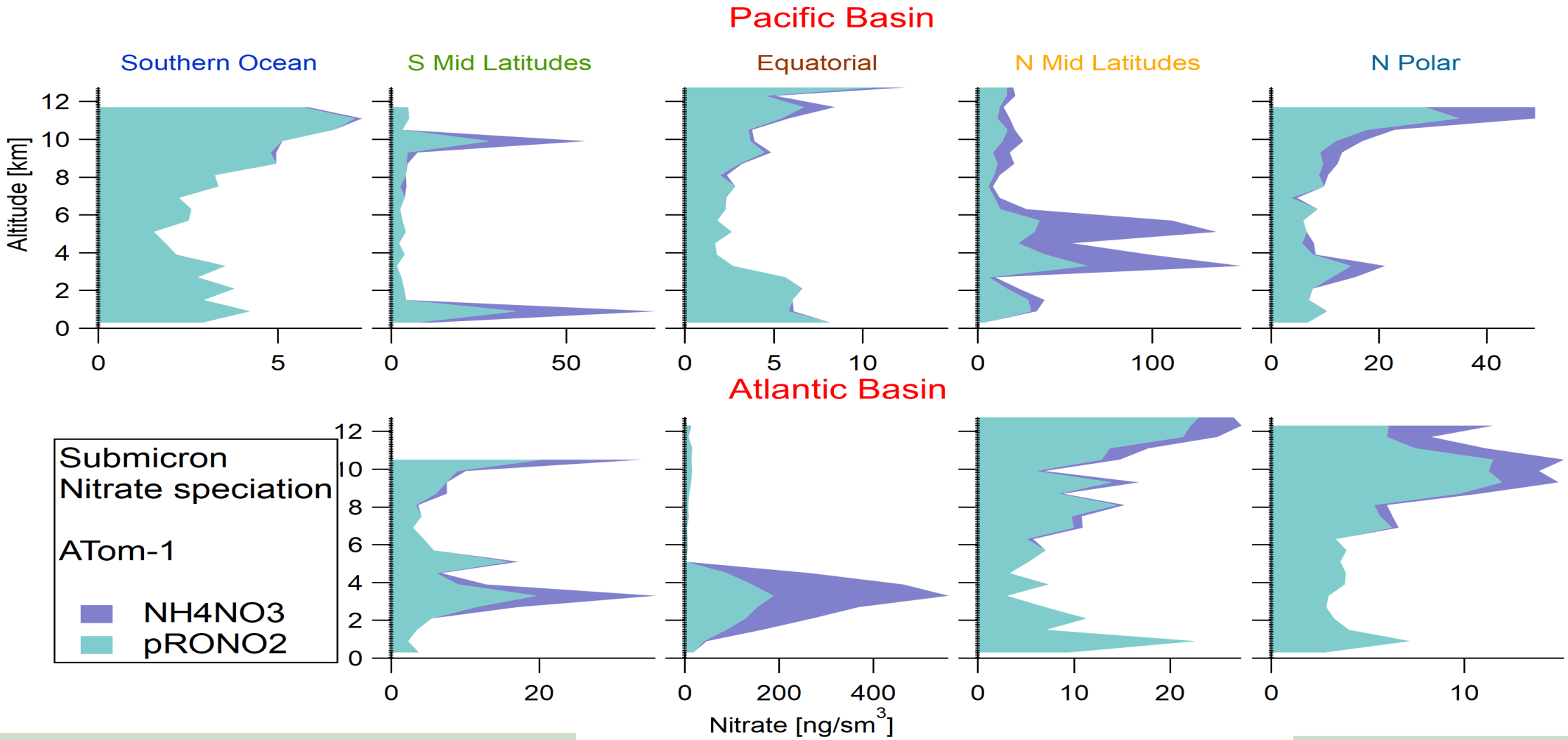


$$NH_3 + H_2O \Leftrightarrow NH_3 \cdot H_2O$$

$$NH_3 \cdot H_2O \Leftrightarrow NH_4^+ + OH^-.$$

Remaining issues for modeling

What forms of nitrate: inorganic or organic?
Where nitrate come from: primary and/or secondary?

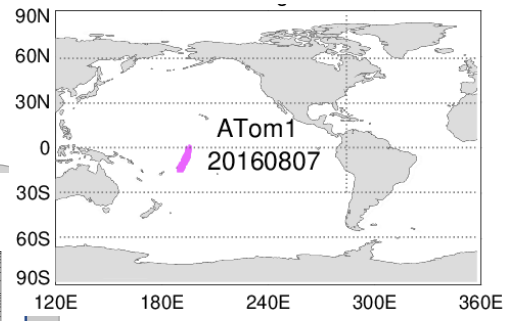


Pedro Campuzano_Jost & Jose Jimenez

Do not distribute

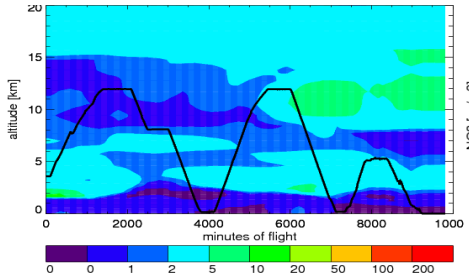
Remaining issues for modeling

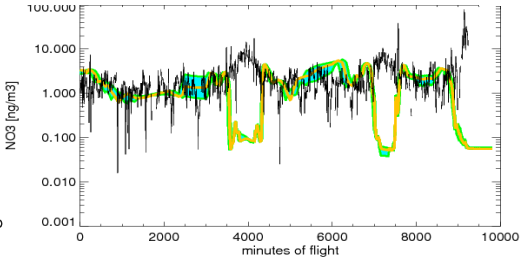
Missing oceanic sources?



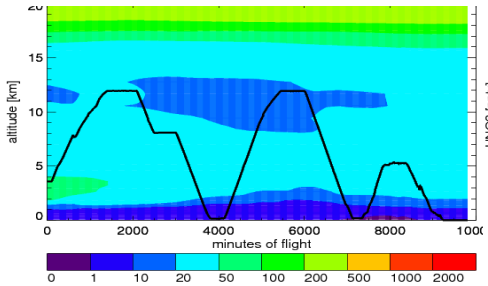
GEOS5-GMI

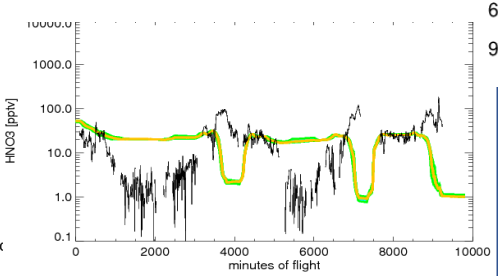
NO3



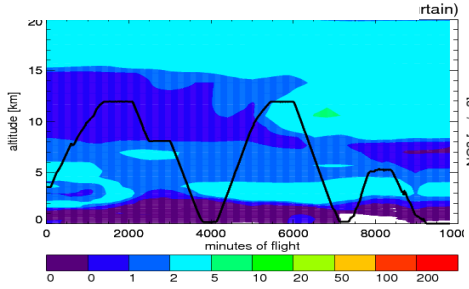


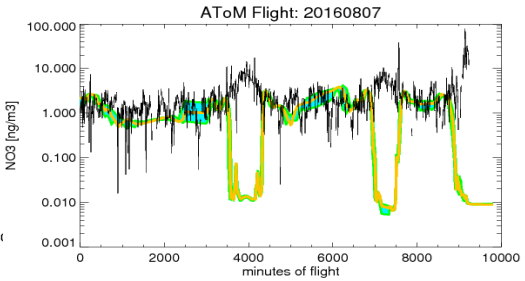
HNO3

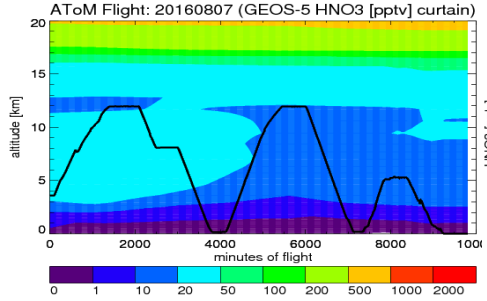


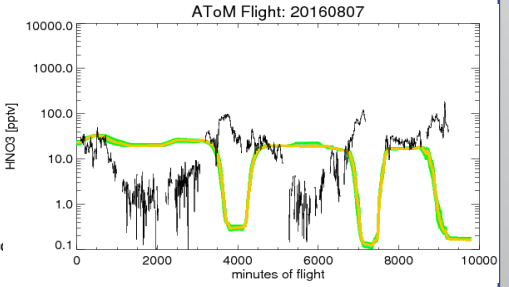


GEOS-Chem

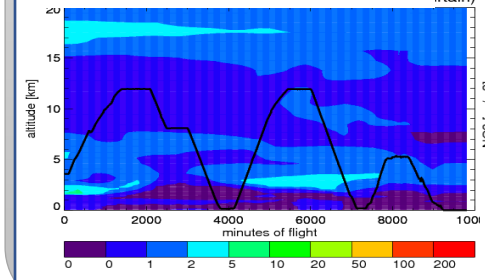


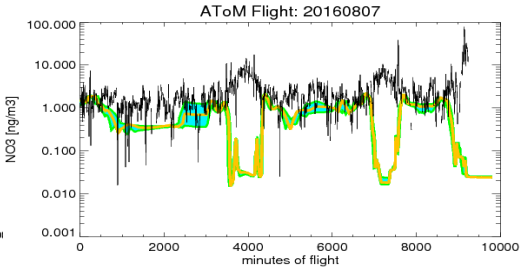


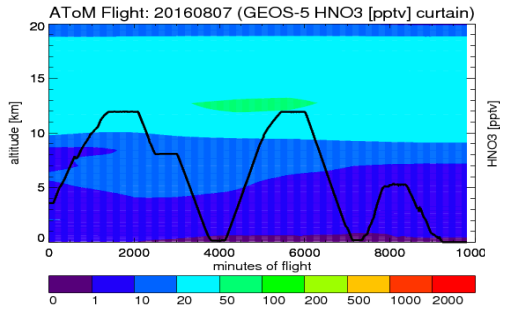


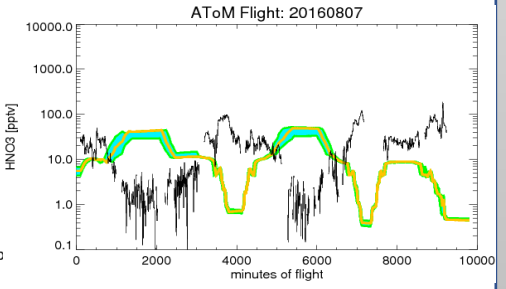


EMAC









Evaluation issues

1. in-situ ground measurement and airborne measurement: difficulty in NH3 measurement
2. Remote satellite measurements (e.g. NH3 products from IASI, TES and AIRS)

Recommendation and future work

1. Based on AeroCom III nitrate study, modelers should pay particular attention to incorporating dust and sea salt and treating NH3 wet deposition to improve nitrate simulation.
2. Include organic gas/aerosol in study since they are important source to atmospheric nitrates and impact on nitrate chemistry such as reduction of the NH3 uptake.
3. Examine how aerosol pH changes and its influence on the atmospheric acid/base gas–particle system.
4. how sensitive nitrate formation is in response to possible future changes in emission and meteorological fields.