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A thermodynamic equilibrium ammonium nitrate scheme in UKCA-mode

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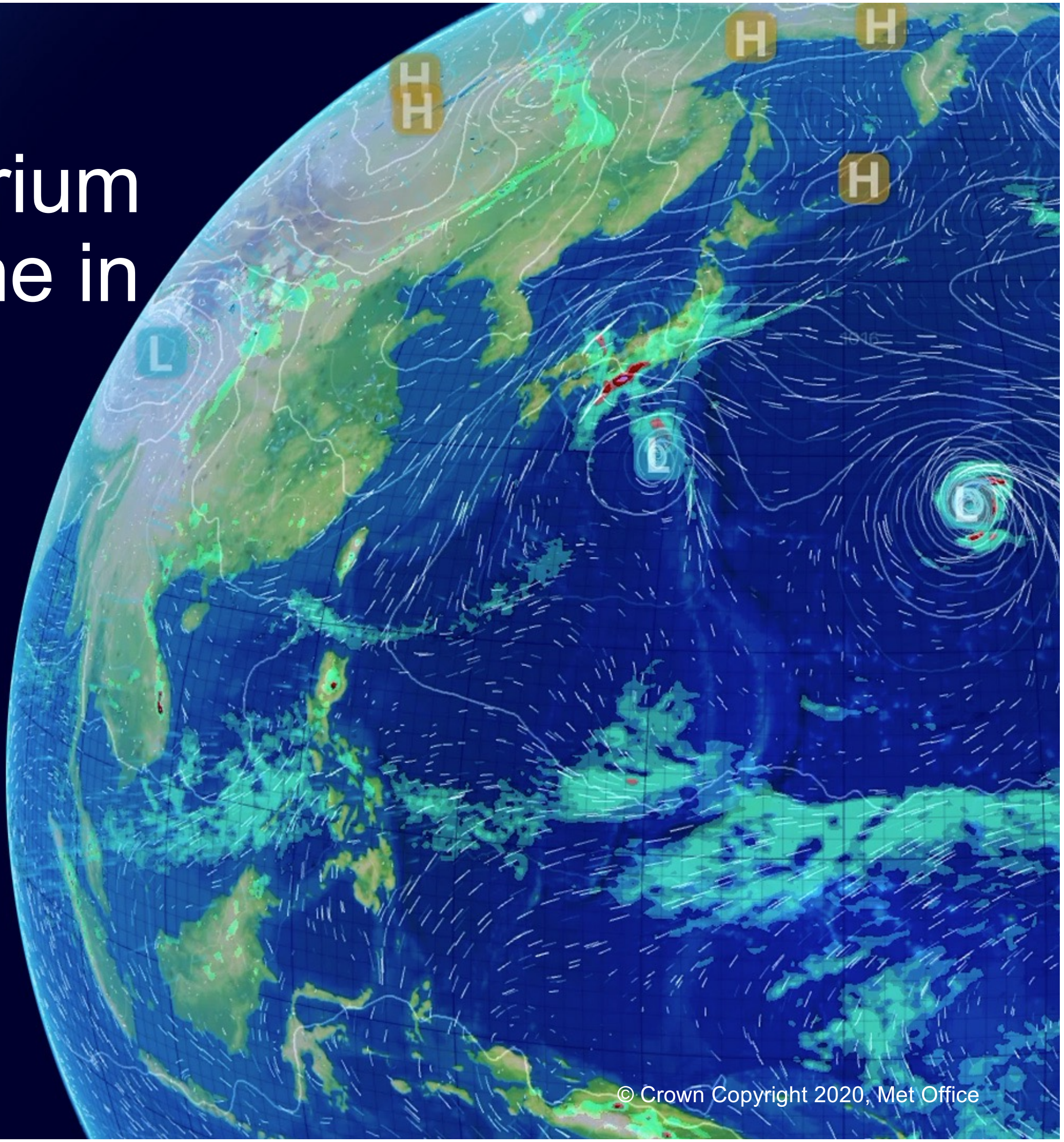

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Overview of nitrate scheme

- Semi-volatoile NH_4 and NO_3 emitted into Aitken and accumulation soluble modes using Mozurkewich (1993) parameterisation
- Rate at which $NH_4{\cdot}NO_3$ reaches equilibrium is limited by first order uptake theory, i.e.

$$k = \frac{2\pi D D_g}{1 + \frac{4K_n}{3\gamma} \times \left(1 - \frac{0.47\gamma}{1 + K_n}\right)}$$

- The uptake coefficient (γ) is altered between FAST (0.193) and SLOW (0.001) in sensitivity simulations
- HNO_3 uptake on dust and sea-salt also simulated with first order uptake in ACC sol. and COA sol. modes
- This scheme is on the trunk at UM11.8 (see ticket 5262) in mode setup 10

Mode	Species
NUC SOL	SO_4, OM
AIT SOL	SO_4, BC, OM, **NH_4, NO_3**
ACC SOL	SO_4, BC, OM, SS, **NH_4, NO_3, $NaNO_3$**
COA SOL	SO_4, BC, OM, SS, **NH_4, NO_3, $NaNO_3$**
AIT INS	BC, OM

<u>$NH_4{\cdot}NO_3$ equilibrium theory</u>

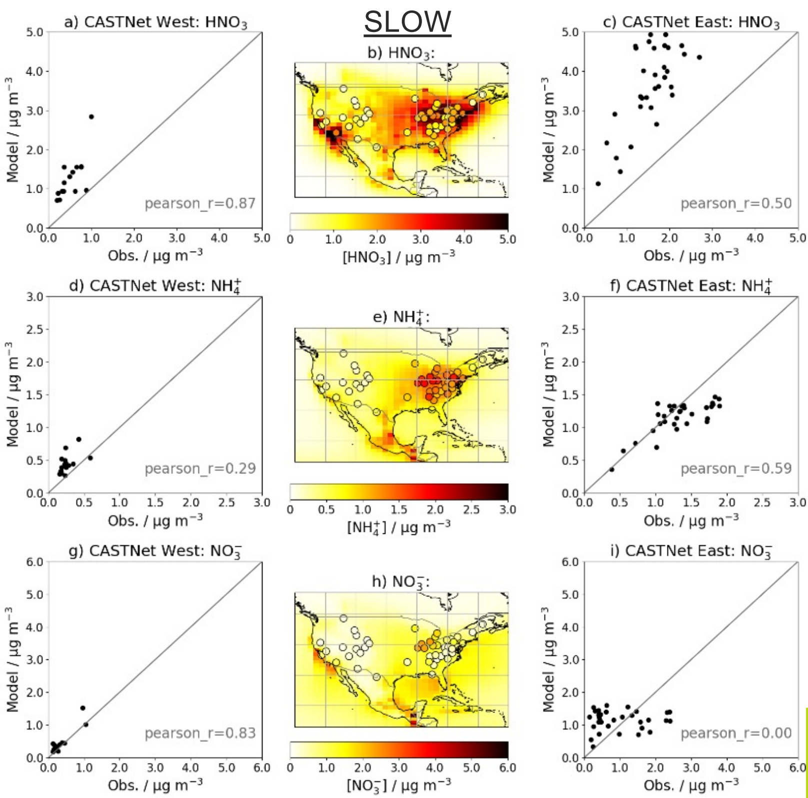
$$\mathrm{HNO_3} + \mathrm{NH_3} \overset{K_p}{\leftrightarrow} \mathrm{NH_4NO_3}$$

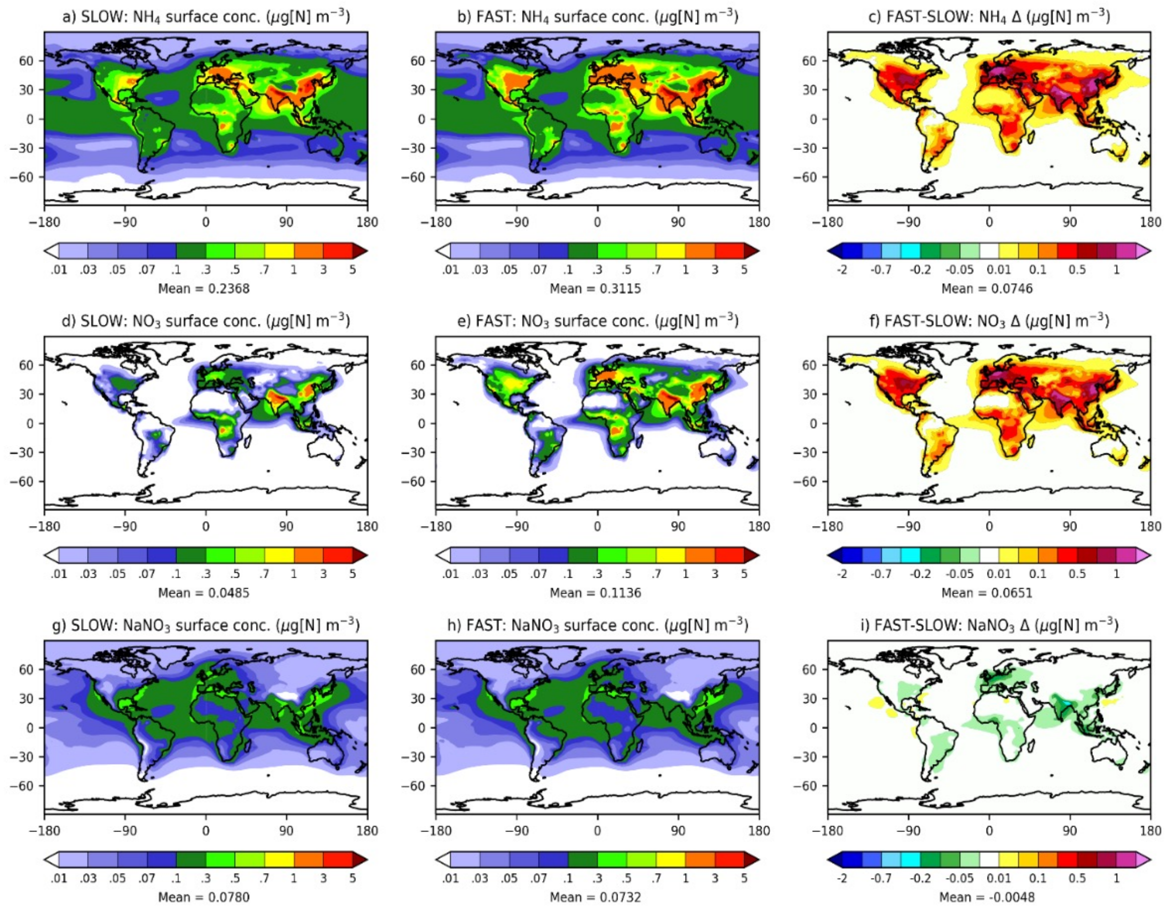
$$\{\mathrm{NH_4NO_3}\}_{eq} = \frac{1}{2}\left[T_A^* + T_N - \sqrt{(T_A^* + T_N)^2 - 4\left(T_N T_A^* - K_p\right)}\right]$$

Simulation	Rose Jobid	Description
CNTL	u-bz552	No nitrate – AMIP, UM11.7, N96, Strattrop
INSTANT	u-ca284	Nitrate – instant equilibrium
FAST	u-bz424	Nitrate – fast uptake ($\gamma = 0.193$)
SLOW	u-bz615	Nitrate – slow uptake ($\gamma = 0.001$)

Near surface concentrations

- Twice as much NO_3 in FAST as in SLOW
- CASTNET observations suggest NO_3 better matched with SLOW, too much in FAST





Credit: Catherine Hardacre

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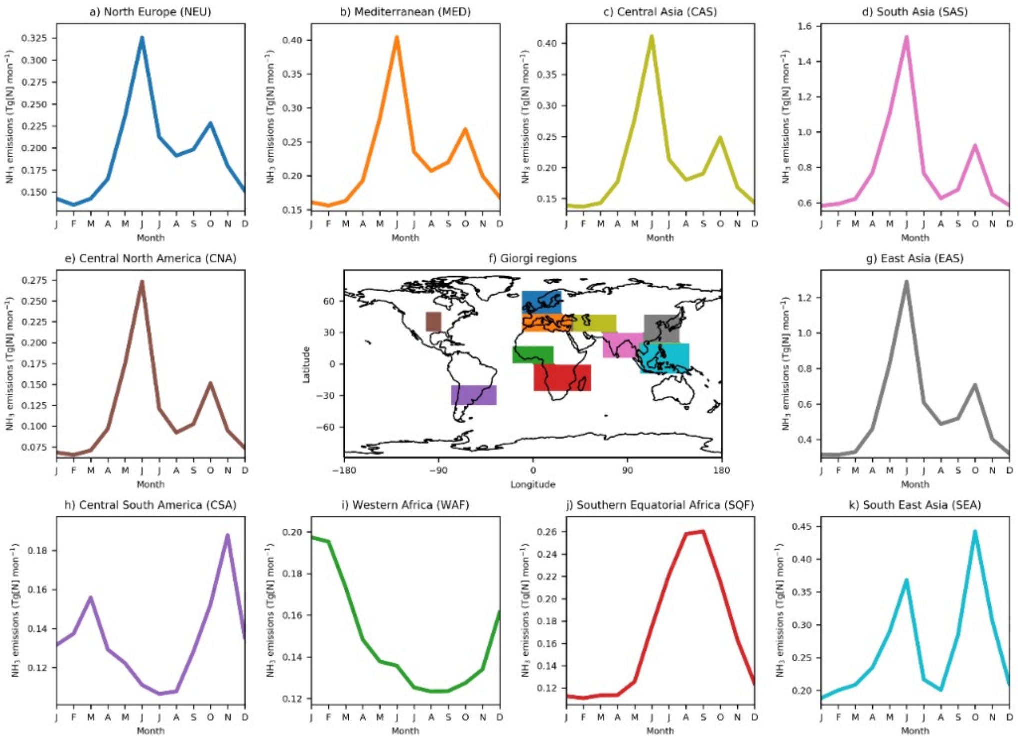
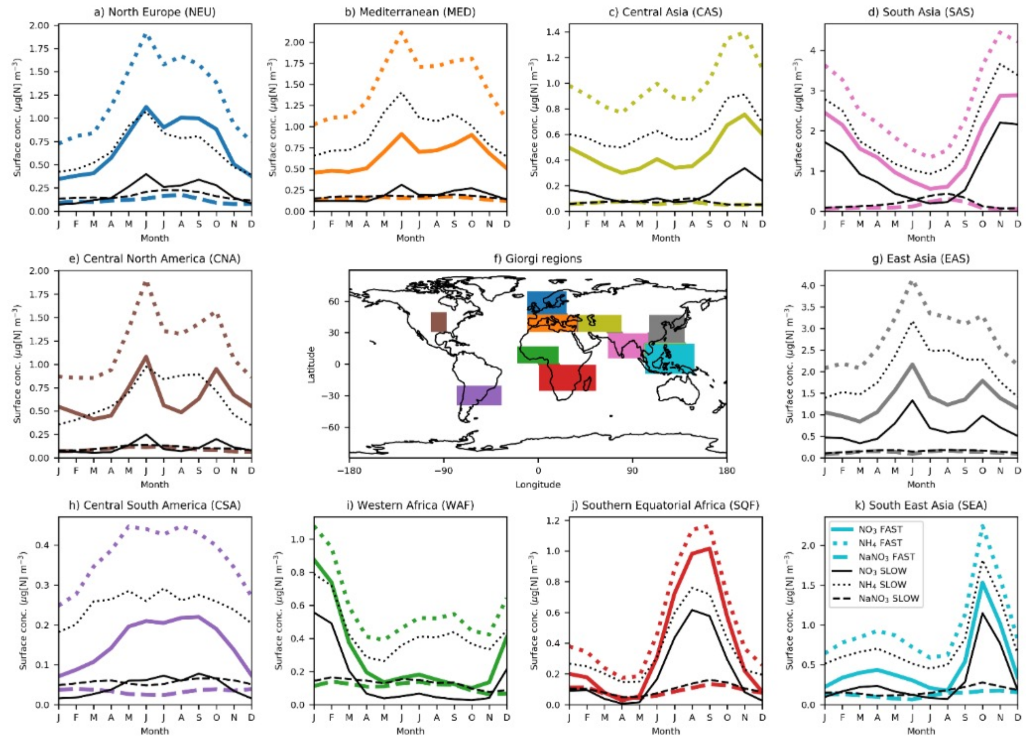
Near surface concentrations

- Seasonal trends in $NH_4{\cdot}NO_3$ concentrations are highly sensitive to NH_3 emissions in most regions

Ammonia emissions



Aerosol surface concentrations



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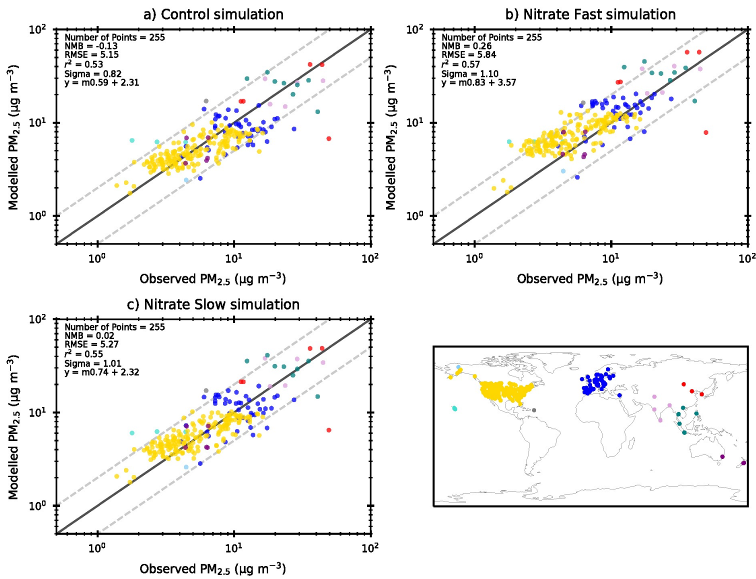
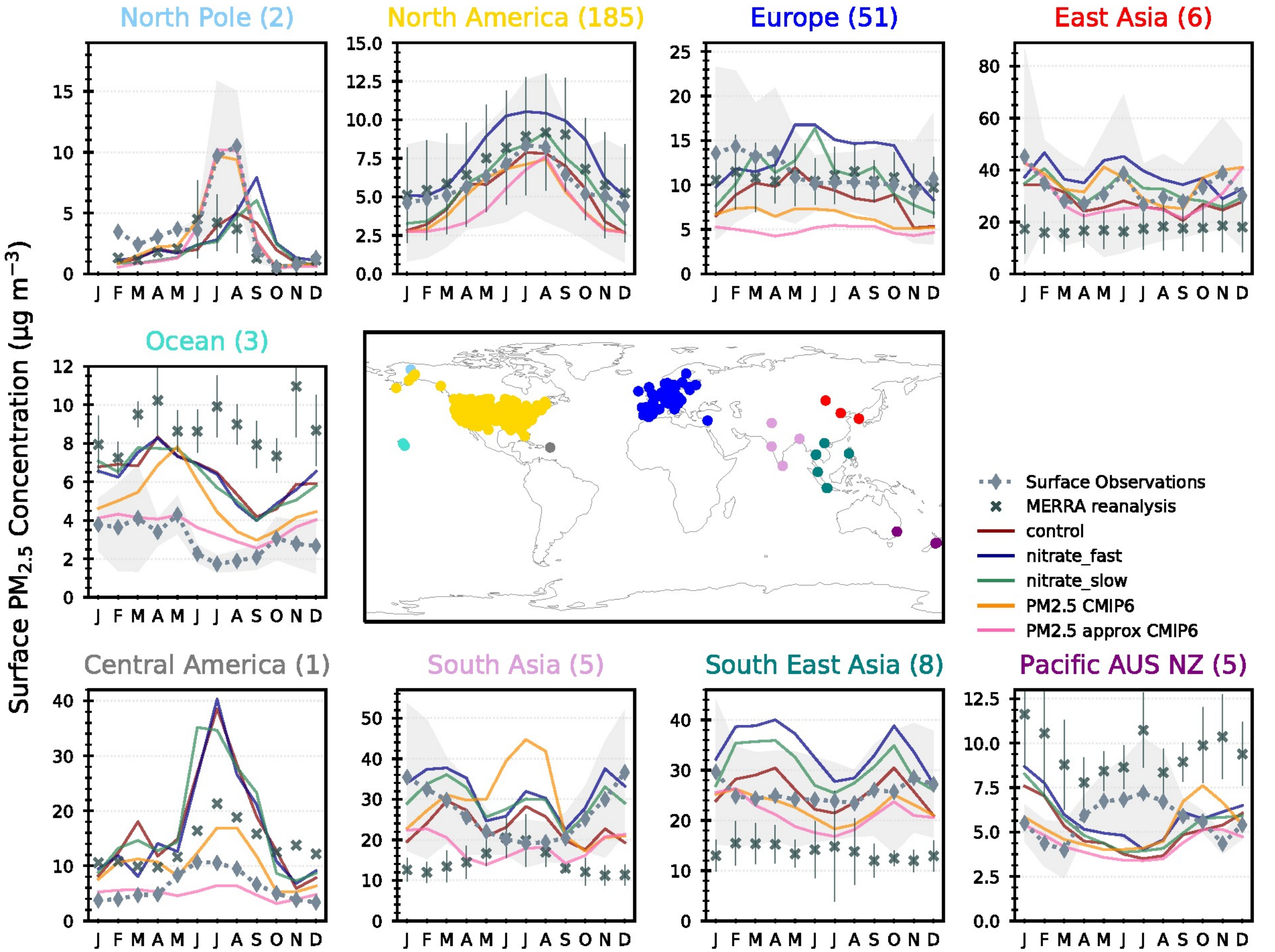
$PM_{2.5}$ concentrations

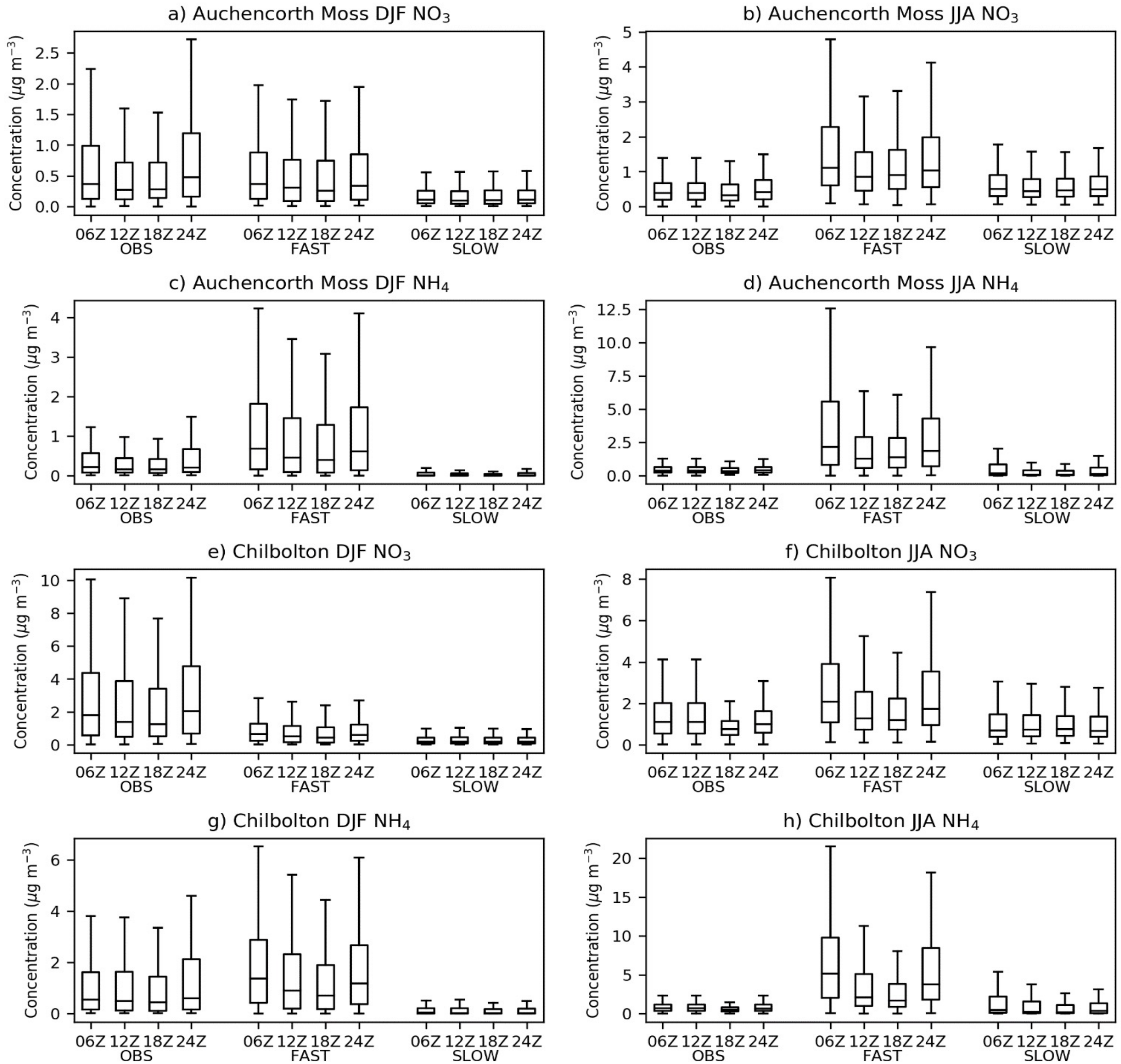
- Anomalous JJA increase in $PM_{2.5}$ over Europe linked to spurious NH_3 emissions?
- $PM_{2.5}$ not broken by $NH_4 \cdot NO_3$





Credit: Steve Turnock

• Diurnal cycle of $NH_4 \cdot NO_3$ concentrations peaking at night and lows in the afternoon largely captured by model and seen in UK observations



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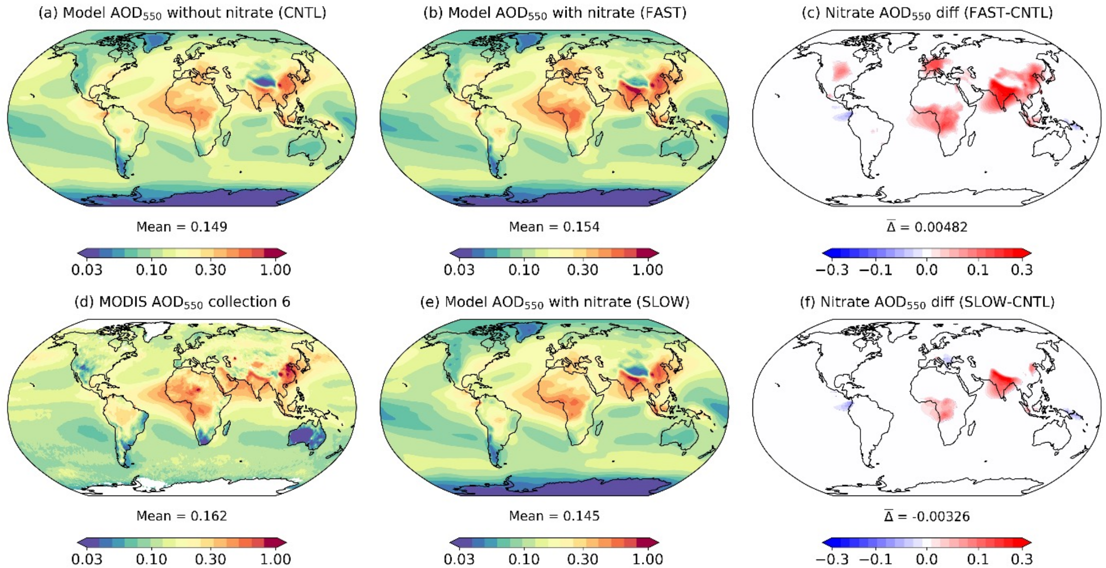
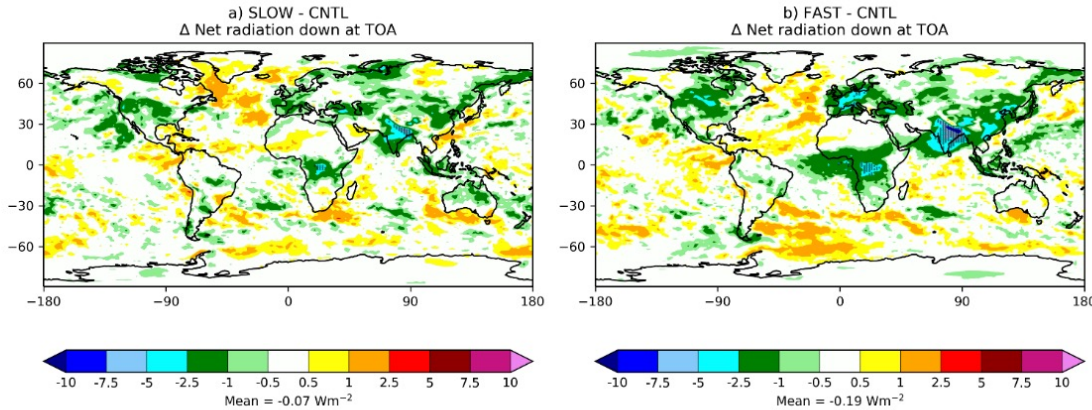
Radiation and AOD

- Δ AOD between -0.003 in SLOW and 0.005 in FAST
- Effective radiative forcing between -0.07 Wm^{-2} in SLOW and -0.19 Wm^{-2} in FAST
- Significant negative forcing over India, Europe and the DRC



Credit: Ben Johnson



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Exploring the sensitivity of atmospheric nitrate concentrations to nitric acid uptake rate using the MetUM at vn11.7

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