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Direct effects of particle precipitation and ion chemistry in the middle atmosphere

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2. Sodankylä Ion and Neutral Chemistry Model (SIC)

   – Analysis of the ion chemistry scheme

   – Parameterization of EPP-related changes in HO_x and NO_y

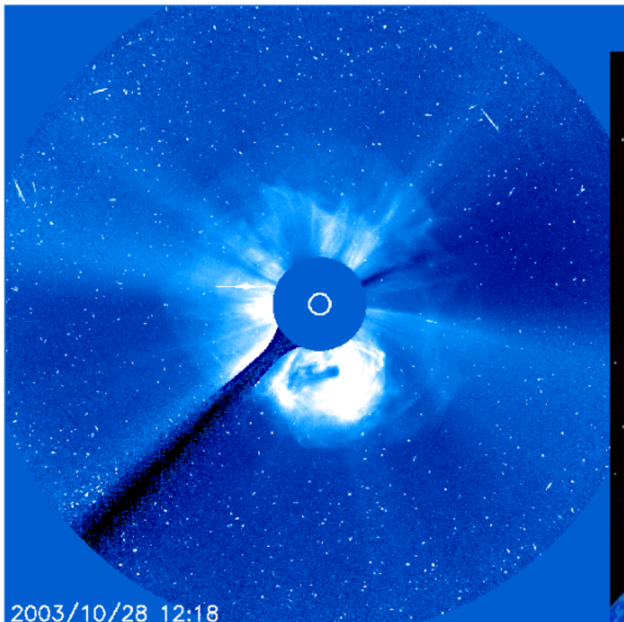
3. SIC model versus MLS/Aura observations:

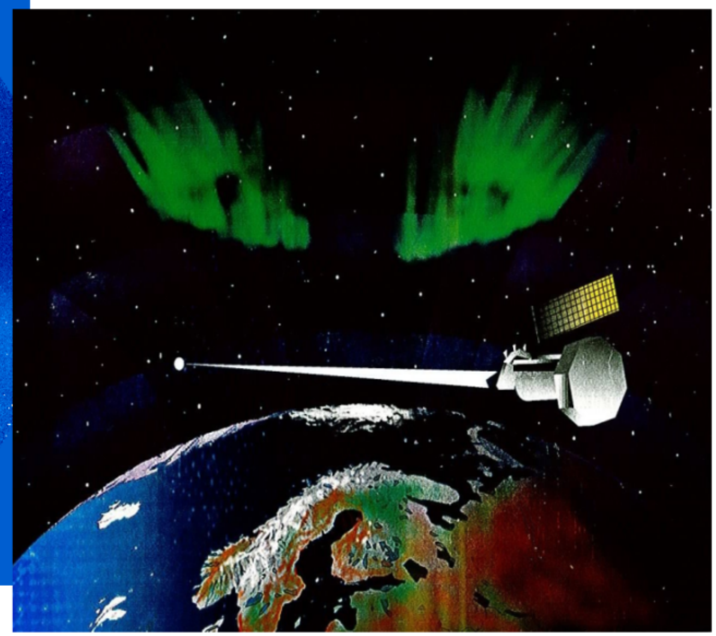
   – SPEs of January 2005 and December 2006

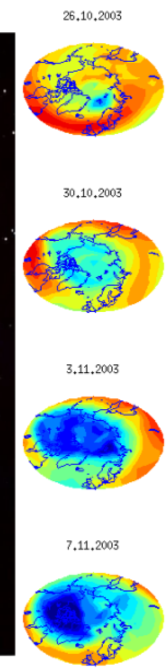
   – Production of HNO_3 and OH

4. Summary

Energetic particle precipitation



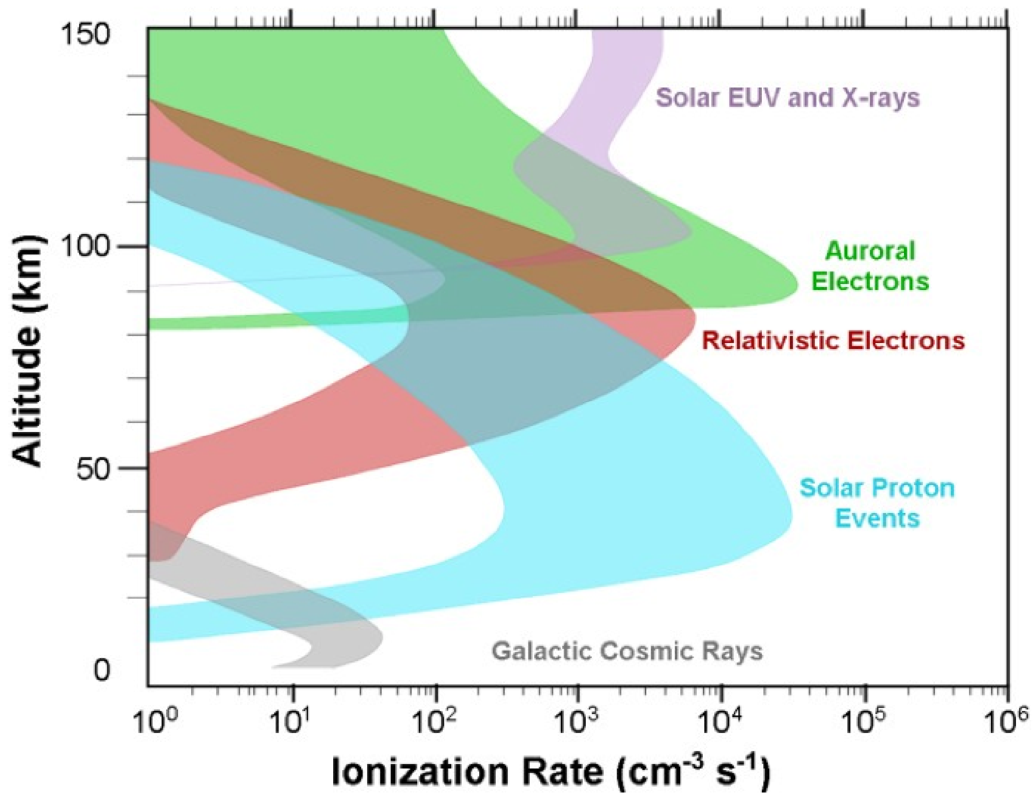




Earth's magnetic field directs charged particles into polar regions

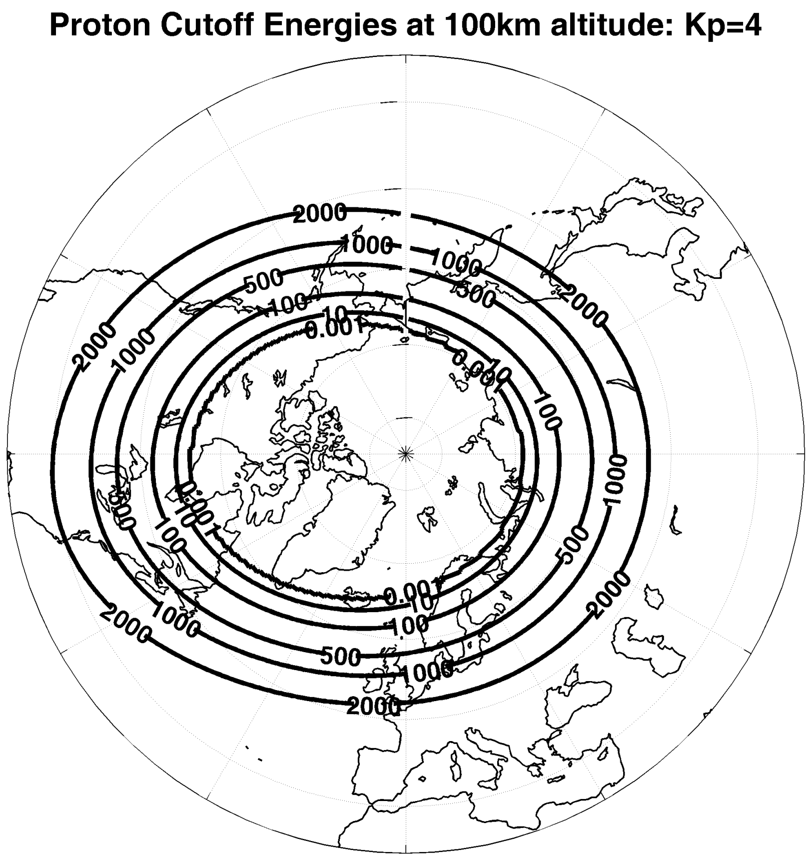
EPP affects both ionosphere and middle atmosphere

Different types of particle precipitation



From a presentation by Randall et al., 2008

SPE: example of geomagnetic cutoff



Rodger et al., Journal of Geophysical Research (2006)

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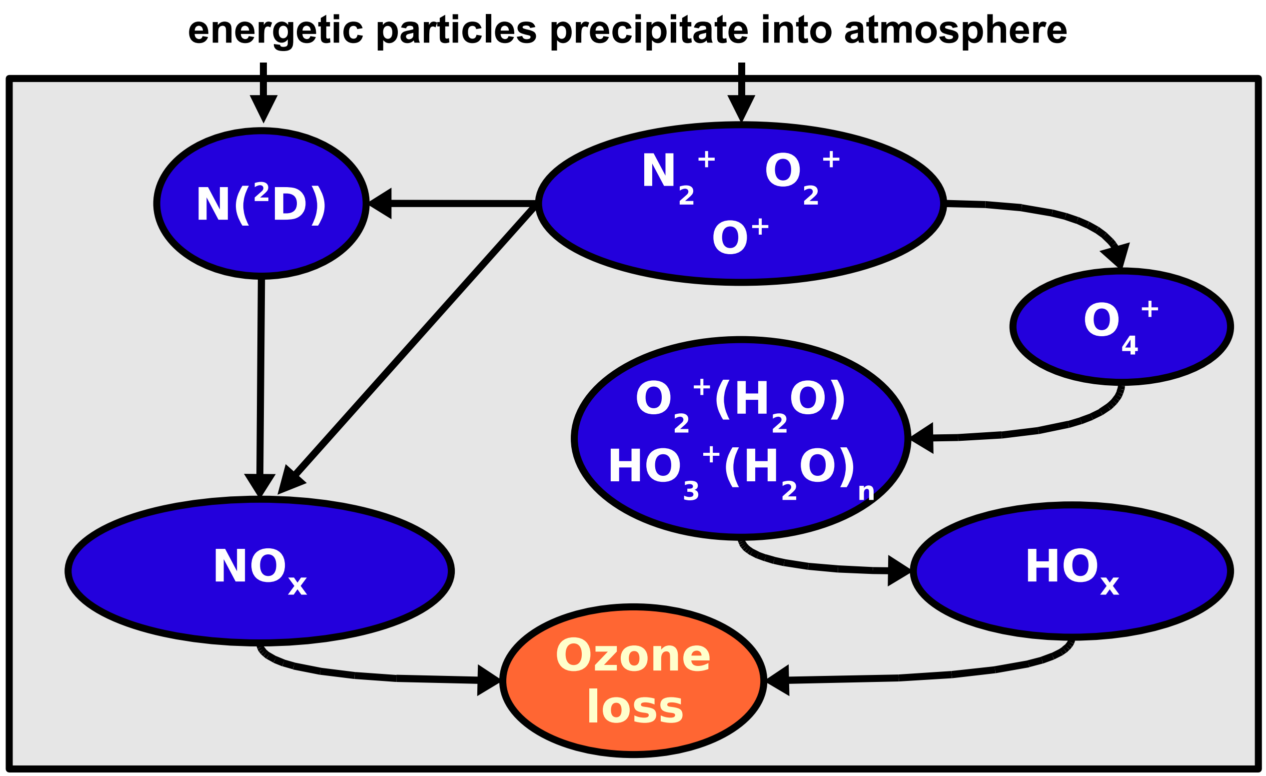
Effects of energetic particle precipitation (EPP)



Ozone connects to temperature and dynamics

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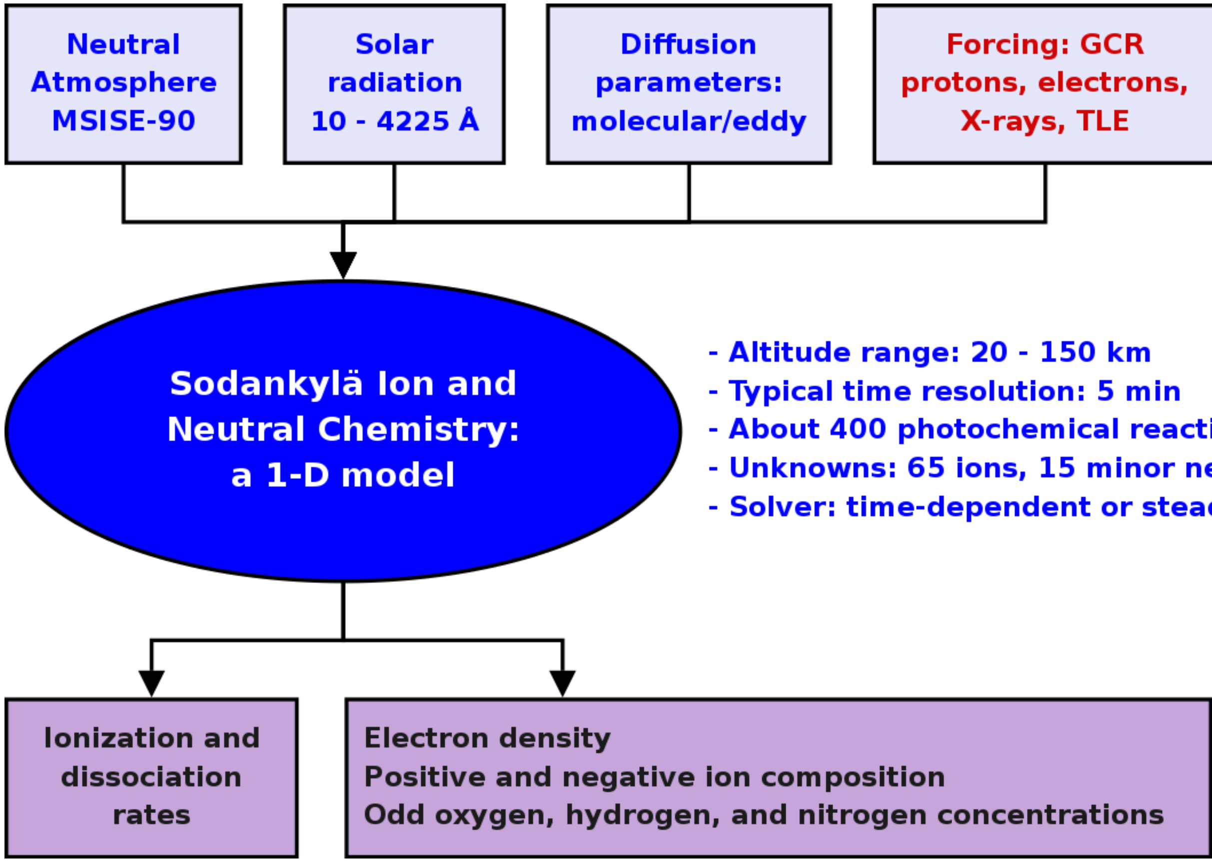
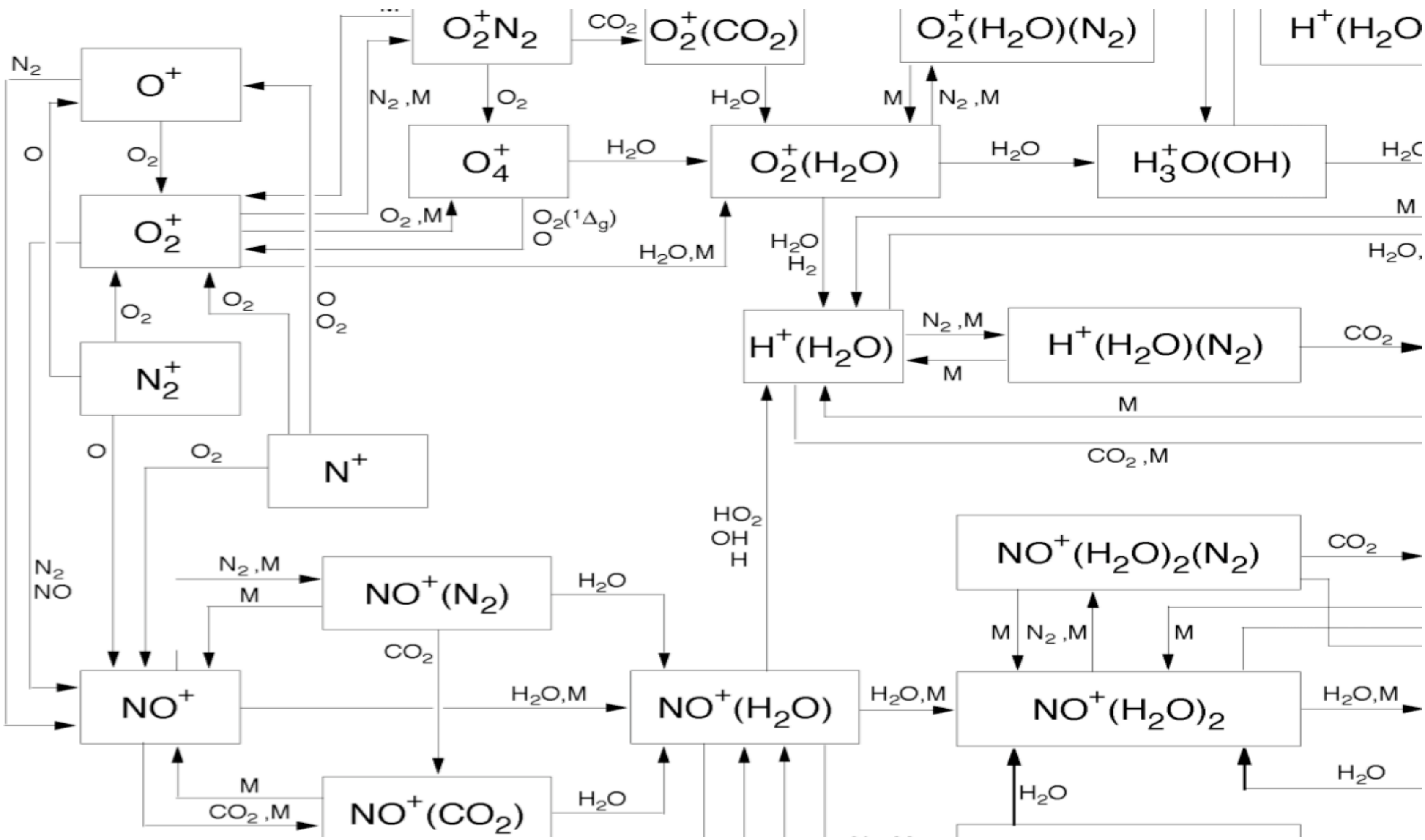
Sodankylä Ion and Neutral Chemistry (SIC)



- Altitude range: 20 - 150 km
- Typical time resolution: 5 min
- About 400 photochemical reactions
- Unknowns: 65 ions, 15 minor neutrals
- Solver: time-dependent or steady-state

SIC: D-region ion chemistry

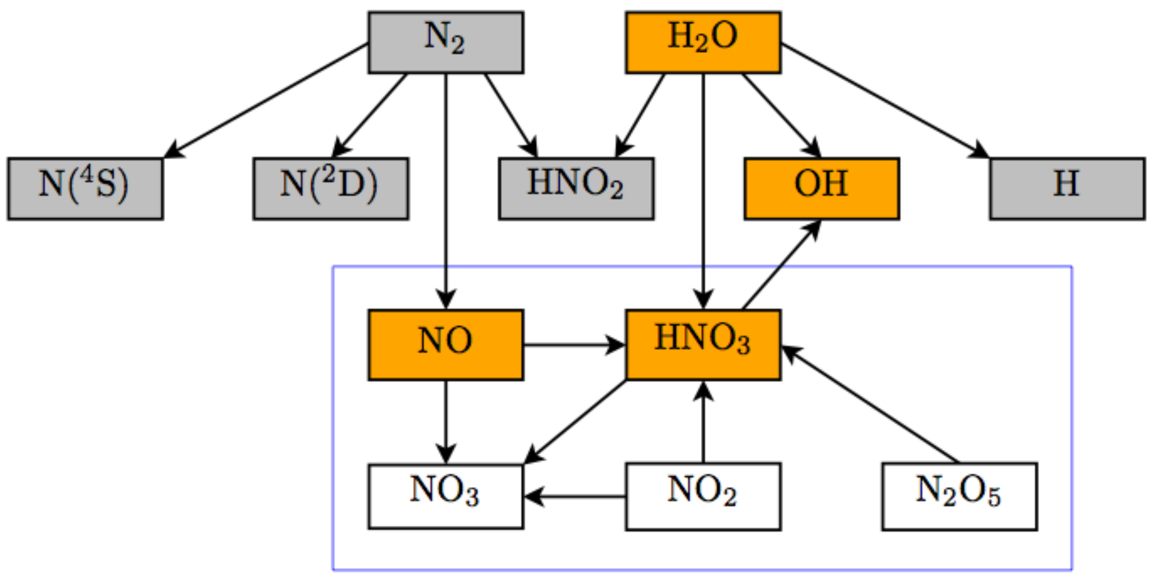


36 positive ions, 29 negative ions, 400 reactions

Changes in hydrogen and nitrogen species

Particles precipitate into middle atmosphere

↓ ↓ ↓ ↓ ↓



– Positive ion chemistry dissociates N_2 and H_2O

– Negative ion chemistry redistributes NO_y (inside the blue box)

– From Verronen and Lehmann, *Ann. Geophys.*, 2013.

SIC: example of HO_x production paths

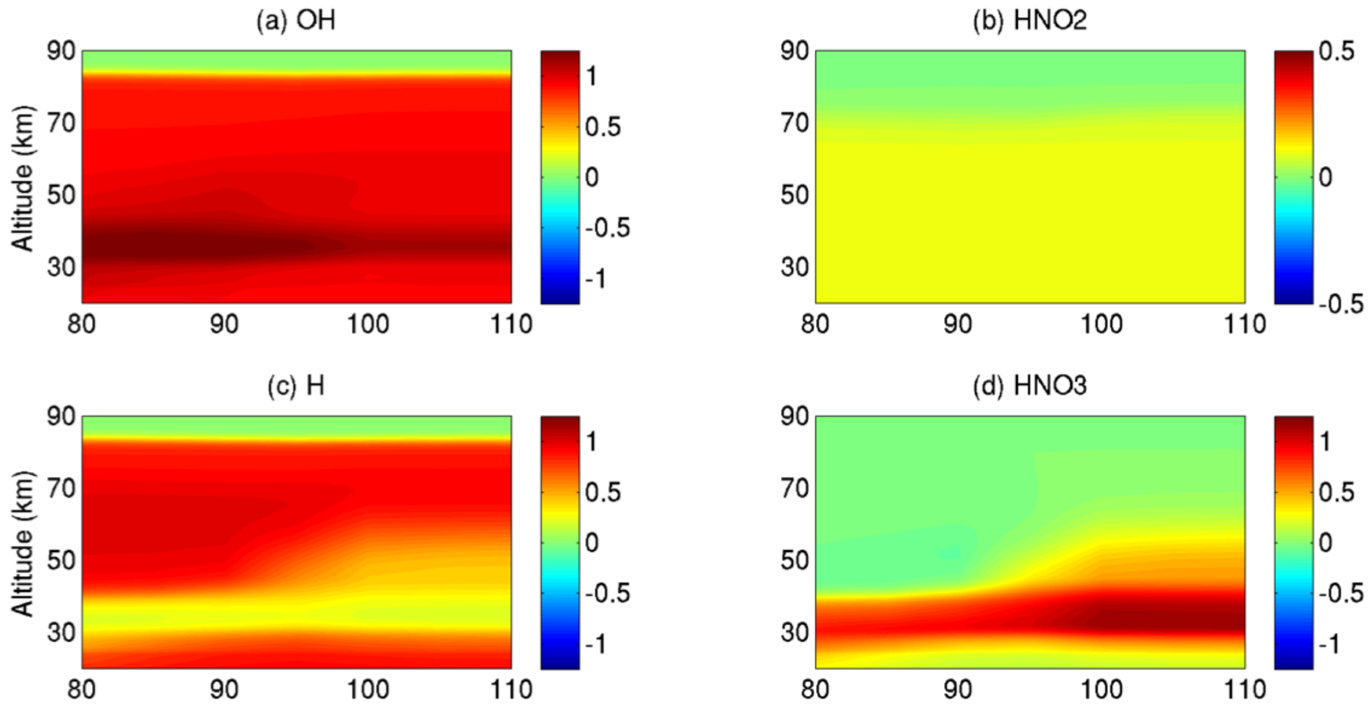
$$
\begin{aligned}
N_2 + p^+(E) &\rightarrow N_2^+ + e^- + p^+(E - \Delta E) \\
N_2^+ + O_2 &\rightarrow O_2^+ + N_2 \\
O_2^+ + O_2 + M &\rightarrow O_4^+ + M \\
O_4^+ + H_2O &\rightarrow O_2^+(H_2O) + O_2 \\
\ldots & \\
O_2^+(H_2O)_2 + H_2O &\rightarrow H_3O^+(OH)H_2O + O_2 \\
H_3O^+(OH)H_2O + H_2O &\rightarrow H^+(H_2O)_3 + \mathbf{OH} \\
H^+(H_2O)_3 + H_2O + M &\rightarrow H^+(H_2O)_4 + M \\
H^+(H_2O)_4 + e^- &\rightarrow \mathbf{H} + 4H_2O \\
--- &\quad --- \\
\mathbf{Net}: H_2O &\rightarrow OH + H
\end{aligned}
$$

SIC: example of HNO_3 production paths

$$
\begin{aligned}
N_2 + p^+(E) &\rightarrow N_2^+ + e^- + p^+(E - \Delta E) \\
O_2 + O_2 + e^- &\rightarrow O_2^- + O_2 \\
O_2^- + O_3 &\rightarrow O_3^- + O_2 \\
O_3^- + CO_2 &\rightarrow CO_3^- + O_2 \\
CO_3^- + NO_2 &\rightarrow NO_3^- + CO_2 \\
NO_3^- + H_2O + M &\rightarrow NO_3^-(H_2O) + M \\
NO_3^-(H_2O) + HNO_3 &\rightarrow NO_3^-(HNO_3) + H_2O \\
NO_3^-(HNO_3) + \mathbf{H^+(H_2O)}_4 &\rightarrow \mathbf{HNO_3} + HNO_3 + 4H_2O \\
- - - &\quad - - - \\
\mathbf{Net} : \mathbf{H_2O} + O_3 + NO_2 &\rightarrow \mathbf{OH} + HNO_3 + O_2
\end{aligned}
$$

P/Q: relative production/loss rates from SIC

$P/Q =$ (ionic production - ionic loss) / ionization rate

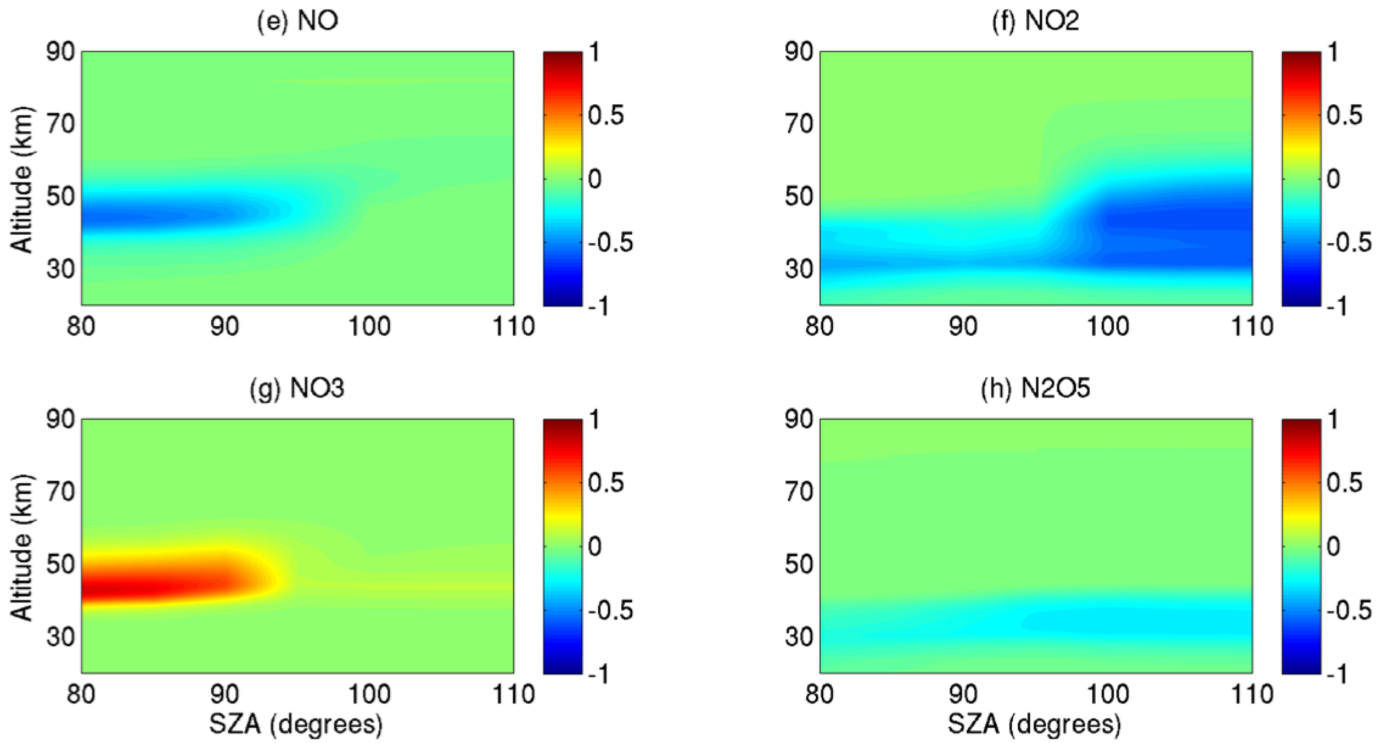


– H_2O becomes the limiting factor at upper altitudes

– At night: more negative ions, more HNO_3 production

P/Q: relative production/loss rates from SIC

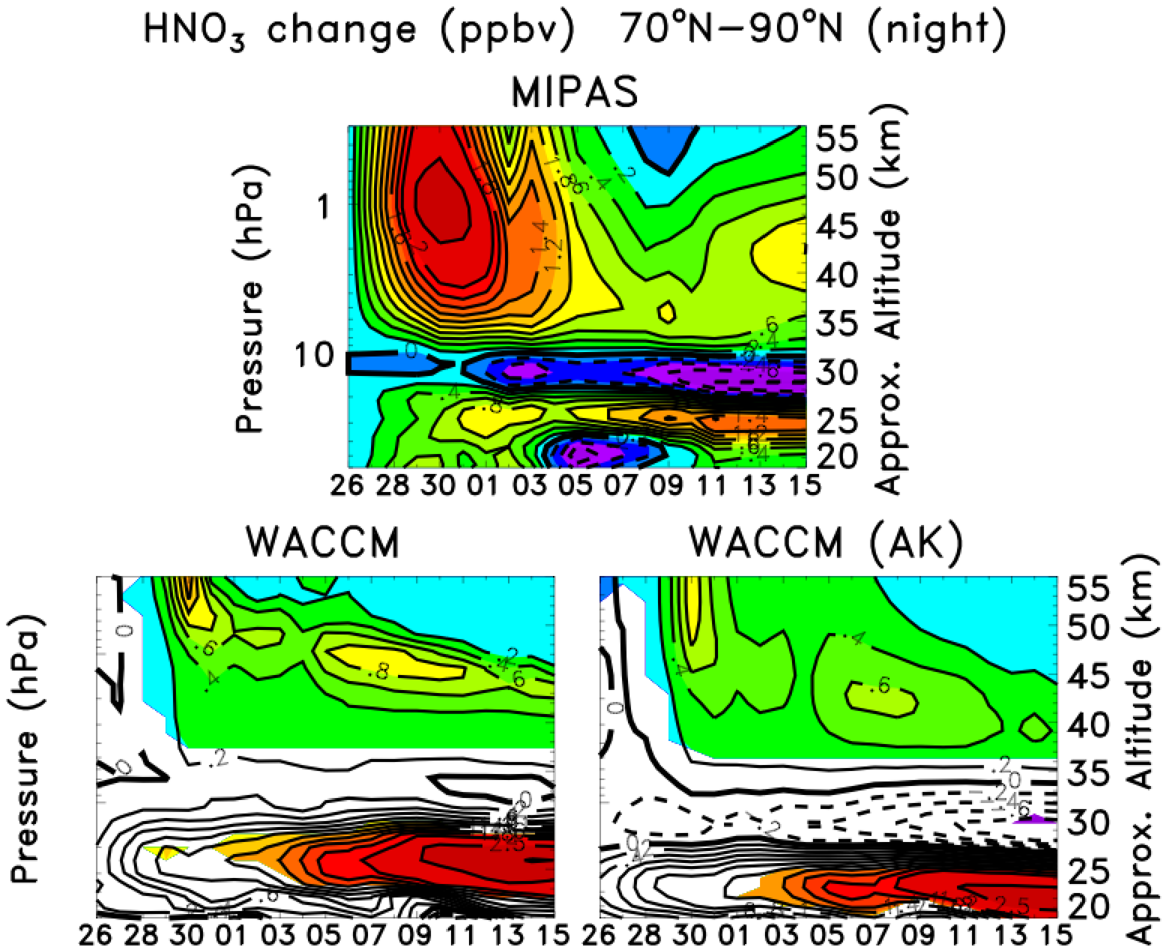
$P/Q =$ (ionic production - ionic loss) / ionization rate



– Note: Zero net change of NO_y (incl. HNO_3) by negative ion chemistry

– Net production of NO_x is by positive ion chemistry

Outstanding issue: nitric acid in CCMs



– From Jackman et al., *Atmos. Chem. Phys.*, 2008

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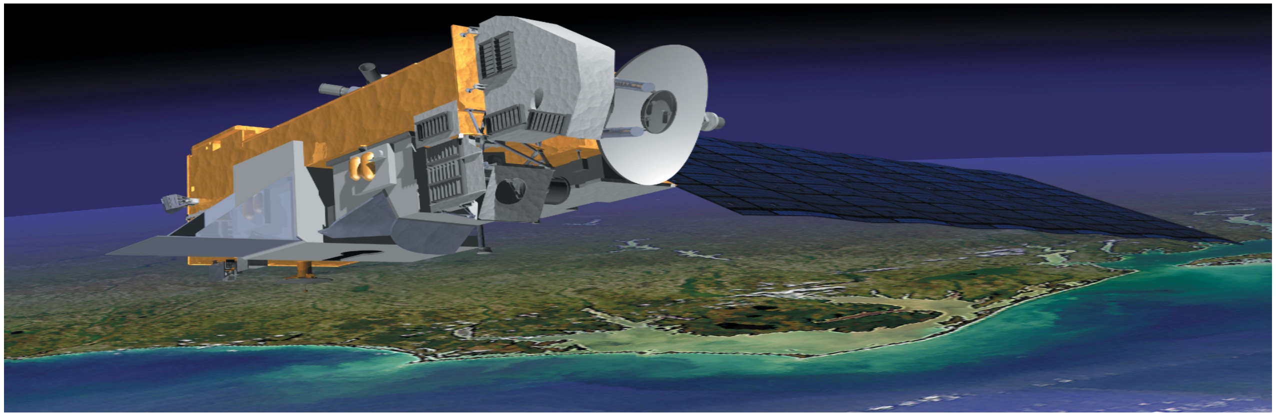
MLS/Aura observations



- Microwave Limb Sounder, measures emissions at mm and sub-mm wavelengths
- Launched in July 2004 into a near-polar orbit, observations cover latitudes between 82°S – 82°N, day and night
- Can be used to monitor temperature and more than 15 trace gases, including O_3, OH, and HNO_3
- First satellite instrument providing continuous observations of mesospheric OH and HO_2

Nitric acid: comparisons

Modeling: Sodankylä Ion and Neutral Chemistry

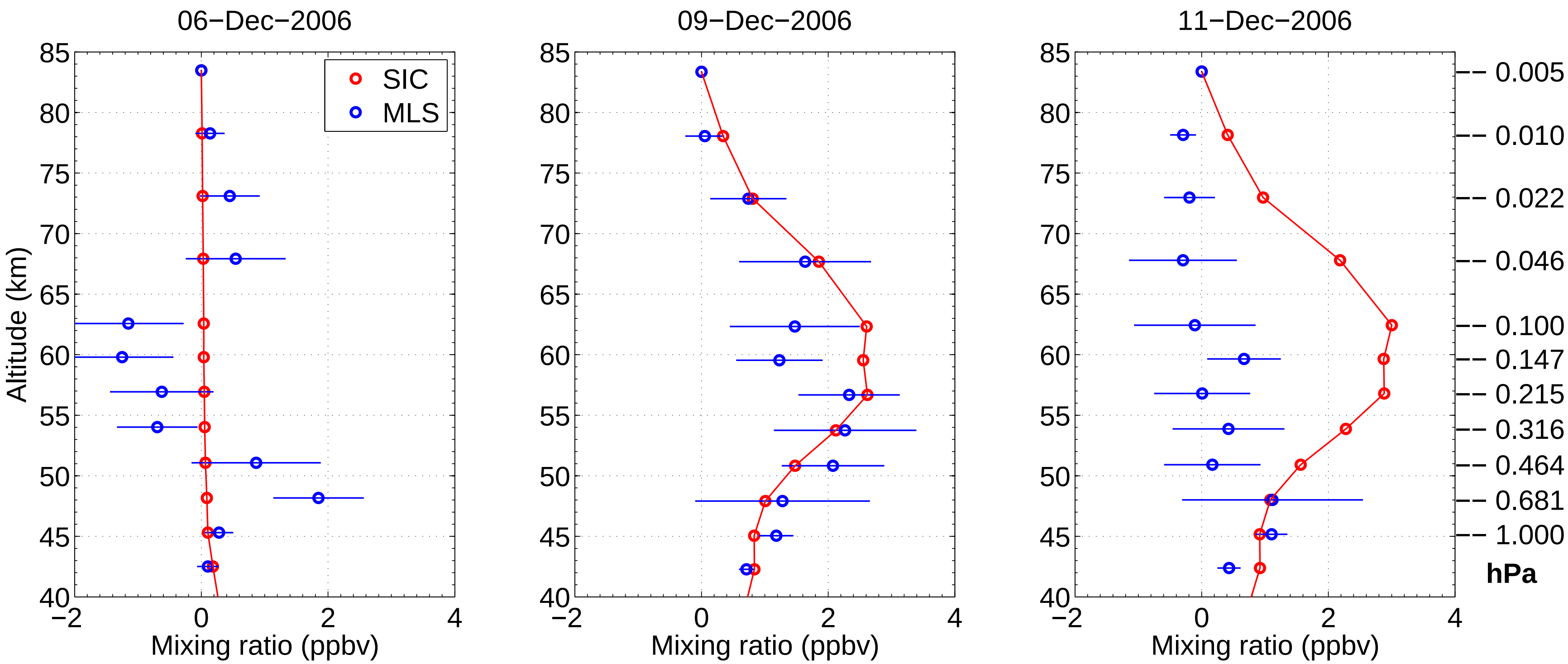
- Uses MLS temperatures, neutral density, and water vapor.
- 80°N/December–January, no diurnal variations.
- Results reduced to MLS altitude resolution using averaging kernels.

Observations: data version 3.30, SZA $> 100^\circ$ (night-time)

- Data are daily means, uncertainty is standard error of the mean.
- Useful range up to 1.5 hPa ($\approx$50 km) in normal conditions, but can be extended into mesosphere when high amounts are observed.
- Mesospheric HNO_3 data have not been validated.
- Comparison is made with the highest amount of HNO_3 observed after the peak of SPE forcing, assuming that it is least affected by dynamics.

SIC vs. MLS: nitric acid, December 2006 SPE

Before (left), during (middle), and after (right) the SPE forcing



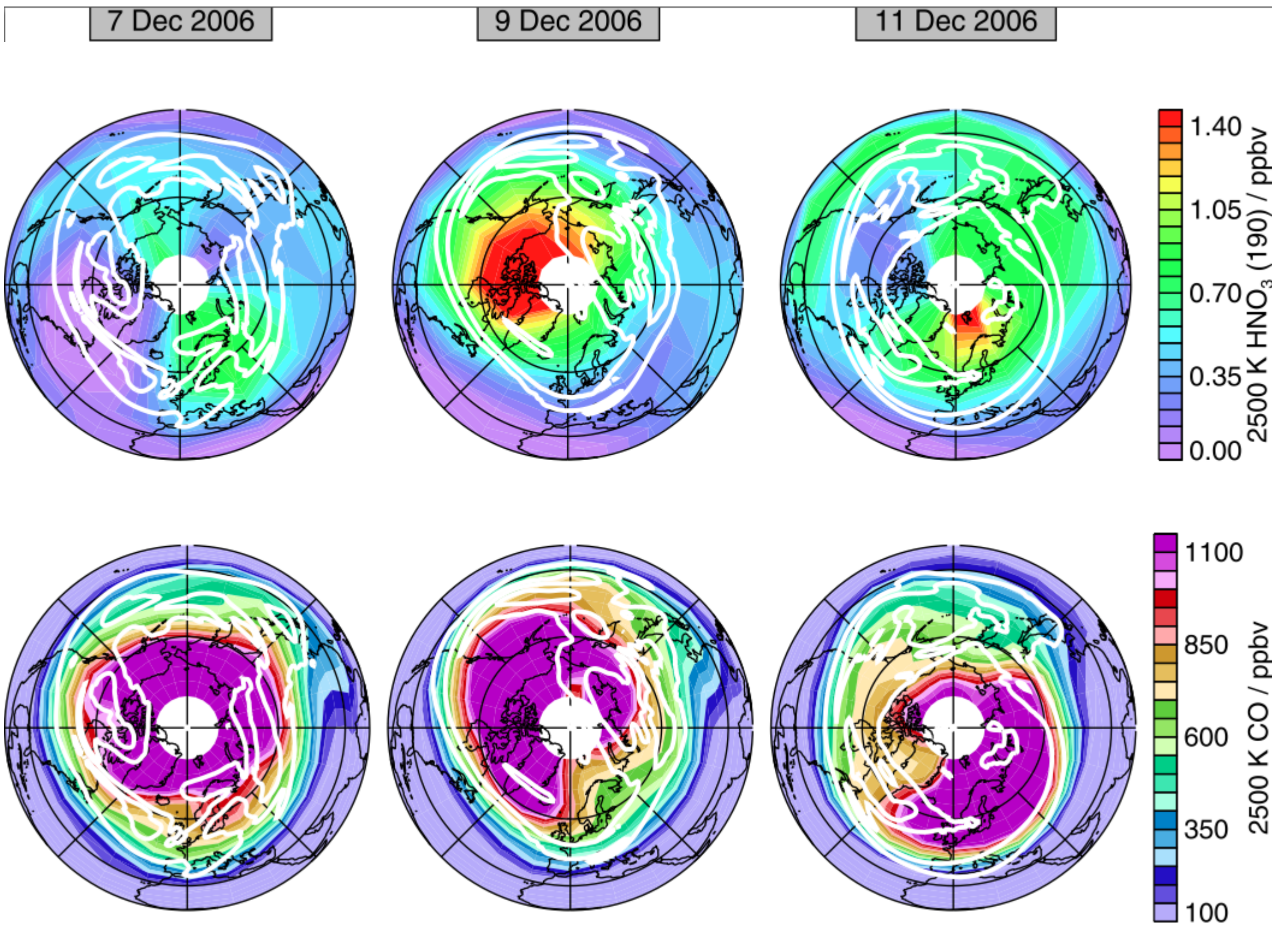
– The model overestimates the HNO_3 increase on Dec 9 at 60–65 km.

– Below 50 km the agreement is OK.

– For more details, see Verronen et al., *J. Geophys. Res.*, 2011.

MLS: HNO_3 (top) and CO (bottom)

Daily avarages at approx. 60 km (2500 K)



Odd hydrogen: comparisons

Modeling: Sodankylä Ion and Neutral Chemistry

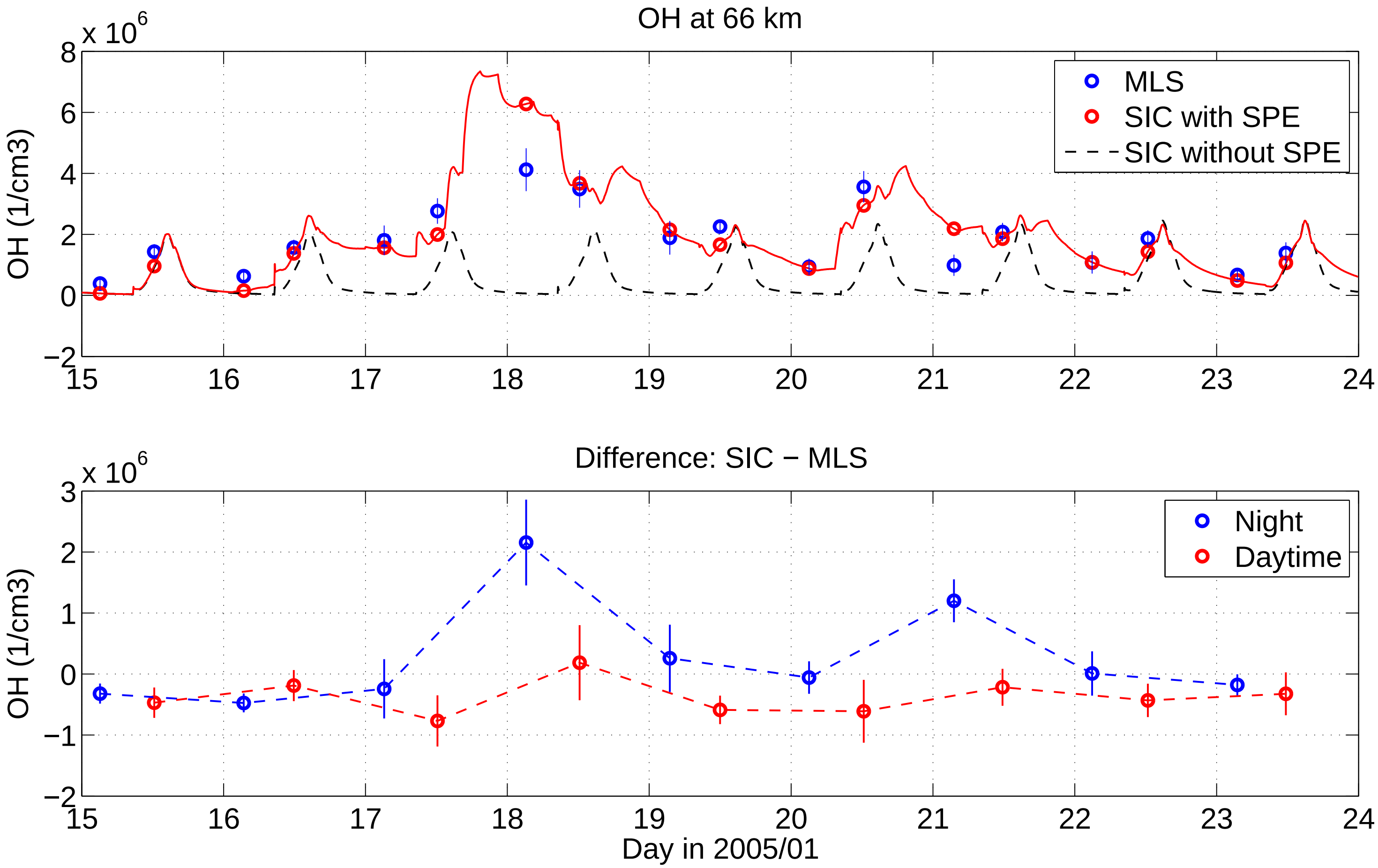
– Uses MLS temperatures, neutral density, and water vapor.
– Latitudes $>60^\circ$N, solar proton events of January 2005 and December 2006.

OH observations: data version 3.30

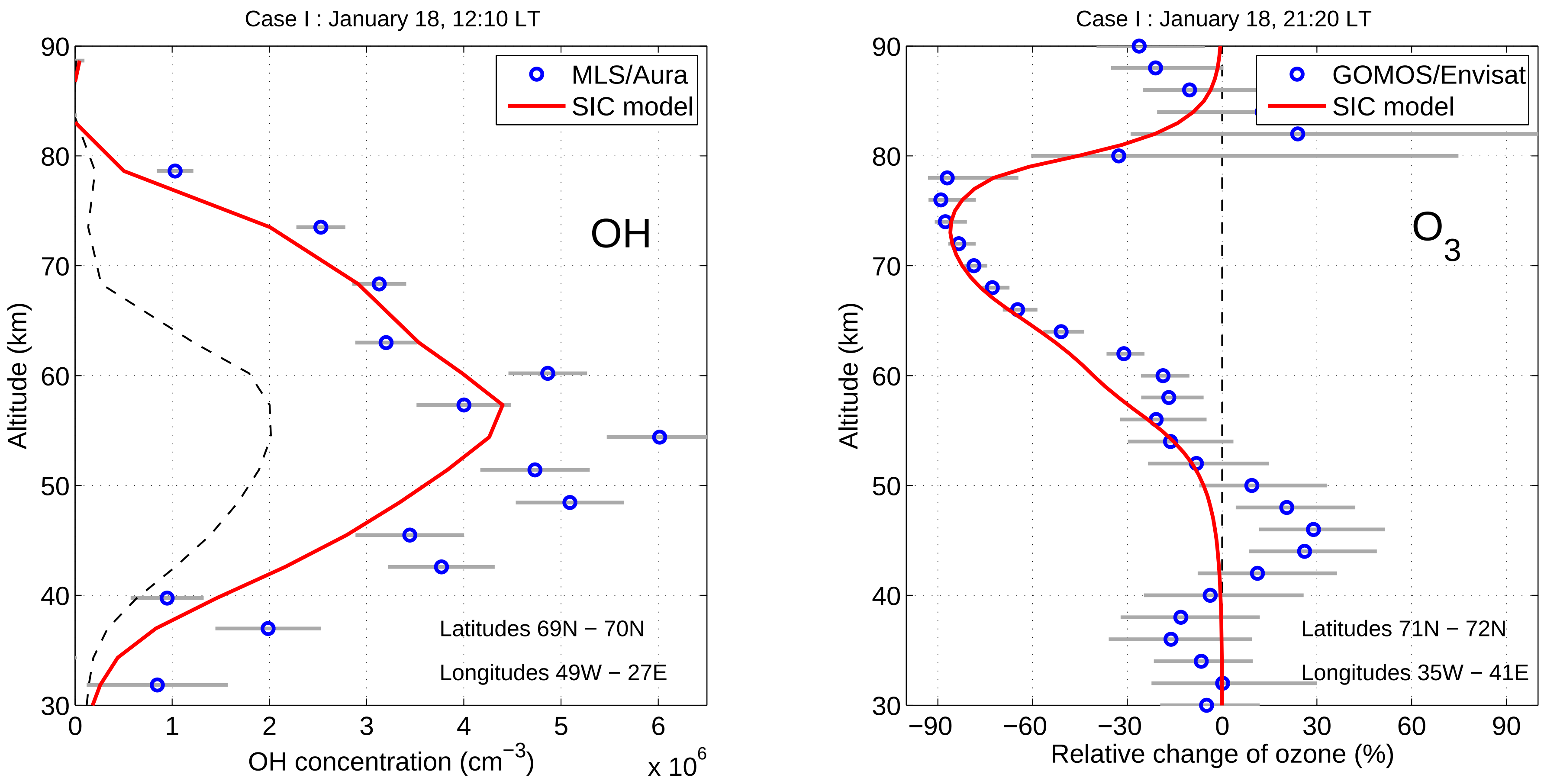
– Useful range up to 0.0032 hPa ($\approx$90 km).
– Mesospheric data have been validated by Pickett et al., JGR, 2008.
– Data are averaged at 65–75°N, for day and night separately.

MLS was the first instrument that provided continuous and global observations of mesospheric HO_x.

SIC vs. MLS: hydroxyl, January 2005



SIC vs. MLS: OH



– From Verronen et al., *Geophys. Res. Lett.*, 2006

Ion chemistry and its effects in models

- Although there are uncertainties, the understanding of ion chemistry seems reasonably good for particle effect modelling.

- Our full knowledge is not used when parameterizing ion chemistry in 3-D atmospheric models, typically:
  – HO_x and NO_x production is included,
  – HNO_3 and HNO_2 production is not included,
  – Chlorine activation is not included

  (Winkler et al., *Geophys. Res. Lett.*, 2009).

- Two ways to include ion chemistry:
  – Parameterization. Simple and good in all situations?
  – Full ion chemistry. Computationally too expensive?