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

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   - Production of $\text{HNO}_3$ 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

Proton Cutoff Energies at 100km altitude: Kp=4

Effects of energetic particle precipitation (EPP)

Energetic particles precipitate into atmosphere

\[ N_2 + O_2 + O^+ + NO_x \]

\[ O_4^+ \]

\[ O_2^+(H_2O) \]

\[ HO_3^+(H_2O)_n \]

\[ NO_x \]

Ozone loss

Ozone connects to temperature and dynamics
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

- Ionization and dissociation rates
- Electron density
  Positive and negative ion composition
  Odd oxygen, hydrogen, and nitrogen concentrations

- Forcing: GCR protons, electrons, X-rays, TLE
- Diffusion parameters: molecular/eddy
- Solar radiation 10 - 4225 Å
- Neutral Atmosphere MSISE-90
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)
SIC: example of HO$_x$ production paths

\[
N_2 + p^+(E) \rightarrow N_2^+ + e^- + p^+(E - \Delta E)
\]

\[
N_2^+ + O_2 \rightarrow O_2^+ + N_2
\]

\[
O_2^+ + O_2 + M \rightarrow O_4^+ + M
\]

\[
O_4^+ + H_2O \rightarrow O_2^+(H_2O) + O_2
\]

\[
\ldots
\]

\[
O_2^+(H_2O)_2 + H_2O \rightarrow H_3O^+(OH)H_2O + O_2
\]

\[
H_3O^+(OH)H_2O + H_2O \rightarrow H^+(H_2O)_3 + OH
\]

\[
H^+(H_2O)_3 + H_2O + M \rightarrow H^+(H_2O)_4 + M
\]

\[
H^+(H_2O)_4 + e^- \rightarrow H^+ + 4H_2O
\]

\[
\text{Net: } H_2O \rightarrow OH + H
\]
SIC: example of HNO$_3$ production paths

\[
\begin{align*}
N_2 + p^+ (E) & \rightarrow N_2^+ + e^- + p^+ (E - \Delta E) \\
O_2 + O_2 + e^- & \rightarrow O_2^- + O_2 \\
O_2^- + O_3 & \rightarrow O_3^- + O_2 \\
O_3^- + CO_2 & \rightarrow CO_3^- + O_2 \\
CO_3^- + NO_2 & \rightarrow NO_3^- + CO_2 \\
NO_3^- + H_2O + M & \rightarrow NO_3^- (H_2O) + M \\
NO_3^- (H_2O) + HNO_3 & \rightarrow NO_3^- (HNO_3) + H_2O \\
NO_3^- (HNO_3) + H^+ (H_2O)_4 & \rightarrow HNO_3 + HNO_3 + 4H_2O
\end{align*}
\]

Net: \( H_2O + O_3 + NO_2 \rightarrow OH + HNO_3 + O_2 \)
P/Q: relative production/loss rates from SIC

\[ P/Q = \frac{\text{ionic production} - \text{ionic loss}}{\text{ionization rate}} \]

- H\(_2\)O becomes the limiting factor at upper altitudes
- At night: more negative ions, more HNO\(_3\) production
P/Q: relative production/loss rates from SIC

\[ \frac{P}{Q} = \frac{\text{ionic production} - \text{ionic loss}}{\text{ionization rate}} \]

– 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

HNO₃ change (ppbv) 70°N–90°N (night)

MIPAS

WACCM

WACCM (AK)

– From Jackman et al., *Atmos. Chem. Phys.*, 2008
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 O₃, OH, and HNO₃
- First satellite instrument providing continuous observations of mesospheric OH and HO₂
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° (night-time)

- Data are daily means, uncertainty is standard error of the mean.
- Useful range up to 1.5 hPa (≈50 km) in normal conditions, but can be extended into mesosphere when high amounts are observed.
- Mesospheric HNO₃ data have not been validated.
- Comparison is made with the highest amount of HNO₃ 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 averages 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$90 km).
– Mesospheric data have been validated by Pickett et al., JGR, 2008.
– Data are averaged at 65–75$^\circ$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

**OH at 66 km**

- MLS
- SIC with SPE
- SIC without SPE

**Difference: SIC − MLS**

- Night
- Daytime
SIC vs. MLS: OH

Case I: January 18, 12:10 LT
Latitudes 69N − 70N
Longitudes 49W − 27E

Case I: January 18, 21:20 LT
Latitudes 71N − 72N
Longitudes 35W − 41E

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:
  – $\text{HO}_x$ and $\text{NO}_x$ production is included,
  – $\text{HNO}_3$ and $\text{HNO}_2$ production is not included,
  – Chlorine activation is not included

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