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Changes in HO_x and NO_y Species During Solar Proton Events: Analysis and Parameterization

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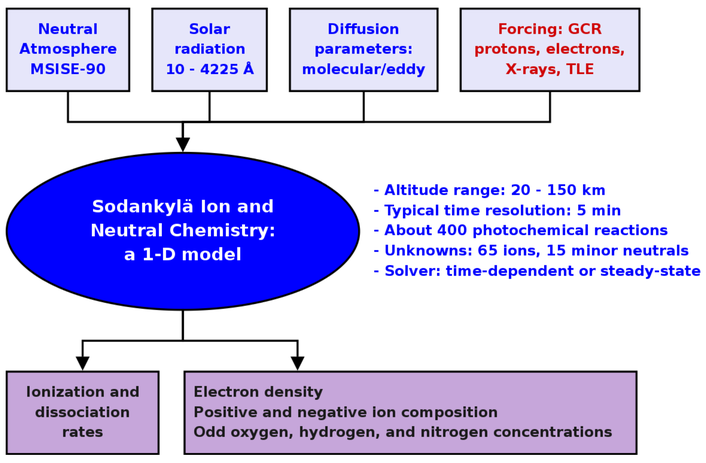
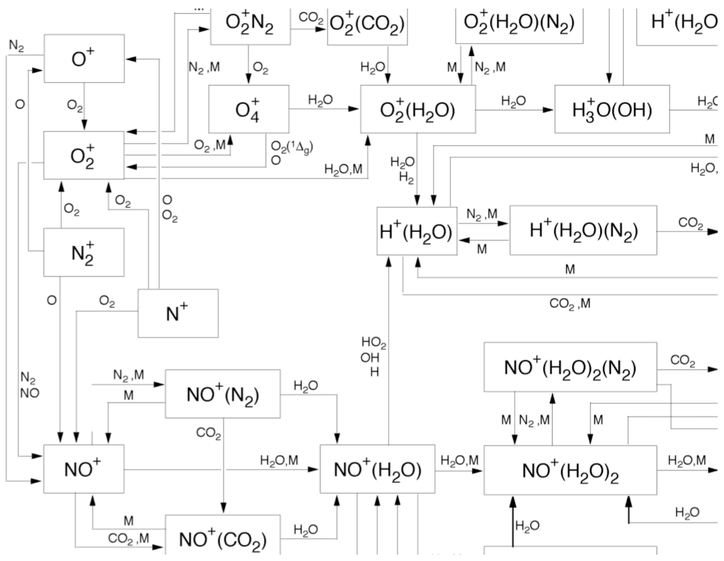
Abstract. In the middle atmosphere, enhanced ionization by precipitating particles leads to changes in minor neutral composition through ion chemistry. For example, nitrogen and water vapor molecules are dissociated, and odd hydrogen (HO_x = H + OH + HO_2) and odd nitrogen (NO_x = N + NO + NO_2) species are produced. Increase in HO_x and NO_x concentrations can then boost the catalytic reaction cycles that destroy ozone.
In this paper, we utilize the Sodankylä Ion and Neutral chemistry model (SIC), which combines ion and neutral chemistry for particle precipitation studies. Based on an analysis of the SIC chemistry, we demonstrate how positive ion chemistry produces NO_x and HO_x, while negative ion chemistry redistributes NO_y species by converting NO_x and N_2O_5 to HNO_3 and NO_3). Recent SIC results on OH and HNO_3 during solar proton events are presented, including comparisons with satellite instruments. We put forward an improved parameterization, which takes into account both positive and negative ion chemistry and can be used to model the effects of particle precipitation.

THE SIC MODEL



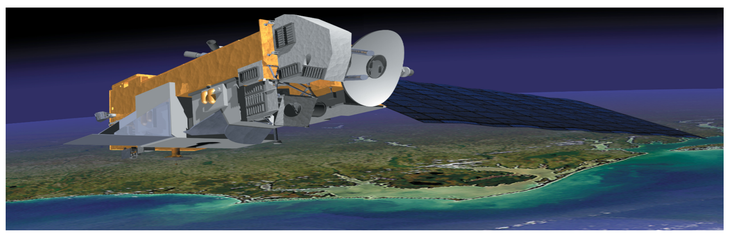
Above: SIC model input/output diagram. **Below:** part of the SIC positive ion scheme, and two examples of reaction pathways leading to H, OH, and HNO_3 production.



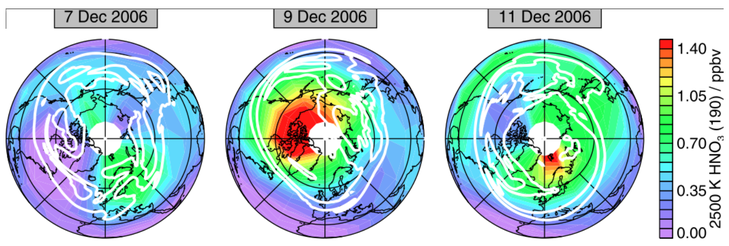
$$N_2 + p^+(E) \rightarrow N_2^+ + e^- + p^+(E - \Delta E)$$
$$N_2^+ + O_2 \rightarrow O_2^+ + N_2$$
$$O_2^+ + O_2 + M \rightarrow O_4^+ + M$$
$$O_4^+ + H_2O \rightarrow O_2^+(H_2O) + O_2$$
$$\dots$$
$$O_2^+(H_2O)_2 + H_2O \rightarrow H_3O^+(OH)H_2O + O_2$$
$$H_3O^+(OH)H_2O + H_2O \rightarrow H^+(H_2O)_3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

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

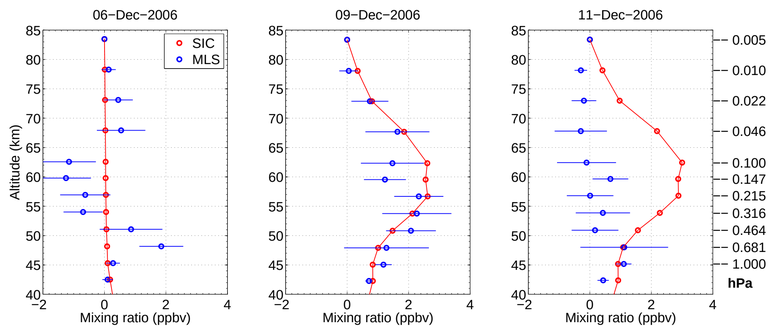
MODEL-SATELLITE COMPARISON



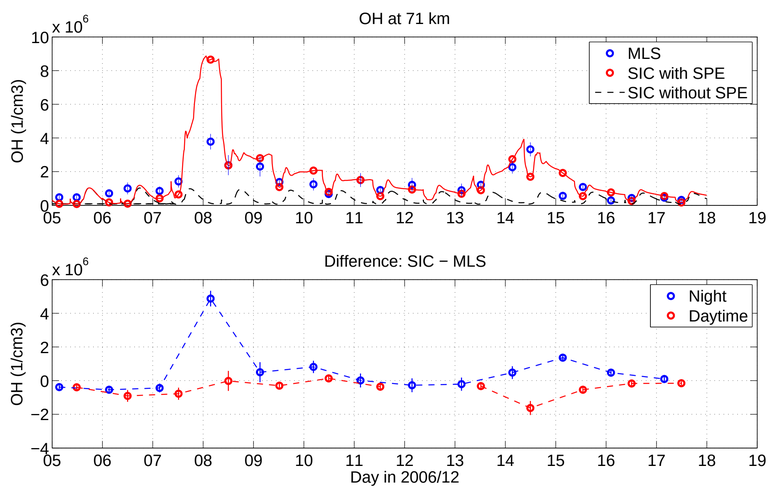
Above: Aura satellite on orbit with Microwave Limb Sounder (MLS) on board. **Below:** NH polar HNO_3 from MLS. Note the increase during the solar proton event (middle panel).

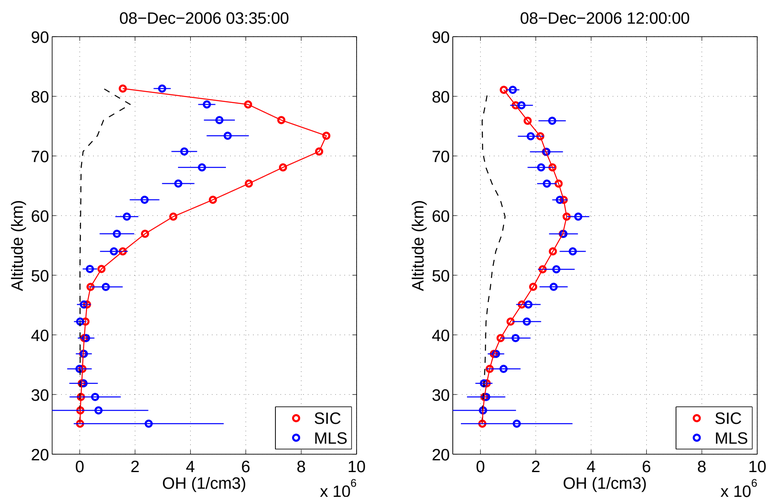


Below: SIC-MLS comparison of HNO_3 at 80°N/75°W.



Below: SIC-MLS comparison of OH in December 2006. Note the good agreement in daytime. SIC overestimates OH at nighttime on Days 8 and 15.

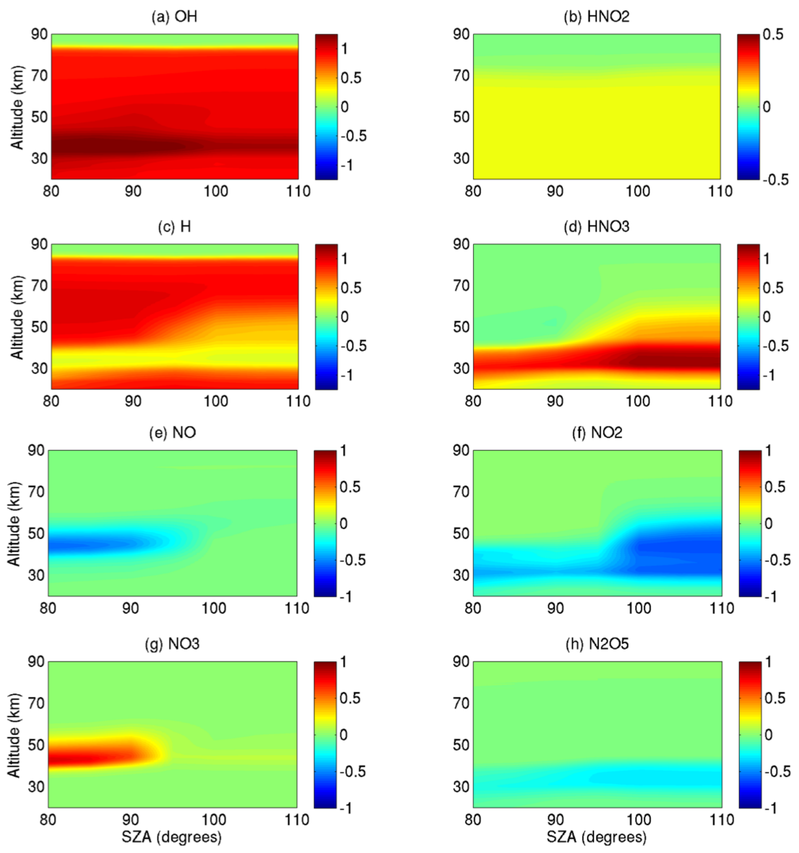




ION CHEMISTRY PARAMETERIZATION

$$P/Q = \frac{(P_{spe} - L_{spe}) - (P_{ref} - L_{ref})}{Q}$$

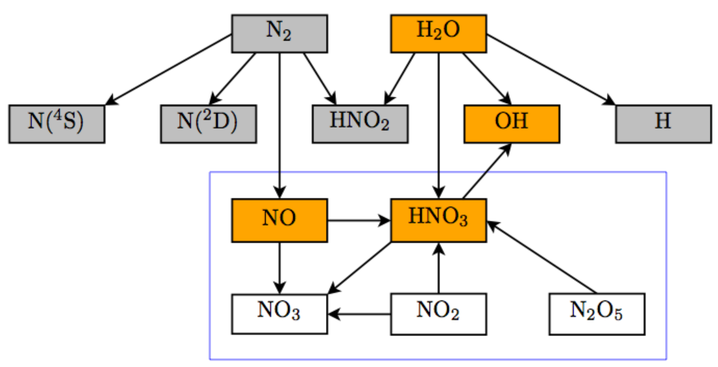
Above: The production rates of, e.g., OH and HNO_3 can be calculated from SIC model results considering production (P) and loss (L) processes. **Below:** Examples of P/Q number, NH, January, Q = 100 $cm^{-3}s^{-1}$.



Below: Example of P/Q tables, numbers given with respect to altitude, ionization rate, solar zenith angle, and season of year.

Q	10^1	10^2	10^3	10^4	10^5	10^1	10^2	10^3	10^4	10^5	10^1	10^2	10^3	10^4	10^5
km		SZA	≤	90°			SZA	=	95°			SZA	≥	100°	
90	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00	−0.00
85	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00
80	+0.00	+0.00	+0.00	+0.00	−0.01	+0.00	+0.00	+0.00	+0.00	−0.01	+0.00	+0.01	+0.01	−0.00	−0.01
75	−0.00	−0.00	−0.00	−0.00	−0.01	−0.00	−0.00	−0.00	−0.00	−0.01	+0.00	+0.01	+0.01	+0.01	−0.00
70	−0.00	−0.00	−0.00	−0.00	−0.01	+0.00	+0.00	+0.00	−0.00	−0.01	+0.03	+0.02	+0.04	+0.04	+0.02
65	−0.00	−0.00	−0.00	−0.00	−0.00	+0.02	+0.01	+0.01	+0.02	+0.01	+0.16	+0.10	+0.12	+0.12	+0.05
60	−0.01	−0.00	−0.01	+0.00	+0.03	+0.08	+0.04	+0.04	+0.08	+0.07	+0.38	+0.23	+0.20	+0.23	+0.15
55	−0.02	−0.01	−0.01	+0.02	+0.10	+0.20	+0.14	+0.10	+0.15	+0.17	+0.54	+0.38	+0.27	+0.32	+0.29
50	−0.06	−0.02	−0.00	+0.05	+0.19	+0.35	+0.28	+0.19	+0.21	+0.27	+0.57	+0.49	+0.34	+0.35	+0.42
45	−0.12	−0.04	+0.03	+0.12	+0.28	+0.50	+0.40	+0.29	+0.27	+0.35	+0.65	+0.52	+0.40	+0.38	+0.48
40	+0.27	+0.23	+0.19	+0.22	+0.34	+0.55	+0.49	+0.37	+0.32	+0.40	+0.66	+0.59	+0.46	+0.40	+0.50
35	+0.42	+0.39	+0.34	+0.29	+0.35	+0.52	+0.49	+0.43	+0.37	+0.41	+0.67	+0.64	+0.56	+0.49	+0.54
30	+0.41	+0.38	+0.34	+0.30	+0.32	+0.53	+0.50	+0.44	+0.37	+0.39	+0.71	+0.68	+0.60	+0.50	+0.49
25	+0.36	+0.34	+0.28	+0.23	+0.24	+0.49	+0.47	+0.38	+0.29	+0.29	+0.70	+0.65	+0.54	+0.37	+0.35
20	+0.34	+0.31	+0.22	+0.16	+0.15	+0.43	+0.38	+0.27	+0.17	+0.16	+0.59	+0.50	+0.33	+0.17	+0.16

Below: A diagram of hydrogen and nitrogen conversions due to ionic reactions. The species in the gray boxes are affected by positive ion chemistry, while NO_y redistribution by negative ion chemistry affects the species inside the blue box. NO, HNO_3, and H_2O are directly affected by both positive and negative ion chemistry. Note that all-neutral reactions, e.g. production of NO from $N(^2D)$, are not included in the diagram.



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- P.T. Verronen et al., Production of Odd Hydrogen in the Mesosphere During the January 2005 Solar Proton Event, *Geophys. Res. Lett.*, *33*, L24811, doi:10.1029/2006GL028115, 2006.