## Space weather impact in the D-region ionosophere: observations and modelling

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## CHAMOS (http://chamos.fmi.fi)



# $$\begin{split} \mathrm{NO}_{\mathrm{x}} &= \mathrm{N} + \mathrm{NO} + \mathrm{NO}_{2} \\ \mathrm{HO}_{\mathrm{x}} &= \mathrm{H} + \mathrm{OH} + \mathrm{HO}_{2} \\ \mathrm{O}_{\mathrm{x}} &= \mathrm{O}_{3} + \mathrm{O} \end{split}$$

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#### WACCM-D model video



#### Ionisation sources



## CMIP with (and without) the medium energy electrons (E=30...1000 keV)



From: Andersson et al., JGR (Atmos.), http://doi.org/10.1002/2017JD027605, 2018

#### APEEP precipitation model, van de Kamp et al., 2016



#### Tyssøy et al., 2021: HEPPA III intercomparison experiment on electron precipitation impacts



Figure 4. Latitude corrected hemispheric mean poleward of 45°S for the eight ionization rate estimates. The legends list the detector(s), upper energy limit, background atmosphere and ionization rate method applied.

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#### EISCAT data available for 15th April 2010 (doy 105)!



#### <sup>1</sup>https://doi.org/10.1029/2021JA029128

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## EPP inversion: $\phi(E) \rightarrow Q(h) \rightarrow N_{\rm e}(h)$

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- Calculate  $Q(h) = \int A(h, E)\phi(E)dE$
- Matrix A(h, E) contains the atmospheric response<sup>1</sup>

$$Q(h) \to \mathrm{SIC} \to N_{\mathrm{e}}(h)$$

- Pre-calculate  $N_e$  at a sufficiently fine grid of Q and interpolate  $Q 
  ightarrow N_e$
- Inversion
  - Proposal  $\phi(E)$  is an arbitrary piece-wise log-log (here: 7 nodes)
  - Minimise in MCMC chain (N=100 000):  $\chi^2 = \sum_h ((\log(N_e(h)) - \log(N_{e:data}(h)))/W)^2$

<sup>1</sup>Fang, X., C. E. Randall, D. Lummerzheim, W. Wang, G. Lu, S. C. Solomon, and R. A. Frahm (2010), Parameterization of monoenergetic electron impact ionization, Geophys. Res. Lett., 37, L22106, doi:10.1029/2010GL045406.

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#### EPP: energy vs. ionisation



<sup>1</sup>Fang et al., Parameterization of monoenergetic electron impact, GRL, 2010

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#### Ionisation impact on electron density (SIC model)



#### Inversion analysis of EISCAT VHF, 15 April 2010



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#### Comparison: EISCAT vs. APEEP



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- APEEP seems to be in the right ballpark with the EISCAT data
- Slight overestimation at the relativistic fluxes is likely due to "stiffness" of the spectral shape
- This case study does not seem to provide an easy solution for the NOx dilemma, i.e., there's *no drastic underestimation* of the ionisation.
- All EISCAT D-region data available for similar comparisons to validate & improve the model.

### Part 2/3: Modelling of consequences of ionisation



### $\text{lonisation} \rightarrow \text{plasma}$



Chemical reactions introduce a set of differential continuity equations: The most simple: just 1 positive ion type  $N_{ip}$ :

$$\frac{dN_e}{dt} = Q - k_1 N_e N_{ip} = Q - k_1 N_e^2 \tag{1}$$

For one type of positive  $N_{ip}$  and one type of negative  $N_{in}$  ions:

$$\frac{dN_e}{dt} = Q - k_1 N_e N_{ip} - k_2 N_e + k_3 N_{in} \tag{2}$$

And so forth ...

### Sodankylä lon (and neutral) Chemistry model (SIC)

Detailed 1-D time dependent chemistry model

- 63 ions (27 negative) & 13 neutrals
- 20-150 km in 1 km resolution
- several hundred reactions (370+)
- vertical transport

Input

- MSIS
- solar EM flux
- proton and electron precipitation
- cosmic rays



#### SIC species

	POSITIVE IONS	NE	GATIVE IONS	N	EUTRALS
1	O <sup>+</sup>	1	0-	1	N <sub>2</sub>
2	$O_{2}^{+}$	2	02	2	$O_2$
3	$O_4^+$	3	03	3	0
4	N <sup>‡</sup>	4	04	4	Ar
5	$N_2^+$	5	OH-	5	He
6	NÕ <sup>+</sup>	6	CO <sub>3</sub>	6	NO
7	$NO^+(N_2)$	7	$CO_4^{-}$	7	$O_2(^{1}D_g)$
8	$NO^+(CO_2)$	8	NO <sub>2</sub>	8	H <sub>2</sub> O
9	$NO^{+}(H_2O)$	9	NO3	9	N
10	$NO^+(H_2O)_2$	10	NO <sup>*</sup>	10	н
11	$NO^+(H_2O)_3$	11	HCO <sub>3</sub>	11	$CO_2$
12	$NO^{+}(H_2O)(N_2)$	12	$O_{2}^{-}(H_{2}O)$	12	$O_3$
13	$NO^+(H_2O)(CO_2)$	13	CĨ-	13	OH
14	$NO^{+}(H_2O)_2(N_2)$	14	$OH^{-}(H_2O)$	14	$NO_2$
15	$NO^{+}(H_2O)_2(CO_2)$	15	$O_{3}^{-}(H_{2}O)$	15	$HO_2$
16	$O_{2}^{+}(H_{2}O)$	16	$NO_3^-(H_2O)$	16	NO <sub>3</sub>
17	$H_{3}O^{+}(OH)$	17	$CO_3^{-}(H_2O)$	17	$HNO_2$
18	$H^{+}(H_{2}O)$	18	$Cl^{-}(H_2O)$	18	$CO_3$
19	$H^{+}(H_{2}O)_{2}$	19	C10 -	19	M
20	$H^{+}(H_{2}O)_{3}$			20	$H_2$
21	$H^{+}(H_{2}O)_{4}$			21	HCl
22	$H^{+}(H_{2}O)_{5}$			22	HNO <sub>3</sub>
23	$H^{+}(H_{2}O)_{6}$			23	CI
24	$H^+(H_2O)_7$ $H^+(H_2O)_7$			24	CIO
25	$O^{+}N$			25	CH4
20	$U_2 N_2$ $H^+(H_2 O)_2(CO_2)$			20	$O(^{1}D)$
28	$H^{+}(H_{2}O)_{2}(CO_{2})$			28	NoO
20	$H^{+}(H_{0}O)CO_{0}$			20	$N(^{2}D)$
30	$H^{+}(H_{2}O)N_{2}$			30	H <sub>2</sub> O <sub>2</sub>
31	$O^+_{0}CO_2$			31	cõ
32	$O_{2}^{+}(H_{2}O)N_{2}$			32	$CH_2O$
33	$O_2^+(H_2O)CO_2$				
34	$O_2^{\tilde{+}}(H_2O)_2$				
35	$H_3O^+(OH)H_2O$				
36	$H_3O^+(OH)CO_2$				

#### Positive ion chemistry scheme



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#### Negative ion chemistry scheme



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#### Solving an arbitrary chemistry scheme

$$\frac{\partial \bar{N}}{\partial t} = \mathbf{B}\bar{N} + \bar{Q} = \begin{pmatrix} -\Lambda_1 & +\Pi_{12} & \dots & +\Pi_{1n} \\ +\Pi_{21} & -\Lambda_2 & & \\ \vdots & & \ddots & \\ & \vdots & & \\ +\Pi_{n1} & & & -\Lambda_n \end{pmatrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ \vdots \\ n_n \end{pmatrix} + \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ \vdots \\ q_n \end{pmatrix}.$$
(4.9)

<sup>1</sup>Courtesy of Verronen, 2006

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- $\bullet$  EPP produces  $O_2^+$  (also:  $N_2^+ + O_2 \rightarrow O_2^+ + N_2$  )
- $\bullet~{\rm NO}_x$  is produced e.g., via:  ${\rm O}_2^+ + {\rm N}_2 \rightarrow {\rm NO}^+ + {\rm NO}$
- $HO_x$ :  $O_2^+$  turns into water clusters  $O_2^+(H_2O)$
- $\bullet$  Recombination with electrons turn  $\mathrm{O}_2^+(\mathrm{H_2O})$  into  $\mathrm{OH}$
- $\bullet$  Recombination with negative ions turn  $O_2^+(H_2O)$  into  $\rm HNO_3,$  which is photodissociated into OH

#### The end of part 2/3: Sensitivity to ionisation (30 minutes)



## Part 3/3: Radio wave methods for observing the ionisation (=electron density)?



Incoherent scatter radars: paradigm change

### **Current EISCAT**

### EISCAT\_3D



UHF-radar at Tromsø, Norway

EISCAT\_3D transmitter site Skibotn, Norway

#### EISCAT\_3D geography



#### EISCAT\_3D concept



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#### HPC-approach needed!

#### Data available:

- "cp6" from 1990-06-13 to 1998-09-24, 76 experiments, ~52 full days (full day = 24h)
- "arcd" —from 2003-05-29, 183 experiments, ~110 full days
- "manda" from 2005-04-14, more than 411 experiments, ~202 full days

Total duration of data available = 364 full days

#### Full computational cost

- MCMC run time for each altitude = ~3.5 sec
- No of altitude steps = 250
- > Computational time for each 5 min average profile = 3.5 x 250 = 875 sec (~ 15 min)
- > 5 min-integrated profiles in 24 hr = 288

#### Estimated computational time :

364 full days x 288 5-min-integrated profiles x 15 minutes per one profile = 1572480 minutes = ~ **3 years of** computational time!).

- Level 0: raw voltage samples
- Level 1: lag-profiles
- Level 2: plasma parameters (density, temperature, composition)
- Level 3: particle precipitation, conductivities, currents ...

### Step 1: Lag-profiles to plasma parameters (level 1 to 2)



Figure: Fingerpori, HS, 7 September 2012

The spectral density of the incoherent scattering is

$$\sigma(\omega_{0}+\omega)d\omega = \frac{N_{e}r_{e}^{2}d\omega}{\pi} \frac{\left(|y_{e}|^{2}\frac{\sum_{j}n_{j}\Re(y_{j})}{\omega-\mathbf{k}\cdot\mathbf{v}_{dj}}\left|\sum_{j}\mu_{j}y_{j}+i\lambda_{D}^{2}k^{2}\right|^{2}\frac{\Re(y_{e})}{\omega-\mathbf{k}\cdot\mathbf{v}_{de}}\right)}{\left(\left|y_{e}+\sum_{j}\mu_{j}y_{j}+i\lambda_{D}^{2}k^{2}\right|^{2}\right)}.$$

Here

n<sub>j</sub> = N<sub>j</sub>/N<sub>e</sub> and μ<sub>j</sub> = n<sub>j</sub>T<sub>e</sub>/T<sub>j</sub> (densities and temperatures),
λ<sub>D</sub> = (ε<sub>0</sub>k<sub>B</sub>T<sub>e</sub>/N<sub>e</sub>e<sup>2</sup>)<sup>1/2</sup> (Debye length)
k = 2π/λ (wave number).

What is needed for calculating the IS spectrum?

- Radio wave parameters:  $\omega$ ,  ${\bf k}$
- Plasma composition, temperatures, ion masses, coll. frequencies and drift velocities: N<sub>j</sub>, T<sub>j</sub>, m<sub>j</sub>, ν<sub>j</sub> and v<sub>j</sub>
- Magnetic field B

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#### Input profiles (based on the SIC model)



#### Incoherent scatter ion line: 90 and 130 km



#### Plasma parameter fit to the ACFs measured



#### Step 2: Energetic particle precipitation inversion



#### Electron precipitation driven ionisation: height vs. altitude



<sup>1</sup>Fang et al., Parameterization of monoenergetic electron impact, GRL, 2010

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- A non-linear problem
- Easy to construct the  $\chi^2$  error function (e.g., in log-scale)
- Easy to limit the solution (e.g., only positive fluxes are allowed)
- Kick-ass MCMC toolbox available<sup>1</sup>

<sup>1</sup>Search: 'Marko Laine + MCMC'  $\rightarrow$  http://helios.fmi.fi/~lainema/mcmc/

#### Example case: 28–29 March 2017



<sup>1</sup>Miyoshi et al. (2021), Penetration of MeV electrons into the mesosphere accompanying pulsating aurorae, Scientific Reports (Springer-Nature). https://doi.org/10.1038/s41598-021-92611-3

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- Inversion of the precipitation characteristics  $(\phi, Q, N_e)$  from the incoherent scatter radar data
- Full time-dependent ion chemistry of the SIC model is used in the forward model  $\rightarrow$  chemical consequences
- Results provide means to constrain better the particle forcing input to the climate models (such as WACCM-D)