Chemistry of the D-region, VLF propagation and HF modelling

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Abstract

High Frequency (HF, 3 - 30 MHz) waves are used for long-distance communications. These waves are partially absorbed when they reach the ionosphere, causing communication losses. A large part of this absorption is driven by the electron density in the D-region, the lowest part of the ionosphere (60 - 90 km, [Zawdie et al., 2017]). This density is impacted by different sources, and in particular solar flares, which are fast increases in the Sun's energetic radiation. Thus, it is crucial to understand the D-region response to forcing to mitigate any communication loss.

At those altitudes, the combination of different ionisation sources and the variety of neutral species present renders the chemistry complex. Chemistry schemes are necessary to understand the interactions between the species created there. The Mitra-Rowe scheme [Mitra & Rowe, 1972] includes the six dominant ion species. It reproduces the main processes in the D-region well, with limited computational cost and without requiring detailed measurements of minor species.
With this model, we reproduce the ionisation of the neutral species by external sources (cosmic-rays, solar Lyman-alpha, EUV, UV, and soft and hard X-ray radiation) to study both quiet periods and perturbed conditions.

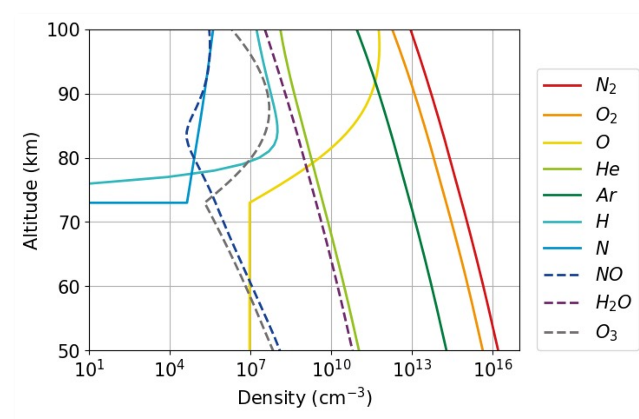
Ionosphere initialisation

Initialisation of the neutrals

Initialisation through MSISE-00 model [Picone et al., 2002]
- $N_2, O_2, O, He, Ar, H, N$

+

- $[O]$ at lower altitudes [Brasseur & Solomon, 2005, p282]
- $[NO]$ [Mitra, 1966]
- $[O_2(^1\Delta_g)]$ (constant at 10^{10} cm^{-3}) [Crutzen et al.,1970; Reid, 1970]
- $[H_2O]$ [Reid, 1971]
- $[O_3]$ [Levine, 1985, p176]



Initialisation of the ionisation sources and computation of ionisation rate

Four sources of ionisation in the D-region:
- Cosmic rays (< 65 km) (e.g. [Lehtinen et al., 2007])
- Ionisation of NO by Lyman-α
- Ionisation of $O_2(^1\Delta_g)$ by EUV/UV [Paulsen et al., 1972]
- Ionisation of O, N, O_2 and N_2 by X-rays (SXR and HXR)

Two major challenges

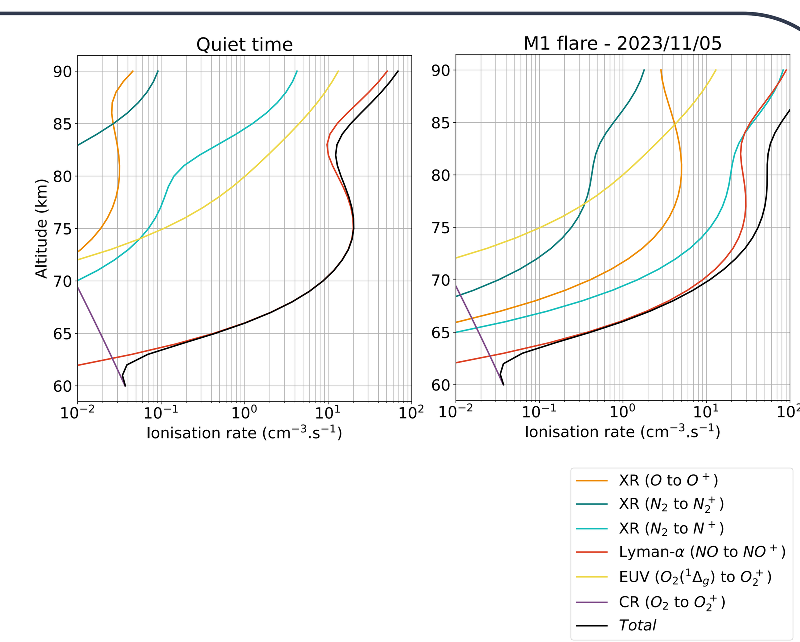
① The X-ray flux is absorbed at high altitude

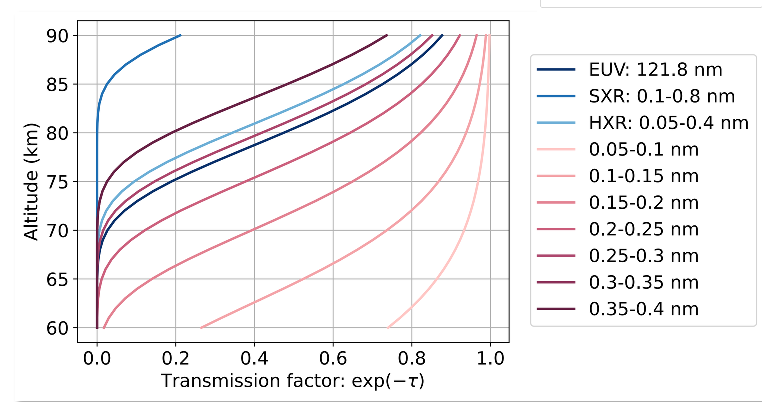
$$\Rightarrow F(z,\lambda) = F(\infty,\lambda)\exp(-\tau(\lambda))$$

1. The soft X-ray fluxes are absorbed before reaching the D-region.
2. GOES hard X-ray flux should be binned. Otherwise, we miss ionisation at lower altitude.

② [NO] is not well-known, but it is ionised by Lyman-α:

$$Q = \sigma^i_{NO}[NO]F(\lambda,z)$$

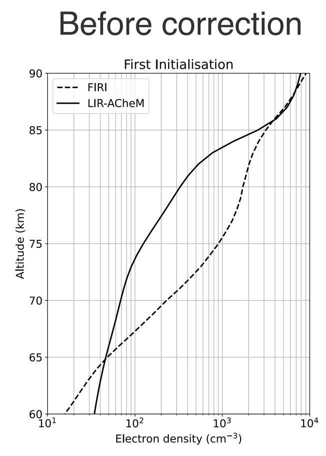




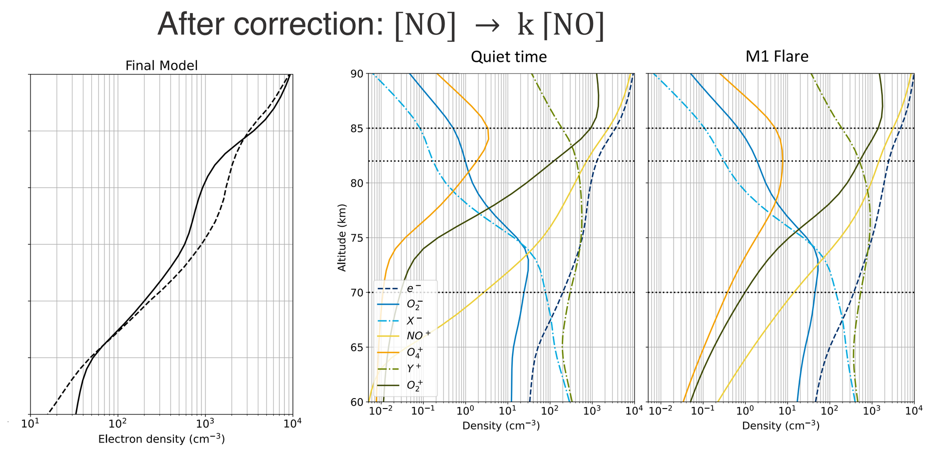
Initialisation of ions and electrons

The ions and electron density are initialised twice from the ionisation sources on the neutral atmosphere and the Mitra-Rowe scheme.
The second initialisation is done after applying a correcting factor to [NO] (see ②) to match FIRI [Friedrich et al., 2018] electron density values at 75 km

Before correction

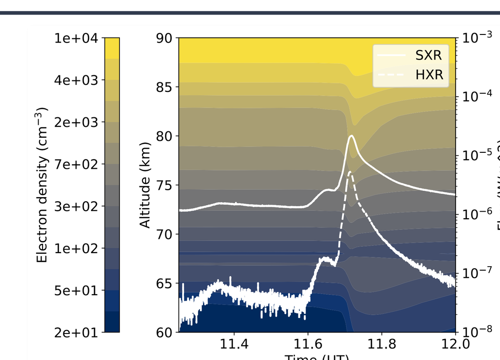


After correction: [NO] → k [NO]



Forcing and D-region response

During solar flares, the SXR and HXR fluxes increase, thus enhancing the production of ions and electrons. This can be modelled using the Mitra-Rowe scheme, recomputing the absorbed fluxes and corresponding ionisation rates at each step



Example: M1 flare on 2023/11/05

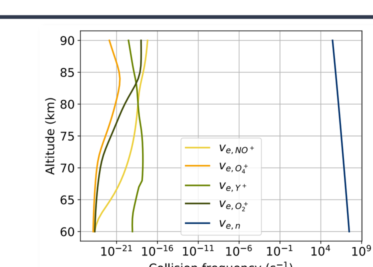
HF absorption

Collision frequencies

Two types of collision frequencies: (e.g. [Zawdie et al., 2017])

1. Electron-ions [Schunk & Nagy, 1978]
2. Electron-neutrals [Schunk & Nagy, 2009]

Electron-neutrals collisions are dominant in the D-region



Refractive index

Appleton-Hartree formula: [Appleton, 1932]

$$n^2 = 1 - 2X\frac{1 - iZ - X}{2(1 - iZ)(1 - iZ - X) - Y^2\sin^2\theta \pm \sqrt{Y^4\sin^4\theta + 4Y^2\cos^2\theta(1 - iZ - X)^2}} = \mu + i\chi$$

with:
X, Y, Z representing the electron density, magnetic field and collisions contributions
θ the angle between the wavevector and the magnetic field

The absorption in the D-region is *non-deviative:* $\mu \approx 1$ and $N_e\nu$ is large [Davies, 1990]

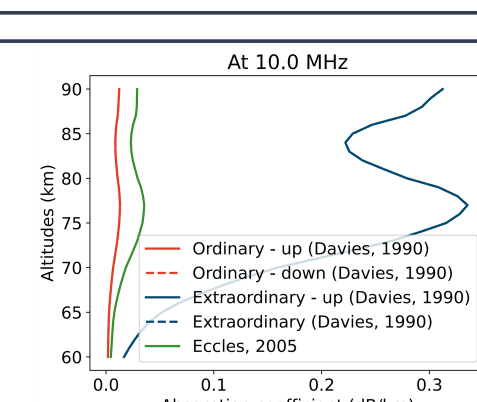
Absorption coefficient

Absorption coefficient: [Davies, 1990]

$$\kappa = 4.6\times10^{-2}\frac{1}{\mu}\frac{N_e\nu}{(\omega^2+\omega_H^2)^2+\nu^2}\ \text{(dB/m)}$$

with ω_H the cyclotron frequency.

Alternative formulations involve setting $\mu = 1$ and ignoring magnetic field (e.g. [Eccles et al., 2005])



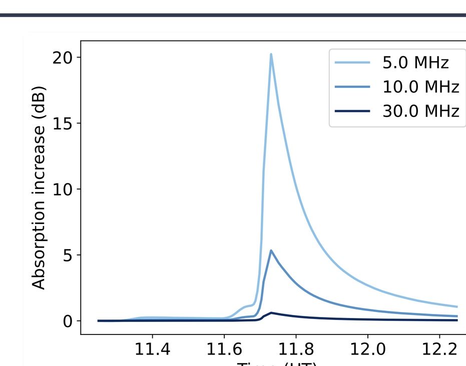
Total absorption coefficient

Total absorption coefficient: [Davies, 1990]

$$L_\alpha = -8.68\int \kappa\, ds$$

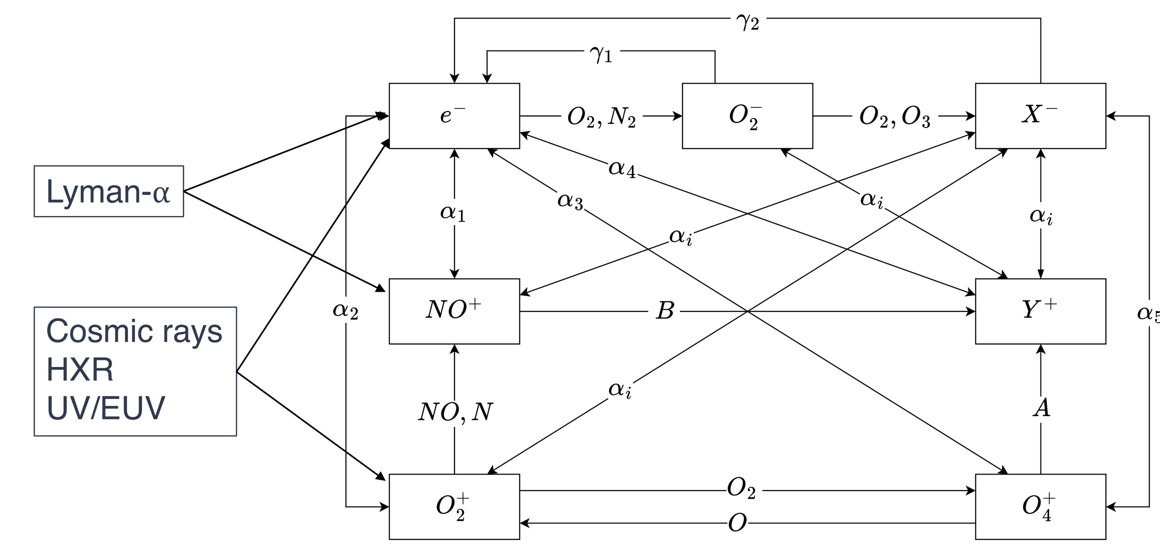
Note: So far, we have considered vertical HF waves, reflected when $f = \omega_p$ with a reflection coefficient equal to 1

This remains to be validated, so any advice is very welcome !



Chemistry scheme

[Mitra & Rowe, 1972; Rowe et al;, 1974; Mitra, 1975]



Main advantages:
- Reproduces well the density variations in the D-region
- Is computationally fast, while conserving individual ion species
- Can be upgraded/downgraded as needed
- Every reaction rate is known

Main assumptions
- All negative ion species are lumped together in X^- (except for O_2^-)
- All heavy positive cluster ion are considered together (Y^+)
- In the D-region, $T_e = T_n$ (e.g. [Verronen et al., 2016])

Benchmarking

We have compared the ions densities we obtained with previous published data [Reid, 1979]. Here are presented the results for simple ions species (not for e^-, Y^+ and X^-).

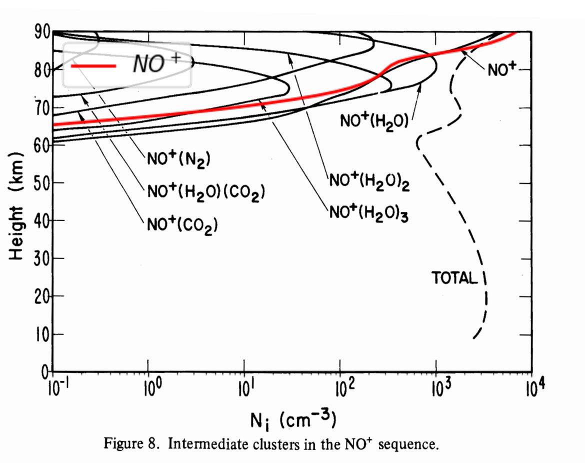


Figure 8. Intermediate clusters in the NO^+ sequence.

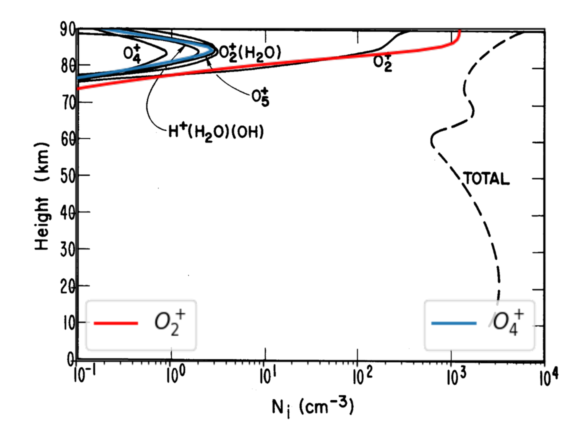


Figure 9. Intermediate clusters in the O_2^+ sequence.

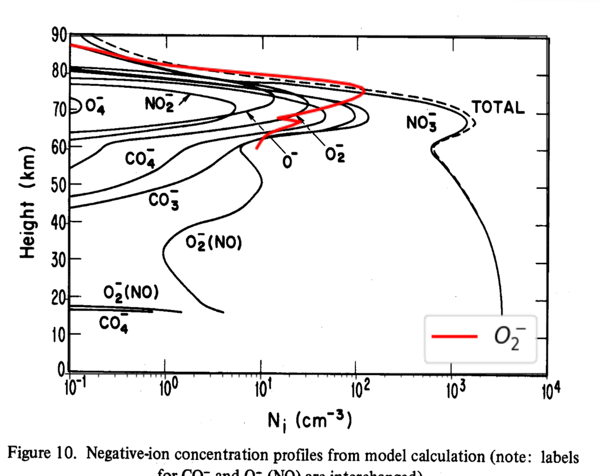


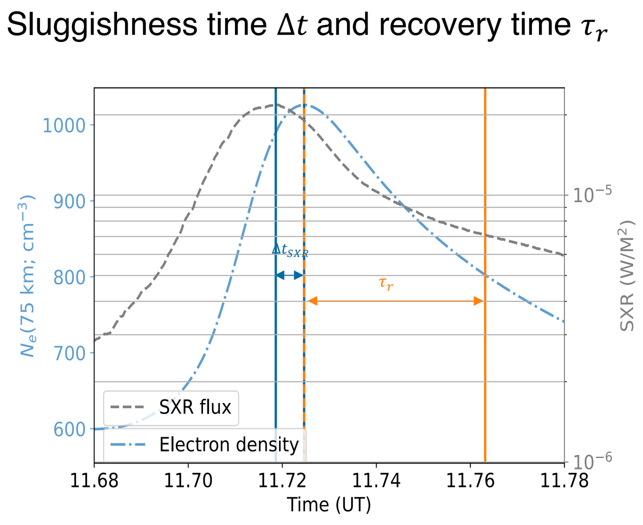
Figure 10. Negative-ion concentration profiles from model calculation (note: labels for CO_4^- and O_2^-(NO) are interchanged).

We plan to validate this work further with WACCM-D results and with comparison to ionosonde and rocket data

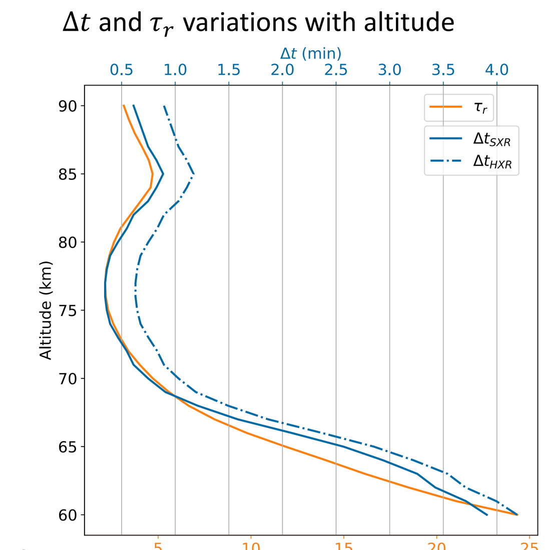
First results

Study of the response to a short M1 flare peaking at 11:43 UT on 2023/11/05.

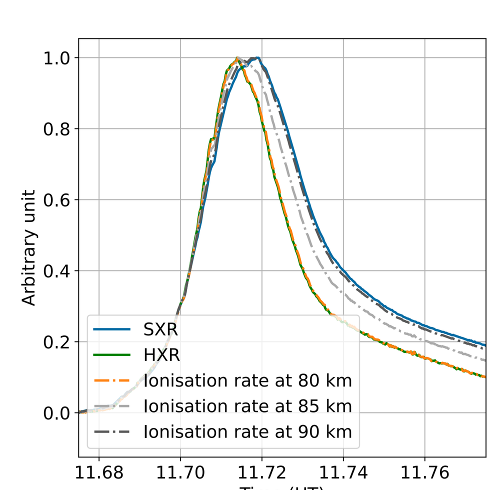
Sluggishness time Δt and recovery time τ_r



Δt and τ_r variations with altitude

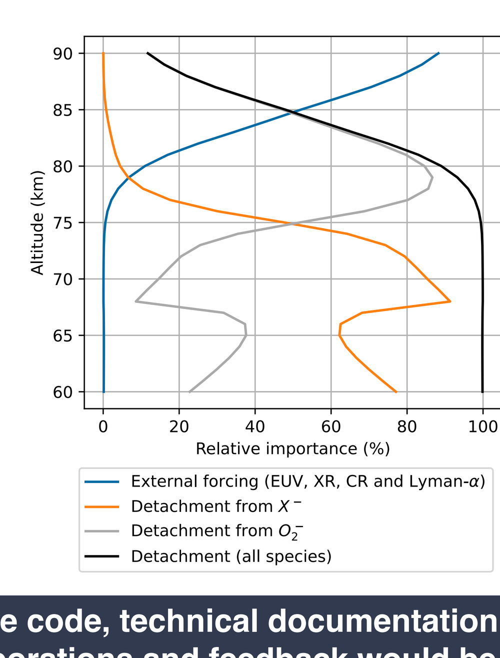


Question: Why do Δt & τ_r increase at low altitude and peak at 85 km ?



At high altitudes, the SXR is not completely absorbed. It occurs later than the HXR, and is the main source of ionisation at the top of the D-region.

At 85 km, both SXR and HXR ionise the neutrals. Thus, Δt increases since the ionisation rises with the (early) HXR flux, and decreases with the (late) SXR flux.



At low altitudes, the majority of electrons come from photodetachment from negative ions. Negative ions thus behave as a reservoir of electrons.

This reactions occurs on a timescale of about 10 min, implying that electrons are produced even after the peak of the flare. This translates as a longer apparent recovery time, and a later peak of N_e.

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Source code, technical documentation and further examples are available. Ask us!
Collaborations and feedback would be greatly appreciated!

Paper accepted for publication in *Atmosphere* (Teysseyre & Briand, 2026)

Note: I am currently looking for a postdoc