

# FYS 3003: Programming task 5

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February 16, 2023

## Ion Chemistry

A simplified way to model the dynamic variation of composition in the ionosphere is to solve the coupled continuity equations for electrons, ions ( $N_2^+$ ,  $O_2^+$ ,  $O^+$  and  $NO^+$ ) and  $NO$  ignoring the effects of transport. This turns the continuity equations into a number of coupled ordinary differential equations. The chemical loss and production reactions for this simplified ion-chemistry are described in table 4.4, on page 211 of Physics of the upper polar atmosphere, note the corrections necessary to the rearrangement reaction where  $N_2^+ + O$  should produce  $NO^+ + N$ , and not  $NO^+ + NO$  as written. Further the radiative recombination-rate  $\alpha_r$  for  $O^+$  should be  $3.7 \cdot 10^{-18} (250/T_e)^{0.7} \text{ (m}^3/\text{s)}$ .

The task is to write a program that solves these coupled ODEs for an arbitrarily time-varying ionization rate for a single altitude – that is for given initial densities of the background atmosphere. The MSIS.dat and IRI.dat files contain the temperatures and densities for the ionosphere/thermosphere necessary to set up the reaction rates and the initial state of the species you need. The fraction of molecular Nitrogen ions per ionization can be approximated by:

$$q_{N_2^+} = q_e * (0.92 * n_{N_2}) / (0.92 * n_{N_2} + n_{O_2} + 0.56 * n_O)$$

where  $q_e$  is the total ionization-rate,  $n_{N_2}$  is the molecular Nitrogen density,  $n_{O_2}$  is the molecular Oxygen density, and  $n_O$  is the atomic Oxygen density. The partitioning of the between the atomic and molecular oxygen ion-productions proceeds with the same weights for the parent-species as are in the denominator - the sum of the ion-production should equal the total production of electrons.

This ion-chemistry-solving program should be tested for two types of time-varying ionization, at altitudes of 110, 170 and 230 km:

0, integrate the continuity-equations for 3600 seconds with a constant ionization-rate of  $1 \cdot 10^8 \text{ (/m}^3/\text{s)}$  to obtain a stable background to use for the initial conditions of the different densities.

1, The response to an ionization pulse with 100 s duration should be modelled over a 600 s long time-period. The ion-electron production rate should be set to  $1 \cdot 10^{10} \text{ (m}^{-3}\text{s}^{-1}\text{)}$  for 100 s followed by absolutely no further ionization. This modelling should be done at altitudes of 110, 170 and 230 km.

2, Same as above but increase the electron and ion temperatures by 1000 K below 150 km, and by 2000 K at the altitudes above 150 km. Compare the ion-composition for the two cases.

- 3, Compare the electron-density decay at 110 and 230 km with the expected decrease-characteristics: " $\alpha$ " ( $(n_e(t_{off})/(1 + \alpha_e n_e(t_{off})))$ ) and " $\beta$ " (exponential decay). Remember to include both the dissociative recombination of  $O_2^+$  and  $NO^+$  when calculating the  $\beta$ -decay.
- 4, The response to ionization that varies as:

$$q_e(t) = \hat{q}_e \sin^2(2\pi t/20)$$

for the first 100 s followed by absolutely no further ionization for the remaining 500 s. The peak ion-electron production,  $\hat{q}_e$ , should be set to  $2 \cdot 10^{10} (m^{-3}s^{-1})$  during the first 100 s followed by absolutely no further ionization. This modelling should be done at altitude of 110, 120 170 and 230 km.

In this task it is imperative for reasonable progress that you utilize ODE-integrating functions to do the actual integration of the differential equations. When writing the programs that produces the results and figures you should also make figures that verifies that the relevant particle and charge time-variations of various species, and make plots of the different loss and source-terms, i.e. the rates of the different reactions. It is also neat if you check that the conservation of charge are satisfied and not only producing plots of the time-variation of the different species for the two ionization-cases.