

Programming Task 3

Photo-ionization

TRYM VARLAND

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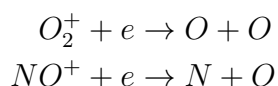
Theory

Ionospheric chemistry

A lot of chemical reactions need to take place in the upper atmosphere to maintain the ionosphere, this means that we need a balance between production of free electrons and their removal. That would say when the ionization is being formed it will immediately be involved in chemical reactions to maintain the equilibrium condition before the ionization took place.

Recombination

One of the most impotent processes in the D, E and F-region is dissociative recombination. A process where electrons attach to a positively charged molecular ions, this forms energetic and unstable neutral molecules. Here the molecules decompose spontaneously, converting internal to kinetic energy. Maybe the most important recombination is of O_2^+ and NO^+ (seen in the bottom), which makes us distinguish objects on a dark and moonless nights on earth.



Rearrangement

Rearrangement is that ions and molecular ions, is rearranging them self with another ion or molecular ion. This rearrangement can give a new product, or we can just have charge rearrangement. This comes clear by looking at the following reactions, from table 1.



Table

Figure 1: Table 4.4. Typical reactions rates relevant for ionospheric processes

<i>Processes</i>	<i>Reaction rates (m³/s)</i>
Dissociative recombination $\text{NO}^+ + e \rightarrow \text{N} + \text{O}$ $\text{O}_2^+ + e \rightarrow \text{O} + \text{O}$ $\text{N}_2^+ + e \rightarrow \text{N} + \text{N}$	$\alpha_1 = 2.1 \times 10^{-13} (T_e/300)^{-0.85}$ $\alpha_2 = 1.9 \times 10^{-13} (T_e/300)^{-0.5}$ $\alpha_3 = 1.8 \times 10^{-13} (T_e/300)^{-0.39}$
Rearrangement $\text{O}^+ + \text{N}_2 \rightarrow \text{NO}^+ + \text{N}$ $\text{O}^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{O}$ $\text{O}_2^+ + \text{NO} \rightarrow \text{NO}^+ + \text{O}_2$ $\text{O}_2^+ + \text{N}_2 \rightarrow \text{NO}^+ + \text{NO}$ $\text{N}_2^+ + \text{O} \rightarrow \text{NO}^+ + \text{NO}$ $\text{N}_2^+ + \text{O}_2 \rightarrow \text{N}_2 + \text{O}_2^+$	$k_1 = 2 \times 10^{-18}$ $k_2 = 2 \times 10^{-17} (T_r/300)^{-0.4}$ $k_3 = 4.4 \times 10^{-16}$ $k_4 = 5 \times 10^{-22}$ $k_5 = 1.4 \times 10^{-16} (T_r/300)^{-0.44}$ $k_6 = 5 \times 10^{-17} (T_r/300)^{-0.8}$
Radiative recombination $\text{O}^+ + e \rightarrow \text{O} + h\nu$	$\alpha_r = 7.8 \times 10^{-14} (T_e/300)^{-0.5}$

Table source: Physics of the upper polar atmosphere, Asgeir Brekke

Task 0: Integrate the continuity equations.

In this task we gone integrate the continuity equations for 3600s with a constant ionization-rate of $1 \cdot 10^8 (m^{-3}s^{-1})$, to obtain a stable background to use for the initial conditions of the different densities. Which we gone do for altitudes at 110, 170 and 230km. To solve the couple ODEs, we need to use the continuity equation for each ion species formed:

$$\frac{\partial n_i}{\partial t} = q_i - l_i \quad (1)$$

Where n_i is the number density of the ion species, q_i is the production (*ionization rate*) and l_i is the loss by chemical and photo-chemical processes. To calculate the production q_i , the task have given use the production of nitrogen ions which we can redefine for O_2 and O . This gives us the following:

$$\begin{aligned}
 q_{\text{N}_2^+} &= q_e \frac{0.92 \cdot n_{\text{N}_2}}{0.92 \cdot n_{\text{N}_2} + n_{\text{O}_2} + 0.56 \cdot n_{\text{O}}} \\
 q_{\text{O}_2^+} &= q_e \frac{n_{\text{O}_2}}{0.92 \cdot n_{\text{N}_2} + n_{\text{O}_2} + 0.56 \cdot n_{\text{O}}} \\
 q_{\text{O}^+} &= q_e \frac{0.56 \cdot n_{\text{O}}}{0.92 \cdot n_{\text{N}_2} + n_{\text{O}_2} + 0.56 \cdot n_{\text{O}}}
 \end{aligned}$$

Now to calculate the loss l_i for each species that we want, this is done by using table 1 and see where the different species is lost in the reaction. If we take N_2^+ as an example, we see from the table 1 that N_2^+ is lost in the reaction on row three, eighth and nine, but we would also need to add the reactions rate on the column to the left. This yields:

$$l_{N_2^+} = -\alpha_3 \cdot n_{N_2^+} \cdot n_e - k_5 \cdot n_{N_2^+} \cdot n_O - k_6 \cdot n_{N_2^+} \cdot n_{O_2}$$

For the calculations of α , T_e is the electron temperature. The calculations of k_i , we have the rearrangement temperature T_r and we see that the rearrangement processes basically takes place due to reaction between an ion and a neutral species, so we can roughly estimate T_r by taking the mean of the ion and neutral temperature.

By doing all of the steps above, we end up with the following couple ODEs:

$$\frac{\partial n_{N_2^+}}{\partial t} = q_{N_2} - \alpha_3 \cdot n_{N_2^+} \cdot n_e - k_5 \cdot n_{N_2^+} \cdot n_O - k_6 \cdot n_{N_2^+} \cdot n_{O_2} \quad (2)$$

$$\frac{\partial n_{O_2^+}}{\partial t} = q_{O_2} - \alpha_2 \cdot n_{O_2^+} \cdot n_e + k_2 \cdot n_{O_2} \cdot n_{O^+} - k_3 \cdot n_{O_2^+} \cdot n_{NO} - k_4 \cdot n_{O_2^+} \cdot n_{N_2} + k_6 \cdot n_{O_2} \cdot n_{N_2^+} \quad (3)$$

$$\frac{\partial n_{O^+}}{\partial t} = q_O - k_1 \cdot n_{O^+} \cdot n_{N_2} - k_2 \cdot n_{O^+} \cdot n_{O_2} - \alpha_r \cdot n_{O^+} \cdot n_e \quad (4)$$

$$\frac{\partial n_{NO^+}}{\partial t} = -\alpha_1 \cdot n_{NO^+} \cdot n_e + k_1 \cdot n_{O^+} \cdot n_{N_2} + k_3 \cdot n_{O_2^+} \cdot n_{NO} + k_4 \cdot n_{O_2^+} \cdot n_{N_2} + k_5 \cdot n_{N_2^+} \cdot n_O \quad (5)$$

$$\frac{\partial n_{NO}}{\partial t} = -k_3 \cdot n_{O_2^+} \cdot n_{NO} + k_4 \cdot n_{O_2^+} \cdot n_{N_2} \quad (6)$$

$$\frac{\partial n_e}{\partial t} = q_e - \alpha_1 \cdot n_{NO^+} \cdot n_e - \alpha_2 \cdot n_{O_2^+} \cdot n_e - \alpha_3 \cdot n_{N_2^+} \cdot n_e - \alpha_r \cdot n_{O^+} \cdot n_e \quad (7)$$

We can then start to implement our ODE-solver, to directly solve our coupled ODEs we gone use library called **scipy** and their package **odeint**. But before this, we define a function which contains our temperature T_e and T_r , reaction rates α_i and k_i , and the ionization rates q_i . Than we implement the couple ODEs 7, and return the ODEs at a specific altitude. Forward, we solve our method/function with the **odeint** package:

```
1 from scipy.integrate import odeint
2 solve = odeint(ODEs, ni0, t, args= (altitude,))
```

Listing 1: odeint implementation

Where **ODEs** is our method/function which contains our ODEs, **ni0** is initial conditions for our species and the last statement is a extra argument for the ODE-solver. This makes the ODE-solver take height into consideration, since we want to return the ion densities at specific heights. This gives us the following plots for the ion densities at different altitudes. Where we have density at y-axis and time on the x-axis, and we have solved the ODEs with a time-interval of 3600s.

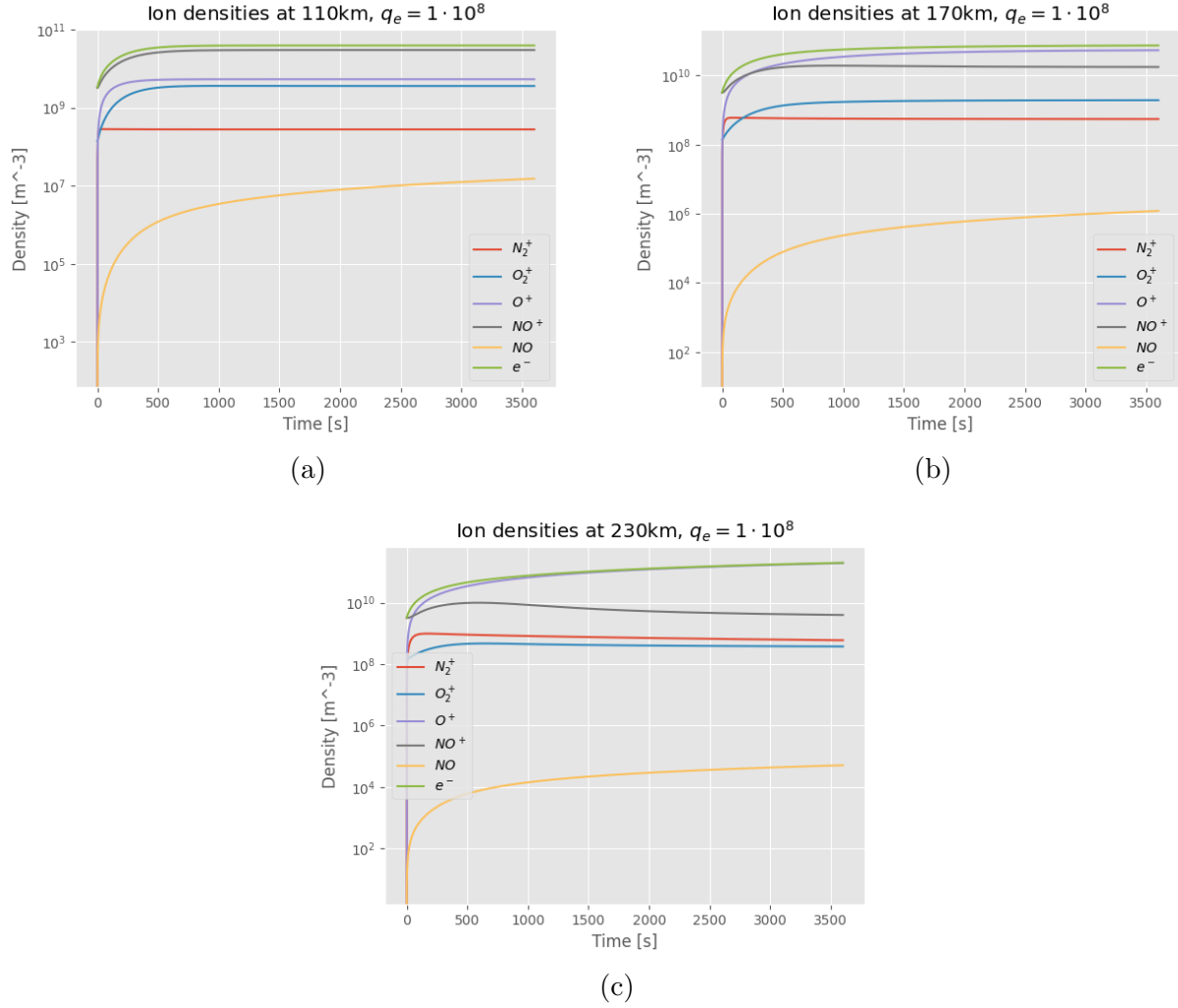


Figure 2: Ion densities at 110, 170 and 230km. In plot a) and b) the graphs look almost horizontal, because of scaling.

We see that the first plot 2a which is at the lowest altitude, is where the different species have the highest density. This makes sense since lower down in the atmosphere we have bigger ion production, further up in the atmosphere we have lower ion production. Below 150km (plot 2a) we see that O_2^+ and NO^+ is the dominant species, above 150km (plot 2b) O^+ is becoming greater and more dominant species and above 200km (plot 2c) we have that the O^+ species is completely dominating. This means that in the E-region

In figure 3, we have plotted the charge conservation, which should be approximately zero. As we can see, it is not totally to zero but pretty close. This is because, we have some rounding in our constants and variables. So we can round this, and set it to approximately zero.

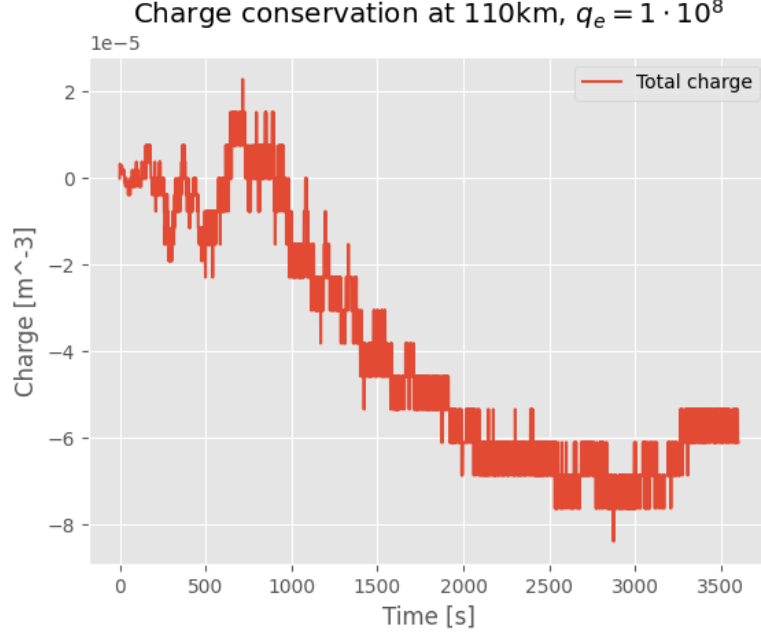


Figure 3: Plot of the charge time-variations conservation

Figure 4, shows the different reactions rates of the loss and source terms. As we can see from the plot, the reaction rates varies with time as we want.

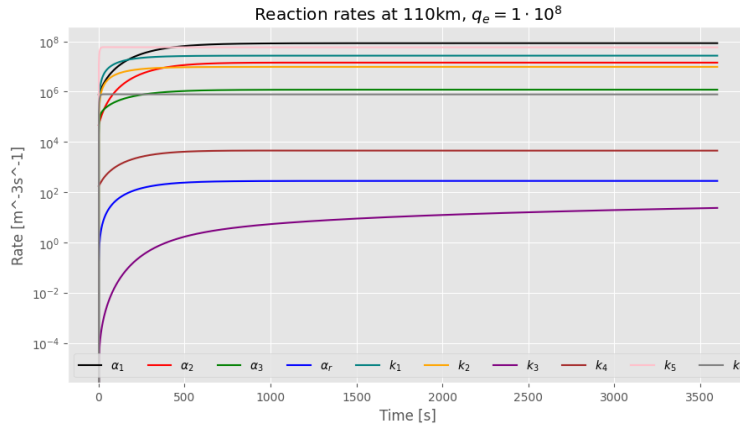


Figure 4: Rates of the different reactions.

Task 1: Ionization pulse with 100s duration over 600s, with ion-electron production rate set to $1 \cdot 10^{10}(m^{-3}s^{-1})$.

In this task we repeat what we did in task 0, but now we have ionization pulse with a duration of 100s over a 600s time span. The ion-electron production rate is set to $1 \cdot 10^{10}(m^{-3}s^{-1})$ for the first 100s and zero else. This gives, following plots:

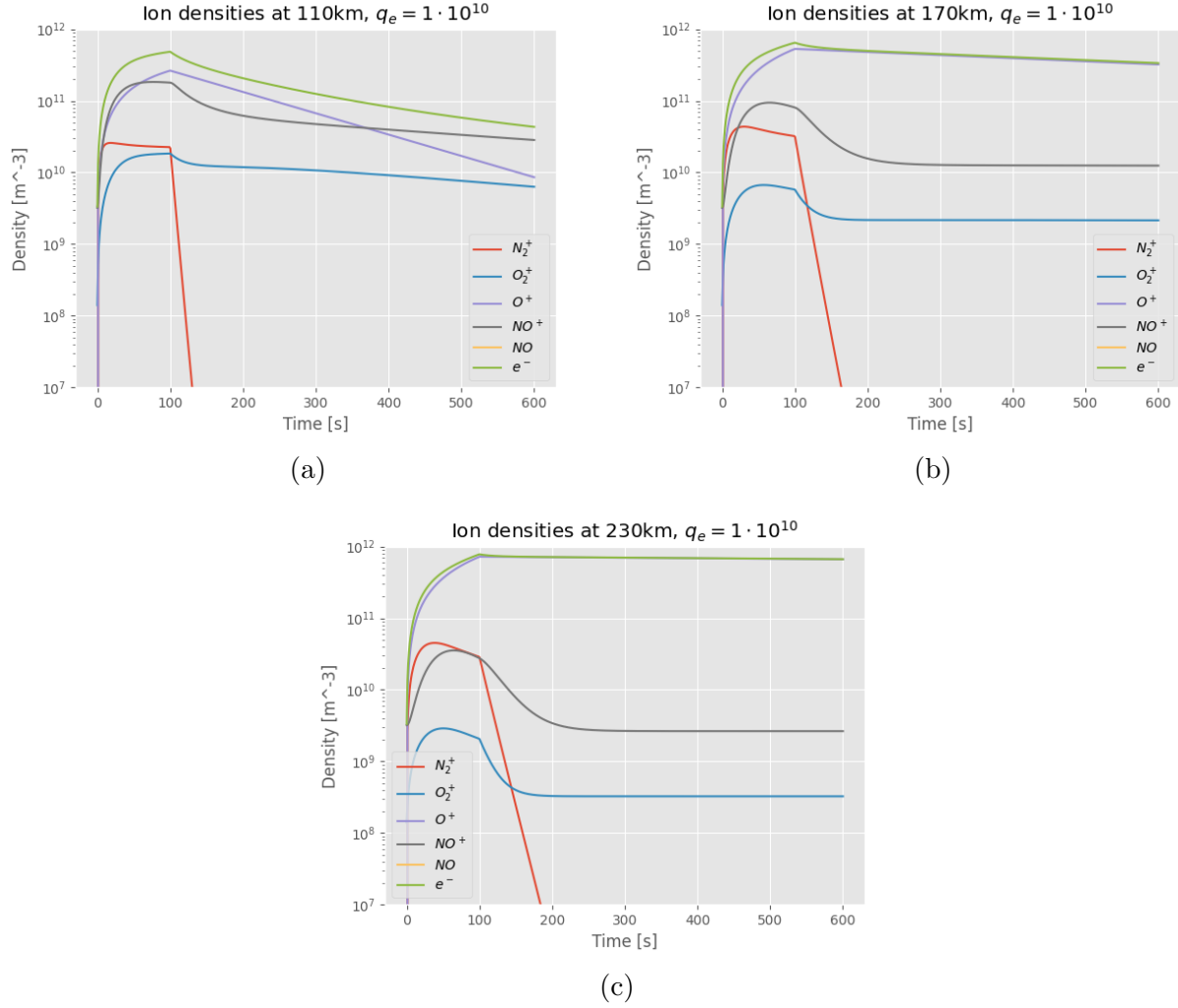


Figure 5: Ion densities at 110, 170 and 230km. With a 100s ion-pulse of a 600s time-span

From the plots, it's clear that the ion-electron production rate is $1 \cdot 10^{10} (m^{-3}s^{-1})$ for the first 100s and zero else. As the ion-pulse is off, we see that the N_2^+ is decreasing way faster than the other molecular ions. This happens since, after the ion-pulse is off, the term for production q_{N_2} is zero and the density falls rapidly. The same yields, for q_O .

Task 2: Same as task 1, with a change.

Now we gone repeat what we did in task 1, but now we increase the electron and ion temperatures by 1000K below 150km, and by 2000K at altitudes above 150km. This gives the following plots:

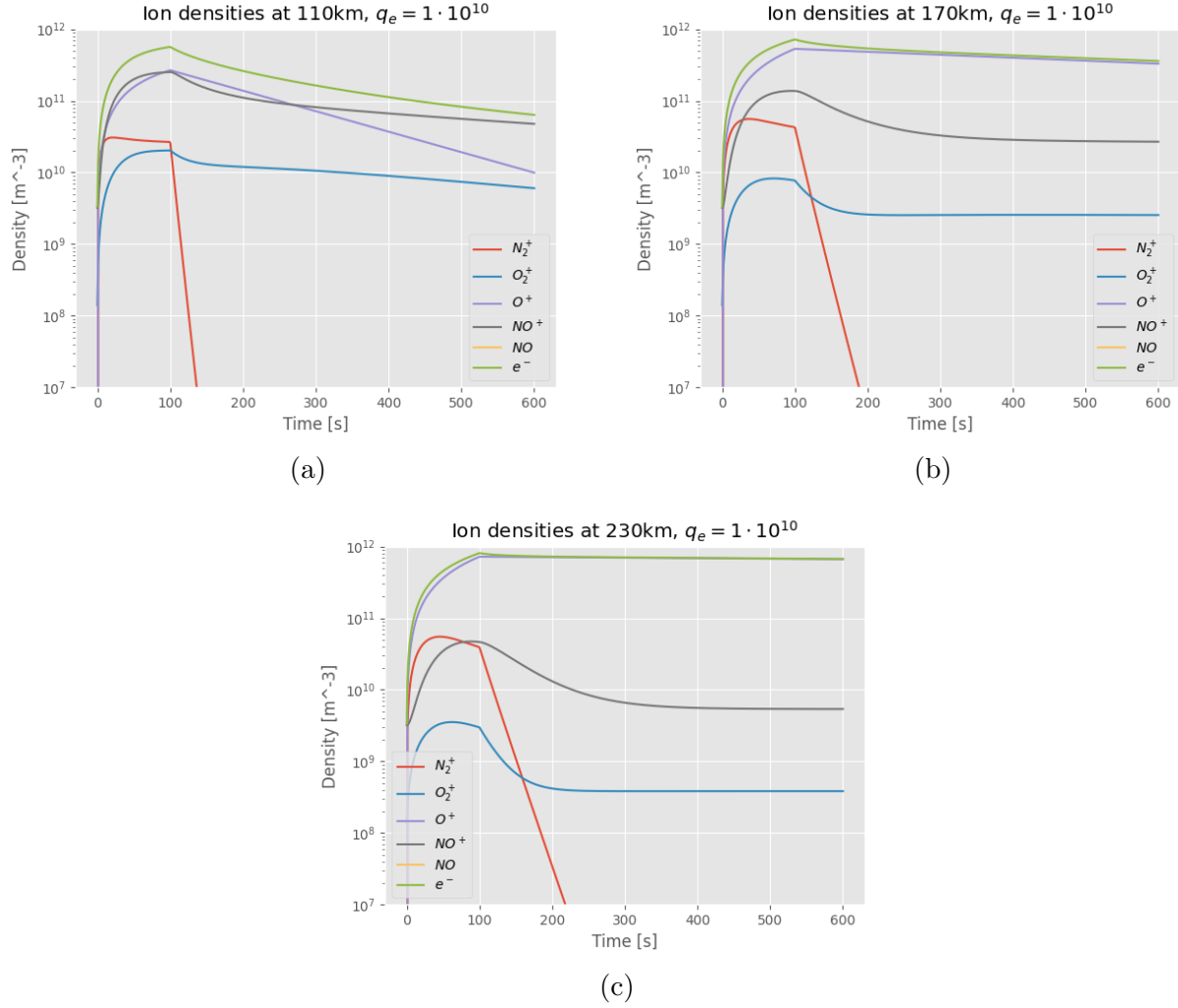


Figure 6: Ion densities at 110, 170 and 230km. With a 100s ion-pulse of a 600s time-span. with increase of temperatures, 1000K below 150km and 2000K above.

As we can see from the plots, the molecular ions now have higher density than the plots shown in task 1. This comes particular clear by comparing the graphs for NO^+ , and we see that now have almost the same peak density as O^+ at the altitude 110km. This is as predicted since, in the equations for reaction rates T_e and T_r is defined so by increasing the temperatures the reaction rates is also increasing. If the reaction rates is increasing the density of the molecular ions, will also increase.

Task 3: Compare the electron-density decay with the expected decrease characteristic α and β .

In this task we gone compare the electron-density decay with the expected decrease characteristic, called α -decay and the β -decay (exponential decay). By using the β -decay model, the decay of electron density with time follows a exponential pattern, where the decay rate is obtained by using a parameter called β' . This model suggest that the loss rate of electrons

is proportional to the electron density itself. The α -decay on the other hand, says that the loss rate is proportional to the square of the electron density.

We gone first consider the β -decay, which is expressed as.

$$\beta = n_e(t_{off}) \cdot \exp(-\beta' t) \quad (8)$$

where $n_e(t_{off})$ is the number density of electrons at where the ion-pulse is switched off, and β' is the decay parameter.

$$\beta' = \frac{k_1 n_{N_2} + k_2 n_{O_2}}{1 + \frac{k_1}{\alpha_1} \frac{n_{N_2}}{n_e} + \frac{k_2}{\alpha_2} \frac{n_{O_2}}{n_e}}$$

As we see, we have all the known information to calculate the β -decay. For the α -decay, we have defined it as.

$$\alpha = \frac{n_e(t_{off})}{1 + \alpha_e n_e(t_{off})} \quad (9)$$

Her the α_e is the decay parameter, which is.

$$\alpha_e = \alpha_1 \frac{n_{NO^+}}{n_e} + \alpha_2 \frac{n_{O_2^+}}{n_e} + \alpha_3 \frac{n_{N_2^+}}{n_e}$$

Than when computing the α - and β -decay, we need to have that all the parameters are using the values from when the ion-pulse is switched off to 600s. This gives the following plots, shown in the figure 7 below.

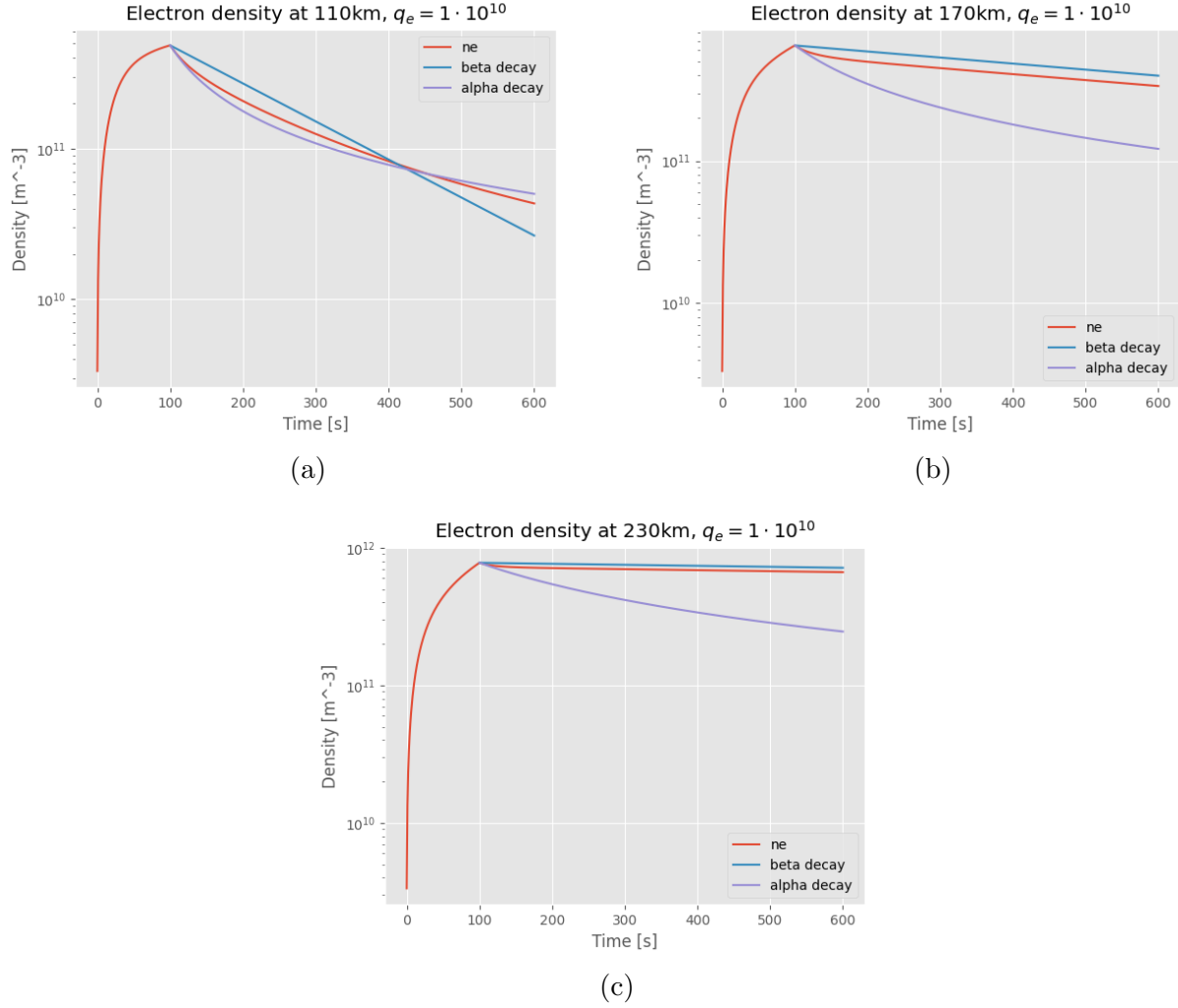


Figure 7: Electron density at 110, 170 and 230km. With a 100s ion-pulse of a 600s time-span, and graphs for α - and β -decay.

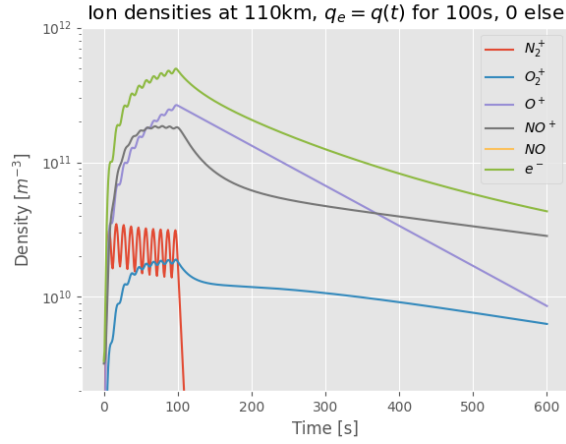
In the E-region we have more recombination going on and the electron loss rate is proportional to n_e^2 , as mention above. In the F-region on the other hand, we that charge rearrangement is dominating. Hence, the α -decay is a good model in the E-region and β -decay is a better model for the F-region. By looking at the plots in figure 7, this comes clear.

Task 4: Ionization that varies

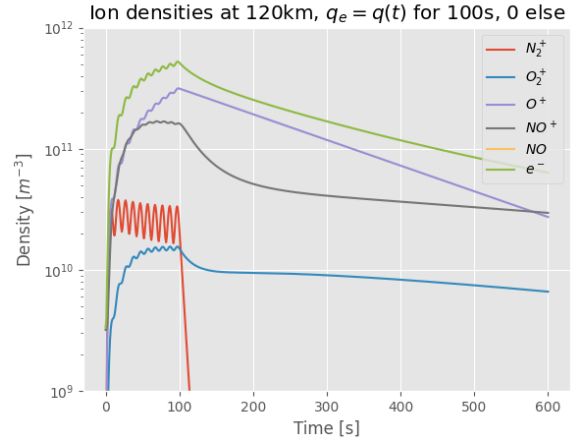
In the last task, we gone have ionization that varies as.

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

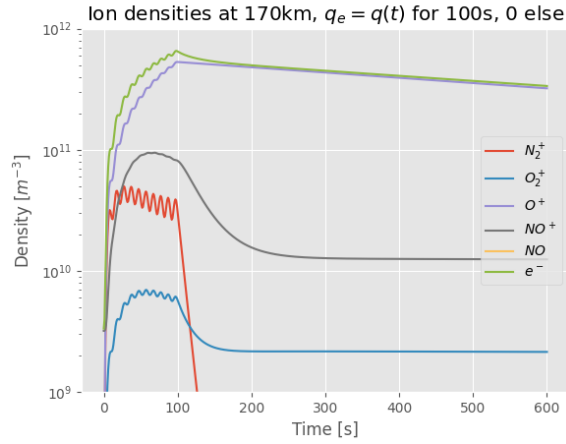
for the first 100s and zero ionization further, the electron production \hat{q}_e is sat to $2 \cdot 10^{10} (\text{m}^{-3} \text{s}^{-1})$ during the first 100s and zero else. This gives the following plots, shown in figure 8.



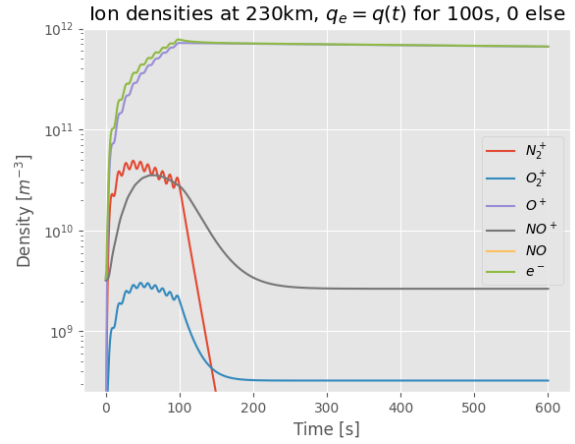
(a)



(b)



(c)



(d)

Figure 8: Electron density at 110, 170 and 230km. With a 100s ion-pulse of a 600s time-span

Here we can see that the ion densities are oscillating forward, to they reach 100s where the ionization is turned off and then rapidly decrease. We see that the N_2^+ is most effected by the varying ionization, and as the altitude is increasing the oscillating decrease for all molecular ions. Which can come from that as the altitude increase the ionization gets decreased and so do the density, which makes the molecular ions oscillate less.