Solutions 5. Running a simple chemical model

a. Examples of the following reaction types are:

- Radiative association: e.g., $H + OH \rightarrow H_2O + h\nu$
- Dissociative recombination: e.g., $HCO^+ + e^- \rightarrow CO + H$
- Photodissociation: e.g., $H_2O + h\nu \rightarrow OH + H$
- Charge transfer: e.g., $OH^+ + H_2O \rightarrow OH + H_2O^+$
- Ion-molecule reaction: e.g., $HCO^+ + H_2O \rightarrow CO + H_3O^+$
- Neutral-neutral reaction: e.g., $H_2 + OH \rightarrow H_2O + H$

b. The water in gas phase decreases (Fig. 1) because it freezes out.

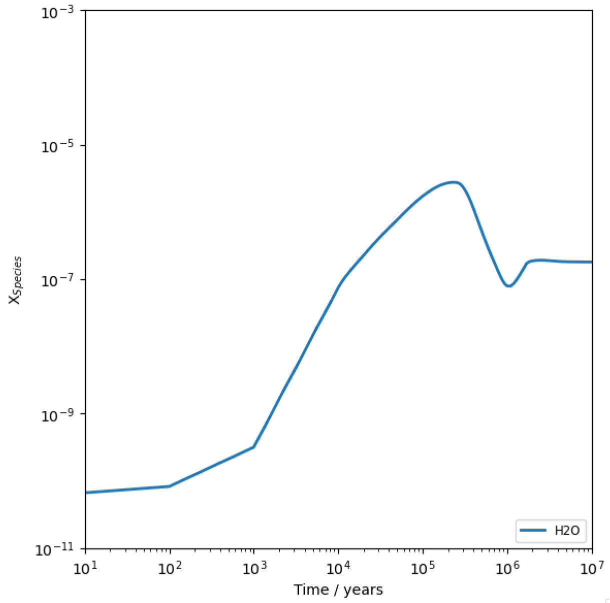

Figure 1: Water abundance in the gas phase.

c. The model predictions for water and O_2 are higher than the observed upper limits (see Fig. 2, top left panel).

d. The abundances can be lowered by decreasing the oxygen abundance from the original 3.34×10^{-4}. A new O abundance of 7×10^{-7} gives abundances consistent with the upper limits after 10^6 years (see Fig. 2, top right panel). You can decrease the oxygen abundance using the command `"fo":7e-7,` in `param_dict` in the `run_astrochemistry.py`. Please note that the observational values are upper limits so we want to get the abundances in the models under the solid black lines in Fig. 2.

e. By setting the `freezeFactor` to 50 the models agree with the observed upper limits at 10^6 years. Here we increase the freeze out rate of gas parcels. See Fig. 2 bottom left panel.

f. Setting `desorb` to False turns off all non-thermal desorption mechanisms and the models agree with observations. See Fig. 2 bottom right panel. This is because in the chemical models efficiency of the non-thermal desorption processes such as photodesorption is uncertain and is likely too high in this case.

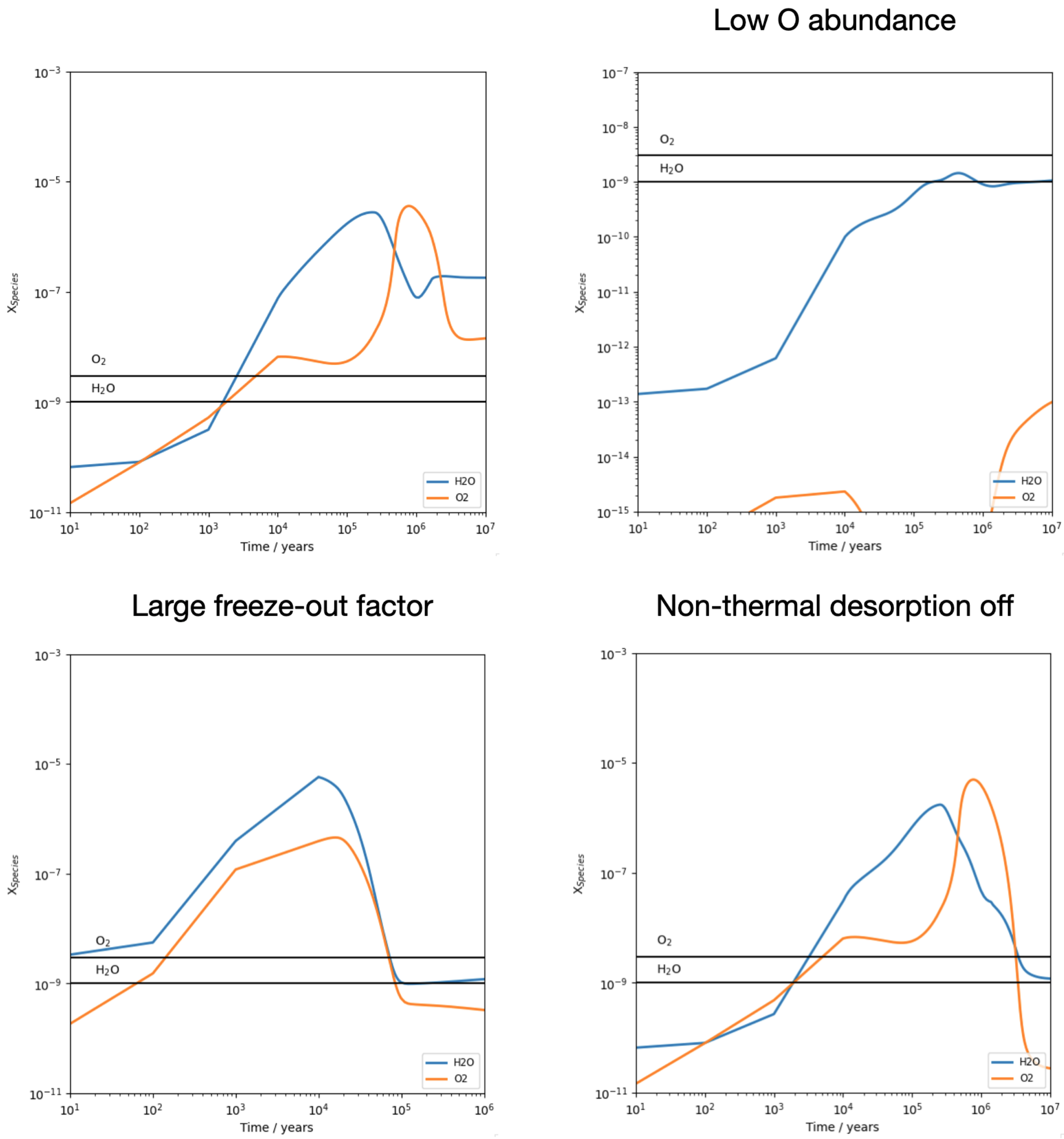

Figure 2: O_2 (orange) and H_2O (blue) abundances as function of time for the fiducial model settings (top left), for an O abundance of 7×10^{-7} (top right), freeze-out factor of 50 (bottom left) and with `desorb` parameter False (bottom right). The observed upper limits are indicated with the solid black lines.

g. HCO^+ has an increase and decrease pattern similar to CO (Fig. 3 left panel) because it is mainly formed though the reaction

$$CO + H_3{}^+ \rightarrow HCO^+ + H_2. \tag{1}$$

Therefore, CO is needed to form HCO^+ and the HCO^+ lags behind the CO.

h. The CO abundance is higher at higher densities at earlier times, but the abundances are lower at later times with a steep drop at around 10^4 years (see Fig. 3 middle panel). The steep drop is due to CO freeze-out. This steep drop also decreases HCO^+ abundance.

i. CO abundance on the grains is plotted in Fig. 4 with orange solid lines. CO ice abundance increases when CO gas abundance decreases indicating its freeze-out.

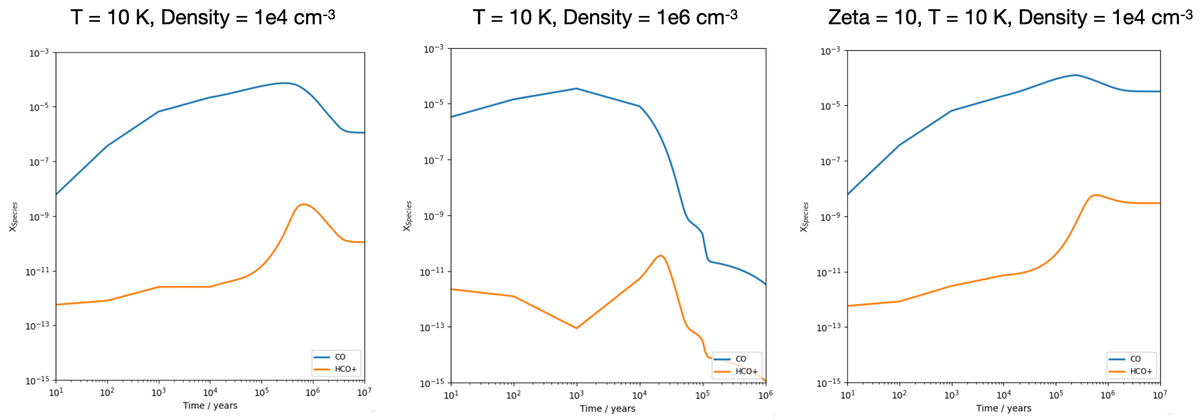

Figure 3: HCO^+ (orange) and CO gas (blue) abundances as function of time for the fiducial model settings (left), high density model (middle) and the fiducial model settings with `zeta` factor set to 10 (right).

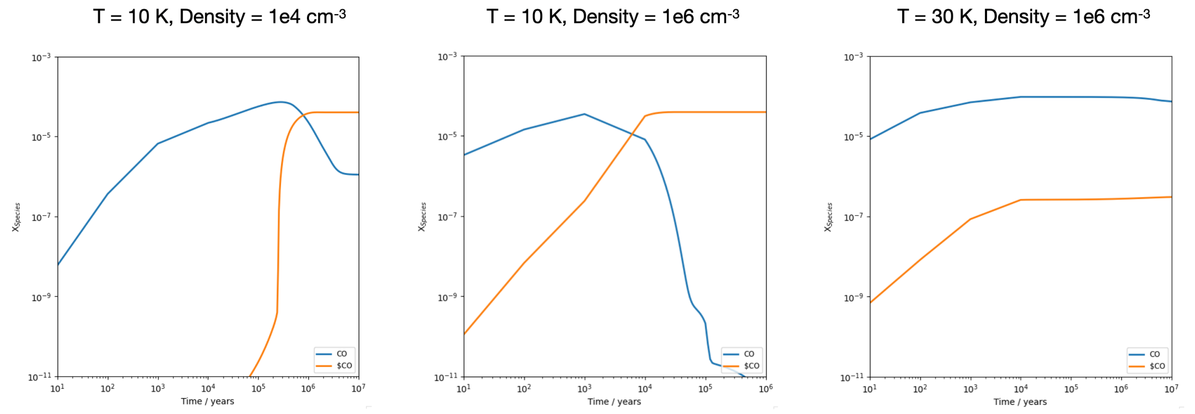

Figure 4: CO gas (blue) and ice (orange) abundance as function of time for the fiducial model settings (left), for higher density (middle) and for higher density and temperature (right).

j. You would expect CO to desorb off the dust grains when the temperature increases. You can see that although the densities are high in Fig. 4 right panel the gas-phase abundance of CO is always larger than the ice abundance of CO.

k. The effect of cosmic ray ionisation on HCO^+ is indicated in Fig. 3 right panel. A 10 times higher cosmic ray ionisation increases the abundance of HCO^+ by a factor $\sqrt{10}$. The reason for this is that HCO^+ is formed from ${H_3}^+$ (see Eq. 1). The formation of ${H_3}^+$ is directly related to the cosmic ray ionization rate. Therefore, also the HCO^+ abundance is governed by the cosmic ray ionization rate.