Problem 5. Running a simple chemical model

For some of the problems one or multiple hints are given in *italics*. Try solving the problems first without the hints!

Downloading and installing the model files.

Download the UCLCHEM network from github
(see also `https://home.strw.leidenuniv.nl/ leemker/astrochemistry`) and install it using the following command:

```
> git clone https://github.com/uclchem/UCLCHEM.git
```

Inspect the input files.

Let us have a look through the various input files. First of all, find the molecules that are included in the network. At the command prompt, type:

```
> nedit src/species.csv &
```

This will open up a file containing the list of chemical species in the network. The file contains the following columns:

1. The species name.
2. The species mass.
3. The number of atoms.
4. The binding energy.
5. The enthalpy.

Note that species appear in the list multiple times. For example, we see `H2O`, `#H2O`, and `@H2O`. The first one is gas-phase water, the second one is water ice on the surface of the grains, and the third one is water ice in the bulk of the ice mantle.

Now open the rates file:

```
> nedit src/reactions.csv &
```

This file contains all the chemical reactions along with the parameters necessary for computing the reaction rate coefficients. The columns show the following:

1-3. The reactants.
4-7. The products.
8-10. The parameters α, β, and γ necessary for the computation of the rate coefficient.
11-12. The temperature range where the parameters are valid.

Scroll through the file and find a reaction listing `FREEZE` as one of the reactants. The UCLCHEM network assumes that a reaction between two gas-phase species is a gas-phase two-body reaction and that a reaction between two ice species is a two-body surface reaction unless denoted otherwise. The `FREEZE` indicates that this is a freezeout reaction where the reactant freezes-out onto a grain. Similarly, the reactions with `DESOH2` are desorption of the reactant from a grain covered in H_2 ice.

a. Find an example of the following reaction types:

- Radiative association.
- Dissociative recombination.

- Photodissociation.
- Charge transfer.
- Ion-molecule reaction.
- Neutral-neutral reaction.

The computer readable version of the `species.csv` and `reactions.csv` are used by the network. Go to

```
> nedit src/fortran_src/chemistry.f90 &
```

And then find the subroutine `integrateODESystem` that updates the abundances in the chemical network and it called at every time step (see `wrap.f90`, subroutine `solveAbundances`). The subroutine `integrateODESystem` calls an ODE solver `DVODE F90` that takes the chemical network, `F`, as a system of ODEs as an input as well as with it's size, `NEQ`, the abundances of the species `abund`, the current time `currentTime`, the time the network needs to evolve to `targetTime`.

Running the code.

If you have not yet done so type the following in the terminal in the main directory

```
> pip install .
```

Make sure that everything goes well by looking for a sentence like: 'Successfully installed uclchem-#VERSION'. Here we run the code at one point for a simple cloud. Go to the course website and download the two python scripts called 'run_astrochemistry.py' and 'plot_astrochemistry.py'. You can find the link to their location here. Save the two scripts in the main directory where the code is located and type the following command in the same directory:

```
> python run_astrochemistry.py
```

You should get a line giving 4 numbers and the first number should be positive otherwise the code has not run correctly. Moreover, you should see the percentage change in total abundances of main species. Those values should all be 0 or less than 1%. They show that the abundances of these elements with respect to the total hydrogen are conserved in the run (and they should be, otherwise something has gone wrong).
Plot H_2O abundance with respect to total hydrogen in the gas-phase as a function of time by typing (Not copy pasting, it will give an error if you copy and paste)

```
> python plot_astrochemistry.py 'H2O' 'dont_plot' &
```

b. Why is there a decrease in gas-phase water abundance at around 10^5 years?

Plot the O_2 and H_2O abundances in the gas-phase as a function of time using the following command:

```
> python plot_astrochemistry.py 'O2' 'H2O' 'dont_plot' &
```

The observed **upper limit** abundances for these molecules in starless cores and cold outer regions of low-mass protostars are: $n(O_2)/n_H < 3 \times 10^{-9}$ and $n(H_2O)/n_H < 1 \times 10^{-9}$. You can add these upper limits to the plot with the following command:

```
> python plot_astrochemistry.py 'O2' 'H2O' 'plot' &
```

c. How do the model's predictions compare to these upper limits?

d. Is it possible to make the model's output agree with the observations by varying the initial oxygen abundance? What abundance of oxygen do you need for the models to agree with observations after 10^6 years? Feel free to change the limits of the figure.

Hint 1: Decrease the oxygen abundance.
Hint 2: The oxygen abundance is controlled via the parameter `"fo"` *in* `run_astrochemistry.py`.

e. Can you make the model's output agree with the observations at 10^6 years by increasing the `freezeFactor` in `run_astrochemistry.py` and keeping the initial oxygen abundance as 3.34e-4? If the model does not converge, decrease the final time in `run_astrochemistry.py` from 10^7 years to 10^6 years.

Note: The `freezeFactor` *increases the rate of freeze out on the grains. So the larger this factor a larger amount of gas parcels at faster speeds freeze out on the grains.*

f. Putting the `freezeFactor` back to 1, can you make the models agree with observations by turning off non-thermal desorption mechanisms using the parameter `desorb`? Make sure to change the final time back to 10^7 years.

Restore the input parameters in `run_astrochemistry.py` to their initial values. Rerun the code and plot the CO and HCO^+ abundance:

```
> python plot_astrochemistry.py 'CO' 'HCO+' 'dont_plot' &
```

g. Explain the relation between CO and HCO^+ abundances over time by the chemical link between the two.

h. Increase the density by two orders of magnitude (the parameter `initialDens` in the `param_dict`). Explain the effect on the CO abundance. Why do you see a steep drop? How does this change affect HCO^+?

i. Check your answer above with plotting CO on the grains (note that the sign $ can be used to indicate the abundance on the grains, i.e. $CO in this case).

j. While keeping the change imposed in (i), increase the temperature to 30 K. Explain the effect of temperature on CO ice abundance.

k. Restore the input parameters to their initial values and increase the `zeta` factor (cosmic ray ionisation factor) to 10. What is its effect on HCO^+ abundance?