



# Modelling the composition of exoplanets

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# 1 Abstract

## 1.1 English

Using a chemical network to model exoplanet atmospheres based on temperature, pressure and initial conditions, the dynamic of the atmosphere as well as quantities of four key molecules ( $\text{H}_2\text{O}$ ,  $\text{CH}_4$ ,  $\text{CO}_2$  and  $\text{O}_2$ ) were studied. The impact of different temperatures, pressures, humidity and nature of the composition were the focus of this project. Comparing simulated Mars atmosphere and Venus atmosphere with empirical data proved the used simplified model effective. The model fails for earth-like planets that include more complex atmospheric chemistry most likely due to the presence of biochemistry.

## 1.2 Dutch

Door gebruik te maken van een chemisch netwerk om exoplaneet atmosferen te modelleren op basis van temperatuur, druk en initialisatie waardes kan zowel de dynamiek van de atmosfeer als de hoeveelheden van vier belangrijke moleculen ( $\text{H}_2\text{O}$ ,  $\text{CH}_4$ ,  $\text{CO}_2$  en  $\text{O}_2$ ) bestudeerd worden. De invloed van verschillende temperaturen, druk, vochtigheid en aard van de atmosfeer was het aandachtspunt voor dit project. Vergelijken van gesimuleerde Mars en Venus atmosfeer met empirische data bewees het model effectief. Het model faalt voor aard-achtige planeten die een meer complexe atmosferische chemie vertonen, waarschijnlijk door de aanwezigheid van biochemie.

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## 2 Introduction

When studying exoplanets, the atmosphere of the planet is an interesting feature to look at, since it does not only tell about the gaseous composition but can also be used to determine how realistic it is that a planet is habitable for earth-like species. The usual method to model exoplanet atmospheres is through transits, in which a dimming of star light is observed for a certain period of time. By observing different wavelengths in which this dimming happens, the atmosphere of the exoplanet can be determined by comparing the wavelength data to the absorption spectra of gaseous molecules. Unfortunately this requires the planet to have a very specific orbit for the observer to apply this transit method, and if it would be, studying atmospheres for terrestrial planets have not yet been effective as it is for hot gas giants. An alternative method to model exoplanets would be through a chemical network.

Chemistry plays a large role in the composition of atmospheres, and governs the balance between the molecules that make up the air around us. A chemical network is a large system build up from many reactions that take place between gaseous molecules, in a way that if an amount of one specific molecule changes, it has impact on the entire system and could shift what the atmosphere is made out of. Additionally, Chemical reactions are very dependent on internal variables (activation energy) and external variables (temperature and pressure) and will impact how the chemical network responds.

Throughout this project there will be experimentation with the variables and molecule abundances with the goal to model and analyse what terrestrial exoplanet atmospheres look like. The chemical network used in this project does not contain all the reactions that take place in atmospheres, as we are working with a simplified model, but does contain all the necessary reactions for a presentable model.

## 3 Method

### 3.1 Chemical Network

When simulating exoplanet atmosphere based on a chemical network, the reactions of the chemical network will be based on the interest of the study. An example would be a chemical network focusing on organic gases would be build up from different reactions than one that focuses on more basic composition elements or molecules such as O<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O,... During the project we studied 2 networks among which the Archibald network and the Vulcan network. The Archibald network was build around O<sub>x</sub>, HO<sub>x</sub> and NO<sub>x</sub> chemical cycles as well as carbon monoxide, ethane, propane, isoprene and chlorine and bromine reactions. The Analysis of the Archibald network was the initial goal of the project but the software in use was still under development and lacked

assumptions needed to run this chemical network with relevant results. The alternative chemical network used to do the modelling of exoplanets was the Vulcan network, a less complex network made up of primarily common reactions occurring between basic molecules composed of primarily oxygen, carbon, nitrogen and hydrogen. Chemical reactions can become very complicated once dry deposition (reactions between atmosphere and dry surface), wet deposition (reactions between atmosphere and water surface) and photochemistry are introduced. Large chemical networks can very quickly cost great amounts of computational energy, thus a simplified and efficient chemical network of only the most crucial reactions is of most importance.

Every reaction in the network has a reaction coefficient rate  $k_{(T)}$  dependent on the temperature given by the modified Arrhenius equation [4].

$$k_{(T)} = A \left( \frac{T}{300} \right)^\alpha \exp\left( \frac{-Ea}{RT} \right) \quad (1)$$

Slow reactions are largely limited due to large activation energies needed, even though a reaction can be energetically favourable. The reaction rate then solely depends on the pre-exponential factor  $A$ , the temperature exponent  $\alpha$  and the exponent factor  $(-Ea/RT)$  depending only on a variable activation energy. When all this information is given, the reaction coefficient rate can be found for that reaction for a specific temperature. This means that the chemical network is entirely dependent on the temperature of the atmosphere. Both the Archibald network and Vulcan network used bi-molecular reactions that could have multiple products.

The software will then run Equation 1 for each reaction in each time-step. This results in a data set of the amounts of each element/molecule in the network at each time-step. This can then be studied as an evolution of time. Reactions that are highly exothermic will form most of the stable molecules within very small time ranges and will remain constant due to the extremely stable state they are in. Other reactions need longer time spans to form molecules and will thus show evolution as large amounts of time passes. These slower acting reactions make the atmosphere that is being modelled dynamic and allows it to change even after long ranges of time.

## 3.2 Parameters

### 3.2.1 Temperature

The main focus of this project is to evaluate atmospheric composition change of exoplanets as temperature changes. The temperature will be varied from 200 kelvin up to 324 kelvin. In this temperature range, the composition of the atmosphere will have drastically changed. As temperature increases endothermic reactions will be favoured more than exothermic reactions. As temperature increases, so will the energy in the system, this allows reactions that need a lot

of energy to still take place.

During the study of other parameters, the 300 kelvin will be used as a control variable for the temperature, as this is a realistic temperature for terrestrial planets. It is also close to earths temperature and is convenient since we will often be using earth-like atmosphere compositions discussed in Section 3.3.

### 3.2.2 Pressure

To calculate a rough estimate of the pressure  $P$  of an atmosphere, the ideal gas law is used

$$P = \frac{nRT}{V} \quad (2)$$

with  $n$  the molar quantity of the gas,  $R$  the gas constant,  $T$  the temperature and  $V$  the volume. The fractional pressure for each gas can then be acquired by looking at their relative molecule count to the total amount of molecules.

$$\frac{P_i}{P_{tot}} = \frac{n_i}{n_{tot}} \frac{RT}{V} \quad (3)$$

In the ideal gas law there is a clear relation between temperature and pressure, meaning hot planets will likely have a high pressure and cold planets will have a lower pressure. Even greenhouse gases impact this relation, as a planet with a high pressure will also increase the effects of greenhouse effect heating up the planet even more.

### 3.2.3 humidity

The humidity of an atmosphere can vary greatly. Even on earth the amount of gaseous  $H_2O$  can differ between 0 and 30 000 ppm (3 percent of the total atmosphere). This humidity study is targeted more towards planets which can dynamically change the amount of H in their atmospheres not caused by a temperature change or pressure change, earth is an example of such planet due to the large surface area covered by water. The humidity will be varied between 0 ppm and 5000 ppm as this is the highest the software allows. In reality, this value for humidity can be set much higher.

## 3.3 Initial Conditions

The initial conditions determine the abundances of elements in the chemical network. Some planet atmospheres are naturally richer in, for example, oxygen while others are naturally richer in hydrogen. In this project, two different initial conditions were used, stellar abundances and earth-like abundances. Stellar abundances is the total proportion of elements that exist in our universe, this abundance, although not directly relevant for atmospheres is a good approximation for a initial condition since planets are made of 'discs of dust' representing stellar abundances [5]. These abundances are more applicable to planets with

atmospheres similar to Saturn, Uranus and Neptune largely composed of mostly hydrogen and smaller amounts of helium. The stellar abundances used are displayed in Table 1

Table 1: Stellar Abundances [6].

| Element | percentage |
|---------|------------|
| H       | 73.9       |
| He      | 24.0       |
| O       | 1.04       |
| C       | 0.46       |
| N       | 0.096      |
| S       | 0.044      |

Unfortunately there are planet atmospheres do not have stellar abundances. Instead there is a wide variation of compositions. Earth-like abundances can be taken to study and simulate for a possibly habitable exoplanet. The earth like abundances are shown in table 2

Table 2: Atomic earth-like Abundances [7].

| Element | percentage |
|---------|------------|
| N       | 78.1       |
| O       | 20.9       |
| C       | 0.042      |
| S       | 0.0001     |
| H       | 0.000005   |

An alternate way to represent an earth-like atmosphere is not with atomic abundances but with molecular abundances. The difference should not be much except when using atomic abundances, all the molecules still need to be formed from the elements, this usually happens in a matter of microseconds. The molecular earth-like abundances are shown in table 3.

Table 3: molecular earth-like Abundances [8].

| Molecule        | percentage |
|-----------------|------------|
| N <sub>2</sub>  | 78.1       |
| O <sub>2</sub>  | 20.9       |
| CO <sub>2</sub> | 0.00042    |
| S               | 0.000001   |
| CH <sub>4</sub> | 0.0000019  |

For molecular earth-like abundances the H<sub>2</sub>O is set as zero since this can vary largely in earth's atmosphere. The impact of H<sub>2</sub>O will be studied and discussed as humidity, a parameter of its own.

### 3.4 Molecules of interest

When looking at the results of the simulation, it is unpractical and unnecessary to discuss every molecule. Only the quantities of the most important and meaningful molecules should be discussed. These molecules are H<sub>2</sub>O, CH<sub>4</sub>, CO<sub>2</sub> and O<sub>2</sub>. These molecule quantities unfortunately do not allow us to determine if life is present since, as a common misconception, O<sub>2</sub> is not a bio-marker and the topic of bio-markers in exoplanets is complex enough to deserve a project of its own. The simulation can give us a rough estimate of the habitability of an exoplanet. For habitability of an exoplanet, the temperature needs to lie between -15 and 122 degrees Celsius and pressure needs to be at least 0.01 bar. For molecular quantities, a adequate amount of N<sub>2</sub> is necessary and at least 1 percent of the atmosphere must consist of O<sub>2</sub>. Finally there must be a high relative amount of carbon compared to heavy metals. This carbon often comes forward in atmospheric CO<sub>2</sub> or CH<sub>4</sub> [9].

### 3.5 Software

The software was partly written in Python and partly in Fortran. All above mentioned parameters are varied to get calculate results. The code also consists of multiple parameters that can influence the outcomes such as different types of solvers and tolerances. When calculating solution to this big set of differential equations, numerical methods are required and used. Finding solutions this way are effective but not exact. The solvers that are used can be tweaked for performance and speed at a loss of precision. The goal here was to find a maximum precision at lowest tolerance for error without loss of speed.

## 4 Results

The following results were calculated by varying a specific parameter to get a good understanding of what changes in initial conditions are of impact on the final atmospheric composition. When varying, the remaining parameters are held at standard values. The following conditions are defined to be 'standard' in the results shown in table 4. Results for the evolution of molecular abundances over time for standard conditions are given in figure 1 and figure 2.

Table 4: Standard conditions.

| Parameter          | Standard value               |
|--------------------|------------------------------|
| Temperature        | 300K                         |
| Pressure           | 1 bar                        |
| Initial abundances | Earth-like atomic abundances |
| Chemical network   | Vulcan network               |
| Humidity           | Earth-like                   |

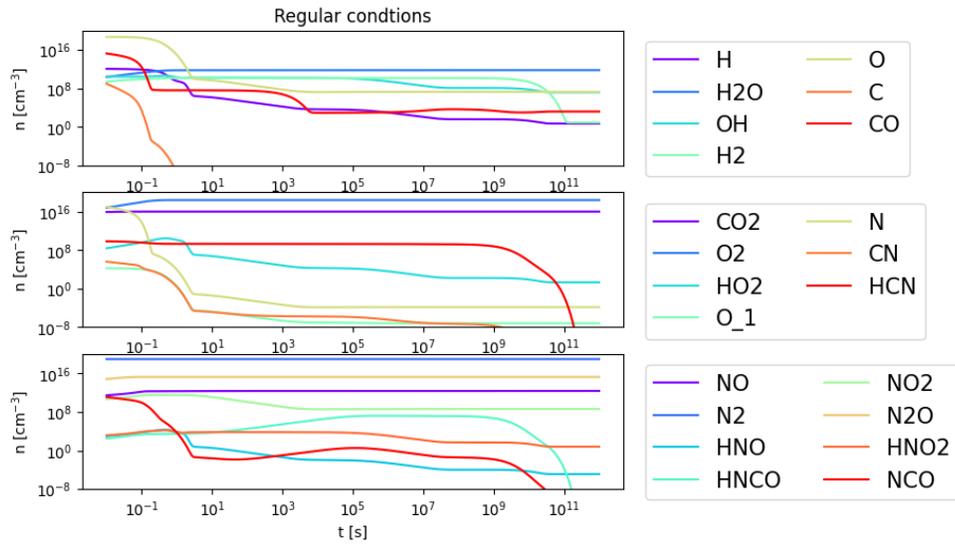


Figure 1: Plotted results for standard conditions.

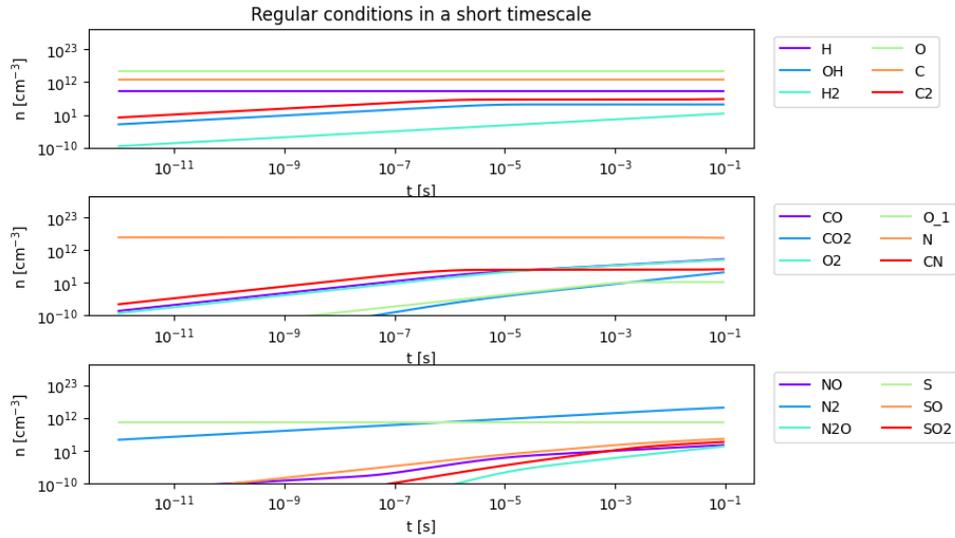


Figure 2: Plotted results for standard conditions in early stages of molecule formation.

#### 4.1 Temperature

When varying only the temperature the abundances of  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  after 100.000 years are plotted in function of temperature in figure below.

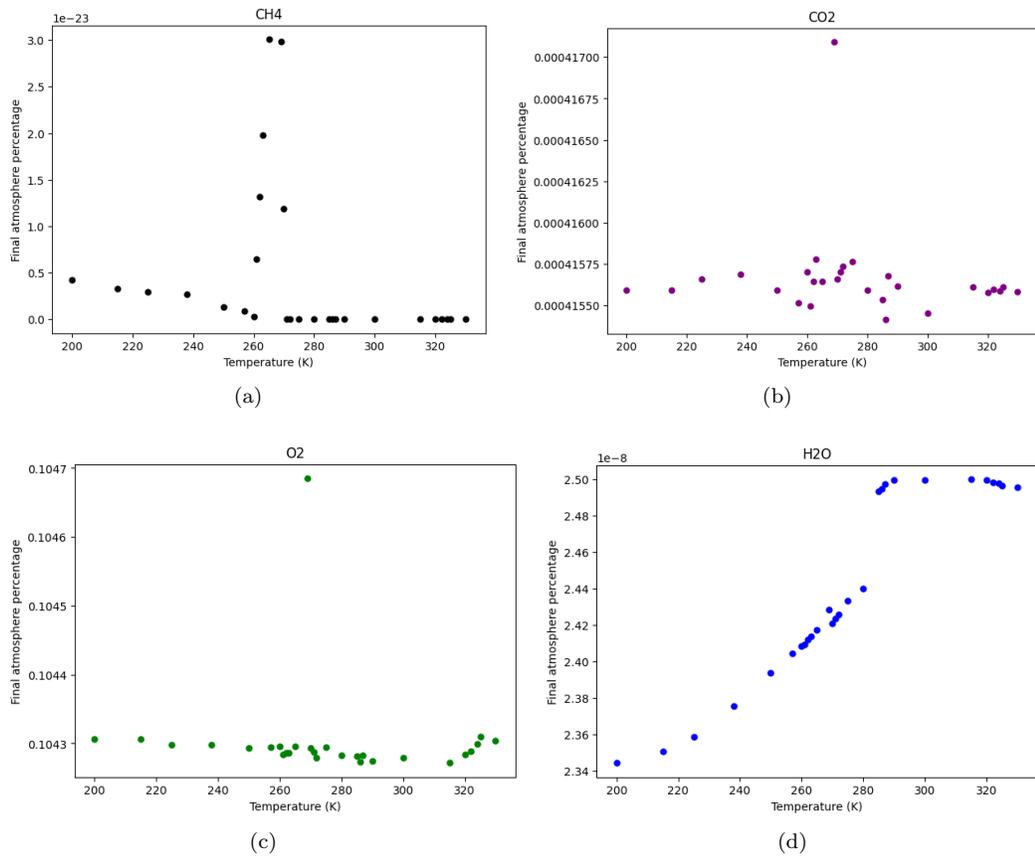


Figure 3: Final CH<sub>4</sub>, CO<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>O abundances in function of temperature.

## 4.2 Pressure

When varying only the pressure the abundances of CH<sub>4</sub>, CO<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>O after 100.000 years are plotted in function of pressure in figure below.

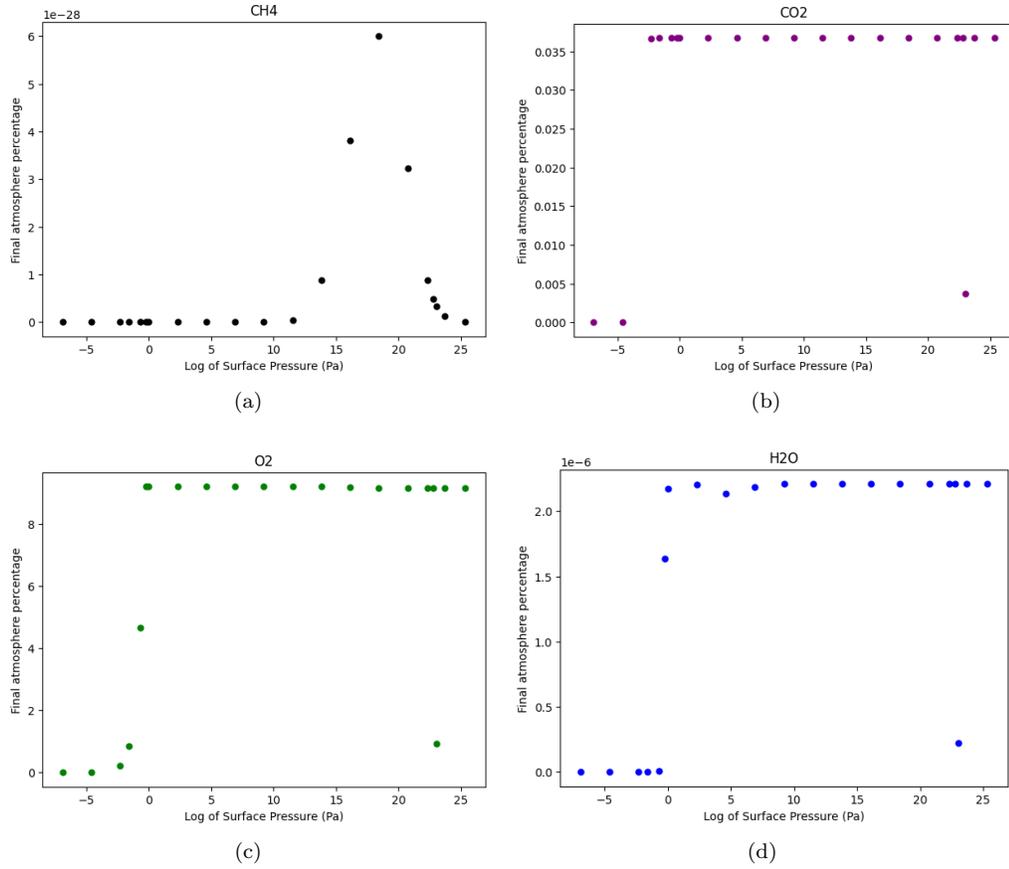


Figure 4: abundances of  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  in function of pressure.

### 4.3 Humidity

When varying only the humidity the abundances of  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  are plotted in function of time in figure 5.

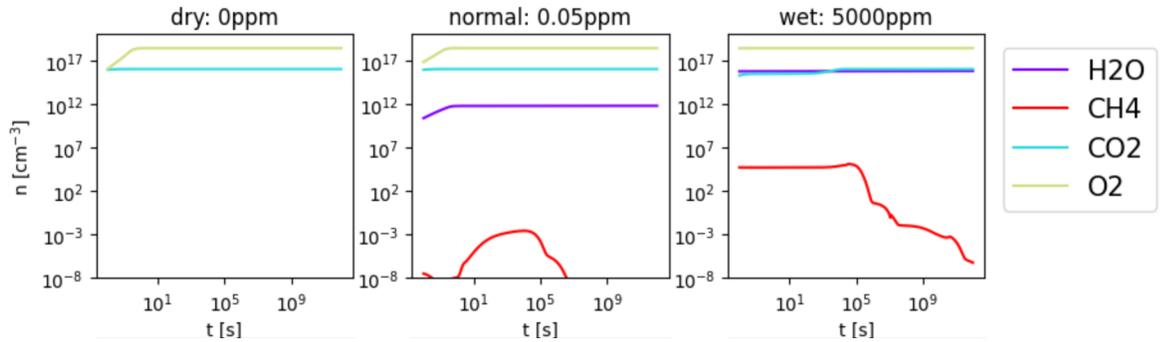


Figure 5: Molecule abundances over time for different initial values of humidity.

#### 4.4 Starting Abundances

When changing initial abundances from earth-like to solar-like the atmosphere dynamic is plotted in figure 6. Abundances of  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  are plotted in function of time in figure 7.

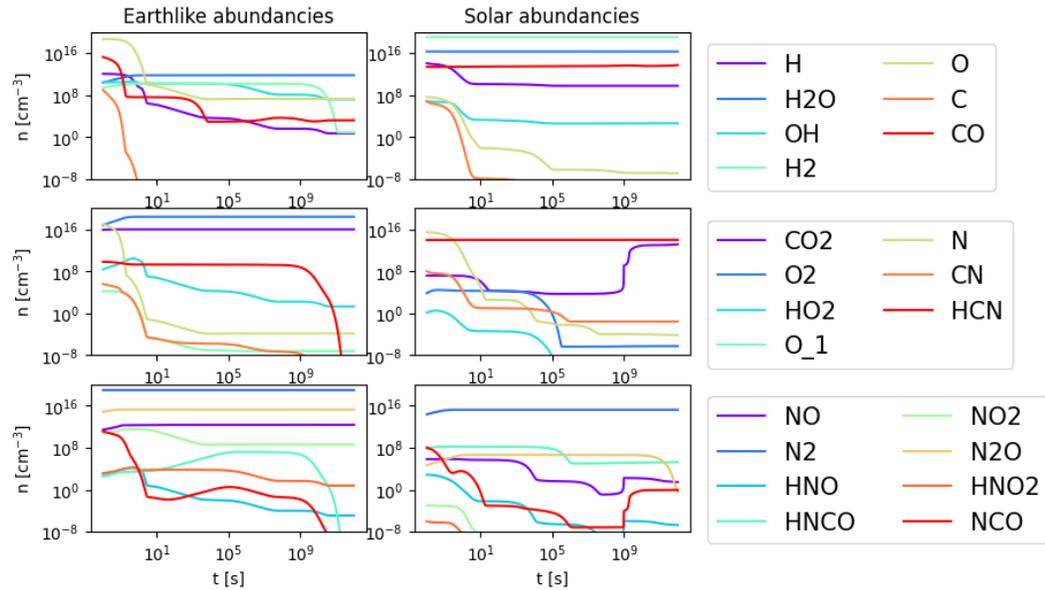


Figure 6: Molecule abundances over time for different initial abundances.

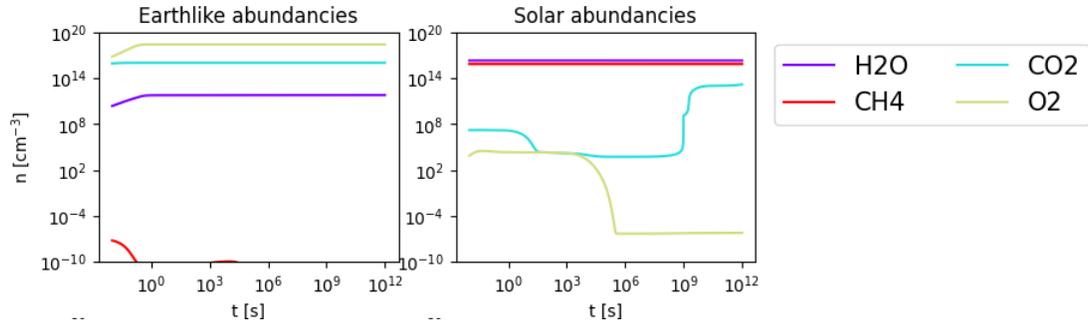


Figure 7: Molecule abundances over time for different initial abundancies. For the four specific molecules.

#### 4.5 Planets in our Solar System

Since earth is not the only interesting planet in our solar system, it is also useful to look at rocky planet's that can be observed more easily than exoplanets. In this section the results are showed when simulating the evolution of the atmosphere for 2 planets within our solar system namely Mars and Venus. The simulation was made with observed abundancies of these planets as well as a pressure of 600 Pascal, a temperature of 200K for mars [10] and a pressure of  $9.3 \cdot 10^6$  Pascal and a temperature of 737 Kelvin for Venus [11]. Due to difficulties calculating the Venus simulation only the final time could only be set to  $10^4$  seconds.

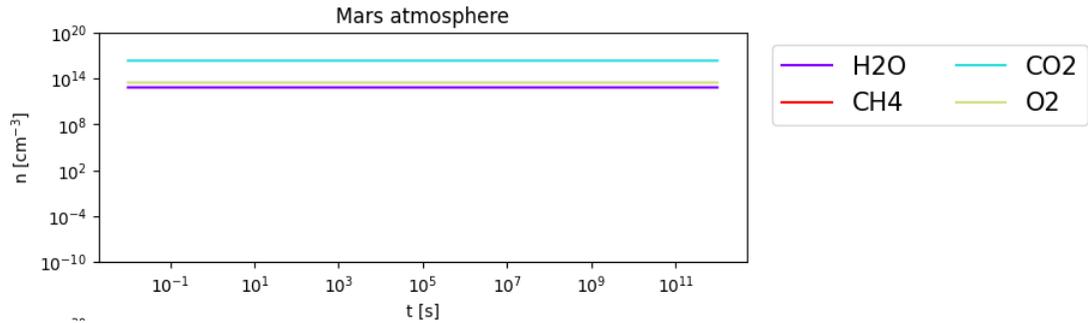


Figure 8: Molecule abundances over time for conditions that equal those of Mars' atmosphere.

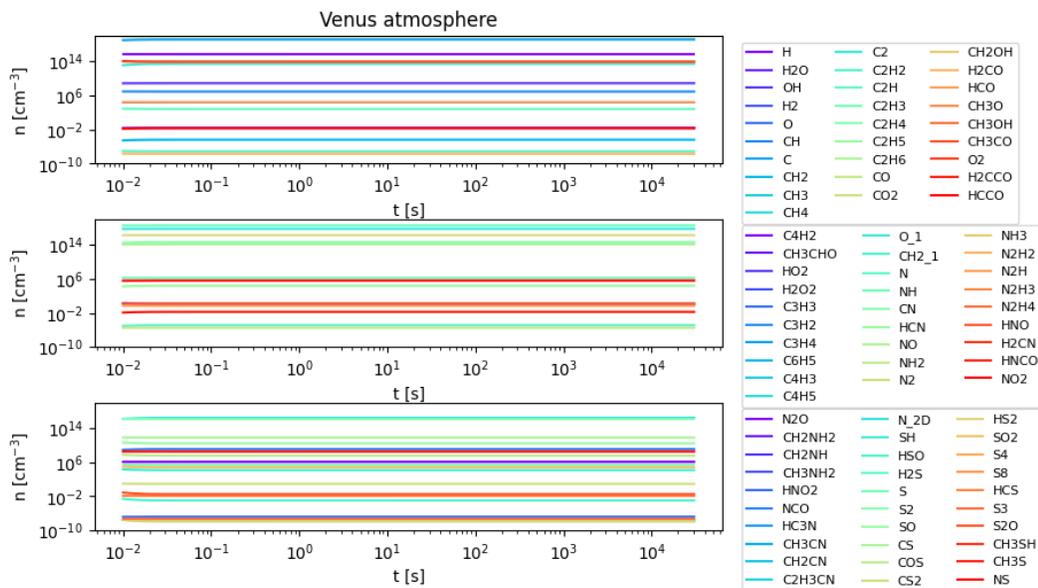


Figure 9: Molecule abundances over time for conditions that equal those of Venus' atmosphere.

## 5 Discussion

### 5.1 Systematic Errors

The nature of the errors comes from systematic errors from the simulation. These systematic errors can stem from multiple places. One of the large contributors to the systematic errors is the assumptions and simplifications made by the simulation. Without these simplifications the simulation would take an impractical amount of time to model atmospheres, and are thus of most importance. Another large contributor of the systematic error is due to the lack of equations provided by the chemical network. The chemical network used in this project has only the most important reactions. Even if the chemical network would be expanded to contain more reactions, there is still photo-reactions, dry deposition and wet deposition reactions. Since all known error on this model is systematic of nature, no error bars can be provided for an insight to the statistical variation.

### 5.2 Standard conditions

The standard conditions have as goal to mimic an earth-like atmosphere as much as possible. Looking at figure 1, one can see that many of the unbonded atoms such as H, O, C and N quickly decrease in quantity. This is due to

the forming of bonded molecules that have a much lower energy when bonded compared to if molecules were separated atoms. The initial conditions for the standard conditions are all atomic but in figure 1 it would appear that large amounts of  $\text{H}_2\text{O}$ ,  $\text{OH}$ ,  $\text{H}_2$ ,  $\text{CO}$  and many other bonded molecules already exist at the beginning of the time frame. These molecules have already formed large quantities before  $10^{-1}$  seconds shown in figure 2. Some of these molecules then proceed to hold a constant quantity for very long periods of time probably due to the extremely stable bond, which does not easily allow the molecule to react and form different molecules.

The atmosphere composition appears to be very dynamic, even allowing changes in molecular quantities thousands of years later. This is thought to be caused by slower reactions that need many years to slowly build up a sufficient molecular quantity to impact other reactions enough to have a non-negligible effect on it's products.

### 5.3 Temperature

During the study of the effect of temperature change, the four most interesting molecules were studied individually.

**CH<sub>4</sub>:** Between temperature 200 kelvin and 260 kelvin, there is a decline in quantity that appears to be linear with temperature. At 260 kelvin, this quantity of  $\text{CH}_4$  appears to peak, increasing its quantity six fold. After this peak the quantity drastically decreases to almost a negligible amount of  $\text{CH}_4$ . This gives reason to presume that there is a maximum temperature for which  $\text{CH}_4$  can exist and be stable enough to not react in any other reaction. We observe this temperature to be around 270 kelvin. When looking at an earth-like atmosphere temperature of around 290 kelvin, we see that no large amounts of  $\text{CH}_4$  should occur. In reality this is not the case and methane can be observed in earth's atmosphere. This is an example of how the simulation can differ from reality due to systematic errors discussed in section 5.1

**CO<sub>2</sub>:** The  $\text{CO}_2$  quantity seems to be generally independent of temperature in the range 200K to 320K, with exception a peak at around 270K. This peak seems to be induced by the concentration of other molecules rather than temperature. This peak is also a very minor deviation from the base value of  $\text{CO}_2$  for different temperature only showing a change of 0.3 percent. This change could seem small enough to be assumed unimportant but is instead a great example of how the the formation of a molecule can impact the formation of a different molecule. In this case, the formation of  $\text{CH}_4$  and  $\text{CO}_2$  seem to be correlated to another.

**O<sub>2</sub>:** Very similar to  $\text{CH}_4$ , a trend appears in the oxygen quantity and the temperature. The general trend between 200K and 300K is a very slight linear decrease, with once again an exceptional peak at around 270K. This decrease is

consistent but between 200K and 300K, the  $O_2$  only changes with an order of 0.01 percent. Like  $CO_2$ , this peak is thought to be induced by the concentration of other molecules rather than temperature and only reaches a height 0.4 percent higher than the expected  $O_2$  level. More interestingly,  $O_2$  quantity seems to increase as temperature increases for temperatures higher than 300K, but the data does not seem conclusive enough to establish this with enough confidence. Unfortunately the simulator used in for this project was not stable enough to run for higher temperatures to investigate this  $O_2$ -temperature relation any further. The increase in  $O_2$  quantity after a consistent decrease seems mysterious. An explanation for such phenomena could be that a particular molecule, let it be called X, is no longer present in the atmosphere at 300K due to an inability to form. This molecule X would inhibit the formation of  $O_2$ . After this molecule X is no longer present in the atmosphere it would allow  $O_2$  to form in larger quantities. This is not a definitive explanation, but rather speculation and should be studied further. Looking at these values, one can see that  $O_2$  at an earth-like temperature of 290K only makes up 10.43 percent of the total atmosphere. In reality, the earths atmosphere is 21 percent  $O_2$ . This could be due to the systematic error of the simulation or could be explained by photosynthesis taking place on our planet which is not accounted for in the simulation.

**H<sub>2</sub>O:** The  $H_2O$  quantity, or rather the humidity of the atmosphere, shows an increasing correlation between 200K and 280K before reaching what appears to be a maximum humidity. At temperature above 300K there seems to be a slight decrease in humidity and need to be studied for higher temperatures to give more conclusive results. comparing simulation values at 290K to observed earth values, the simulated atmosphere is possible. The inclusion of wet deposition reactions in the chemical network would give more realistic results for  $H_2O$  quantities.

## 5.4 Pressure

To see how different surface pressures lead to different molecular abundances in the atmosphere after a long period of time the four key molecules were studied again. Interestingly for all molecules the final abundance remained constant within certain pressure intervals depending on the molecule type.

**CH<sub>4</sub>:** When looking at the abundances of methane some interesting things happen when varying pressure. Even though the initial abundances of all simulations are equal, the final abundances of methane are nonexistent for all pressures except for a peak in a pressure range. This range is roughly between  $10^6$  Pascal and  $10^9$  Pascal. For earth-like initial abundances, in this model, no methane is expected in the atmosphere at a temperature of 300 Kelvin except for pressures between  $10^6$  and  $10^9$  Pascal with a maximum at a value of around  $10^8$  Pascal.

**CO<sub>2</sub>:** For  $CO_2$  a different trend can be seen. Either there is no carbon dioxide

or there is a substantial amount. The former happens when the pressure gets lower than a certain threshold, a critical pressure, of around  $5 \cdot 10^{-3}$  Pascal while the latter happens for all pressures higher than this. It is difficult to simulate what happens in between this regions as this happens quite abruptly and is not stable for our solver. Another interesting point happens at around  $10^9$ - $10^{10}$  Pascal. In this point there is a very sudden drop in atmospheric percentage of carbon dioxide. The same problem occurs in that it is difficult to model points around this one to get a better understanding of how the trend behaves in it's near vicinity. We suspect this is a similar peak as explained in the methane section, but a very sharp one which makes it more difficult analyse. This is a very interesting point and could be interesting to study further. This might just be an anomaly or error by the solver, but it might also be an interesting actual drop in carbon dioxide.

**O<sub>2</sub>:** The oxygen displays an extremely similar trend to the one of carbon dioxide. The main difference being that when it is present in the atmosphere is there in much higher percentages, around 10 percent. Another slight difference is that oxygen gas will be present in the atmosphere at a pressure (just below 1 Pascal) just below the pressure for which carbon dioxide starts (Just above 1 Pascal) to present itself. The transition between these two plateaus does not seem as steep, it was also easier to simulate in this regime.

**H<sub>2</sub>O:** The final water abundances in function of pressure are again similar to the two previous described molecules but again at a different scale. Only small traces of water are found in the earth-like atmospheres in this model. The entire plot not only seems scaled on the y-direction but looks shifted to the right as well. The pressure threshold after which the 'water-plateau' arose (at around 1 Pascal) is slightly higher than the threshold of carbon dioxide and oxygen gas. A less noticeable small dip can be observed in the water data with a minimum around  $10^2$  Pascal.

It is often not easy to determine at what pressures or temperatures all these changes occur. To analyse this better more data points should be collected especially around those interesting ranges. Many different trends can occur and can be observed in these types of plots but are difficult to understand. These dips can occur from long propagation of a small effect in initial conditions that can have impact on the entire atmosphere's composition.

The pressure data points did not deviate a lot from their trend when they looked to be constant. The same can be seen for their peaks and plateaus. This is in direct contrast to the temperature varied data points where there seems to be a lot of noise even when the values seem to follow some clear trend. We suspect that this is because the temperature has direct influence on chemical network as well as the solver which can be very sensitive to small changes. Pressure on the other hand mainly has impact on the initial abundances (gas law), more specifically the initial total amount of particles.

## 5.5 Humidity

Changing the humidity in this case meant changing the initial abundance of the element H. So logically a change in this element's abundance has effects on all molecules containing the element H. It is possible to see in figure 5 how the larger starting abundance of H also has higher final abundances of molecules containing this element, most notably H<sub>2</sub>O. Elements containing H are strongly affected by a change in humidity. What is less straightforward is how other elements are also affected. An increase in H might mean that it becomes favourable to create some molecules that contain H. These molecules then in turn might react with other molecules that contain some other elements and so on. This is clearest seen in how the CH<sub>4</sub> quantity changes as H<sub>2</sub>O abundance is increased, even on long time scales. A more subtle affect of this increase in H could be seen in the formation of O<sub>2</sub>. For starting H abundances of 0 ppm and 0.05 ppm it is seen that at the start of the figure, O<sub>2</sub> is still forming. Meanwhile for starting H abundances of 5000 ppm the O<sub>2</sub> is already formed, implying that the amount of H<sub>2</sub>O in atmosphere can accelerate O<sub>2</sub> production. Small changes can lead to vastly different atmospheres even for molecules that don't look like they have anything to do with humidity.

## 5.6 Starting Abundances

To check how changing general starting abundances leads to different exoplanet atmospheres, the temperature and pressure were held constant as two different abundance models were applied. Two drastically different result are seen for the two starting conditions. This can be seen for the general element evolution as well as in more detail for the interesting elements in figure 7. Some elements have a much higher starting value in one model as opposed to the other. These elements are in return of impact on elements that are not present at the initialisation of the model and so almost all elements and molecules evolve differently over time in the two models.

## 5.7 Planets in our Solar System

For both planets it is clear that all molecules/elements remain constant over time. This is exactly what is expected as the planets pressure and temperature are used as well as their documented molecular abundances. Observations show that these atmospheres are indeed not changing rapidly and this is also what our model predicts.

**Mars:** The plotting functions used in this project only displays molecules with significant changes in quantities. This implies that almost no new molecules were formed in the atmosphere. This could be due to a low interaction rate between the existing molecules due to very low pressure and very low temperature.

**Venus:** The plotting of molecules in Venus's atmosphere shows many molecules

graphed. This is because all molecules present in the figure were made by the atmosphere itself and showed significant change in quantity. All these molecules appear to be constant in quantity between time ranges  $10^{-2}$  and  $10^4$  seconds. All these molecules were made in time ranges smaller than  $10^{-2}$  seconds. This is probably due to large pressures and high temperature driving the reactions to take place quicker. These large pressures and temperature also supplies more energy to this system allowing molecules to form temporarily that need a lot of energy to form. These molecules would not form in these quantities under more earth-like conditions due to the instability of these molecules. These molecules would then react back to more energetically favourable stable molecules holding the unstable molecule quantity in balance and remains constant. It would have been in the best of interest to study the simulation of Venus's atmosphere at longer timescales but due to the high abundances of a wide variation of molecules this is numerically very demanding from the software. More efficient or Venus atmosphere specific software should be used for simulating the atmosphere of Venus for longer timescales.

## 5.8 Archibald Network

Due to earlier mentioned problems results for the Archibald network and our original goal could not be produced. The reason for this was that the numerical solver that was written beforehand had some assumptions in mind that did not go well with just any chemical network. It is still possible to go further with this specific chemical network. However this would require to write a specific numerical solver for this network or find one which is already written that is compatible.

## 6 Conclusion

Making use of a chemical network, the atmosphere for exoplanets can be modelled starting with some initial molecular abundances as well as specific exoplanet parameters such as pressure and temperature. During this project the quantities of four important molecules were plotted and studied as atmospheric conditions changed.

As temperature changes between 200 Kelvin and 324 Kelvin, there are slight changes in  $\text{CH}_4$ ,  $\text{CO}_2$  and  $\text{O}_2$  quantities apart from a peak at around 270 kelvin seen for each of the molecules. As temperature rises there is a clear increase in  $\text{H}_2\text{O}$  before reaching a maximal value at around 290 Kelvin.

During the study of pressure variation,  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{H}_2\text{O}$  each show a step like behaviour, staying low until a critical pressure and reaching a maximum very quickly for pressures larger than this critical pressure.  $\text{CH}_4$  generally stays low for all pressures with the exception of a peak. This occurs at a very high pressure.

Humidity also has a significant impact on the composition of the atmosphere by resulting in a drastic increase in the quantities of other hydrogen containing molecules but also has a smaller affect on molecules not containing hydrogen.

When initial abundances of Mars and Venus are applied with their corresponding temperature and pressure, the atmosphere keeps the molecular quantities constant meaning that the simplified model agrees with empiric data. Unfortunately not the same could be said about Earth as the simulation quickly deviates from empirical data. The main suspect for this are the biochemical reactions used to support life in organisms such as photosynthesis.

Even in this simple model, slight changes in temperature, pressure or initial composition can lead to vastly different exoplanet atmospheres. The model could be further improved by including dry deposition reactions, wet deposition reactions and photo-chemical reactions in the chemical network.

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