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Abstract

Context. If Venus and Earth were Exoplanets that we discovered with our current available methods, we would label them as the same type of Exoplanet. However Venus has a CO₂ rich atmosphere and very high surface temperatures, which is very different to Earth. Venus' upper atmosphere however has quite moderate temperatures, leading to the question, if this was always the case, or if under an evolving Sun it was close to heating up so rapidly for atmospheric loss to be severe.

Aim. This study aims at understanding the effect of heating and cooling mechanisms in Venus' upper atmosphere on the temperature profile, and therefore on the atmospheric loss through Jeans escape. We are not only interested in Venus current situation, but especially in its recent history. We investigate how different atmospheric compositions and solar fluxes affect CO₂ and N₂ rich atmospheres to gain insight in which atmospheres are protected from severe loss rates.

Methods. We performed a set of simulations with a state-of-the-art upper atmosphere model called the Kompot Code developed at the University of Vienna to investigate the effect of initial CO₂ composition and XUV flux on the heating and cooling processes in Venus upper atmosphere.

Results. Depending on the altitude the dominance of the heating and cooling mechanisms changes. Chemical heating dominates at altitudes above 100km and XUV heating below 100km. We find that chemical heating and CO₂ cooling is strongest for atmospheres with 30% CO₂, with lower rates for larger and smaller CO₂ mixing ratios. The total heating through XUV gets stronger with more CO₂, but the 90% CO₂ simulation leads to the lowest rates. Starting from 150km the temperature profiles for different compositions spread out, with CO₂ lacking atmospheres being hotter and more expanded. This is due to XUV, chemical, and photoelectron heating being stronger for atmospheres with less CO₂ at this altitude. The cooling mechanisms on the other hand do not severely change with mixing ratio. At 2/3 of the atmosphere the picture is inverted for almost all heating and cooling mechanisms with CO₂ strong atmospheres leading to higher rates, bringing a stop to the rapid increase of temperature at higher altitudes. At the exobase the effect of the mechanisms is not significantly affected by composition, leading to stable temperatures at higher altitudes for all compositions. Additionally we find that IR heating and CO₂ cooling at the exobase decrease strongly with flux and composition which is most likely to atmospheres being more expanded and therefore looser, resulting in only little CO₂ at these altitudes. We also find that higher X-ray fluxes heat up atmospheres with little CO₂ stronger, expanding them to higher exobase altitudes. The rapid increase in temperature is due to the heating mechanisms at 150km being strongly affected by a changing flux. Despite the rapid increase in temperature and exobase altitude, X-ray flux of below 1.8erg/s/cm² do not lead to significant atmospheric loss.

Kurzfassung

Wenn wir Venus oder die Erde als Exoplaneten beobachten würden, gingen wir davon aus, dass diese beiden Objekte zum selben Typ gehören. Dabei hat Venus eine CO_2 dominierte Atmosphäre mit sehr hoher Oberflächentemperatur. Trotz dieser hohen Temperaturen ist die obere Atmosphäre relativ kühl. Es stellt sich die Frage, ob dies während einer sich entwickelnden Sonne mit stärkerer Röntgenstrahlung anders war, oder ob Venus nie unter Bedrängnis war ihre Atmosphäre zu verlieren.

Ziel dieser Masterarbeit ist es, den Einfluss von wärmenden und kühlenden Prozessen in Venus' oberer Atmosphäre auf Temperaturprofile zu analysieren, und entsprechend auf den Verlust von Atmosphäre durch Jeans-Escape. Dabei achten wir nicht nur auf die Venus in ihrer derzeitigen Form, sondern vor allem in der nahen Vergangenheit. Wir beschäftigen uns mit verschiedenen Zusammensetzungen der oberen Atmosphäre und unterschiedlichen Sonnenflüssen und deren Effekt auf CO_2 und N_2 dominierten Atmosphären. Dadurch möchten wir ein besseres Verständnis gewinnen, welche Atmosphären besser gegen den Verlust von Atmosphäre gewappnet sind.

Um diese Ziele zu erreichen führen wir Simulationen mit dem Kompot Code durch, der obere Atmosphären von beliebigen Planeten berechnet. Wir variieren dabei die anfängliche Menge an CO_2 in der Atmosphäre, sowie das Spektrum der Sonne, um die Auswirkungen dieser Variationen auf die Wärm- und Kühlprozesse zu verstehen.

Die Simulationen zeigen, dass die Temperaturprofile von CO_2 dominanten Atmosphären deutlich konstanter bleiben, während jene mit wenig CO_2 einen extremen Anstieg an Temperatur und Ausweitung aufweisen. Eine genauere Analyse zeigt, dass diese Verläufe durch die Heiz- und Kühlmechanismen bei den jeweiligen Schichten die die entscheidenden Erklärungen liefern.

Der kühlsste Punkt im Temperaturprofil liegt bei allen Simulationen bei 150km, mit weitgehend übereinstimmenden Temperaturen für Atmosphären bei derzeitiger Sonneneinstrahlung. Es zeigen sich dennoch Unterschiede zwischen den Raten der Heiz- und Kühlvorgänge je nach Zusammensetzung. So finden wir höhere Heizraten bei Atmosphären mit geringem CO_2 Anteil, während die Kühlmechanismen kaum von der Zusammensetzung betroffen sind. Tendenziell kühlen CO_2 dominante Atmosphären aber besser. Dies führt insgesamt zu einer gleichbleibenden Temperatur auf dieser Höhe.

Nach 150km folgt ein starker Temperaturanstieg, höchstwahrscheinlich verschuldet durch chemische Heizprozesse, oder Heizung durch Photoelektronen. Diese Höhenlage verschuldet auch die extremen Unterschiede in der Entwicklung mit steigendem Fluss. Bei 2/3 nehmen die Profile wieder konstante Temperaturen ein. Wir finden, dass CO_2 dominante Atmosphären besser kühlen, wodurch der Temperaturanstieg schneller abgebremsst werden kann.

In der obersten Schicht, der Exobase, haben alle Heiz- und Kühlmechanismen praktisch

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dieselbe Stärke, unabhängig von Zusammensetzung und Sonneneinstrahlung. Nur die Erwärmung durch Infrarot und die Kühlung durch CO₂ nimmt drastisch ab je stärker die Sonneneinstrahlung ist.

Zusätzlich beobachteten wir, dass CO₂ schwache Atmosphären durch ihre deutlich wärmeren oberen Schichten auch weiter ausgedehnt sind, und entsprechend höhere Verlusten bzgl Atmosphäre aufweisen. Jedoch konnte in keiner der Simulationen Verlusten festgestellt werden, die hoch genug sind, um die Atmosphäre vollständig zu entfernen - zumindest nicht für X-ray Flüsse unter 1.8erg/s/cm².

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1. Introduction

Before the discovery of the first exoplanet, the term *habitability* was mostly connected with flora, islands, food, the sea or animals, according to the paper network on the astrophysics data system *ads*. But from that point on, planets and exoplanets suddenly became the main topic of many papers, with the paper count rising from just about 60 in 1992 to over 800 in 2021 alone and over 11000 in total, linking topics such as climate, habitable zone, exoplanets, water, moon and many other astronomy related keywords. This shows how important research into habitability has become.

Habitability, which defines requirements that need to be met in order for life to exist (such as liquid water), is, however, bound to many different aspects, such as the distance between a planet and its host star, the planet's temperature, its atmospheric composition, magnetic fields and many more. Thankfully, we neither have to look at a distant exoplanet to study habitable worlds, nor do we need a large sample of exoplanets that are afflicted with observational biases. We can simply look at our own solar system, as there are many interesting objects besides Earth, such as Venus, Mars or Titan.

Venus is of particular interest, as it is very similar to Earth, but far from habitable. The question arises why Venus turned to be like this, and if it could have gone into a direction more hospitable to life with Earth's sibling if its composition was slightly different. This thesis will, therefore, discuss Venus with a focus on its temperature, the heating and cooling mechanisms behind it and how they change depending on composition and solar flux.

For this, the first chapter will introduce the Sun as a host star. It will give a quick overview on its evolution through time and how flux and age are connected, then atmospheres will be the centre of attention. There, the different processes in the atmosphere will be elaborated on, such as photochemistry and diffusion among others, as well as how the upper atmosphere can be lost to space. The last part will talk about the situation on Venus and the current theories on why it is the way it is.

1.1. The Sun

As the main source of energy, understanding the Sun and its evolution as well as the energy budget it provides is essential for understanding the evolution of atmospheres, especially when it comes to the heating and cooling mechanisms and hence also atmospheric escape. Solar radiation penetrates the atmosphere to different depths depending on the atmospheric composition. A more active Sun with more XUV (X-ray: 0.01-10nm, UV: 10-400nm, combined X-ray and UV are called XUV) radiation might, therefore, affect the planet's heating mechanisms differently than a less active Sun.

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1.1.1. Solar radiation and flux

First of all we need to understand where the energy that is given to the planet comes from. The Sun mainly consists of Hydrogen ($\sim 90\%$ of the total atoms and $\sim 70\%$ of the mass) and due to the very high temperatures of $16 \cdot 10^6$ K in the Sun's core, the particles move at very high speeds, which allows them to overcome the electrostatic repulsion and for the attractive nuclear force to be strong enough for fusion to happen. This process combines four atomic H nuclei to form an atomic He nucleus which has higher mass. However, there is a discrepancy in mass when looking at Einstein's energy-mass equation, meaning some mass is converted to energy. This is the energy that the Sun emits in the form of photons. These photons have different wavelengths, mainly in the visible regime, but also in the highly energetic XUV range of the spectrum.

After being created in the Sun's core the photons travel to the Sun's surface for a couple of thousands of years and reach the planet after several minutes. To express this *flow of photons* in a useful way, we imagine that the photons travel through a surface area per time and call it flux. There are different types of fluxes that can be expressed with different units. Luminosity is also a flow of energy, not per surface area, but the total energy lost per second in all directions. There also exists the specific term of surface flux, which is a flux normalised to the surface it is coming from.

We can, therefore, differentiate between surface incident fluxes at various positions, e.g. the flux at the Sun or at the Earth. The surface flux at the Sun is approximately $30000 \text{ erg/cm}^2/\text{s}$.

When measuring the flux at the Sun's surface, the distance d which the light travels is exactly the Sun's radius. Eq. 1.1 results in a luminosity of $1.85 \cdot 10^{27} \text{ erg/s}$, when using $d = R$.

When, however, the flux that arrives at Earth is of interest, we set $d = a = 1AU$, which results in a surface flux of $0.65 \text{ erg/cm}^2/\text{s}$. This means of the original $30000 \text{ erg/cm}^2/\text{s}$, only $0.65 \text{ erg/cm}^2/\text{s}$ arrive at Earth because the flux is being distributed around a bigger sphere (see Fig. 1.1). We can also express a flux density, which is flux per unit wavelength, or frequency.

$$F = \frac{L}{4\pi d^2} \quad (1.1)$$

1.1.2. Rotation and activity

Deep inside the convective zone of a star, a dynamo generates a magnetic field. The magnetic field itself is influenced by differential rotation and convective motion, and therefore, the rotation rate affects the magnetic activity in general (Güdel [2020]).

Because the Sun, just like other stars, span down through its evolution, it evolved from magnetically active at young ages to less active at older ages. Depending on the initial rotation rate the Sun could have followed different evolution tracks, as pointed out by

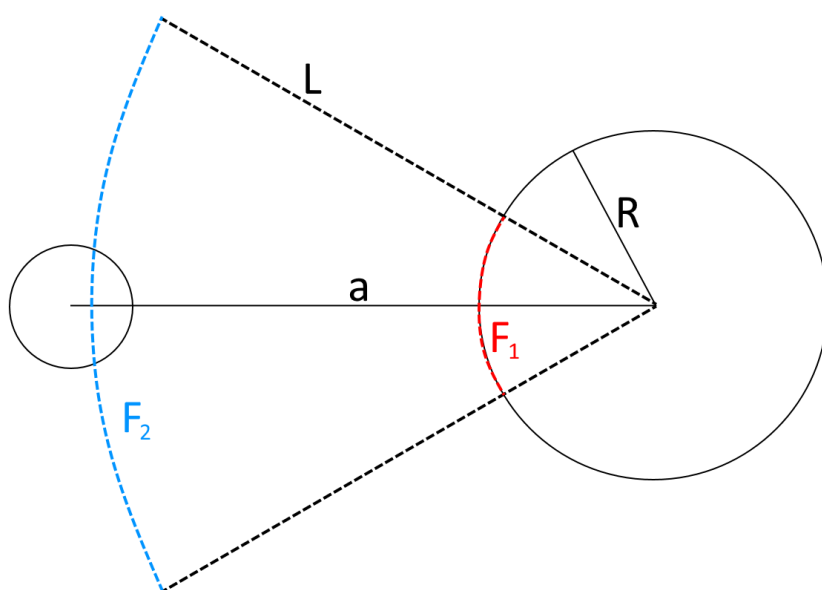


Figure 1.1.: The figure shows a schematic view of the Sun with radius R and a planet at a distance a . The flux at the surface of the Sun (F_1) is different than at the planet (F_2), as it is distributed over a larger area.

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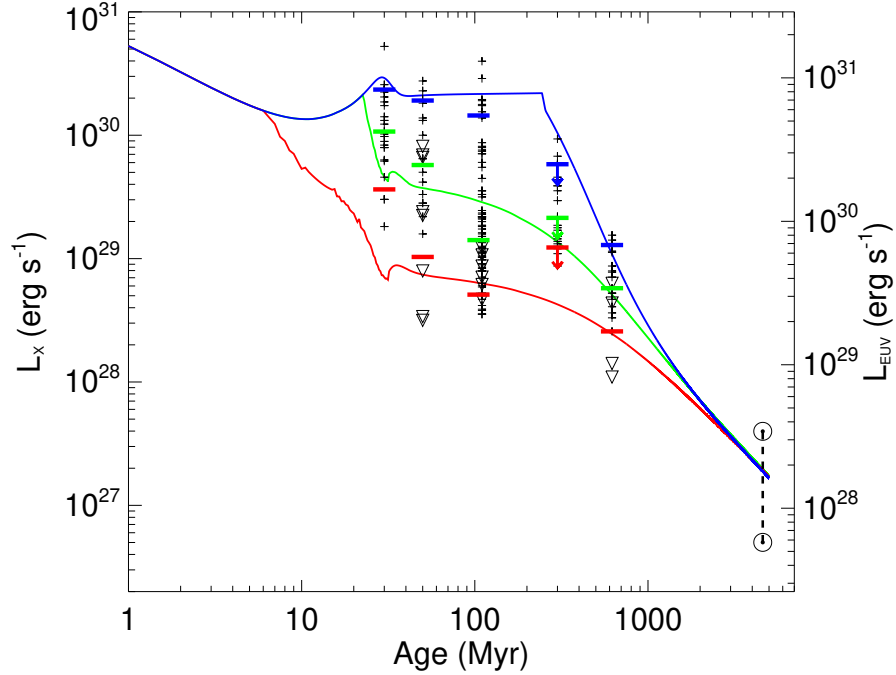


Figure 1.2.: Depending on the initial rotation rate, the Sun’s luminosity evolves differently. The three coloured lines show evolution tracks for a Sun with slow (red), mediocre (green) and fast (blue) initial rotation. The symbols show observed X-ray luminosities of various stars. The difference in luminosity due to the solar cycle are represented by the two solar symbols at 4.5 Gyr.

Tu et al. [2015]. As rotation rate is connected to the activity of a star and therefore, also to X-ray luminosity, a fast rotating star has a higher X-ray luminosity than a slow rotating star (see Fig. 1.2 taken from Tu et al. [2015]). When looking back in time the solar spectrum will, therefore, mostly show differences in the XUV part of the spectrum, but not in the optical and infrared (IR) part.

A recent study by Johnstone et al. [2021a] discovered that the Sun most likely started as a slow rotating star as otherwise CO_2 in Earth’s atmosphere would have been lost too rapidly due to the strong XUV radiation and a lack of CO_2 would have led to insufficient cooling for habitable conditions.

As the Sun evolves with time the X-ray luminosity drops, but can still be related to the extreme ultraviolet (EUV) flux via the relationships shown in Eq. 1.2 and 1.3. EUV1 refers the first segment of EUV wavelengths (10-36 nm) and EUV2 to the second segment (36-92 nm). It is very hard to constrain EUV tracks from observations as the interstellar medium absorbs most of it. Luckily, even though the X-ray luminosity changes with time, the relation between EUV and X-ray seems to stay constant. To derive the EUV part of the spectrum for an earlier stage of the Sun, equations 1.2 and 1.3 can be used (Johnstone et al. [2021b]).

$$F_{EUV1} = 110 \cdot F_X^{0.681} \quad (1.2)$$

$$F_{EUV2} = 0.924 \cdot F_{EUV1}^{0.92} \quad (1.3)$$

1.1.3. Flux and age

As stated in the previous section the activity of the Sun changes depending on the initial rotation period, as does the flux. Therefore, the use of age is ambiguous and we should strictly only speak of fluxes. It is possible, however, to calculate the corresponding age for a given flux, either by using Eq. 1.4 from Tu et al. [2015], which is valid for a slowly rotating Sun with an initial rotation rate of about $\Omega_0 = 1.8 \Omega_{\odot}$.

$$L_x = 2.0 \cdot 10^{31} t^{-1.12} \text{ erg/s} \quad (1.4)$$

1.2. Atmospheres

Atmospheres form alongside their planets and, therefore, have the same source of matter. While a planet grows through collisions of smaller sized bodies, its gravitational sphere of influence grows, and it accretes more and more gas of the surrounding protoplanetary disk. If the planet exceeds a certain size it will end up as a gas giant. If, however, the planet is approximately Earth sized or slightly larger, the result will be a core-atmosphere combination similar to Earth. The exact composition and density of the atmosphere depends on different factors, e.g. the solid size distribution in the disk (Khorshid et al. [2021]), distance to the Sun and, therefore, temperature of the planet, as well as magnetic fields, which protect the atmosphere against the solar wind.

However, an atmosphere can be lost through time. Solar radiation can heat the atmosphere in a way that causes the atmosphere to expand and gas to be lost to space. Impacts and the solar wind can strip away the atmosphere as well. Due to geological processes like outgassing, however, the atmosphere is not necessarily completely lost (Catling and Kasting [2017]). The question is always how fast the atmosphere is lost to space.

In this theses we are especially interested in the heating mechanisms induced by the Sun, which might show a difference in strength depending on the composition of the atmosphere. More heating might lead to higher temperatures (depending on the cooling mechanisms that act against it), which has a direct effect on atmospheric loss. Therefore, this chapter will give an overview about the basic physical concepts of atmospheres, their heating and cooling mechanisms, and how atmospheric escape happens.

1.2.1. Structure of atmospheres

In this thesis we divide the structure of the atmosphere into two parts: upper and lower atmosphere. The lower atmosphere is the part where clouds and hazes exist. The upper

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atmosphere does not have such complicated structures. The border between these two layers is the last turning point of the atmospheric temperature profile. The temperature profile not only gives the border between upper and lower atmospheres, it also provides for a finer definition of the different layers of an atmosphere (see Fig. 1.3). Every turning point sets a new base of a layer. Because the definition of the layers depend on the temperature profile, certain layers might not exist in other atmospheres (e.g. the thermosphere on Venus). The last layer is the exosphere, where the density is already so low that collisions between particles rarely happen (Catling and Kasting [2017]). Therefore, the upper limit of the simulation domain used in our calculations will be the boundary between the thermosphere and the exosphere, called the exobase (more in Chapter 2).

Scale Height

The scale height H is an important parameter when working with atmospheres. It describes the distance in which the pressure of the atmosphere decreases by a factor of e and gives us a good understanding of how the curve for the pressure profile behaves. A small H implies that the pressure decreases rapidly. However, H is not a constant as it varies with altitude (see Eq. 1.5) (Lissauer and de Pater [2013]).

$$H(z) = \frac{kT(z)}{g_p(z)\mu_a(z)m_{amu}} \quad (1.5)$$

Here $g_p(z)$ is the gravitational acceleration at altitude z , $T(z)$ is the temperature at altitude z , and $\mu_a(z)m_{amu}$ is the molecular mass.

1.2.2. Processes in the atmosphere

The solar radiation travels through space towards the planet and hits its atmosphere. Depending on the composition, different parts of the spectrum will penetrate to certain depths triggering different processes, such as photochemistry or heating and cooling processes.

Photochemistry

Photochemistry - as the name suggests - deals with the the effects of light on chemistry. Reactions that fall under this term are caused by absorption of photons in the wavelength regimes of UV, visible or IR.

According to the Grotthuss-Draper law, a species first needs to absorb light so that a photochemical reaction can take place. This can happen when the frequency of the light matches the natural frequency at which the bonds connecting two atoms vibrate. This excites the electrons, which can disrupt the chemical bonds, allowing an electron to break free. If this happens the atom/molecule will be ionised (= photoionisation). It can, however, also disrupt the chemical bonds between atoms which could lead to the breaking up of the molecule (= photodissociation), depending on the wavelength (Reusch, 2013).

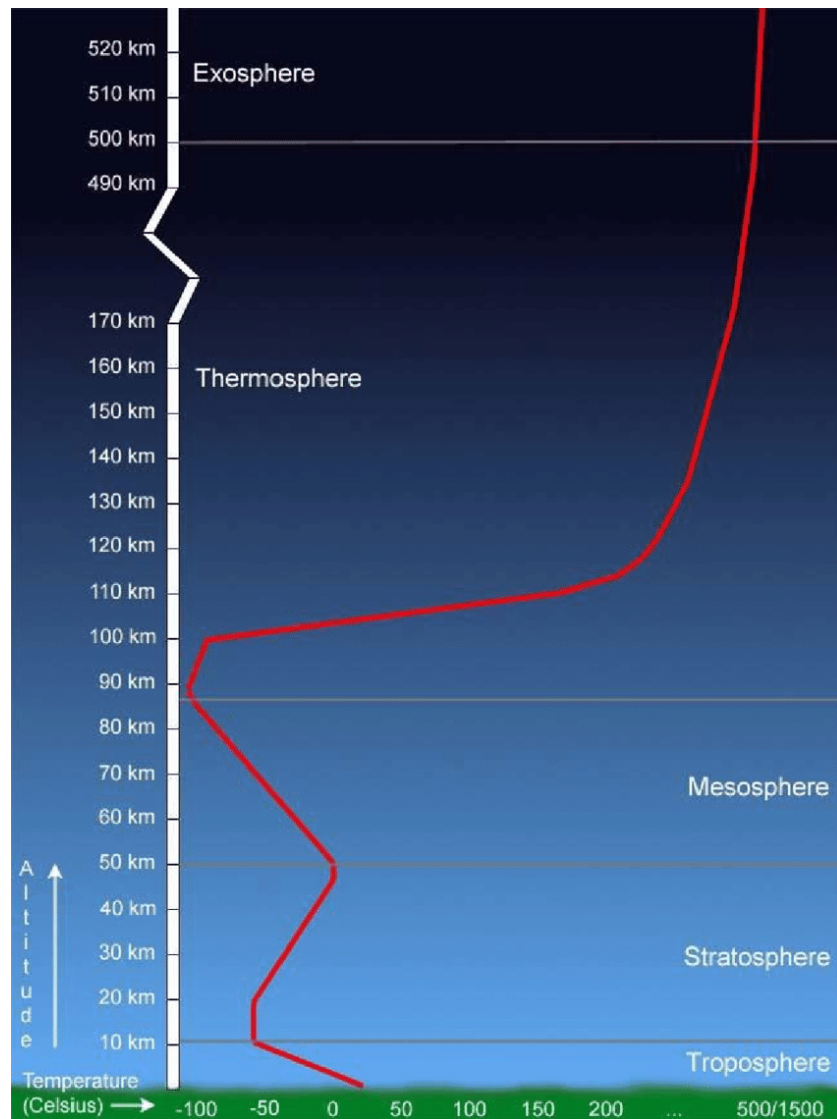


Figure 1.3.: Figure showing the layers of Earths atmosphere, figure taken from Rao [2018].

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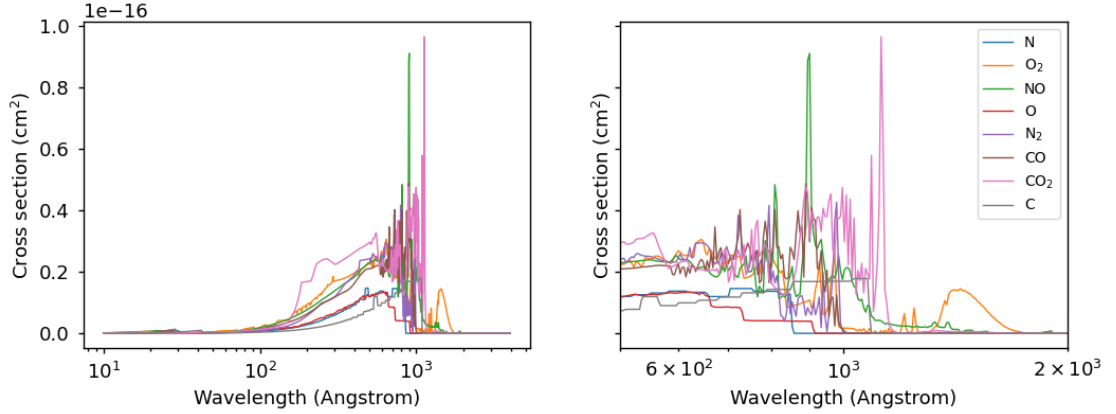


Figure 1.4.: Both figures show the cross sections of the main species in Venus's atmosphere. The right plot presents the same data as the left plot over a smaller wavelength range, and, therefore, shares the same y-axis scale.

As every molecule vibrates at a different frequency, each one absorbs clearly defined levels of electromagnetic radiation. How likely it is that a certain wavelength is absorbed by a molecule or atom is given by the cross section, shown in Fig. 1.4.

If the reactants only absorb radiation with specific frequencies, photodissociation and photoionisation also depend on the species and their natural frequency. CO₂ is a very good IR absorber. Its cross section shows, however, that it also absorbs XUV very well. In Earth's atmosphere CO₂ absorbs UV radiation above 85 km which leads to the heating of the CO₂ molecule. Lissauer and de Pater [2013] explain that the optical depth is larger for high energy photons and that photodissociation or photoionisation are more likely to occur at higher altitudes. At lower altitudes on the other hand, recombination dominates, which is the reverse reaction to photodissociation. Vertical transport acts as a balancing mechanism between dissociation and recombination.

Diffusion

Diffusion can be seen as the motion of particles from a region of high concentration to a region of low concentration and has nothing to do with the properties of the particles themselves. While atoms and molecules are lost to space, diffusion supplies the atmosphere with more particles. Therefore, the speed with which diffusion happens puts a limiting factor on how much of a species is lost to space. We distinguish between two different diffusive processes: eddy diffusion and molecular diffusion.

In a gas of moving particles, swirls can occur. These swirls, also called eddies, cause mixing on a wide scale range, depending on the kinetic energy. Over time, kinetic energy is lost, and the eddies get smaller until viscosity becomes a limiting factor. This type of mixing is called eddy diffusion. It is the dominating process in the homosphere, as this is the atmospheric layer where turbulence occurs.

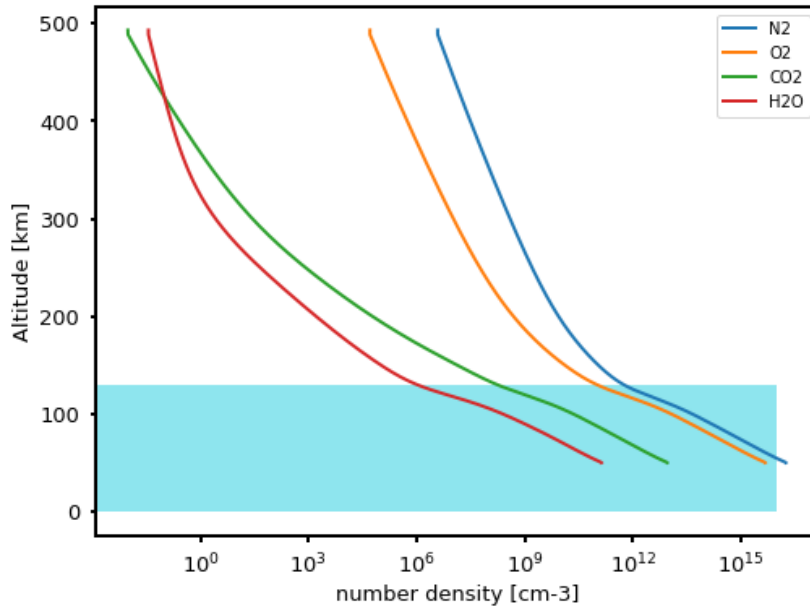


Figure 1.5.: The cyan area indicates the layers below the homopause, where the gas is well mixed, with each species following the pressure scale height of the whole gas. Above the homosphere the species follow their own pressure scale height and lighter species like H_2O become more abundant than heavier ones like CO_2 .

Eddy diffusion is the mixing of particles due to turbulence. Molecular diffusion comes from the random motion of individual particles. As lighter species are less affected by gravitational forces, they can move higher in the atmosphere, separating heavier from lighter species, as can be seen in Fig. 1.5. This process additionally depends on the temperature and pressure of the gas (García Muñoz [2007a]). This is known as molecular buoyancy diffusion, where heavier species have higher concentration at lower altitudes (Lissauer and de Pater [2013]).

Heating and cooling

There are many different processes that lead to heating or cooling of the atmosphere. The main source for heating is solar radiation, in the upper atmosphere specifically XUV (Kang et al. [2019]), which is mostly absorbed by neutral atoms and molecules. The quantum state of the molecule will be excited when it absorbs XUV radiation and a small amount of energy will be transformed into kinetic energy which will result in heating. The molecule or atom might also get ionised.

Joule heating creates heat when an electric current passes through a conductor. In the case of the atmosphere, the friction between moving ions and the neutral gas causes this

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electric current. Photoionisation enhances the ionospheric conductivity by increasing the ion and electron densities. This affects the ionospheric currents and, therefore, Joule heating also feels a positive effect from XUV radiation.

Additionally, solar radiation provides the energy for exothermal chemical reactions, and the increase of kinetic energy leads to heating through collisions.

Cooling can happen when an excited molecule, such as CO_2 or H_2O , emits radiation to get back into a lower state of energy.

Both of these processes will be analysed in detail in Chapter 3.

Two important mechanisms that balance heating and cooling are conduction and convection. Conduction transfers energy through collisions: If one region has an excess of energy this will be transported to a cooler region through conduction. Convection on the other hand is caused by a density gradient due to temperature differences. Both processes transfer energy from a warm region to a cooler region, which results in equalising the temperatures of those two regions (Lissauer and de Pater [2013]).

1.2.3. Atmospheric escape

As mentioned in the previous sections, solar radiation transfers kinetic energy to a particle. If the kinetic energy is larger than the gravitational binding energy and the particle moves in an upward direction, the particle may escape from the atmosphere if no other particles are in its way. This region where potential escape happens is called the exosphere (Lissauer and de Pater [2013]).

However, particles cannot only be lost to space due to thermal (Jeans) escape caused by solar radiation, but also due to non-thermal escape. Additionally, impacts play a big role in stripping away large chunks of the atmosphere, and the role of hydrodynamic escape is important when it comes to losing species that would usually be too heavy to be lost via Jeans escape.

For this thesis the escape mechanism of interest is Jeans escape, as this is what is calculated by the model we are using (see Chapter 2).

Jeans Escape

Particles move with velocities according to a Maxwellian probability distribution. Even though the distribution covers velocities up to infinity, one can say that the largest velocities are four times higher than the most probable one to simplify the problem, given by the following equation:

$$v_0 = \sqrt{\frac{2kT}{m}} \quad (1.6)$$

If the velocity of a particle becomes larger than the planet's escape velocity it could potentially be lost to space. Jeans Escape is based on the probability with which a particle moves a distance larger than the atmospheric scale height, without colliding with another particle (Rouan [2015]). This tendency to escape is represented by the Jeans parameter λ_{Jeans} in Eq. 1.7, with the mass of the planet M , the mass of the particle m ,

temperature T , radius R and altitude z .

$$\lambda_{Jeans} = G \cdot \frac{Mm}{k_B T(R+z)} \quad (1.7)$$

This can further be expressed as the ratio between the escape velocity and the Jeans velocity squared: $\left(\frac{v_e}{v_0}\right)^2$.

Since it is of interest to derive the number of particles that escape to fully understand the consequences of Jeans escape, it is helpful to introduce the Jeans flux:

$$F_{Jeans} = \frac{n_{exo} v_0 (1 + \lambda_{Jeans})}{2\sqrt{\pi}} \cdot e^{-\lambda_{Jeans}} \quad (1.8)$$

The Jeans flux gives an escape rate in atoms per area per second. It is usually calculated for a specific species with mass m that goes into the Jeans parameter and number density at the exobase n_{exo} .

Note that Jeans escape is not significant for heavier species as $\lambda_{jeans} \propto m$. By looking at Eq. 1.8 it can be easily seen that the higher the mass, the larger the Jeans parameter and, therefore, the smaller the Jeans flux.

1.2.4. Non-thermal and Hydrodynamic Escape

In most atmospheres that are not fully hydrodynamic (no extreme temperature and pressure), the dominant escape mechanism is non-thermal escape. This includes dissociation of molecules, charge exchange, and sputtering.

The X-ray part of the solar spectrum can induce enough energy for ionisation and dissociation to happen, which in turn changes the composition but also heats up the atmosphere, leading to higher escape rates (Lammer et al. [2009]).

Atmospheric loss through charge exchange happens when a hot ion (e.g. H^+) - hot meaning fast moving - collides with a neutral atom (H). The hot ion becomes a neutral atom, but it continues to move fast and, therefore, can be lost to space (Catling and Kasting [2017], Lissauer and de Pater [2013]).

The solar wind can knock atoms out of the atmosphere by transferring enough energy through collisions with fast moving atoms or ions. This process is called sputtering and is more likely caused by ions than atoms as they can be accelerated for example by a magnetic field in a much easier way than atoms (Lundin et al. [2007]).

Planets with magnetic fields like Earth can lose atoms over the magnetic poles, where the field lines are open. Ions (especially H^+) can easily escape along the field lines, when accelerated upwards through Landau resonance with kinetic Alfvén waves by XUV radiation of the Sun (Bingham et al. [2013]). This is called polar wind. On Earth approximately 15% of H escapes in this way (Catling and Kasting [2017], Yung et al. [1989]).

On planets without a global dipole magnetic field, the solar wind interacts primarily with the ionosphere, which can lead to severe atmospheric loss, in case of a small planet like

1. Introduction

Mars (Catling and Kasting [2017]).

Hydrodynamic escape plays an important role in the early Solar System, where the energy input is high enough for this mechanism to occur. Here, lighter species drag heavier species with them which would not escape by themselves according to the Eq. 1.7. According to Tian et al. [2008a] this is the case for an Earth-like atmosphere once the solar UV intensity is greater than five times the current solar UV intensity. This scenario only occurred during the Hadean epoch on Earth, assuming the Sun was a slow rotator (Johnstone et al. [2018]).

1.3. Venus

Venus is a rocky planet that is slightly smaller and less massive than Earth, which formed 4.5 - 4.6 billion years ago by accretion of surrounding disk material. Even though the formation history might be very similar to the Earth's, Venus still ended up with much higher surface temperatures (up to 740 K) due to its thick atmosphere and slow retrograde rotation. An additional effect of the slow rotation and the lack of internal thermal convection is that Venus does not have a significant magnetic field ($7.0 \cdot 10^{-5} G$ according to Zhang et al. [2016]).

These characteristics lead to uninhabitable conditions, giving rise to the question of where it went "wrong" and if Earth might have a very similar future ahead.

1.3.1. Surface, Volcanism and Plate Tectonics

Venus has a crust thickness of between 8 - 25 km according to James et al. [2013], while Williams et al. [2020] specify a lithosphere of 12 - 35 km. This is more than twice as much as Earth's oceanic crust (3 - 10 km) but thinner than the 35 - 40 km continental crust (Perfit [2016]). The surface pressure of 92 bar leads to the fragmentation of impacting bodies smaller than 1 km, explaining the lack of recent smaller impact craters on Venus (Odert et al. [2018], Salvador et al. [2017]). Due to the thickness of its crust and the lack of water (which would lower the viscosity of rocks, helping plates to slide around), there is no plate tectonics, leaving few options for the heat of the interior to escape.

Venus shows a large number of volcanoes in different sizes and shapes, meaning global volcanism is one method for the planet to release trapped heat. Heat accumulates until the upper mantle liquefies and breaks through the surface. Once the heat is released, the upper mantle will solidify again, leaving a new surface. Because of its volcanic activity Venus' atmosphere is N and C rich. If Earth didn't have plate tectonics it would probably have a lot of N and C in the atmosphere too (Catling and Kasting [2017]).

Even though Venus does not harbour liquid water it is not clear yet whether it started wet and lost it over time, or if it had always been dry. The high ratio of Deuterium and Hydrogen (D/H) supports the wet Venus theory: As H escapes over time the D/H ratio increases, because D is more difficult to lose. This does not mean, however, that large amounts of water are required to get these values. Impacts could have resupplied the water content or hydrodynamic escape of hydrogen could have carried away the deuterium.

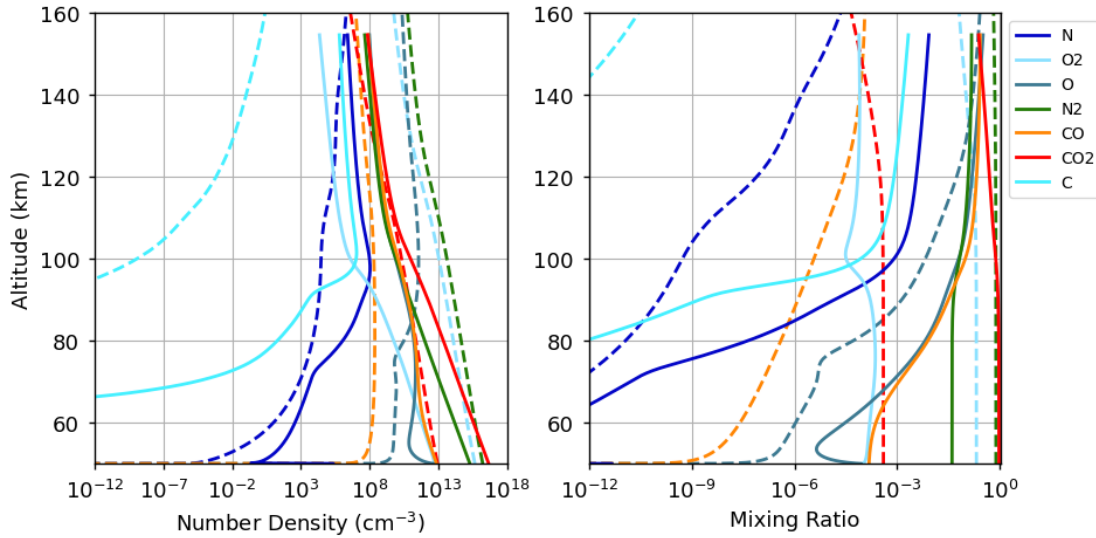


Figure 1.6.: The dashed lines show Earth's profiles, solid lines are Venus profiles. Generated by Kompot for base densities of modern Venus and modern Earth.

The dry young Venus theory, however, was widely dropped after the first publications of the D/H ratio (Catling and Kasting [2017]).

1.3.2. Atmosphere

Even though Venus formed in the same protoplanetary disk as Earth, its atmospheric composition is very different in terms of mixing ratios. According to Chassefière et al. [2012] the Nitrogen and Carbon mixing ratios are twice as high as Earth's atmosphere, hydrosphere and sediments, and in terms of column mass we find values that are even more extreme: The N_2 column mass of Venus is three times higher than on Earth, and CO_2 columns mass is 3500 times higher.

At first glance this seems like a lot. However, it can be easily explained when looking at Earth's rocks, where most of the near-surface N and C is locked. If the C and N in all the rocks on Earth would suddenly convert to their gaseous forms in the atmosphere, we would end up with similar values for the partial pressures as on Venus.

On Venus these constituents are not locked up due to the lack of water (Catling and Kasting [2017]), and, therefore, it is no option for the slow carbon cycle to remove CO_2 from the atmosphere. Even though Venus might have had Hydrogen at the beginning of its life, most of this was lost due to hydrogen escape.

To visualise the difference in composition, models for the species profiles of Earth and Venus were generated by the Kompot code (see Chapter 2) as shown in Fig. 1.6.

Venus is only hot on the surface, as can be seen in Fig. 1.7. The temperature rapidly

1. Introduction

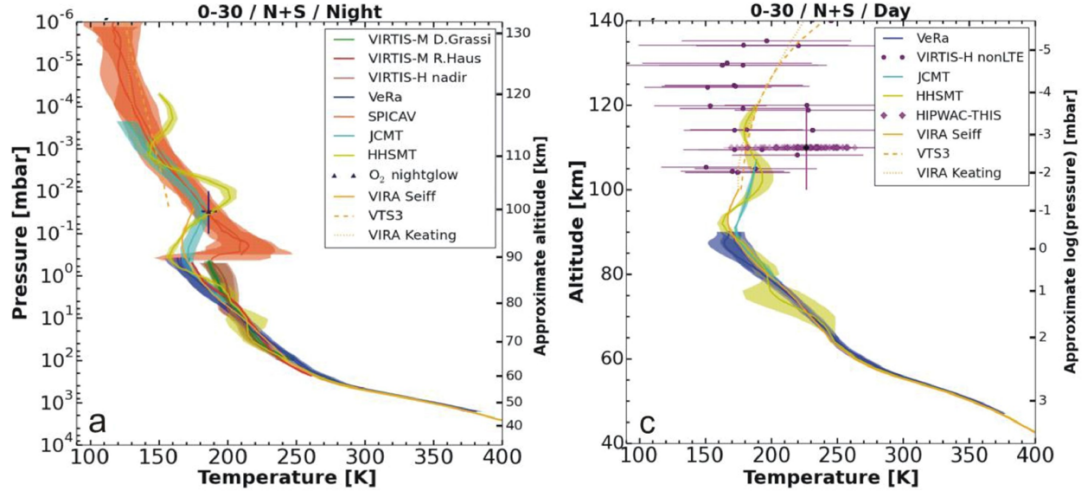


Figure 1.7.: The figures show the temperature profiles of Venus for the nightside (left) and the dayside (right) between latitudes of 0 - 30° adapted from Limaye, 2017.

declines until approximately 100 km and then has a turning point where it starts increasing slightly. There is a difference between the day and the nightside in the upper atmosphere temperature, as during the night no solar XUV radiation hits the atmosphere on this side, allowing the thermosphere to cool down. This already indicates that XUV heating has a strong impact on the upper atmosphere - a hypothesis which will be tested in Section 3.1.

Greenhouse effect

The temperatures in Venus's lower atmosphere can be ascribed to the greenhouse effect, which is a feedback loop in which the temperature keeps increasing. The most important greenhouse gases on Earth are CO₂, CH₄, O₃ and H₂O. On Venus CO₂ and - if there was water present - H₂O take on this role. H₂SO₄ acts as an opposing, cooling key factor. Sulfur gases condense exothermically into H₂SO₄ clouds, which reflect almost 80% of the incoming radiation (Crisp [2012]) and, therefore, keep the surface temperatures at about 730K.

No matter whether there was water in the past or not, it was eventually lost. But without water as a sink for CO₂, the temperatures can increase unhindered, resulting in a runaway greenhouse.

2. The Kompot Code

In recent years, a 1D first-principles physical planetary atmosphere model, called The Kompot Code, has been developed that calculates the thermal, chemical, and hydrodynamic processes taking place in the upper atmospheres of planets in response to the XUV spectral flux of stars. Additionally it takes the planet's mass and radius as well as its atmospheric properties at the base of the simulation as input parameters. Its simulation domain reaches from an arbitrary altitude up to the exobase and breaks the gas within this domain down into species, including electrons, neutrals, and ions.

There are three assumptions taken:

- The gas has one bulk advection speed, which the entire gas shares.
- Neutrals, ions and electrons have their own temperatures.
- Electrons and ions have the same density (= quasineutrality).

Depending on the changes in temperature and composition due to the radiation, the atmosphere expands or contracts within a predefined grid (see Section 2.1.1). X-ray, UV and IR radiation are transported through the atmosphere, where photoionisation reactions can produce non-thermal electrons. Apart from photoionisation, other atmospheric chemical reactions which are driven by impacts with non-thermal electrons are included. Molecular and eddy diffusion as well as different heating and cooling mechanisms such as neutral heating, electron heating, infrared cooling, and conduction are handled by the code. Johnstone et al. [2018] provide a detailed explanation of these processes in their benchmark paper.

2.1. Parameters

The Kompot code provides a parameter file where the most important parameters can be adjusted such as the grid parameters, chemical composition, input spectrum, physical parameters of the planet (radius R , mass M , semi-major axis a), as well as heating and cooling mechanisms used. This section will introduce the most important parameters, and how they are implemented in the code.

2.1.1. The Grid

The 1D grid (illustrated in Fig. 2.1) is defined through four main properties: lower limit of the simulation domain in km (z_{min}), upper limit of the simulation domain also in km

2. The Kompot Code

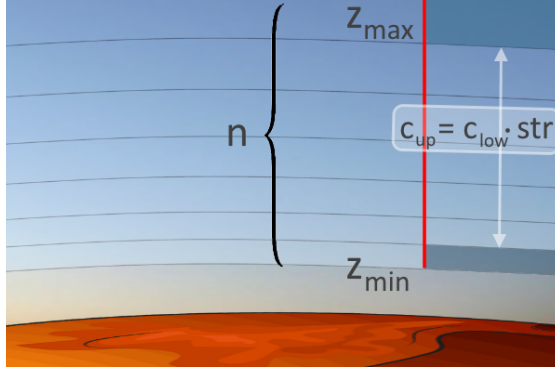


Figure 2.1.: The parameters that make up the grid are shown: z_{max} and z_{min} give the upper and lower limits of the grid in km, n gives the number of cells ($n = 7$ in this example). The stretch factor str gives the proportion of the lowermost c_{low} and the uppermost cell c_{up} . Note, that the code is a 1D code and this figure only acts as an illustration of the basic concept.

(z_{max}), number of cells (n), and the stretch factor (str), which gives the factor of how much bigger the uppermost cell is compared to the lowermost cell.

The stepsize dx is the distance between two neighbouring cells and increases linearly in altitude as shown in Fig. 2.2. There it is also clearly visible that fewer cells require a more rapid increase in stepsize, than grids with more cells. The gradient in stepsize Δdx , therefore, is also very large, while grids with a larger number of cells tend to have a smaller gradient. The figure also shows that the effect of the number of cells dominates over the stretch factor, as the stepsize at the exobase dx_{exo} spans over a wider range than for grids with constant stretch factor but changing number of cells. The example of $str = 100$ shows that for 550 cells dx is approximately 1.1, but for 200 cells dx is 4, which is a difference of $\Delta dx \approx 2.9$. Keeping the number of cells constant, on the other hand, will produce a $\Delta dx \approx 0.75$ for 550 cells.

Another thing that can be seen in this figure are the ghost cells. These are the first three cells with fixed sizes that set the base of the simulation. The smaller the stretch factor, the larger those ghost cells.

Once the grid is set up, the atmosphere can expand into it. The code will calculate initial profiles and within small timesteps determine whether the atmosphere expands or contracts. If the altitude of the exobase reaches or exceeds z_{max} , the simulation will stop because there are no more grid cells the atmosphere could expand into. Then z_{max} needs to be increased manually, and the simulation restarted. However, if one wants to keep the proportions of the cells the same, the number of cells and stretch factor need to be adjusted as well.

Lets imagine we have an old grid, with a defined lowermost cell $d_{old,1}$, an uppermost cell $d_{old,m}$ and number of cells m , as well as a stretch factor s_{old} . Then we want our new grid to have a lower most cell $d_{new,1}$ with the same size as $d_{old,1}$. We also assume that the m 'th cell of the new grid has the same size as the m 'th cell of the old grid. The new grid,

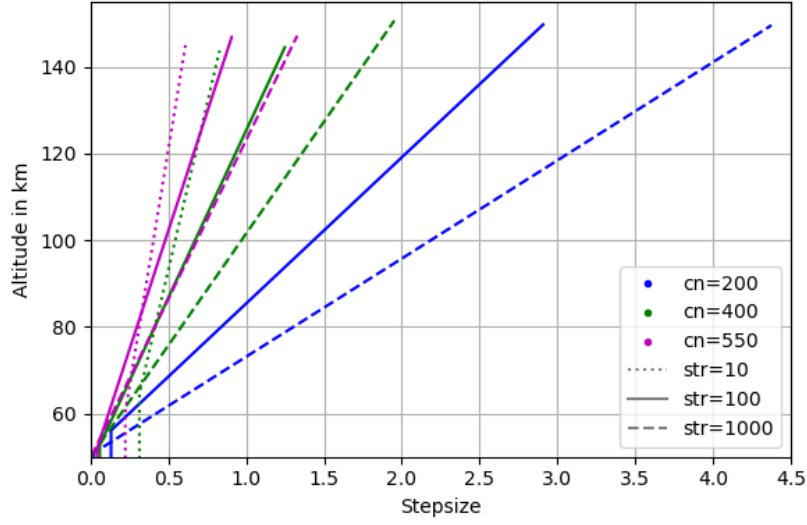


Figure 2.2.: Different colours represent different numbers of cells, while the linestyle indicates the stretch factor. One can see, that the stretch factor has a dominating effect over the number of cells. The straight lines in the first few kilometers are due to the ghost cells, which have a fixed size.

however, has a higher number of cells (n) than the old one, $n > m$. We define:

$$d_{old,m} = s_{old} \cdot d_{old,1}, \quad d_{old,i} = \frac{i}{m} \cdot s_{old} \cdot d_{old,1} \quad (2.1)$$

As mentioned before, we want the lowest cell of the old and the new grid to be the same, as well as the m 'th cell:

$$d_{old,1} = d_{new,1}, \quad d_{old,m} = d_{new,m} \quad (2.2)$$

With $d_{old,i} = d_{new,m} = \frac{m}{n} \cdot s_{new} \cdot d_{new,1}$ and $d_{old,1} = d_{new,1}$ we get:

$$\begin{aligned} d_{old,m} &= d_{new,m} \\ s_{old} \cdot d_{old,1} &= \frac{m}{n} \cdot s_{new} \cdot d_{old,1} \\ \frac{s_{old}}{m} &= \frac{s_{new}}{n} \end{aligned} \quad (2.3)$$

From this equation we see that the only thing we need to worry about, when changing the size of the grid, is the ratio between stretch factor and number of cells. To calculate these, we first need to define the maximum altitude of the grid z_{max} , which can be simply found by summing up the cells:

$$z_{old,max} = \sum_i^m d_{old,i} = \sum_i^m \frac{i}{m} \cdot s_{old} \cdot d_{old,1} = \frac{m+1}{2} s_{old} \cdot d_{old,1} \quad (2.4)$$

2. The Kompot Code

With the ratio of stretch factors just found and with the lowest cells having the same size, we rearrange until we end up with a quadratic equation as shown in Eq. 2.5 and its solution Eq. 2.6:

$$n^2 + n - \frac{z_{new,max}}{z_{old,max}}(m+1)m = 0 \quad (2.5)$$

$$n = -\frac{1}{2} \cdot \left(1 \pm \sqrt{1 + 4m(m+1)\frac{z_{new}}{z_{old}}} \right) \quad (2.6)$$

A test example shows that a grid of originally 500 grid cells ($m=500$), a stretch factor of 350 ($s_{old} = 350$) and a maximum altitude of 1200 ($z_{max} = 1200$) which ran out of space, can easily be restarted: Setting the new maximum altitude to 2400, and inserting the old values into Eq. 2.6, we derive $n_1 = 707$ and $n_2 = -708$, with the latter one being an unphysical solution, which can be dropped. The corresponding stretch factor would then be 495, gained from Eq. 2.3.

2.1.2. Spectra

Kompot takes an input spectrum in the form of tabulated values of energy (eV) and irradiance ($\text{eV s}^{-1} \text{ cm}^{-2} \text{ Hz}^{-1}$), and already provides a set of Sun spectra created by Claire et al. [2012], which carry solar fluxes at Earth. The spectra can be easily changed by adding files to the folder and then referring to them in the parameter file.

The spectra provided are labeled with the age of the Sun in gigayears ago (Gya). This, however, assumes a certain evolutionary track of the Sun, and is normalised to Earth's distance. For this thesis, the crossmatch between fluxes and ages is, therefore, not valid, as the fluxes first need to be normalised to Venus distances. Only then the solar fluxes and ages can be matched.

A conversion from fluxes at Earth to fluxes at Venus can be done by simply multiplying $f_x \cdot \left(\frac{a_E}{a_V}\right)^2$ (see Fig. 1.1), where a_E is the distance of Earth to Sun, and a_V is the distance of from Venus to the Sun.

2.1.3. Chemistry

The chemistry can be set in the parameter file by specifying the initial composition in terms of mixing ratios. Kompot - if not told otherwise - will assume that all species exist in the atmosphere, even if not specifically set in the parameter file. It will assume the minimum number of particles needed for the calculations to not diverge, which is of order of 10^{-30} cm^{-3} . This means that even in atmospheres with initial compositions of $N_2 + CO_2 = 100\%$, hydrogen species will appear. There is, however, the option of turning specific species off completely with the parameter *maskspecies*.

Kompot combines the chemical Networks of Fox and Sung [2001], Verronen et al. [2002], Yelle [2004], García Muñoz [2007b], Tian et al. [2008b], Richards and Voglozin [2011], Fox [2015], Fox et al. [2015], as well as rate coefficients and some reactions of the KIDA

database (Wakelam et al. [2012]). The photoreactions are taken from the PHIDRATES database by Huebner and Mukherjee [2015].

2.1.4. Heating and Cooling

The atmosphere can be heated up and cooled down in different ways. Kompot comprises five different heating mechanisms, and three different cooling mechanism. The heating mechanisms included are the following:

1. XUV heating
2. Chemical heating
3. IR heating
4. Photoelectron heating
5. Joule heating

XUV heating comes from the excess energy after absorbing a photon and using it for photochemistry. Let's say a CO_2 molecule absorbs a 10 eV photon - which is not in the XUV range, but we just choose this for the sake of the example. For it to create CO and O 3 eV are needed, so the additional 7 eV go to heating. Chemical heating is the heating through exothermic reactions, and as photoreactions are already being treated in XUV heating they are excluded from this mechanism. IR heating comes from the energy that is removed from the IR field as it passes through the atmosphere, and only includes CO_2 , due to Venus' composition. Photoelectron heating is created by absorption or collision with non-thermal electrons, while Joule heating is caused by friction of the ions that travel through the gas of neutral species. The latter one will only heat up the neutral gas.

The three cooling mechanisms implemented in the code are:

1. CO_2 cooling
2. O cooling
3. NO cooling

O and NO cooling are implemented in a quite simple way, where the number density of the species is multiplied by some coefficient.

CO_2 cooling is slightly more complicated. Here the CO_2 particle has absorbed some energy, and will emit it in IR in all directions. Therefore, half of the heat radiated away will go in the direction of space, and the other half will remain on the planet. Of course this heat could be absorbed by other CO_2 molecules again, which would again radiate half of it away. On average the assumption of half of the heat being radiated to space is, therefore, a good approximation. The remaining heat stays in that specific cell, and will not be redistributed.

2. The Kompot Code

2.2. Initialization, Flow, and End Criterion

Kompot initialises a grid based on the grid parameters in the parameter file. The grid at this point only holds information about the radius. In the next step, the temperatures are set to the base temperature in all cells, likewise for the species structure which is set to the base densities, assuming a hydrostatic structure.

As this can be a rather poor representation of an atmosphere it is advised to restart simulations from previous runs, where a good solution has already been found. This will drastically improve the runtime.

The timestep in which Kompot updates the atmosphere is dynamically adjusted. It goes through the entire atmosphere looking at the size of the cell and the advective speed, which gives the speed with which a particle could leave a cell. It then takes the smallest possible time, so that a particle will never "randomly" leave a cell. The timestep represents actual time in which chemistry, diffusion and energy exchange happen.

The criterion on which ending the simulation is based has to do with the mixing ratios: When the mixing ratios remain the same over a long period of time, we speak of a steady state, and the simulation can, therefore, be stopped. Currently this is not automated, so one needs to check and end the simulation by hand.

2.3. Output

Kompot produces a large volume of data, saving temperature and species profiles, as well as heating and cooling rates for reactions and species, among others. For more details see the benchmark paper Johnstone et al. [2018]. Here we will only briefly show how energy deposition and loss rates are calculated.

2.3.1. Energy deposition

Energy deposition is an important quantity when the goal is to understand where the received energy from the Sun is used. It is calculated by summing over the energy bins, at a specific altitude per species (see Eq. 2.7). The indices i , j , and k refer to radius, species, and energy bin respectively. σ is the cross section, which depends on the species and the energy bin that is currently being looked at, n gives the number density of that species, and F_{XUV} represents the flux of an energy bin k at radius i .

$$Q_{photoreactions,i,j} = \sum_k \sigma_{j,k} \cdot n_{i,j} \cdot F_{XUV,k,i} \quad (2.7)$$

The flux gets updated every few hundreds of timesteps. Kompot looks at how much flux is received in a specific layer by using the equation of radiative transfer.

The irradiance received by one cell lower in the grid is equal to the received irradiance of the current cell multiplied by a factor which includes the opacity and the thickness of the layer:

$$I_{j-1} = I_j \cdot e^{-\kappa \cdot dx} \quad (2.8)$$

The term κ represents the XUV absorption coefficient of each energy bin and is calculated by multiplying the number density of each element with its cross section and summing over all absorbing species.

2.3.2. Atmospheric loss

Loss rates are a very important property when talking about the stability of atmospheres. A quick estimate can be obtained by Jeans loss, which was already mentioned in Section 1.2.3. The three equations Kompot uses to determine the loss rates are Eq. 1.6 for the thermal velocity at the exobase, Eq. 1.7 for the Jeans parameter, and Eq. 1.8. All three equations are calculated for all species. It is, therefore, possible to track how quickly a specific species will be depleted. By summing the loss rates it is, however, also possible to estimate the time until the whole atmosphere would be lost. This of course assumes that the atmosphere is not replenished by processes on the surface, like volcanism, and also assumes the loss rates do not change as species escape, because it is assumed that the underlying atmospheric composition stays constant.

2.4. Grid study

In order to understand in which ways the setup of the grid might affect the results, a grid study was performed. For this we tested the number of cells as well as the stretch factor, and specifically looked at the species altitude profiles as well as the temperature profiles as a comparison factor.

2.4.1. Grid study 1: A rough estimate

The setup for the first study was chosen to be a modern Earth case, meaning the planet was located at Earth's distance, with one Earth mass and radius and irradiated by the current Sun, but with a chemical composition of $N_2=50\%$ and $CO_2=50\%$. In Fig. 2.3 the full parameter space of the tested simulations is shown. One can easily see that simulations with small stretch factor and small number of cells produce errors, while large stretch factors at high numbers of cells exceed the runtime we set as reasonable (runtime should not exceed 10 days, as most simulations are done within a day). While we have not tested for the exact reason for this to happen, it is safe to say that in the first case the cells and, therefore, also the gradients are simply very big, which always leads to calculation problems. In the second case there are too many cells that also are unnecessarily small at the bottom, which leads to an excessive number of calculations.

To test the effect of different stretch factors, the number of cells was fixed while comparing the resulting profiles of simulations with number of cells $cn = [200, 300, 400, 450, 550, 600, 700]$. The choice of 450 and 550 (instead of $cn = 500$) was taken due to an error occurring, when setting cn to 500. This issue only occurs when running the simulations on the Vienna science cluster (VSC) 4, but not for VSC3 or local runs, and is still under investigation.

2. The Kompot Code

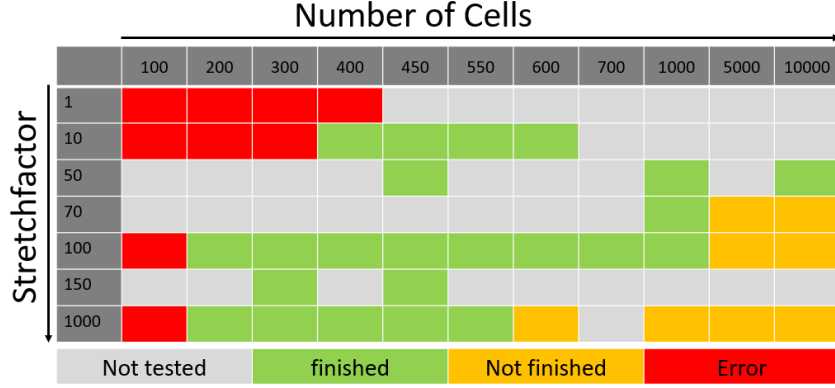


Figure 2.3.: This figure shows the tested parameter space for Grid study 1.

The temperature profiles of all runs are very similar, the maximum difference being at the exobase with $\Delta T = 20$ K (see Fig. 2.4). A linear correlation between larger cn and accuracy of the results can not be found. While the cases of $cn = 200$ and $cn = 400$ result in different temperatures at the exobase, the temperature profiles of $cn = 300$ overlap perfectly, while $cn = 450$ gives better results than $cn = 400$. It should also be noted that $cn = 550$, 600 , and 700 give similar results as $cn = 450$.

To test the effect of different number of cells cn , the stretch factor was set to 10, 100, and 1000, and cn was set to six different values: 300, 400, 450, 550, 600, 700. When looking at the temperature profiles none of the cases seem to differ by much. Only when the stretch factor is very large, differences at the exobase appear. Interestingly the changes do not linearly increase or decrease with the number of cells, but seem to be distributed rather randomly (see Fig. 2.5).

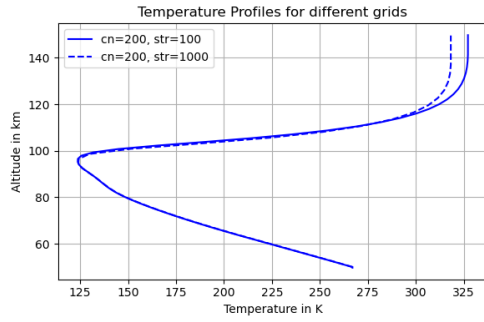
The lowest temperature is obtained in a grid with $cn = 200$, while $cn = 400$ results in the highest temperatures, with a difference of $\Delta T_{200,400} \approx 30$ K. If one compares the Jeans parameters for these temperatures one sees that a difference of 30 K affects the Jeans parameter by almost 10%, as pointed out in Eq. 2.9.

$$\frac{\lambda_{200}}{\lambda_{400}} = \frac{(T + 30)}{T} \quad \underline{T = 320K} \rightarrow = 1.09 \quad (2.9)$$

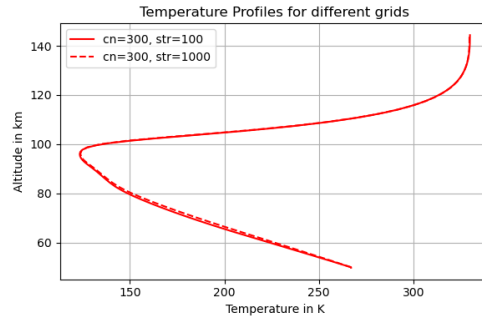
This is a rather large difference and, therefore, it is not advised to use stretch factors in the order of 1000.

When comparing the density profiles of different species, the upper part of the atmosphere (above 100 km) stays mostly unaffected by the choice of grid as well as the density profiles of the two most common species in Venus's atmosphere: CO_2 and N_2 . O_2 was chosen as an example species where the grid does seem to make a difference, however, only for stretch factors of 100 and 1000 (see Fig. 2.6). In both cases we see differences of about two orders of magnitude.

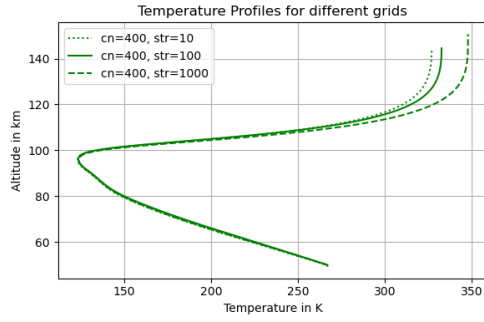
2.4. Grid study



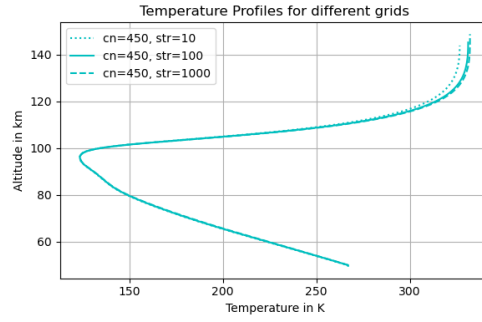
(a) $cn = 200$



(b) $cn = 300$



(c) $cn = 400$



(d) $cn = 450$

Figure 2.4.: The four figures show temperature profiles for Earth simulations, with $N_2=50\%$ and $CO_2=50\%$ as starting conditions. The only difference is in the setup of the number of cells cn .

2. The Kompot Code

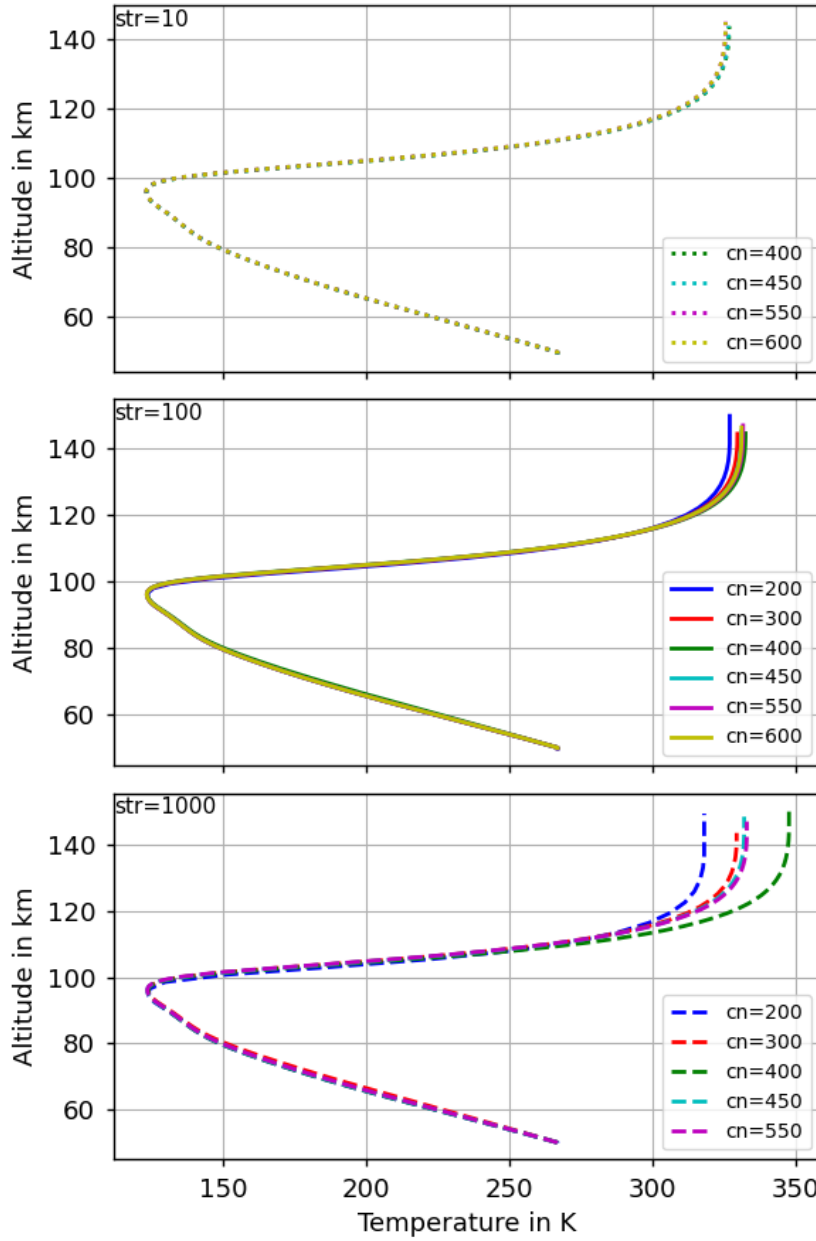


Figure 2.5.: This figure shows the temperature profiles of different grids. The setup is again for Earth with $N_2=50\%$ and $CO_2=50\%$ (normalised to total = 1). The figures fix the stretch factor at $str = 10$ (top panel), $str = 100$ (middle panel), and $str = 1000$ (bottom panel) and vary only the number of cells.

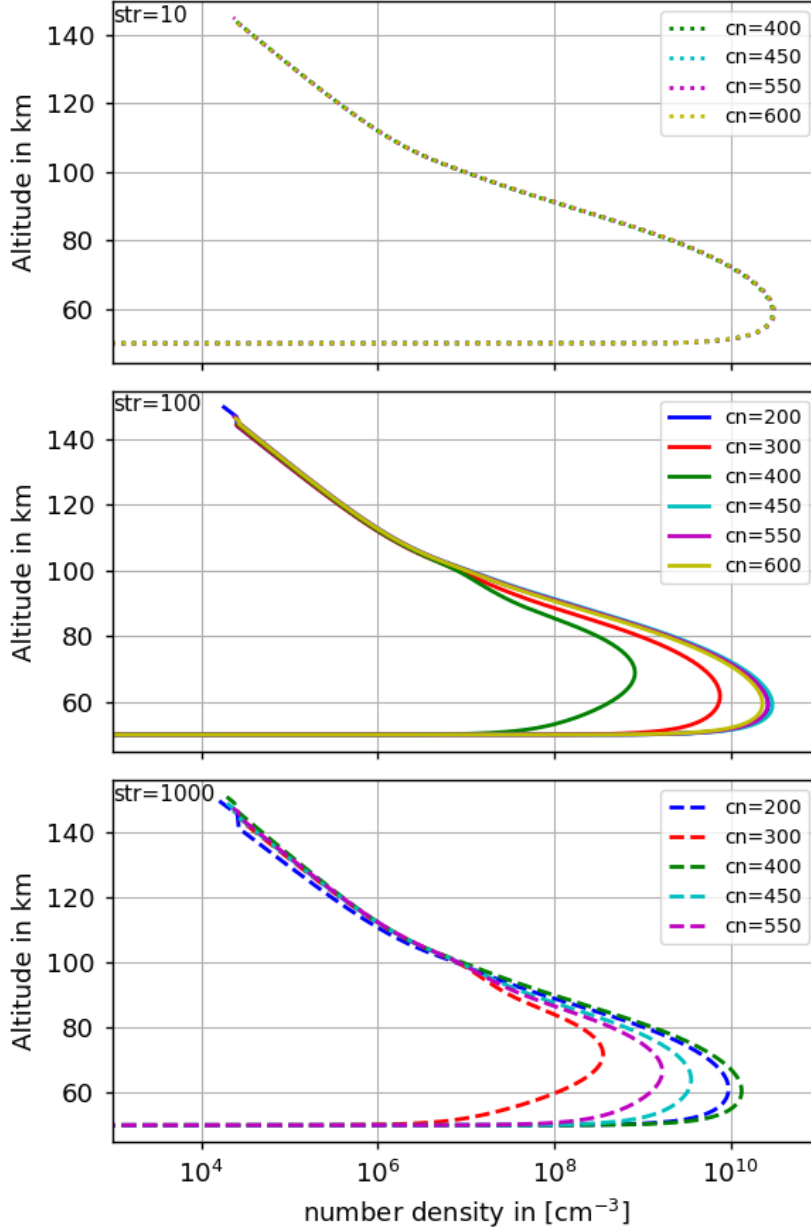


Figure 2.6.: The figures show the O_2 density profiles for different grids. The figures fix the stretch factor at $str = 10$ (top panel), $str = 100$ (middle panel), and $str = 1000$ (bottom panel) and varies only the number of cells. O_2 for different numbers of cells seems to be fine above 100km, but below this altitude the lines diverge, except for small stretch factors.

2. The Kompot Code

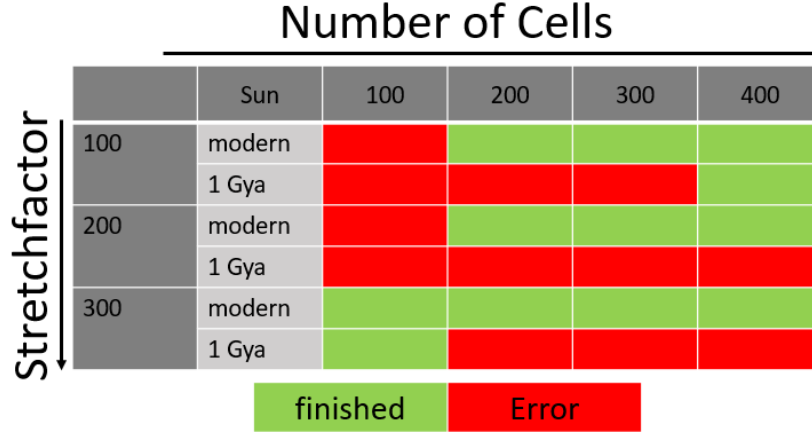


Figure 2.7.: Grid study performed for Venus, with 90% N₂ and 10% CO₂ for spectra of the modern Sun ($F_{X-ray}=0.75$ erg/s/cm²) and the Sun 1 Gyr (XUV Flux of 0.7 erg/s/cm²) ago. Simulations of the latter case mostly ended in errors, limiting the options for a grid strongly.

The analysis of possible reasons for this behaviour is left for further studies, as this would exceed the scope of this thesis. The grid study, however, does show, that stretch factors in the order of 1000 are not recommended, and that stretch factors of 100 only give accurate results with specific numbers of cells (see Fig. 2.6). Additionally, it was shown that a higher number of cells seem to result in more stable results. In terms of runtime, a combination of stretch factors of around 100 and number of cells between 300 and 600 are best suited, excluding $cn = 400$.

2.4.2. Grid study 2: A more detailed analysis

The second study was based on the results of the first one, limiting the range for the number of cells and stretch factors. It was performed for Venus, hence distance, mass and radius were changed to Venus values. This time the chemical composition was set to N₂=90% and CO₂=10%. Additionally, we tested each grid for the modern Sun, as well as the Sun 1 Gyr ago (Gya), which corresponds to XUV fluxes of about 3.78 and 4.98 (or X-ray fluxes of 0.75 and 1.01) erg/s/cm² respectively.

One recurring problem was that for higher fluxes the simulations ended in errors (see Fig. 2.7).

As the previous grid study already ruled out the combination of small number of cells with a large stretch factor, the only option for the grid setup for future simulation runs was the combination of $cn = 400$ and $str = 100$.

During the first scientific simulations, however, we found that the code also runs for $cn = 500$ and $str = 350$, and, therefore, decided to use this setup.

Radius	Mass	a	F_{sun}	init. composition	T	n
0.952	0.815	0.723	$0.75 - 2$	N ₂ ,CO ₂	177	$7.641866 \cdot 10^{14}$

Table 2.1.: The table shows the parameters chosen for the Venus simulations. Radius R in units of $R_{\oplus}$, Mass M in units of $M_{\oplus}$, semi major axis a in AU, flux in erg/s/cm². The initial composition constituents add up to 100%, base Temperature T is in K, base density n is in cm⁻³.

2.5. Setup

This thesis focuses on Venus and how different solar spectra and chemical compositions affect this planet's evolution, and explores the underlying mechanisms that lead to this precise evolution. Therefore, the planetary radius and mass are set to Venus values, as well as the distance to the Sun. N₂ and CO₂ are the most dominant species, and hence we limit the chemical constituents to these two species, meaning that if the atmosphere consists of 40% N₂ the other 60% are CO₂. Limiting the initial chemical composition to these two species does not mean that there will be no other species in the atmosphere at a later point, as the implemented chemical and physical processes will trigger different reactions leading to a variety of species within the atmosphere, based on the initial composition. As we do not have any hydrogen species in our setup we will also conduct atmospheres without any hydrogen species.

Due to the limitations of the code presented in the grid study, we used solar spectra between $F_{X-ray} = 0.75 - 2$ erg/s/cm².

The full set of simulations that have been done can be seen in Fig. 2.8, the choice of parameters is listed in Tab. 2.1. Green dots are simulations that ran successfully, red (or missing) dots are simulations that ran into a problem or did not find a solution. This shows the current limitations quite clearly: High fluxes with low CO₂ content create problems, which could to this point not be solved and are, therefore, still under investigation.

2. The Kompot Code

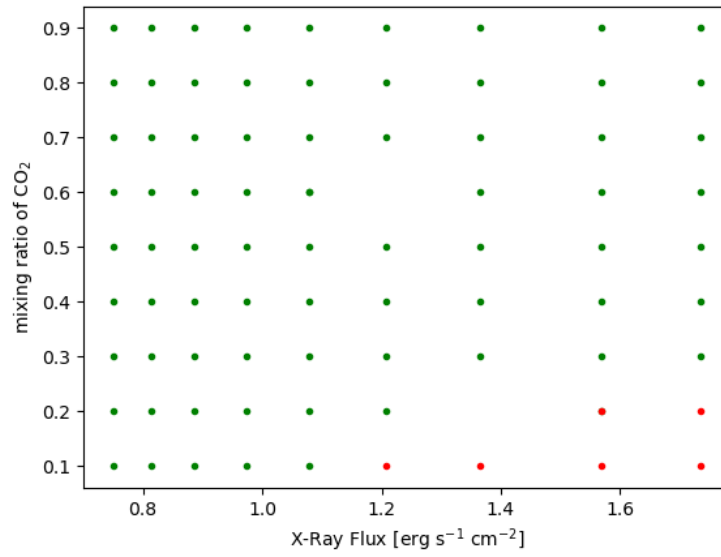


Figure 2.8.: This figure shows the parameter space of the simulation runs. The x-axis shows the X-ray flux of the input spectrum. On the y-axis the initial composition can be seen. A value of 0.1 refers to 10% CO₂ and 90% N₂. Green dots are simulations that finished successfully, red dots either did not find a steady state or resulted in an error. The two missing dots occurred due to wrong choice of parameters.

3. Results

Up to this point this thesis gave an overview of the interaction between host star and planetary atmospheres, as well as a scientific model which can be used to obtain simulated spectra of any planetary atmosphere. It also stressed that Venus is an especially interesting object owing to the upper atmosphere being relatively cool despite Venus' very high surface temperatures. This leads to three science questions, which shall be addressed in this chapter:

1. What are the dominant heating and cooling mechanisms in Venus' upper atmosphere?
2. How does the composition of the upper atmosphere affect the heating and cooling mechanisms, and hence the temperature?
3. How does an evolving Sun (e.g. more X-ray luminous) play into this picture?

To answer these questions we need to look back in time which is - out of obvious reasons - not possible with observation. Therefore a several sets of simulations were performed with the Kompot Code for different times as described in Chapter 2. The simulations were divided into three categories, mirroring the questions listed above:

1. The first set focused on processes taking place in modern Venus' upper atmosphere, to set a basic understanding of the influence of certain species and chemical reactions on the mechanisms.
2. The second set addressed Venus' atmosphere for different initial compositions, to get a clearer picture on how composition affects the heating and cooling mechanisms.
3. The third and last set of simulations was performed with different solar spectra which represent the Sun over the past gigayear (Gyr) as well as different initial compositions to create an idea on how the evolution of such planets might have taken place.

3.1. Modern Venus

Before being able to talk about the evolution of Venus the present or modern Venus needs to be understood. Of course the complete understanding of the interplay between all mechanisms would require much more space than could ever be provided by a master's thesis, however this section will still give a good overview of how the heating and cooling mechanisms affect Venus' upper atmosphere, and how the temperature profile is impacted by them.

3. Results

N	N ₂	O ₂	HE	O	CO	CO ₂
$4.67 \cdot 10^{-12}$	$4.06 \cdot 10^{-2}$	$9.03 \cdot 10^{-5}$	$2.09 \cdot 10^{-6}$	$9.03 \cdot 10^{-5}$	$1.52 \cdot 10^{-4}$	0.96

Table 3.1.: The initial composition for the modern Venus simulation.

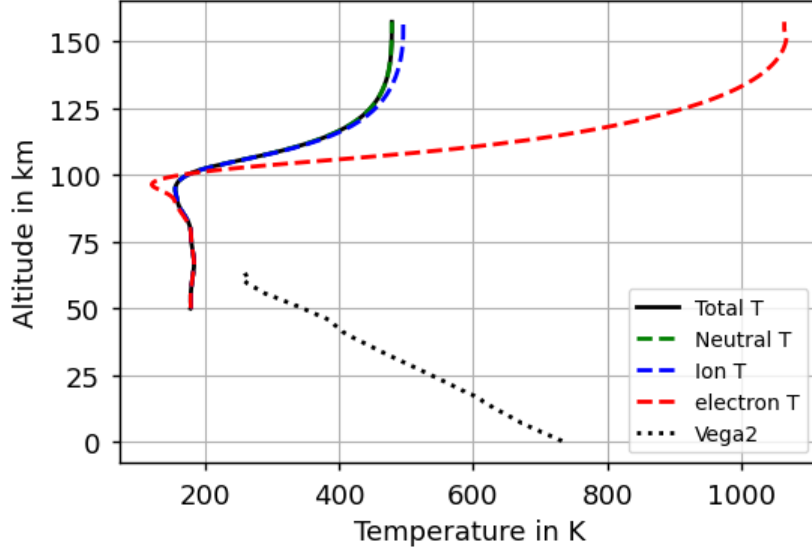


Figure 3.1.: The temperature profiles for neutrals (green), ions (blue) and electrons (red) start at 200 K and then diverge at 100 km, where the electron temperature becomes more than twice as high at the exobase. The model results were gained through a simulation for modern Venus as described in the text. The black dotted line shows the measured temperature profile temperatures from the Vega mission.

Additionally this thesis will try to connect this basic picture to a more detailed analysis of how species abundances and chemical reactions affect the heating and cooling mechanisms.

As mentioned previously this thesis works with the Kompot Code to simulate Venus' upper atmosphere. For this, certain parameters need to be set, which are listed in Tab. 2.1, as well as an initial chemical composition at the base of the simulation given by Hedin et al. [1983] and shown in Tab. 3.1.

3.1.1. Temperature

Venus is known to be a very hot and unfriendly place, however this is only true at lower altitudes, close to the surface, as can be seen when looking at the Vega data in Fig. 3.1. Within the first 50 km from the surface to higher altitudes the temperature drops from over 700 K to about 300 K, which is not so far from Earths temperature at the same

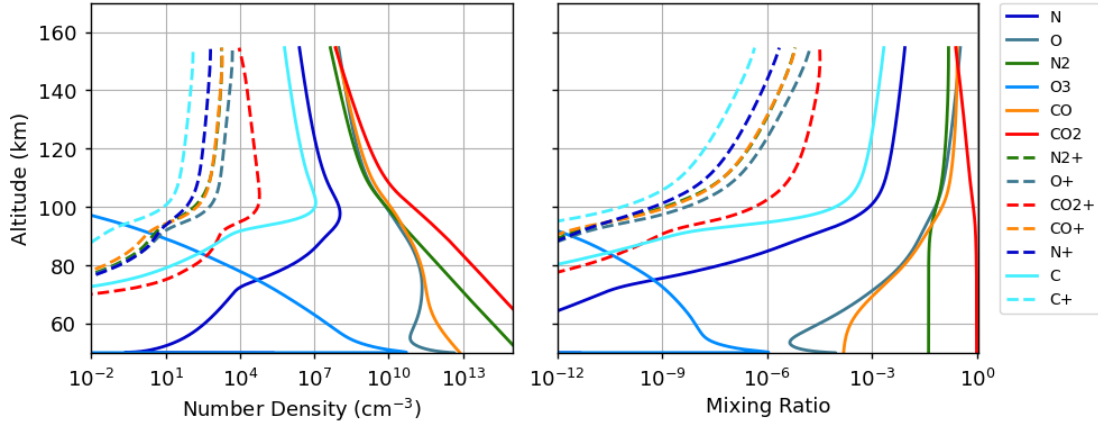


Figure 3.2.: Both the number density profiles and mixing ratios were gained from simulations using Kompot with modern Venus parameters. The colors indicate different species, the dashed lines highlight specific ion species.

altitude (about 250 K). Skeptics might look at the observed and modeled temperature profile and immediately notice the missing overlap between the two curves. This however can easily be explained by the differences in day and night side measurements, and general uncertainties of the observations.

After the sharp drop in temperature between the surface and the 50 km mark, the temperature stays rather steady, leading to a drop to the coldest region at 100 km, followed by a rapid increase in temperature. The electron temperature increases much more rapidly, leading to an exobase temperature more than twice as high as the ion and neutral temperatures, which will be discussed at a later point in this chapter. The difference between neutral and ion temperatures is very small, and the total temperature aligns with the neutral temperature, which is due to Kompot only taking neutrals into account for the calculation of the total temperature.

The temperature inversion beginning at around 100 km was already pointed out by authors like Limaye et al. [2018]. When we compare the temperature structure with the density profiles of species of interest in Fig. 3.2, we see that this temperature inversion, which is usually triggered by O_3 , must have other reasons, as O_3 is barely present at these altitudes. This is not only shown by our simulations, but has also been discussed by Montmessin et al. [2011]. According to Limaye et al. [2018] aerosols and subsidence might be the reason behind this temperature inversion. A sneak peek to Fig. 3.4 provides other ideas where this inversion might come from: At the 100 km mark chemical heating is almost at its maximum, photoelectron heating just started to increase again, and XUV heating is still strong. IR heating and Joule heating might be decreasing, but in total we see an increase of overall heating.

3. Results

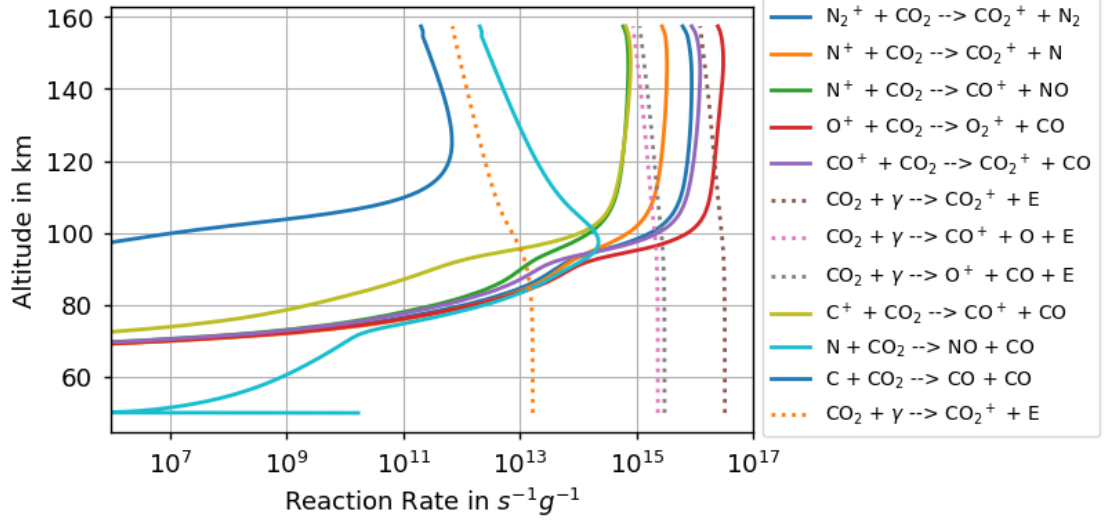


Figure 3.3.: The plot shows the main contributing reaction rates involving neutral CO_2 . The dotted lines highlight photoreactions.

Reaction	Energy (eV)
$\text{N}_2^+ + \text{CO}_2 \rightarrow \text{CO}_2^+ + \text{N}_2$	1.81
$\text{N}^+ + \text{CO}_2 \rightarrow \text{CO}_2^+ + \text{N}$	0.78
$\text{N}^+ + \text{CO}_2 \rightarrow \text{CO}^+ + \text{NO}$	1.57
$\text{O}^+ + \text{CO}_2 \rightarrow \text{O}_2^+ + \text{CO}$	1.20
$\text{CO}^+ + \text{CO}_2 \rightarrow \text{CO}_2^+ + \text{CO}$	0.24
$\text{C}^+ + \text{CO}_2 \rightarrow \text{CO}^+ + \text{CO}$	3.02
$\text{N} + \text{CO}_2 \rightarrow \text{NO} + \text{CO}$	1.06
$\text{C} + \text{CO}_2 \rightarrow \text{CO} + \text{CO}$	4.53

Table 3.2.: The table shows the energy that is being released by certain reactions. As comparison, charge exchange between He^+ and O_2 results in the highest energy of 12.57eV among the reactions in the network.

3.1.2. Species Densities and Reaction Rates

Heating and cooling come - roughly speaking - from atoms and molecules absorbing and emitting energy, respectively. It is, therefore, of great interest to investigate the species densities (Fig. 3.2) and the chemical reactions (Fig. 3.3) taking place in the atmosphere. It is not surprising to see CO_2 as the dominant species up to approximately 150 km as this is something we already know from observations. For the last few km (above 150 km) O takes over. As CO_2 decreases the mixing ratio of CO, O and C increase, indicating that photodissociation breaks up CO_2 into its constituents. However we find that the reaction rate of CO_2 photodissociation (orange dotted line in Fig. 3.3) is negligibly small. There are however many other reactions that break apart CO_2 , through neutral-neutral or ion-neutral collision (particularly collisions of O^+ with CO_2), as well as photoionization. While the photoreactions seem to stay relatively stable through all altitudes, which is most likely due to XUV reaching far down in the atmosphere as will be show later, reactions through collision show a strong increase from bottom to top. This also explains why in the lower parts of the atmosphere CO_2 does not decrease so fast with altitude, but does so in the upper parts.

The reaction rates strongly correlate with the species density profiles, which can be seen on the example of $\text{N} + \text{CO}_2$: The rates increase rapidly between 50-100 km, which coincides with the number density of N increasing, and then decreases with the same trend, as N and CO_2 both decrease. It can also be seen that the reactions involving N^+ follow the density profile of this ion very strongly.

The dominant photoreaction is the photoionization of CO_2 , closely followed by CO_2 being broken down into O and CO where one of both is an ion and the other one is a neutral (pink dotted, and gray dotted lines).

It should be noted that the horizontal line at 50 km is a computational artifact most likely due to the ghost cells, which are set to a fixed density.

3.1.3. Heating Mechanisms

As discussed in chapter 2 there are five main heating mechanisms included in the code: XUV heating, which comes from the excess energy after absorbing a photon, chemical heating, through exothermic reactions, IR heating, coming from the energy that is removed from the IR field as it passes through the atmosphere (only includes CO_2 , due to Venus' composition), photoelectron heating through absorption or collision with non-thermal electrons, and Joule heating, caused by friction between the ions and neutrals.

These five heating mechanisms are shown as a function of altitude in Fig. 3.4. Chemical heating dominates the upper atmosphere, but drops sharply from 100 km downwards, from where XUV heating takes over. Joule heating contributes in the least amount.

To discuss the chemical heating we look back at the reaction rates in Fig. 3.3 and focus on the solid lines, as photoreactions are not included in chemical heating. The plot only includes reactions containing CO_2 , as this is the most abundant species and, therefore, will have the highest reaction rates by default. Reactions with ions happen more frequently than neutral reactions, which does not necessarily mean that they contribute the most

3. Results

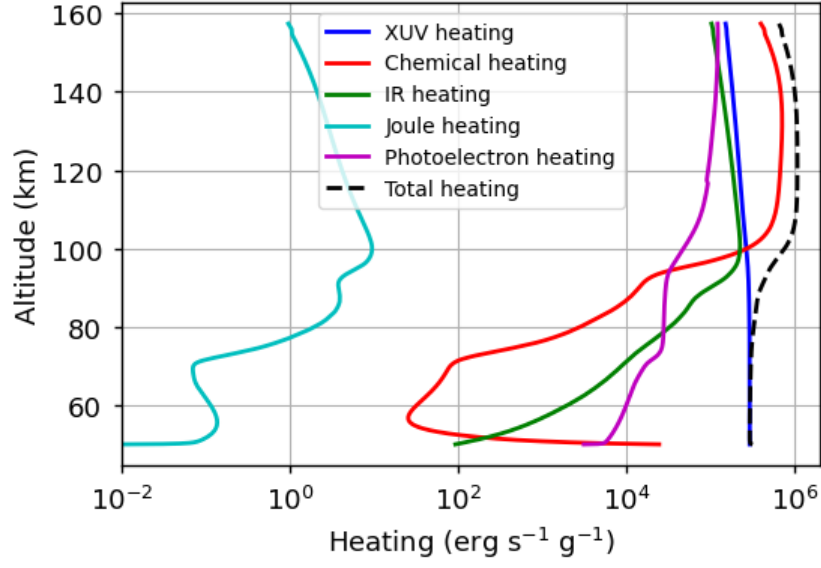


Figure 3.4.: Each color represents one of the five heating mechanisms contributing in the modern Venus simulation. The black dashed line shows the total heating over all altitudes (=the sum of all heating mechanisms). Depending on the altitude different heating mechanisms are dominant.

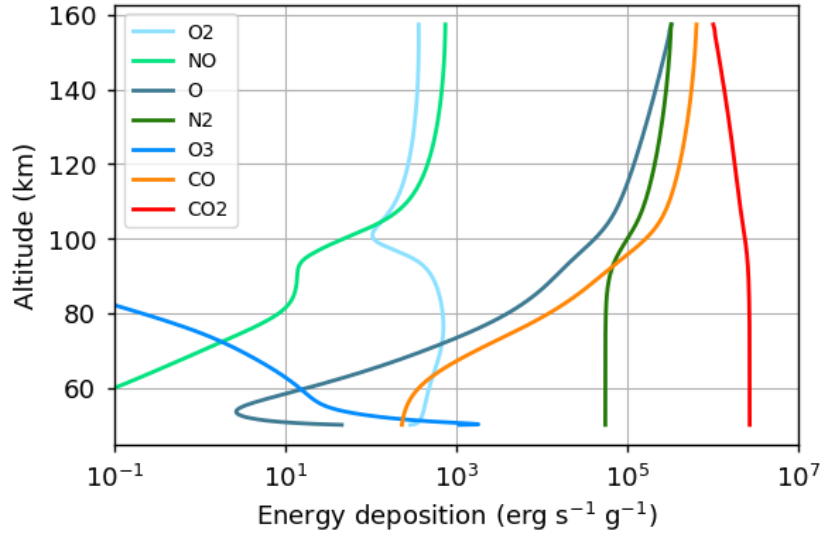


Figure 3.5.: The energy deposition reflects how much energy the species holds at this specific altitude. It correlates very strongly with the species density/mixing ratio profile. Unsurprisingly the most energy is deposited in CO₂ as it is the most abundant species in this simulation.

heating. How much heating is being contributed depends on the energy released by the reaction, as listed by Johnstone et al. [2018] and shown in Tab. 3.2. From the numbers we see that they are too small to make a significant impact on the importance of one reaction over another, only if they are very similar in reaction rate. This means that the order of the reactions will not really change and we can state that charge exchange reactions shown in Fig. 3.3 are a large factor in contributing to chemical heating.

Fig. 3.3 shows a sharp drop in reaction rates below 100 km, which coincides with the sharp drop of ion number density, and also of chemical heating. The density profiles of C and N - which are the main neutral reactants - also follow this trend.

Note that the simulation includes 20 absorbing species. It is, therefore, highly unlikely that a certain behavior in the heating curve can be directed to one specific reaction. Through general analysis above we however find that ions are the most important species for chemical heating.

The rapid decline at the first few km is due to the ghost cells having fixed values again.

The second most important heating mechanism is direct XUV heating. It is the dominant contributor below 100 km and has the second highest heating rate above this altitude. To track where this heating comes from we direct our attention to Fig. 3.5, where we see the energy coming from XUV being deposited in species as a function of altitude.

From the species density profiles in Fig. 3.2 we saw that CO_2 is the dominant species. It is, therefore, not surprising that it is also the species in which most of the energy is being deposited. Because the energy deposition depends on how much of the species is actually present in the atmosphere it strongly correlates with the *shape* of the density profiles, which also results in the contribution of each species following the same order as for the densities. We hence find that after CO_2 , CO, N_2 and O carry the most energy. The slight decline in XUV heating in the upper atmosphere can, therefore, be explained by the lower density atmosphere containing less species.

When looking at the spectrum and its penetration depth it becomes clear why XUV heating is still so strong in the lower regions. Even though the X-ray part of the spectrum has already been absorbed there is still enough UV to reach the lowest regions (see Fig. 3.6).

Infrared heating is almost as strong as XUV heating in the first half of the upper atmosphere, but rapidly decreases starting from 100 km downwards. This most likely comes from how far IR reaches down to those low altitudes - the corresponding penetration depths for IR are not provided by Kompot and can, therefore, not be plotted. It is very likely, though that the reason for the IR trends are as follows: In the upper regions we find less CO_2 and hence less heating. In the lower regions IR has most likely already been depleted, so the heating effect declines despite there being enough CO_2 present.

Photoelectron heating decreases only by two orders of magnitude from the exobase to the lower end of the simulation domain, while IR and chemical heating decrease by more than four and five orders of magnitude, respectively. This might be due to radiation

3. Results

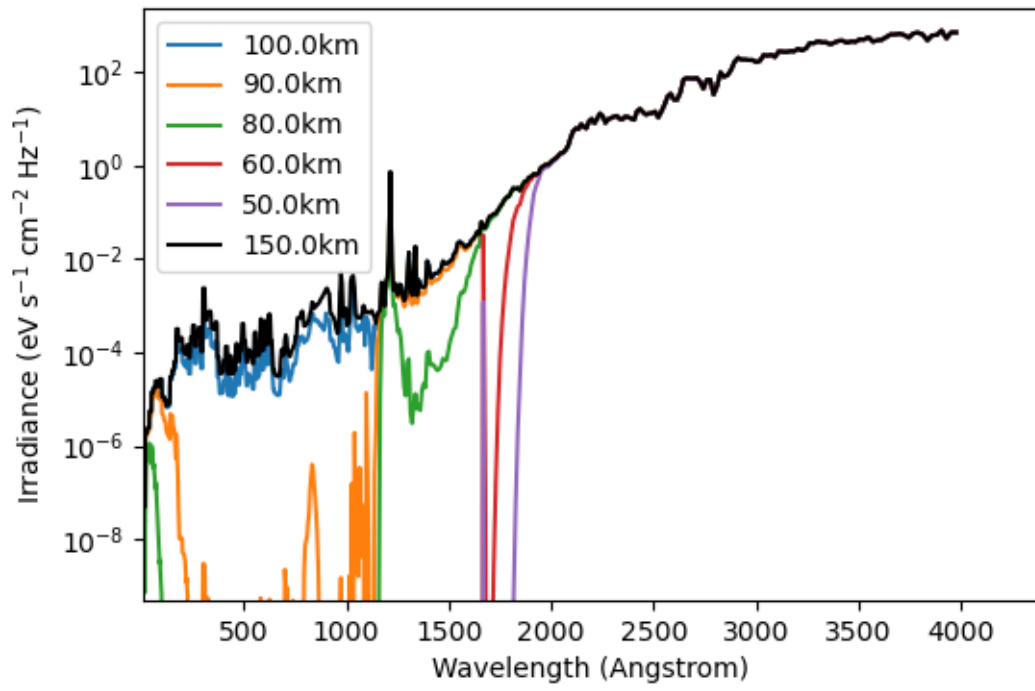


Figure 3.6.: Spectrum at different altitudes of Venus' atmosphere showing the penetration depth of XUV.

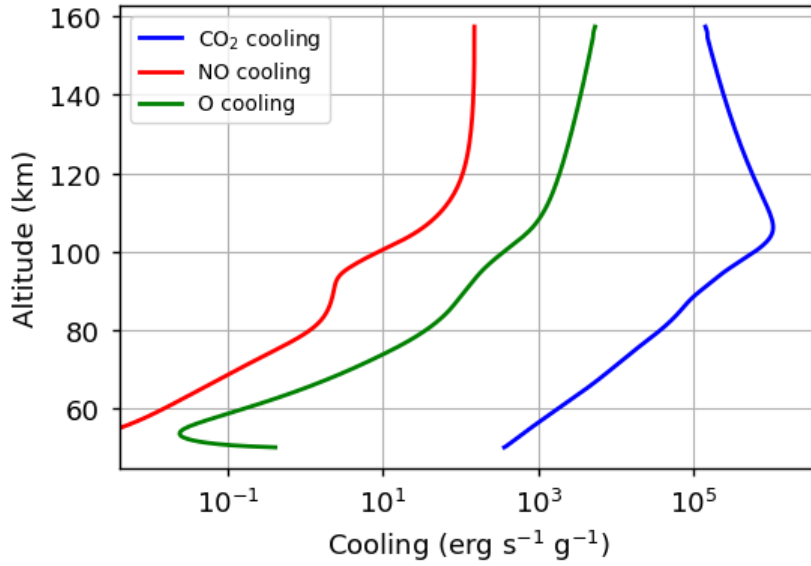


Figure 3.7.: Cooling mechanisms for modern Venus.

reaching far down in the atmosphere, kicking out electrons of species that reside at lower altitudes (see Fig. 3.2). The free electron thus created can be absorbed or can collide with another particle, where it will turn its kinetic energy into thermal energy, leading to heating. A consequence of this is the large difference in electron temperature compared to ion or neutral temperature, as already noted at the beginning of this chapter.

We note that the magnetic field was not changed from the default value of 0.5 G to Venus values of $7 \cdot 10^{-5} G$. The resulting Joule heating is, therefore, much stronger than it would be, but the shape should remain the same. It shows several turning points, the highest one at 100 km. The movement of particles through collisions, diffusion or advection are contributing factors, as well as the distribution of ions and electrons. As we can see it is contributing not as much as the other heating mechanisms, and would have even less of an impact if we had used the value of Venus' magnetic field. Hence, we will turn off Joule heating in the following simulations and will, therefore, not analyse this mechanism in more detail.

3.1.4. Cooling mechanisms

The cooling mechanisms acting against the above presented heating mechanisms, are the dominating CO_2 cooling, O cooling and NO cooling, which can be seen in Fig. 3.7. The way these mechanisms work is through emission of IR. Let's picture a CO_2 molecule that just absorbed some energy and is now in a state of excitation, where its bonds are vibrating strongly. By emitting IR radiation itself it can fall back into a lower state of

3. Results

energy. The IR radiation is emitted in all directions. We can, therefore, say half of it is going downwards in the direction of the surface (=Greenhouse effect), and the other half is going towards space. Of course other CO₂ molecules can absorb this emitted IR radiation again, but it will again emit half of it upwards.

At the top of the atmosphere we have lower optical depth, with less CO₂. The further down we go the more CO₂ we find. This resonates with CO₂ cooling, which increases from the top to 100 km, where we find the peak. The optical depth is moderate here and CO₂ has increased by almost 3 orders of magnitude. Compared to the temperature profile we see that the temperature gradients here are very large. From that point on CO₂ cooling decreases downwards, despite the still increasing number densities of CO₂. This might be due to there being so much CO₂ in the above layers that the lower layers can't effectively cool.

The other two cooling mechanisms, O and NO cooling scale linearly with their species profiles. This is related to how cooling is implemented in the code (see Section 2.1.4).

3.1.5. Conduction

The temperature profiles are not only influenced by the heating and cooling mechanisms, but also by conduction, which can transport heat from a warmer to a cooler cell. To show how modern Venus is affected by this, the change in energy at a given point due to conduction was plotted alongside the total cooling and total heating curves (see Fig. 3.8). At approximately 100 km the cooling effect is strongest and the temperatures are the lowest. The above layers only show conduction transporting heat away. At 100 km the atmosphere, therefore, acts as a sink for heat.

Between 110 km and 80 km heat is being received, but not in a uniform way. We find three peaks, the first one at 100 km, where total cooling and heating have the same rates, but cooling being at its peak. This is, therefore, the coldest region, receiving the most heat. As cooling rates drop the respective region is comparatively warmer, therefore receiving less heat.

At around 80 km there is an area where heat is taken away again that can't really be ascribed to behaviors in heating or cooling, followed by regions of positive and negative conduction. To explain this behavior one must remember that conduction is dependent on the temperature gradients as well as the thermal conductivity, which in turn depends on the detailed gas composition, including ionization state and electron density. It is difficult to see conduction as a stationary effect, because while conduction transports heat away from a region, it will flatten the gradient, which in turn affects conduction again. However in this situation we see some slight wiggles in the temperature profile around that area which explain the sequence of positive and negative conduction over several areas. If we recall that conduction is based on the second derivative of temperature, it can be easily seen that the slightest wiggles in the slope will drive the second derivative from positive to negative or the other way round. Also, the derivative of the conductivity matters.

In this sense conduction in the lower regions is more of an effect due to the temperature

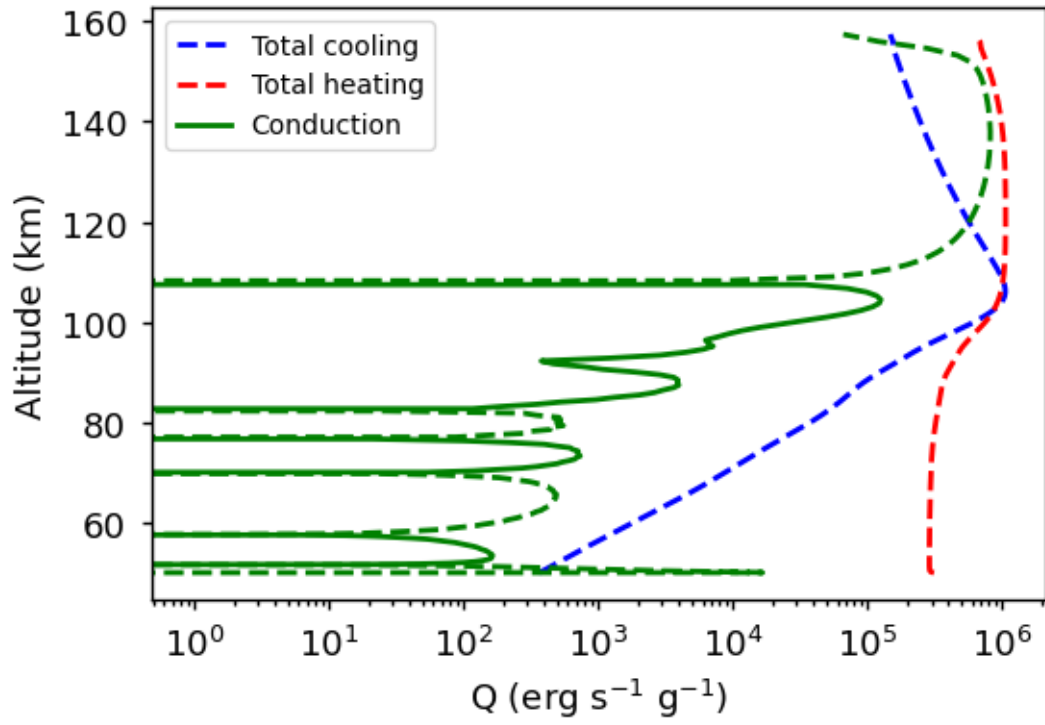


Figure 3.8.: The figure shows the total heating and cooling rates alongside the change of energy due to conduction. The dashed green line is heat being transported away from a cell (negative conduction), while the solid line shows heat being received through conduction (positive conduction).

3. Results

gradients, while the upper region can explain why the atmosphere does not heat up infinitely.

3.1.6. Linking heating, cooling and conduction to the temperature

We find that at lower altitudes the cooling rates for all mechanisms increase from 50 to 100 km, resulting in the lowest temperature at that point. The heating mechanisms up to that point are slowly increasing as well, and from 100 km the overall heating rates are at a maximum. At the same time CO₂ cooling declines again, but the other two cooling mechanisms are still increasing, which balances out the lack of CO₂ cooling slightly. Additionally conduction takes away heat from the upper region, distributing it to the colder parts of the atmosphere below 100 km, which prevents a runaway temperature increase.

3.2. Effect of CO₂ mixing ratios on the modern Venus

Now that it is clear which effect the present day Sun has on Venus with present day composition (modern Venus), the next question can be addressed, namely, how the temperatures in Venus' upper atmosphere would change if the mixing ratio of CO₂ decreased. One would expect the atmosphere to be hotter, as the dominant cooling mechanism (CO₂ cooling) is likely to decrease if there was less CO₂ present. However other cooling mechanisms, such as NO cooling, might start to take over as there will be more N present which could lead to the production of more NO.

On the other hand the effect of IR heating is expected to be stronger with more CO₂, because IR heating is only happening through absorption by CO₂ on Venus. It is, therefore, of great interest if and how these two opposing factors balance each other out.

The simulations have the same setup as the modern Venus scenario, where grid and input spectrum stayed the same, as well as the heating and cooling mechanisms allowed, with the exception of Joule heating, which was turned off as explained in the previous part of this thesis. To see the effects of CO₂ and N₂ - the two dominant species in the Venusian atmosphere - better, a simplified composition was chosen, where these two molecules are the only constituents in the initial composition, adding up to 100% always. Within this setup a range of parameters between 10% to 90% in 10% steps was tested. One should emphasize that the previous simulation in Section 3.1 cannot be compared to this simulation one-to-one, as the atmosphere now is a simplified version and Joule heating is turned off. However the basic concepts stay the same, and the simplified simulation will give good insights on how the changes would affect modern Venus.

One effect we immediately see when comparing the temperature profiles is that the temperatures indeed increase with less CO₂ present, as visible in Fig. 3.9. Additionally, we see that the lines of the temperature profiles reach up to a higher altitude, which means that the exobases extend to higher altitudes. This shows that with higher temperatures

3.2. Effect of CO₂ mixing ratios on the modern Venus

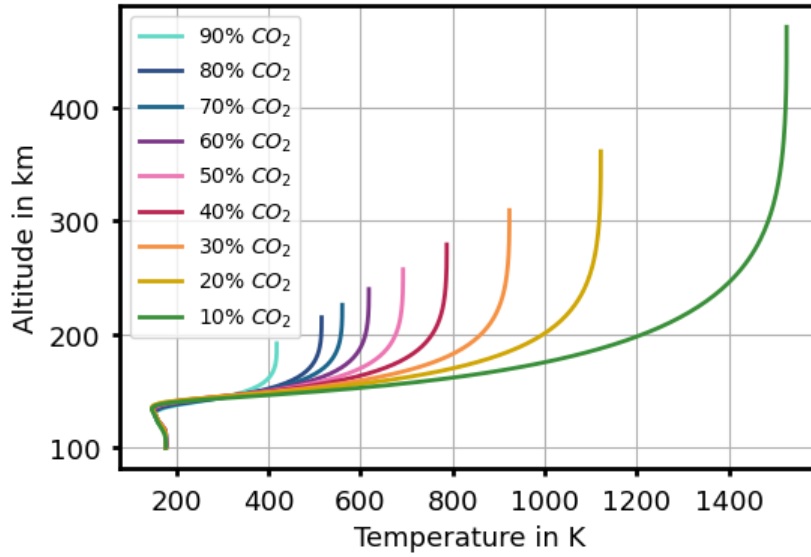


Figure 3.9.: Temperature profiles for a modern Venus with different CO₂ N₂ mixing ratios

atmospheres tend to expand, which was already mentioned in Section 1.2.

It is interesting, however, that the profiles only start to diverge after the point of minimum temperature at around 140 km. Below that, the profiles overlap. Additionally the differences in exobase temperature arise from the much more rapid increase in temperature between 150 km and approximately 2/3 of the atmosphere's altitude. After that, the lines evolve in parallel again.

The heating mechanisms which have been included in these simulations are heating through XUV and IR radiation, chemical heating from exothermic reactions and photoelectron heating. In the comparison of the temperature profiles for different CO₂ mixing ratios we saw a smooth transition from low to high ratios. The same can be seen in the heating and cooling mechanisms, which is why only the extreme cases of 10% and 90% as well as the intermediate 50% CO₂ mixing ratio were selected to be shown in the following sections.

3.2.1. Venus with 90% CO₂ and 10% N₂

The 90% CO₂ simulation shows the smallest temperature difference from bottom to top (Fig. 3.9) of just $\Delta T = 200$ K, which is comparable to the modern Venus, which is Venus with present day composition at present day solar Flux (see 3.1).

In Fig. 3.12 it can be seen that the total heating rate at the exobase stays the same compared to the modern Venus simulation from the previous section - despite the simplified version of the atmosphere. Below 130 km however, photoelectron and XUV heating drop rapidly, which does not happen in any other simulation.

The number densities (Fig. 3.11) of the 90% CO₂ atmosphere are quite like the modern

3. Results

Venus profiles, where O and O₃ are the only species that strongly diverge from the modern Venus profiles. However, the energy deposition in Fig. 3.14 of some species show the same rapid drop as photoelectron and XUV heating. Especially N₂, O and CO rapidly decline below 130 km, and CO₂ declines below 140 km. This rapid drop off does, therefore, not seem to be a computational error, but might be due to the simplified version of this atmosphere. Hence, this particular case is advised to investigate further, as it is not clear, why this rapid drop off occurs in the 90% CO₂ Venus but not in modern Venus, which has a similar CO₂ content. The 90% CO₂ Venus will, therefore, only be noted as special case here, as the analysis is outside the scope of this thesis.

We can still however analyse the heating mechanisms above 130 km and find that XUV heating contributes second most above this altitude.

Chemical heating (see left panel in Fig. 3.12) is the dominant heating mechanism above 130 km, and follows the XUV heating profile below this altitude. In Fig. 3.10 we see that the reaction rates in the upper parts are high, but drop drastically below 130 km. This was seen for reactions other than photoreactions in modern Venus as well, but here the photoreactions also show the same trend, explaining the strange behavior of XUV heating. The reason for why exactly this happens is however still unclear, but it seems as if something is blocking XUV from reaching down to layers below 130 km. This, however, is refuted by the penetration depths of the spectrum at different altitudes shown in Fig. 3.6. The order of importance of the different reactions stays mostly unaffected.

One of the differences between the 90% CO₂ Venus and modern Venus is the reaction of ionized nitrogen with CO₂, which above 130 km does not happen as often as in the modern Venus. There might be a lack of energy present for N⁺ to be created. However, when comparing the number density with the modern Venus we see that there is actually more N⁺ present in the 90% Venus. This means that the lower rate of charge exchange reactions leads to the accumulation of more N⁺. However there is no clear reason for why this happens.

Most of the reaction rates are quite similar to the modern Venus, so the chemical heating profile stays similar as well.

The profile of IR heating (see left panel in Fig. 3.12) stays the same compared to the modern Venus but is overall shifted to higher heating rates. The effects that cause this shape have already been discussed in Section 3.1. As IR heating depends only on the CO₂ number density, it stays mostly unaffected in its behavior through the atmosphere compared to IR heating in the modern Venus, while XUV and photoelectron heating depend on many other species. Due to this they might be much more sensitive to change in species mixing ratios, than IR heating. It is interesting to see, however, that photoelectric heating follows a similar behavior as XUV heating that is mostly responsible for the free electrons needed for this mechanism.

Unlike the heating mechanisms there is basically no change to be seen in the cooling

3.2. Effect of CO₂ mixing ratios on the modern Venus

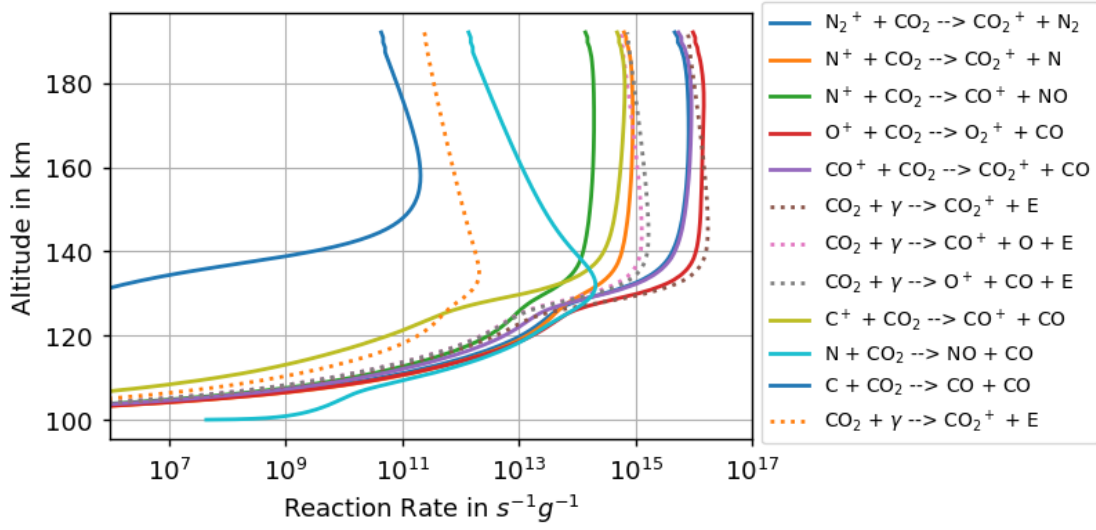


Figure 3.10.: These are the main reaction rates for the 90% CO₂ Venus simulation. The dotted lines highlight photoreactions.

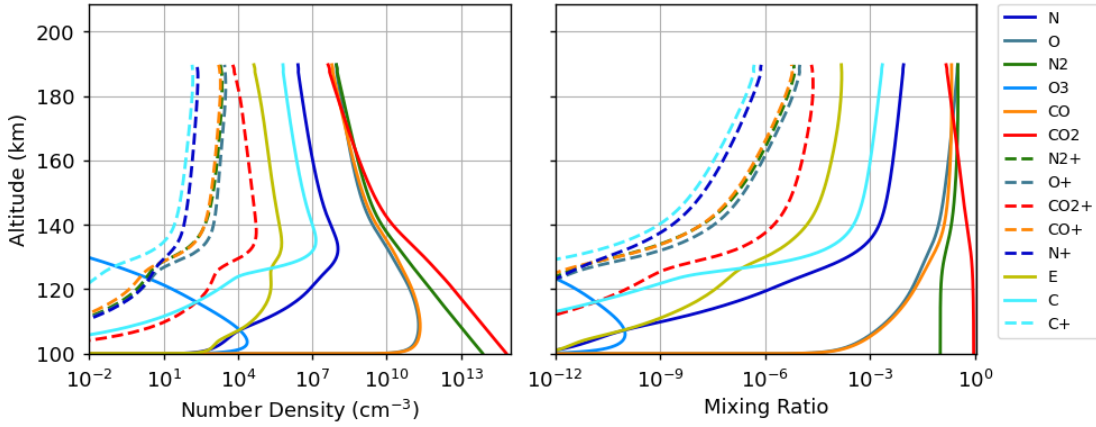


Figure 3.11.: Number Densities of species in the 90% CO₂ Venus simulation on the left side and mixing ratios on the right side.

3. Results

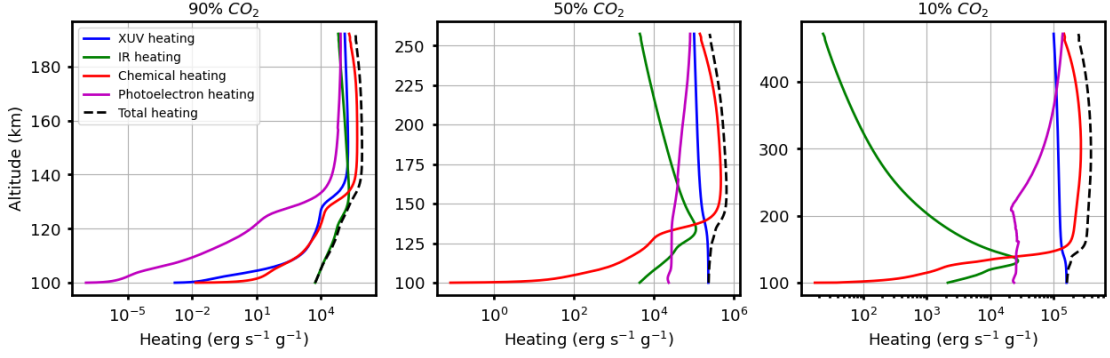


Figure 3.12.: Heating mechanisms for a Venus with CO₂ mixing ratios of 90%, 50% and 10% at present day solar flux.

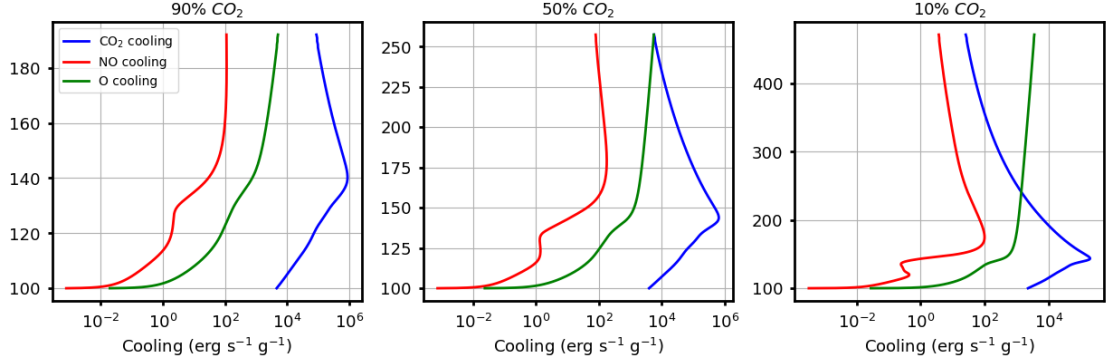


Figure 3.13.: Cooling mechanisms for a Venus with CO₂ mixing ratios of 90%, 50% and 10% at present day solar flux.

mechanisms compared to modern Venus (see Fig. 3.13). CO₂ cooling is still the dominant mechanism with its step increase from base towards its peak at 150 km, and the decrease above that altitude. O cooling is also still contributing in the same amount, as well as NO cooling. The concepts that cause these behaviors of the cooling mechanisms have also already been discussed in the previous section.

3.2.2. Venus with 50% CO₂ and 50% N₂

If we look at a Venus with 50% CO₂ and N₂ at its base, the temperature structure is already significantly different. The exobase temperature increased by 300 K and the exobase altitude by approximately 50 km .

For the heating mechanisms in the middle figure of Fig. 3.12 we see that IR heating becomes less strong, as CO₂ stopped being the dominant species. XUV heating is as strong as in the modern Venus simulation, and chemical heating as well as photoelectron heating are not much different.

3.2. Effect of CO₂ mixing ratios on the modern Venus

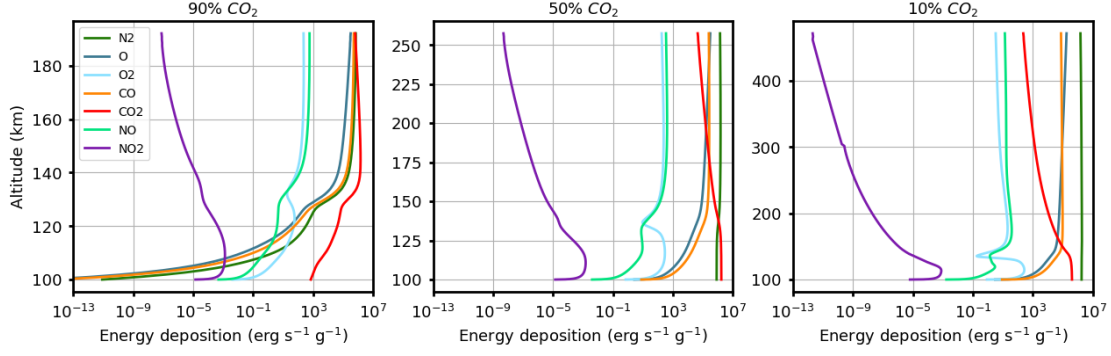


Figure 3.14.: Energy deposition for a Venus with CO₂ mixing ratios of 90%, 50% and 10% at present day solar flux.

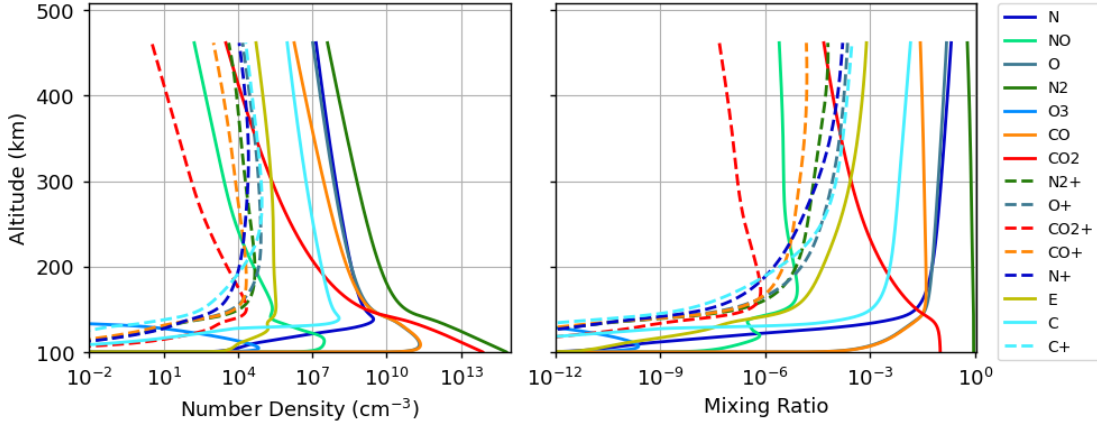


Figure 3.15.: Species densities and mixing ratios of the 10% CO₂ Venus simulation for a present day solar flux.

For CO₂ cooling we see a similar effect as for IR heating. It becomes clearly visible when comparing the rates at 200 km in Fig. 3.13, where the 90% Venus shows a cooling rate of 10^5 erg/s/g, and the 50% Venus cooling rate is clearly below this value. When comparing with the IR-heating rate again we see a similar difference, which is self-consistent.

3.2.3. Venus with 10% CO₂ and 90% N₂

The setup with 10% CO₂ results in the most extreme temperatures with the most extended atmospheres with almost 1500 K at an exobase of 480 km. This is an increase in exobase temperature of 350%. IR heating now shows an overall shift of almost one order of magnitude compared to modern Venus, while chemical heating stays dominant between 150 km up to the exobase. XUV heating stays the second most contributing heating source up to 370 km, where photoelectron heating becomes more important. Interestingly, the electrons become more abundant than CO₂ even lower down, at 300 km (see Fig.

3. Results

3.15). Also noteworthy is that the ion number densities have decrease slower in the higher regions than the neutral number densities. This indicates that neutral species are too heavy to exist in the higher up regions. However, the total number of particles per species might still stay the same, but stretched over a larger atmospheric range.

Among the cooling mechanisms in Fig. 3.13 we also see some changes. CO₂ cooling, just as IR heating, is, compared to the 90% Venus, now by one order of magnitude weaker (visible in the shift by one order of magnitude to the left), and O cooling replaces it as largest contributor at the exobase. We also see an interesting trend in NO cooling in the same figure, where from 160 km upwards the cooling rate starts decreasing again. This reflects the species density profile very well, as NO starts decreasing at a similar altitude (see Fig. 3.15). Interestingly O dominates over CO₂ from 150 km onward, but only becomes the dominating cooling source at 250 km. We therefore take a look at the energy deposition plot in Fig. 3.14 to see if O might not have absorbed enough energy to be re-emitted for the cooling effect to be strong enough. We find that the profiles reflect the species densities very well: There is less energy deposited in O below 160 km than in CO₂, whereas above 160 km it dominates over CO₂.

3.3. Effect of a Changing Solar Flux on a Venus with different CO₂ mixing ratios

Next we are interested in the evolution of a Venusian atmosphere. Kompot is not a tool for long-term evolution; however, we can simulate an evolution in time by providing different spectra that resemble the Sun at a younger age. With this we are tackling the question on how a younger Sun might have affected Venus' atmosphere, and what would have happened if it had had less CO₂. In the previous section we found that a lower CO₂ content leads to rapidly increasing temperature between 150 km and 2/3 of the atmosphere up to the exobase, with hot and therefore expanded exobases. This was due to chemical heating staying strong above 150 km as well as photoelectron heating increasing from 200 km onward. Expanded atmospheres are easy targets for solar wind to strip away. Even though the solar wind is not included in the code, we can calculate Jeans escape and provide lower limits in terms of loss rates, which will be done in Chapter 4.

As was shown in Fig. 2.8 we tested different compositions from X-ray fluxes between 0.7 and 1.7 erg/s/cm², but for the extreme cases of 10% and 20% CO₂ the higher end resulted in errors. For our detailed analysis of the effects of the solar XUV flux on the heating and cooling mechanisms we therefore look at the 90%, 50% and 30% CO₂ Venus.

3.3.1. Temperatures

In the foregoing sections we showed that the temperature profiles don't show changes in their turning points but only in terms of a sudden increase after them, resulting in hotter,

3.3. Effect of a Changing Solar Flux on a Venus with different CO₂ mixing ratios

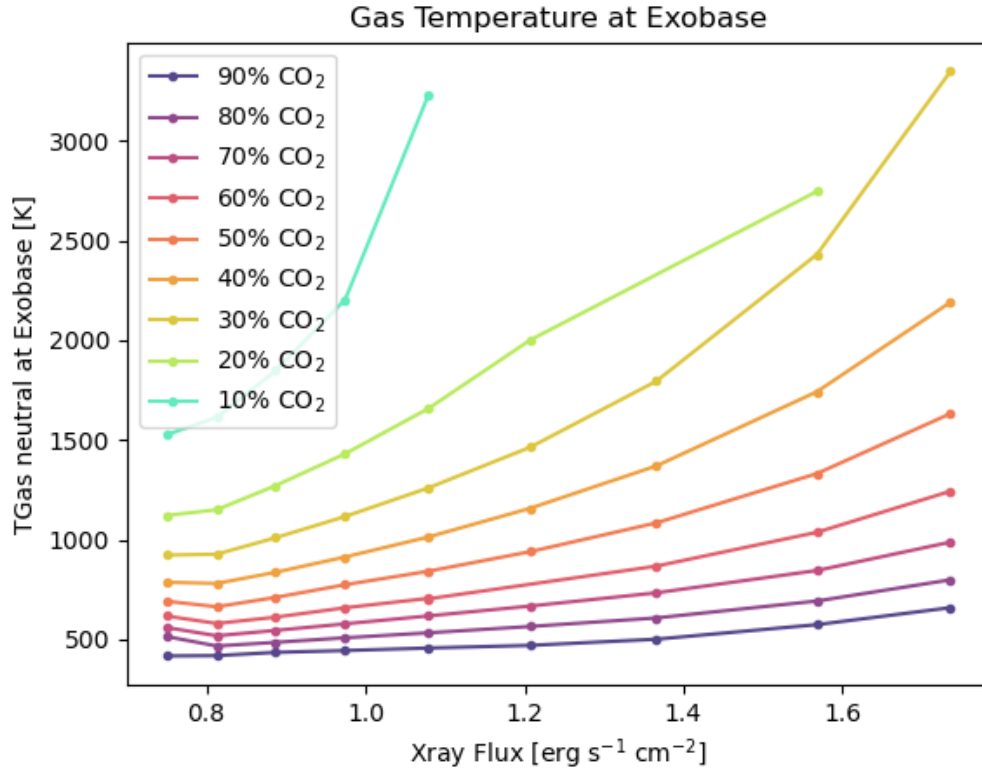


Figure 3.16.: The Temperature at the exobase for different compositions and different solar X-ray fluxes are shown. The 20% case seems to follow a different trend, which might be due to the fact that the last simulation used the simulation at a Flux of 1.2erg/s/cm² as initial condition, and not not as the other ones at ≈ 1.35 .

highly expanded atmospheres for less CO₂. Because the overall shape stays the same the most interesting key point is the exobase temperature, as this is a good indicator on how much the atmosphere underwent heating. The exobase temperatures for all successful simulations are shown in Fig. 3.16. There we see that for atmospheres with less CO₂ the temperature increases much faster with flux than for atmospheres with more CO₂. Additionally, we found the same trends and behaviors in ion temperatures with similar temperature ranges. To understand why higher fluxes have this effect we will take a closer look at the heating and cooling mechanisms one more time.

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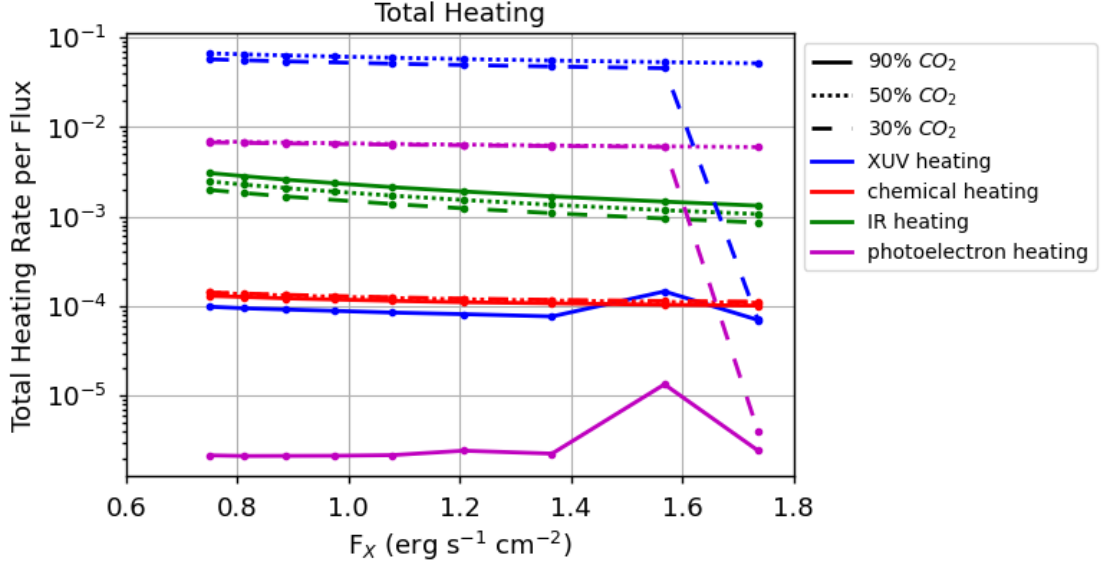


Figure 3.17.: Evolution of the total heating rates for different mechanisms (colour) for different compositions (linestyle) depending on the solar X-ray flux. The heating rates are normalized to the flux to get an efficiency, and are therefore unitless.

3.3.2. Heating

The heating mechanisms included in the simulation are the same as in the previous simulations: Heating through XUV and IR due to solar radiation, chemical heating due to exothermic reactions, and photoelectron heating. We compare how the contributions of these mechanisms change depending on composition and X-ray flux. One way to investigate the change in heating rates is by calculating the total heating rate for each mechanism. This is done by integrating over the heating rate in each cell. We additionally normalized the total heating rates to the incoming flux, to get something that can be interpreted as heating efficiency.

The general trend for XUV, photoelectron and chemical heating is increasing with flux, only IR seems to stay constant. This can easily be explained with the nature of the solar spectrum itself. When going back to a younger Sun it is the XUV part that changes. This is why instead of using heating rates per solar flux the use of an efficiency gives a much clearer picture of how the heating rates are affected by the atmospheres composition, as the contribution of the flux is canceled out by the normalisation (see Fig. 3.17). In this Figure the efficiency of the different configurations do not significantly change over time, with IR heating being an exception. This is however due to the normalization that has been done, as the IR spectrum itself does not change significantly over time but XUV gets stronger.

3.3. Effect of a Changing Solar Flux on a Venus with different CO₂ mixing ratios

Very interesting to see is the varying effect of composition. For chemical heating the different compositions do not seem to have much impact on the total heating rate, however, if we take a look at just chemical heating by itself, we see a tendency for atmospheres of higher CO₂ content to have lower chemical heating rates. A very low content of CO₂, however, also leads to lower rates (see Fig. A.4). It would be interesting to investigate the limit of how much CO₂ is needed to still lead to higher rates in the future.

XUV and photoelectron heating are strongly affected - though the effect is rather strange. Here the 90% CO₂ Venus results in drastically smaller rates, than the other compositions. Additionally for the 30% Venus we see a sudden drop in XUV and photoelectron heating rates for a flux of 1.7erg/s/cm². We double-checked the setup of our simulation, but did not find any mistake. Additionally we checked these two heating mechanisms for other simulations as well (see Fig. A.2) and found a sudden drop in the 10% CO₂ case as well, but not in the 20% case. If we compare with the exobase altitudes (see Fig. A.1), we see that indeed the two simulations with rapidly dropping rates have similar exobase altitudes, while the 20% case did not reach these altitudes yet. This suggests that the reason for the rapid drop lies in the expanded altitudes.

IR heating shows a clear trend of higher CO₂ content resulting in higher heating rates, which is pretty much self-explanatory, as CO₂ is the only IR absorber in the simulated atmosphere. If CO₂ increases it is clear that the overall IR heating also increases. We also looked at the other simulations to see if the change has a linear effect, and find this to be true (see Fig. A.3). The difference in heating rate for different compositions gets slightly larger the less CO₂ the atmosphere has, however, the differences are much smaller than expected. It would be interesting to further investigate whether there is a critical value of CO₂ where IR heating rates suddenly drop off.

Despite the differences of the effect of composition on the heating mechanisms, we do not find a big impact of flux on them.

In the previous sections we have already seen that the effect of heating mechanisms depends on the altitude at which we look as well. While at 150 km the temperature profiles do still overlap for all compositions (compare Fig. 3.9), we already find differences in the heating and cooling rates. We therefore look at the mechanisms at three different altitudes: 150 km, 2/3 of the atmosphere (which results in different altitudes for each simulation), and the exobase.

At 150 km (see Fig. 3.18) we see a clear tendency for lower CO₂ atmospheres to be heated more, with IR being an exception. Note, that here the heating rates are not normalized to the flux. The increase with flux is therefore again the straightforward correlation between more energy being put into the atmosphere, resulting in more heating. In this figure we also see that chemical heating is the most contributing mechanism, while photoelectron heating contributes the least. However, above a flux of 1.4 erg/s/g IR heating rates become even less important.

Above 150 km the atmospheres increase in temperature rapidly until approximately

3. Results

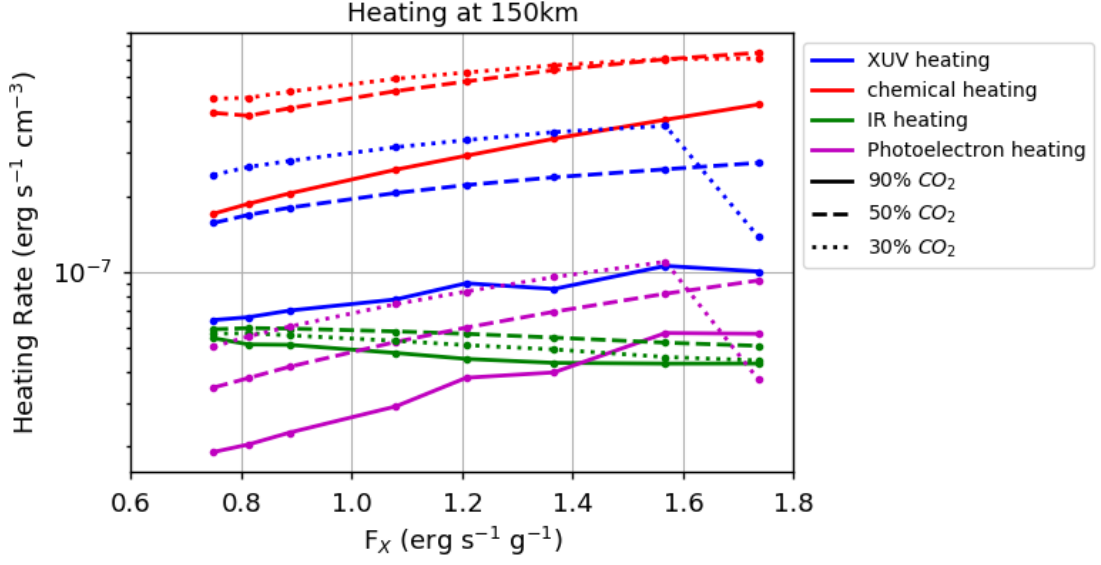


Figure 3.18.: Different heating mechanisms are shown for the 90% CO₂ Venus (solid) the 50% CO₂ Venus (dashed) and the 30% CO₂ Venus (dotted) for different X-ray fluxes at 150 km.

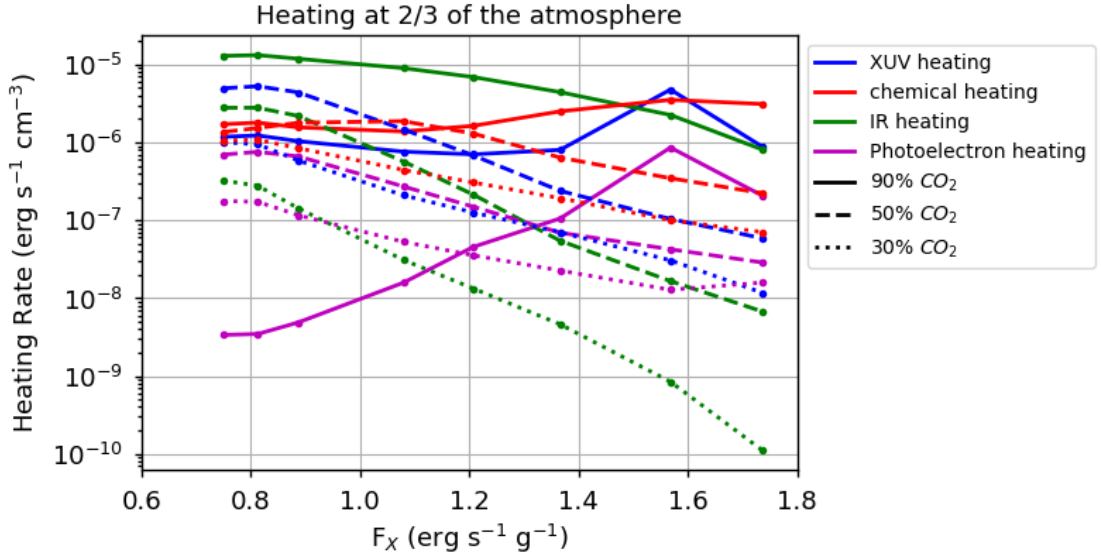


Figure 3.19.: Different heating mechanisms are shown for the 90% CO₂ Venus (solid) the 50% CO₂ Venus (dashed) and the 30% CO₂ Venus (dotted) for different X-ray fluxes at 2/3 of the atmosphere.

3.3. Effect of a Changing Solar Flux on a Venus with different CO₂ mixing ratios

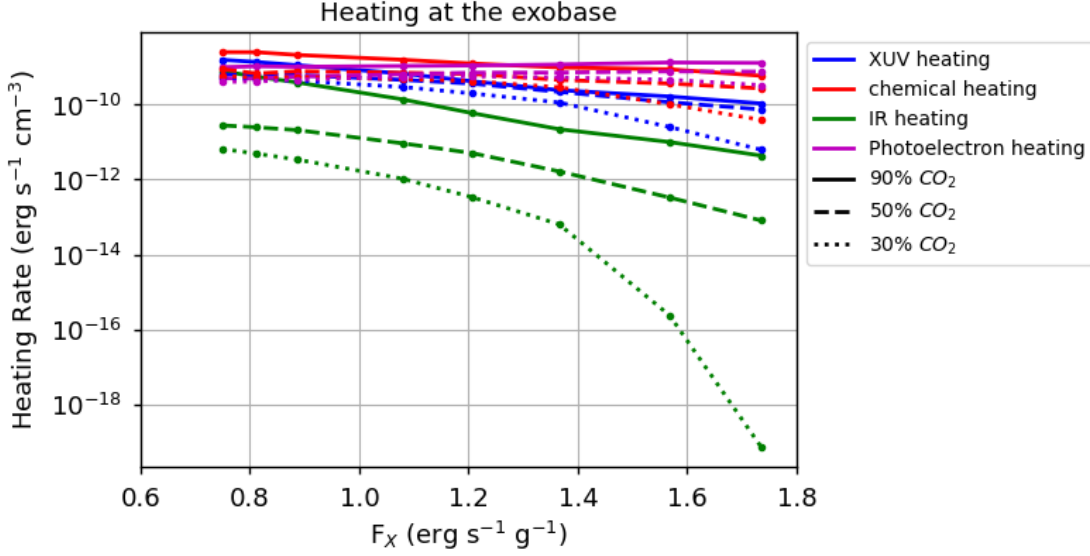


Figure 3.20.: Different heating mechanisms are shown for the 90% CO₂ Venus (solid) the 50% CO₂ Venus (dashed) and the 30% CO₂ Venus (dotted) for different X-ray fluxes at the exobase.

two thirds of the atmosphere's exobase altitude. Here they stabilize again. The heating mechanisms, however, seem very chaotic at first glance (see Fig. 3.19). This might be very much due to the arbitrarily chosen altitude. We do see some tendencies, however, such as IR heating following a clear trend of high CO₂ atmospheres having higher IR heating rates, and - as before - dropping with flux. XUV and photoelectron heating show some interesting behaviour, where the high CO₂ case starts with lower rates, but has higher rates than the other compositions for fluxes exceeding 1.3 erg/s/g. For photoelectron heating this might be explained by the atmospheres of high CO₂ ratios still being rather compact compared to the others, which would give particles the chance for more collisions, leading to more heating. The rates for chemical heating start off very similar for small fluxes, but then spread out with higher CO₂ leading to higher heating rates.

At the exobase we see equal heating rates for almost all heating mechanisms (see Fig. 3.20), with IR heating being an exception once again. We see the same tendency as previously, where atmospheres with higher CO₂ mixing ratio lead to higher heating rates, and the heating rates staying almost unaffected by the increasing flux. IR heating rates however drop with flux, and do so more strongly for smaller CO₂ ratios. As we mentioned several times IR heating depends on the CO₂ content, so it is already expected to see IR heating rates dropping for smaller CO₂ ratios. Additionally, the atmospheres are expanded with lower densities at the exobase and therefore have even less CO₂ number density.

3. Results

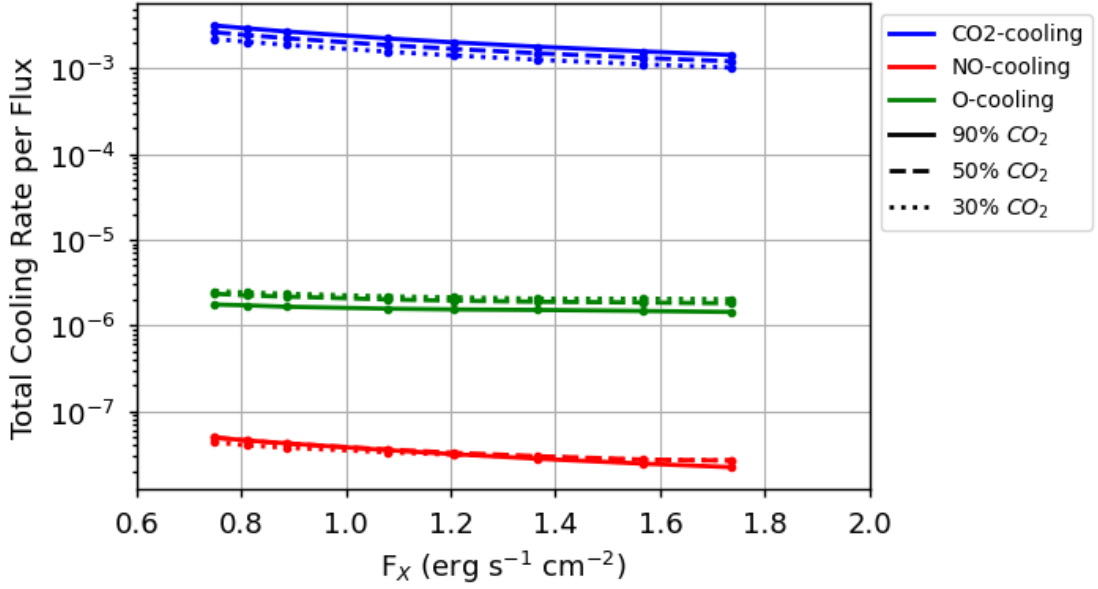


Figure 3.21.: Evolution of the total cooling rates for different mechanisms (colour) for different compositions (linestyle) normalised to the solar X-ray flux, and therefore unitless.

3.3.3. Cooling

The cooling mechanisms that can contribute in the performed simulations are the same as previously: CO₂, O, and NO cooling. As with the heating rates we compare how the contributions of these mechanisms change depending on composition and flux by calculating a total cooling rate for each mechanism in the same way as before. The resulting rates are presented in Fig. 3.21.

In Fig. 3.21 the total cooling rates for 90%, 50% and 30% CO₂ are shown for different fluxes. We see that the mechanisms scale with the composition albeit only slightly. CO₂ has higher total rates for atmospheres with higher CO₂ composition, while O cooling shows the opposite effect. NO cooling starts off with high CO₂ being more efficient at cooling, but then at 1.2 erg/s/cm² the lower CO₂ atmospheres take over. It is very surprising how little the composition plays into the cooling effect, especially for CO₂ cooling. The cooling mechanisms also do not significantly change with an increasing solar flux; however CO₂ and NO cooling show trends of lower efficiency towards higher fluxes, which add up to the picture of expanded and hotter atmospheres at higher fluxes. One possible reason for CO₂ cooling to only show little change is that the IR flux does not change drastically over time.

The efficiency of O cooling, on the other hand, stays constant, but because it is negligible compared to CO₂ cooling, it can't be solely responsible for balancing out the increased heating when solar XUV flux increases. However, we have seen at an earlier stage of this

3.3. Effect of a Changing Solar Flux on a Venus with different CO₂ mixing ratios

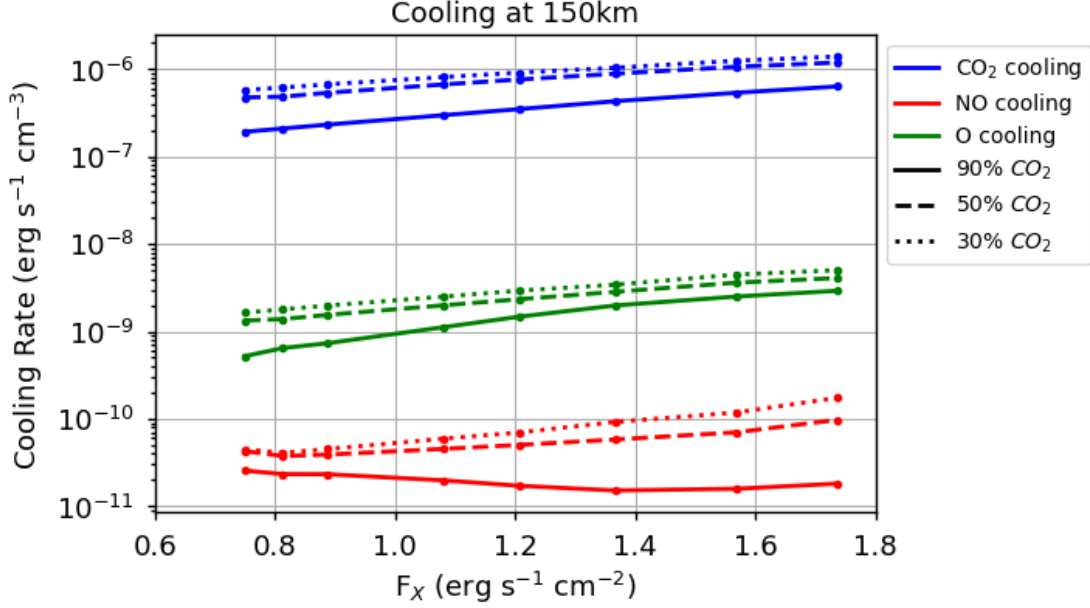


Figure 3.22.: Cooling rates for different compositions at 150 km for varying fluxes.

thesis that conduction is very efficient in transporting heat from the upper parts of the atmosphere, to lower regions. Interestingly, in these lower regions at around 150 km the trend for the cooling rates change (see Fig. 3.22). Note that here the cooling rate is shown and not the cooling efficiency.

Similar to the heating mechanisms in the previous section, it is interesting to investigate the cooling mechanisms at 150 km, which is the point of lowest temperature. At this point CO₂ cooling results in the highest rates, while NO cooling has the smallest rates; however, the effect of the composition is reversed, as high CO₂ atmospheres have less cooling. When investigating the mechanisms further we find that O and NO cooling show a clear correlation between higher CO₂ rates resulting in less cooling at 150 km. This might be due to the fact that there is less O and NO present at these altitudes, compared to lower ratios of CO₂. CO₂ cooling, however, does not show this clear correlation, as the 10% case produces the same rates as the 60% case for smaller X-ray fluxes (see Fig. A.5).

At two thirds of the atmospheres height higher CO₂ ratios lead to higher cooling rates again (see Fig. 3.23), where CO₂ cooling follows a trend that has already been seen for IR heating earlier and most likely also follows the same explanation. With less CO₂ the atmospheres are more expanded, leading to lower densities and less CO₂ at higher altitudes, which in turn leads to less cooling. O cooling stays stable for different fluxes, but NO cooling shows some interesting behavior. There seems to be a non-linear correlation between flux and composition, where atmospheres with less CO₂ have higher cooling rates for lower fluxes, quickly increasing, but then decreasing again. This would be interesting

3. Results

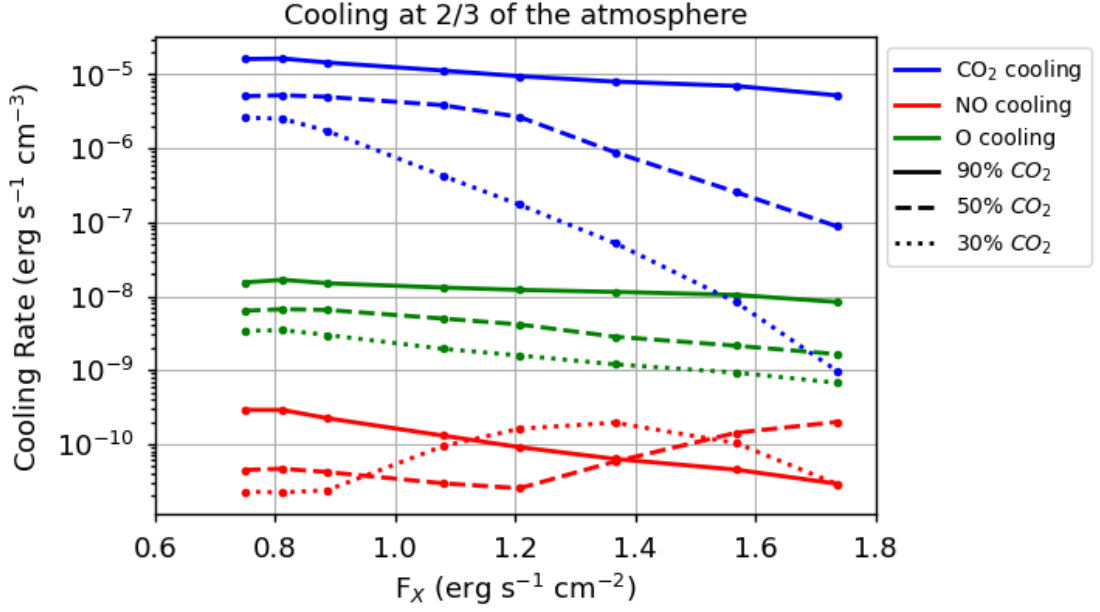


Figure 3.23.: Cooling rates for different compositions at 2/3 of the atmospheres height for varying fluxes. The absolute altitude therefore changes, for each simulation, as the atmosphere will expand for higher flux.

to investigate further in future work.

Lastly, the exobase shows similar rates for all cooling mechanisms, all of them having higher rates for higher CO_2 compositions. But while the rates for O cooling increase with flux, NO and CO_2 cooling decrease. This is most likely again due to expanded atmospheres having less heavy species at the exobase than light species such as O. The rapid drop in CO_2 cooling has been explained before.

3.3. Effect of a Changing Solar Flux on a Venus with different CO_2 mixing ratios

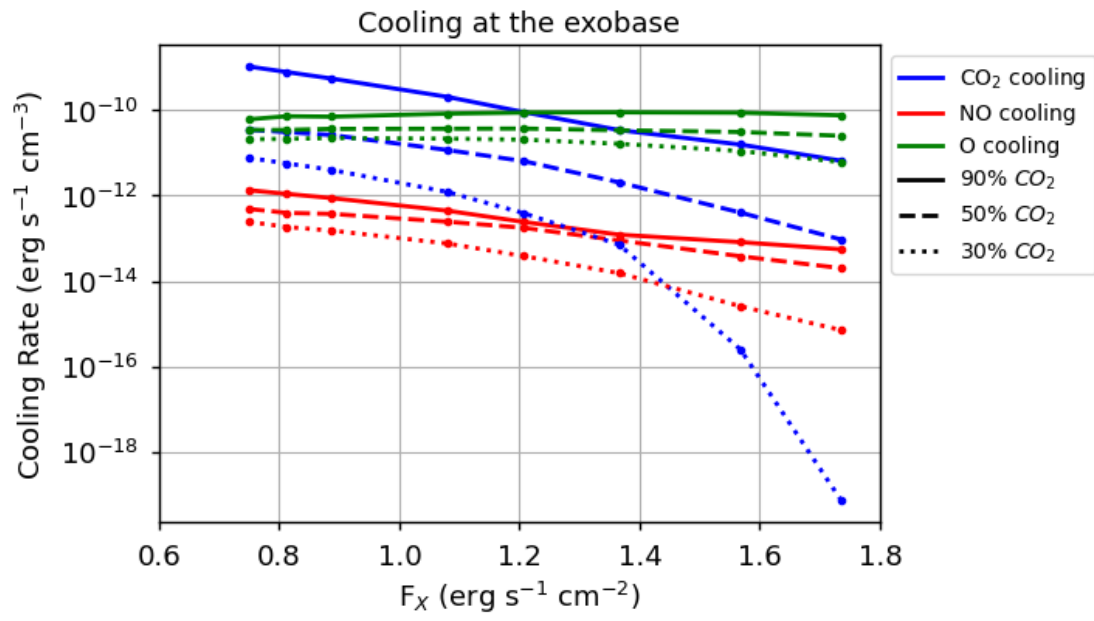


Figure 3.24.: Cooling rates for different compositions at the exobase for varying fluxes.

4. Discussion

Venus' surface temperature is about 750 K hot and the lower atmosphere has therefore very high temperatures as well, but it is dropping rapidly to 200-250 K at 60 km altitude, a temperature comparable to Earth values at similar altitudes. However, the high abundance of CO₂ on Venus might be the key to this, as CO₂ contributes a lot to the cooling effects in the upper atmosphere.

This research provided simulations of upper atmospheres to investigate how the CO₂ abundance affects the temperature of Venus' upper atmosphere, with a focus on the heating and cooling mechanisms.

Overall, a tendency was seen that for a lower abundance of CO₂ the resulting atmospheres are hotter and more expanded. However, none of the simulations led to a runaway increase of temperature.

The heating mechanisms show a maximum effect at around 150 km (see Fig. 3.12), which is mainly due to the increase of reaction rates of neutral and ion chemistry up to this level, resulting in higher chemical heating rates. At the same altitude, CO₂ cooling has its maximum (see Fig. 3.13) and its cooling rates decline towards the exobase. O cooling increases at this point, but slower than CO₂ cooling decreases, and with the rates being negligible compared to CO₂ cooling. Due to this difference the atmosphere experience a rapid increase in temperature for the next 50 - 150 km, depending on the composition. A modern Venus simulation shows that conduction plays a big role in redistributing heat in this area as well (see Fig. 3.8).

Between 50 and 150 km above the rapid increase of temperature slows down again, which is approximately where O cooling starts to dominate over CO₂ cooling and conduction becomes larger than the cooling rates, indicating that the transport from the hotter upper parts to the lower parts of the atmospheres is very efficient. Additionally cooling by NO also decreases, but doesn't contribute as much as the other two mechanisms and does therefore not impact the overall situation too much. It would be interesting to investigate the effect of NO further, to understand the importance of NO cooling better. It does, however, not seem to increase by much, even when providing more N₂ in the atmosphere.

These general findings are true for all compositions over all tested fluxes. To highlight possible differences between the heating rates, another set of simulations was performed with different solar spectra between X-ray fluxes of 0.7 - 1.8 erg/s/cm² (see Fig. 3.16). As an indication of how much the atmosphere temperatures changed, the exobase temperatures were compared between all tested compositions for the used fluxes. Atmospheres with higher CO₂ mixing ratios were found to have stable temperatures against a varying flux, whereas low CO₂ mixing ratios resulted in rapidly increasing exobase temperatures, even for small changes in flux.

4. Discussion

To find the cause of these differences, the heating efficiencies, which are calculated by integrating over all altitudes and normalizing them to the X-ray flux, for the four most important heating mechanisms were compared (see Fig. 3.17).

The heating efficiencies for photoelectron and XUV heating stay constant, which is consistent with findings from Johnstone et al. [2021a] where it was shown that the X-ray flux only starts having a big impact on atmospheres from 2 erg/s/cm^2 upwards, whereas the simulations performed for this thesis were stopped at that point. However, XUV heating shows large differences for different chemical compositions: The 90% CO_2 atmosphere results in heating rates that are almost three orders of magnitude smaller than the 50% and 30% CO_2 cases, while the difference between the two latter ones is negligible. Additionally, it is not the 30% CO_2 Venus that results in the highest heating rates, but the 50% Venus, suggesting a non linear correlation between composition and XUV heating rate. When investigating this further (see Fig. A.2) we find that the heating rates do actually follow a linear trend from 10% to 80% CO_2 , with lower mixing ratios resulting in lower heating rates than higher mixing ratios. The 90% CO_2 case seems to be an outlier. It would therefore be interesting to investigate this behavior in a future study.

Chemical heating shows a similar trend as XUV heating, and a more detailed analysis of the composition tracks (see Fig. A.4) show that a lower CO_2 mixing ratio does not necessarily mean higher heating rates, as the 10% CO_2 Venus arranges itself between the two atmospheres with the highest CO_2 content, for X-ray fluxes between 0.7 and 1 erg/s/cm^2 . From this point on, however, the heating rates increase for the 10% CO_2 case, surpassing the atmospheres between 80% and 40% CO_2 . Due to errors in the outputting (several files were not automatically saved), the analysis cannot be performed in greater detail. The non-linear trend, however, is clearly shown, and should therefore be the focus of a future study.

IR heating is the only heating mechanism that drops in efficiency. This is quite straightforward, as the younger Sun only tends to show noteworthy changes in the XUV part of the spectrum, and not in the IR. Additionally, atmospheres are more expanded for higher fluxes. Combined, this leads to less CO_2 in the upper part of the atmosphere absorbing almost the same amount of IR, which results in lower heating efficiency. Unlike chemical or XUV heating, IR heating follows a nice trend, where higher CO_2 mixing ratios lead to higher heating rates (see Fig. A.3).

Overall, the differences in heating rates are not large enough to be able to explain such large changes in temperature, giving rise to the question if the heating rates are different at specific altitudes.

According to the results of the previous part of this study the fastest increase in temperature happens at around 150 km. Focusing on the heating mechanisms at this altitude (see fig. 3.18), it can be seen that all heating mechanisms increase with compositions in the same way: lower CO_2 ratios lead to stronger heating. The difference in XUV heating is especially large, while IR seems to be mainly unaffected. This leads to the assumption that as long as there is a little bit of CO_2 present, it will lead to IR heating.

There is also an overall trend for heating rates to increase toward higher X-ray fluxes,

except IR heating, which decreases. It can be inferred from Fig. 3.18 that the overall composition also does not have a big effect on how the heating mechanisms evolve, as most of the profiles are parallel - with one exception: chemical heating. Here the 30% CO₂ Venus intersects with the 50% Venus at an X-ray flux of 1.6 erg/s/cm².

When investigating this further, a very interesting behaviour can be found (see Fig. A.6): For lower X-ray fluxes the 30% CO₂ Venus has the highest heating rates, at 1.2 erg/s/cm² the 40% Venus takes over. At approximately 1.6 erg/s/cm² the 30% Venus is surpassed by the 50% CO₂ Venus, which in turn intersects the 40% Venus at a higher flux. We therefore see that with higher fluxes higher mixing ratios result in higher rates for chemical heating. It would be interesting to make more simulations at higher fluxes and a deeper analysis, to figure out where the other mixing ratios would start to dominate.

The cooling mechanisms in Fig. 3.22 also show that at 150 km higher CO₂ ratios result in lower cooling - even for CO₂ cooling. CO₂ cooling however is a special case (just like chemical heating), where there is no clear relation between mixing ratio and cooling rate (see Fig. A.5). We find that 30% CO₂ ratios result in the highest cooling rates and stay dominant, while the 20% case seems to be overtaken by the 40% case, and the 10% case starts 4th lowest with a sudden increase and overtaking the 50% Venus above 1.1 erg/s/cm².

At approximately 2/3 of the height of the atmosphere the rapid increase in temperature reduces (see Fig. 3.19), leading to the necessity to check the trend of the heating mechanisms at these altitudes (which for every simulation now refers to a different absolute altitude). There was no clear correlation between heating mechanisms and composition. IR heating is contributing the most for the 90% Venus below 1.3 erg/s/cm², while photoelectron heating is strongest for the 50% Venus and chemical as well as XUV heating switches between those two. Additionally, for XUV and photoelectron heating the different composition tracks intersect each other, indicating that composition plays a different role at different fluxes. This most likely has to do with the fact that atmospheres with little CO₂ expand more rapidly, which leads to lower densities in the upper parts of the atmosphere.

The cooling mechanisms at 2/3 of the atmosphere (see fig. 3.23) seem to be less chaotic: The high CO₂ Venus has the highest cooling rates - with cooling by NO being an exception at certain fluxes - and here we see the clear dominance of the stability of CO₂ cooling over all fluxes. While the cooling rates of the 30% Venus decline rapidly, the 90% Venus stays almost constant. This is again most likely due to the fact that atmospheres are more expanded if the CO₂ mixing ratio is low, which in turn leads to less CO₂ in the upper parts of the atmosphere. It should also be quickly mentioned that the behavior of NO cooling is very interesting, with the 30% Venus evolving in a non-linear way, emphasising the need to explore NO cooling in further studies.

Lastly, the heating rates at the exobase were checked (see Fig. 3.20), which showed that all heating mechanisms contribute in the same manner - except IR heating, which decreases strongly with lower CO₂ mixing ratios. This is again an effect that can be

4. Discussion

explained with less CO₂ being present at higher altitudes. The cooling mechanisms at the exobase (see Fig. 3.24) also show the trend that with higher CO₂ mixing ratio the cooling effect is stronger, and similarly as at the 2/3 mark CO₂ cooling and cooling by NO decline with flux with a sharp drop for CO₂ cooling for the 30% Venus, whereas O cooling seems to stay overall constant.

In combination we can therefore say that at the 150 km mark there is much more heating going on for lower CO₂ mixing ratios, at similar cooling rates, and we find much higher cooling rates at 2/3 of the atmosphere for higher CO₂ mixing ratios, preventing this strong temperature increase for a high CO₂ Venus. From there on the temperatures do not drastically increase anymore, despite the heating rates being higher than the cooling rates, which is due to conduction redistributing the energy from higher altitudes towards lower altitudes. The profiles expand to higher exobases for lower mixing ratios, but in parallel with all other mixing ratios, which can be explained by the fact that at the exobase there is basically no difference among the contribution of the different heating mechanisms for different compositions.

While these elaborations explain the picture of why certain atmospheres show this quick increase in temperature quite consistently, it is very hard to pinpoint the cause to one specific species or chemical reaction as already pointed out in chapter 3. One little change in chemistry can trigger a whole chain of different outcomes. Some species are elevated in number density, which leads to different reactions happening more frequently and storing more or less energy from XUV radiation, while other species might not impact the overall picture as much as we initially would have thought. One example is that the mixing ratio of CO₂ does not increase the CO₂ cooling rates at all altitudes. Another one is that chemical heating and CO₂ cooling do not show a linear correlation with composition, but rather each mixing ratio seems to be dominant in a different flux range. Additionally to the effect of composition we saw that the heating rates at 150 km increase for higher fluxes for all mechanisms, indicating that this is where the rapid increase in temperature is coming from. To see this more clearly, more simulations would be needed in the higher flux regime.

The final part of this discussion will show why this elaborated research on temperatures and heating mechanisms is important, and how it can be connected to other work. As mentioned at the very beginning of this thesis an important goal when studying Earth-like planets and exoplanets is to understand what makes a planet habitable. Temperature alone is already a very important factor to this, because the temperature decides whether we find liquid water on the surface or not. But there is an additional reason for why temperatures are important: Hot atmospheres expand and lose their atmospheres more easily. The study of temperatures therefore provides the key aspects for understanding the loss rates of atmospheres under different conditions.

A quick analysis was done of how the loss rates would change on Venus under varying composition and flux, which shows that X-ray fluxes below 2 erg/s/cm² can not result in

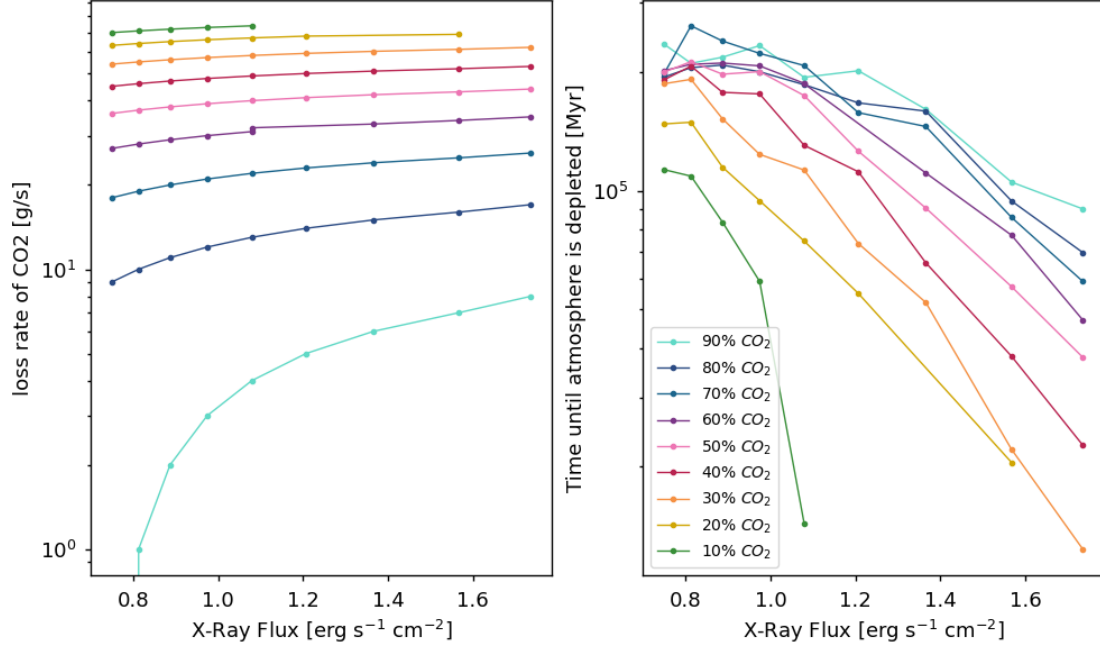


Figure 4.1.: Left: CO₂ loss rates for different compositions (color coded) as a function of X-ray flux. Right: Time until the atmosphere is depleted, for different compositions and evolving X-ray flux.

severe atmospheric loss. This is illustrated in Fig. 4.1, where on the left side the CO₂ loss rates for all simulations are shown, and on the right side the time until the atmosphere is depleted. As can be taken from the figure, the loss rates are negligibly small, as on Earth we have loss rates in the order of 3000 g/s for H, and 50 g/s of He (see Catling and Zahnle [2009]).

The recent study of Johnstone et al. [2021a] already showed that on Earth a certain CO₂ threshold needs to be reached in order for the atmosphere to be sustained at high fluxes. For Venus we were at this point of the study confined to the chosen flux range of 0.7 - 1.75 erg/g/cm², due to limitations of the code. However, in the near future we expect to be able to do a detailed analysis on the impact of higher X-ray fluxes on Venus, to elaborate its possible evolutionary tracks and the role that CO₂ played in it.

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A. Appendix A

We have seen that increasing CO₂ mixing ratio will lead to higher exobase temperatures for higher fluxes. Due to this the exobase altitudes will also be located at higher altitudes, due to the atmospheres being more expanded. This can be seen in fig. A.1.

To investigate the effect of the heating and cooling mechanisms depending on incoming flux, and composition further, we plotted each mechanism by itself for all successful simulations, and present them here (see fig. ??- A.6). For some simulations unfortunately Kompot did not save the necessary data files (for example the 70% and 80% CO₂ Venus), and therefore leaving large gaps in interesting data. The figures still provide an interesting addition to the overall picture, and it is advised to look at the heating mechanisms in greater detail in future studies.

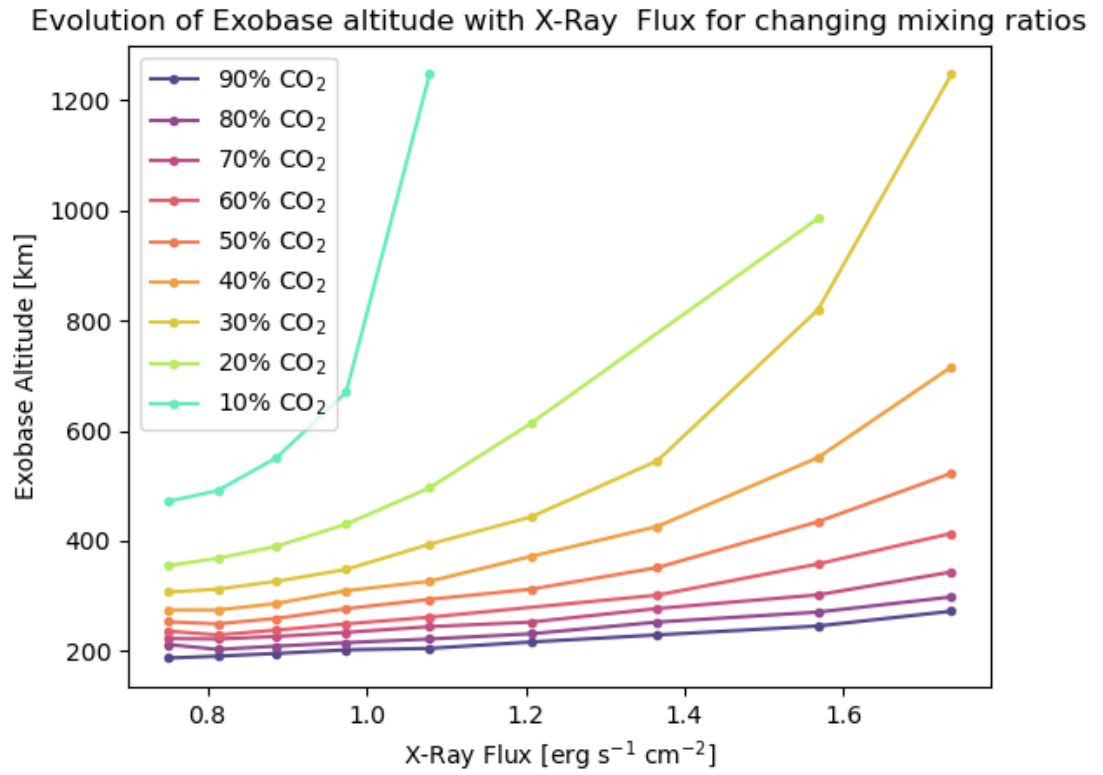


Figure A.1.: The exobase altitudes for different compositions and different solar X-ray fluxes are shown. The 20% case seems to follow a different trend, as previously mentioned. There is a trend of lower CO₂ content leading to rapidly expanding atmospheres.

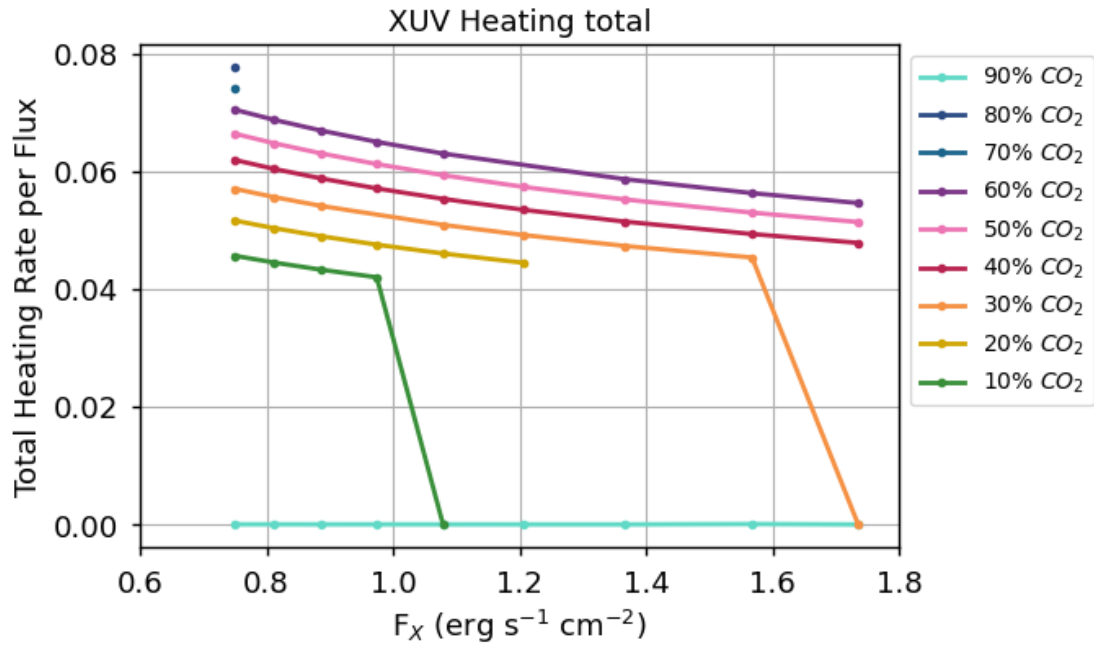


Figure A.2.: The composition affects XUV heating rates proportionally - the more CO₂ the more heating, but for 90% CO₂ we suddenly see way less heating.

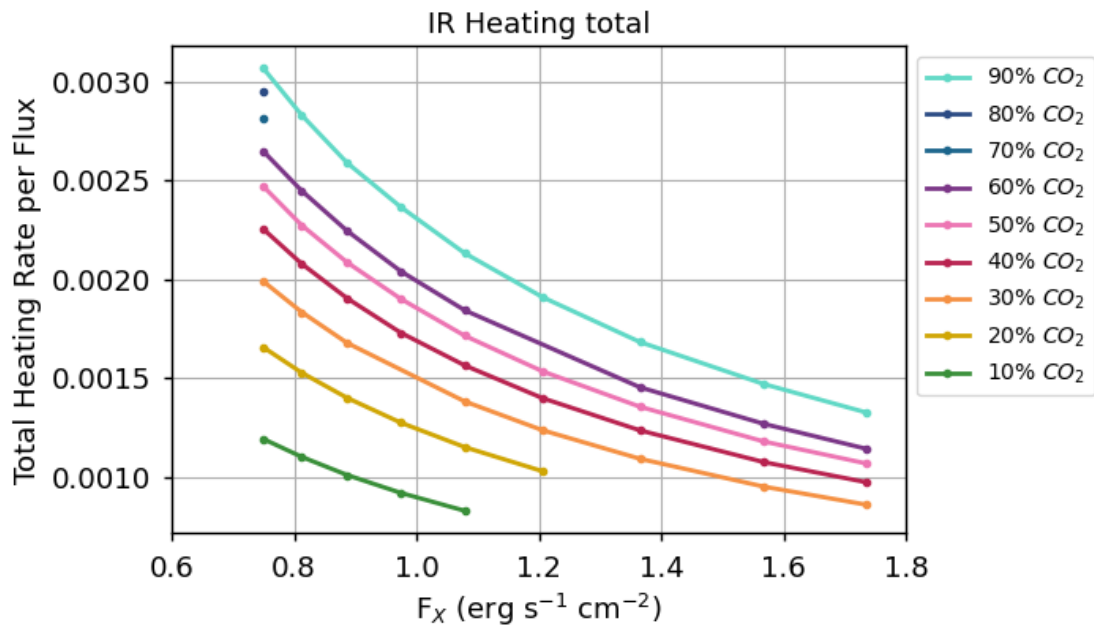


Figure A.3.: The effect of composition on IR heating rates does not seem to be proportional - the curves are not sorted by composition.

A. Appendix A

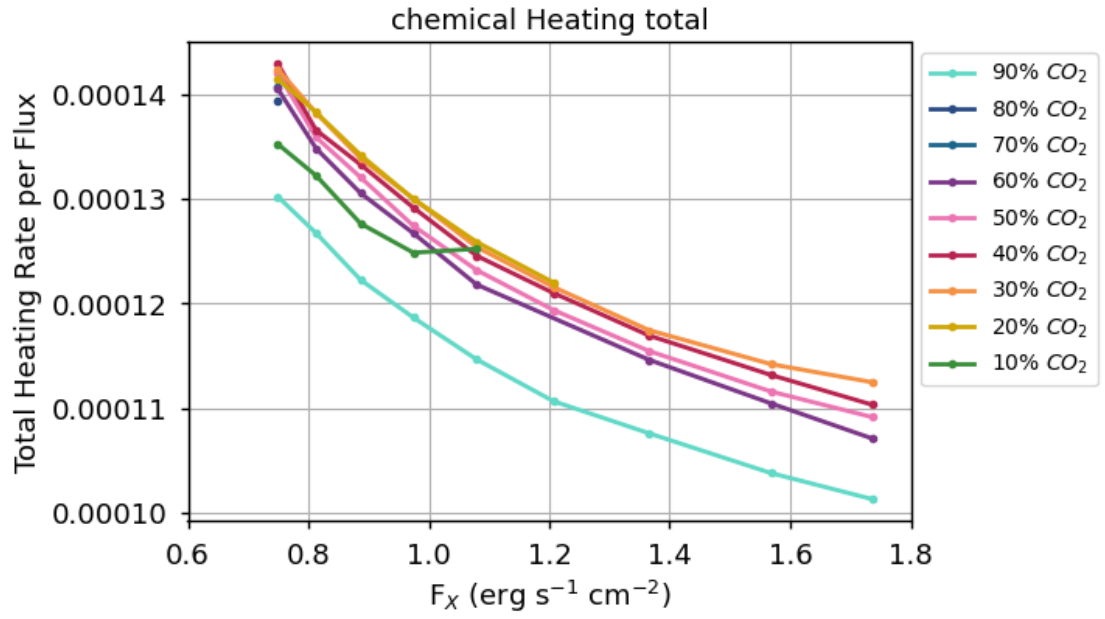


Figure A.4.: Despite the heating rates being quite close together, there does not seem to be a clear correlation between composition and chemical heating, as the lines are not sorted by composition.

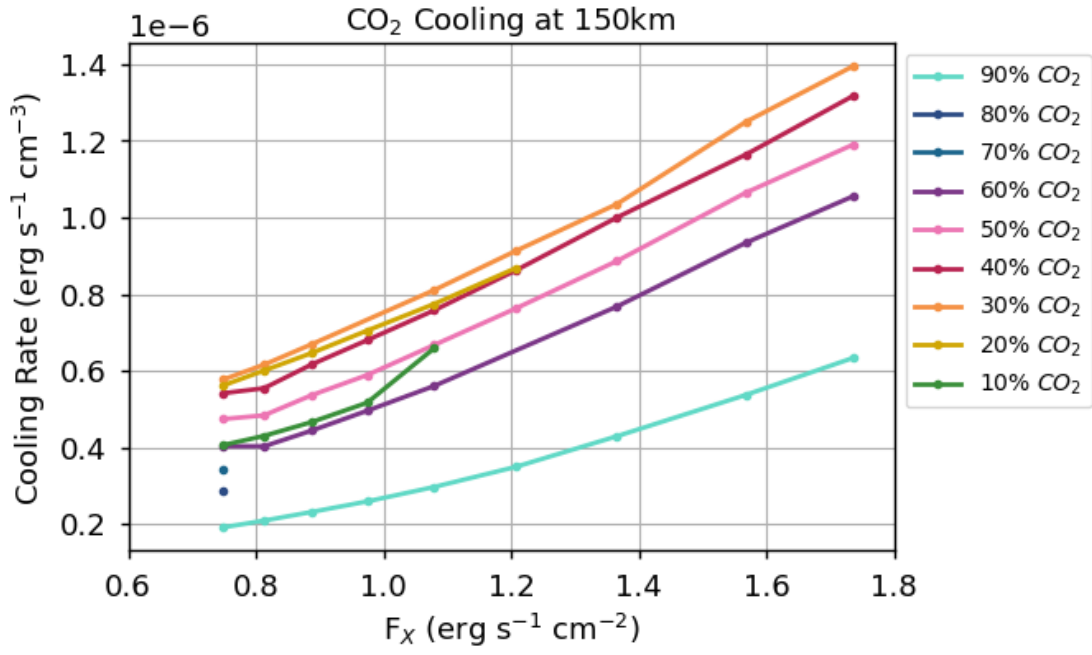


Figure A.5.: Figure shows the cooling rate for CO₂ cooling at 150km, and shows that there are exceptions to the correlation between composition and cooling rates.

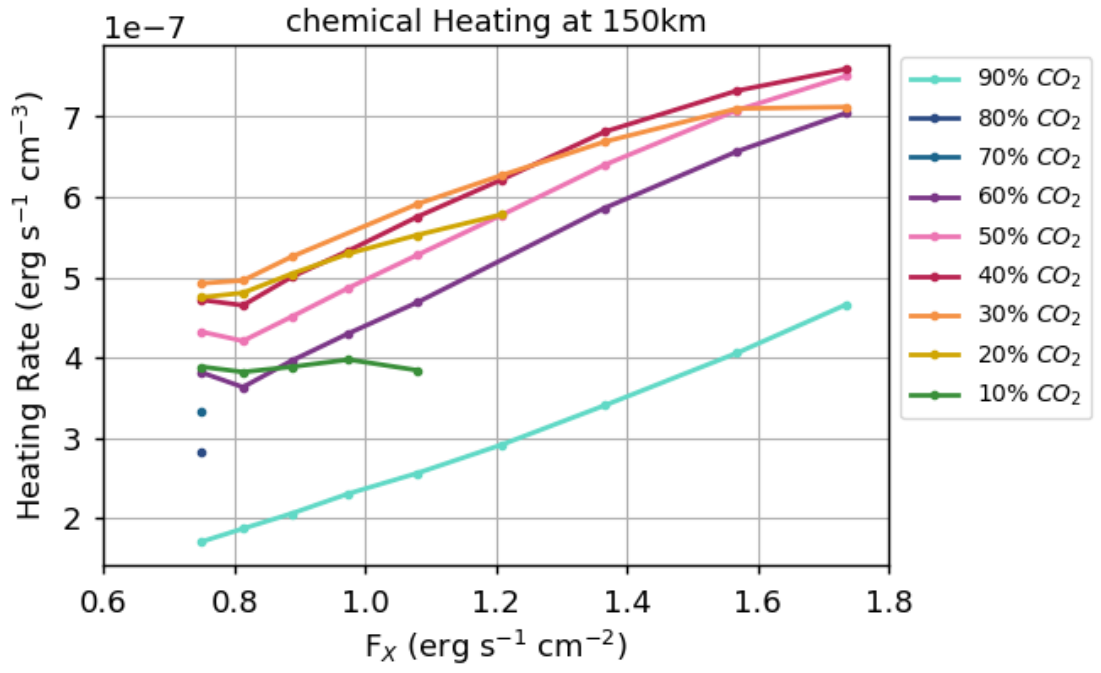


Figure A.6.: Figure shows the chemical heating rate at 150km, and shows that there are exceptions to the correlation between composition and heating rates.