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Exoplanetary Atmospheric Retrieval

Atomspheric Retrieval for planet GJ3470b Implementing Taurex3

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ABSTRACT

Context. More than 7000 planets outside of the solar system (exoplanets) have been discovered, this due to the increment of new technologies, like the James Webb Space Telescope (JWST), allowing for more detailed characterization of their atmospheres.
Aims. Obtain a retrieval spectrum
Methods. We use Taurex, a fully bayesian inverse atmospheric retrieval framework, to construct a forward models and fit its atmospheric parameters such as elemental and molecular abundances. The parameter estimation is carried out using Bayesian inference with Marco Chain Monte Carlo (MCMC) and nested sampling, which can be computationally expensive for complex models. To address this, we employ the MultiNest algorithm to efficiently explore the parameter space
Results. As results, we observe that is very probably that the planet have a stratosphere, additionally the principal molecules in the atmosphere are H20, CO and CH4
Conclusions. This frameworks give us a wide parameter space to fit in the spectrum begging an excellent tool for study the properties of exoplanets

Key words. Atmospheric retrieval, taurex, spectrum, exoplanet

1. Introduction

The exoplanet GJ 3470b is a sub-Neptune that orbits a cool M-dwarf star approximately 96 light-years from Earth in the constellation of Cancer. Discovered in 2012 using radial velocity techniques with the HARPS spectrograph on the ESO 3.6 m telescope, along with transit observations from the TRAPPIST telescope Bonfils et al. (2012), GJ 3470b has since attracted significant interest. Its characteristics offer valuable insights into planetary formation and atmospheric composition, and further study of this system could enhance our understanding and classification of sub-Neptune planets throughout the galaxy.

We rely on the data observed by JWST through the transit method. The Transit Method is one of the most widely used and successful techniques for detecting exoplanets. It involves monitoring the brightness of a star over time and looking for periodic dips in light intensity. These dips occur when a planet crosses our line of sight or "transits" in front of the star, blocking a fraction of the light from reaching Earth. If these dips are repetitive it can be conjectured to be an exoplanet orbiting the star. By detecting these dips in the spectrum, we can identify the absorption lines of the molecules present in the atmosphere.

In this project, we aim to investigate the chemical and thermal structure of its atmosphere using a combination of Bayesian inference and radiative transfer modeling. To do this, we rely on TauREx Al-Refaie et al. (2021) (Tau Retrieval for Exoplanets), an open-source Python library specifically developed for atmospheric retrieval in exoplanetary research.

TauREx supports both forward and inverse modeling and makes use of powerful sampling algorithms such as Nested Sampling and MCMC to effectively explore parameter space and compute posterior distributions of atmospheric variables. Using TauREx we can solve the Schwarzschild radiative transfer equation, which is a fundamental relation that describes how light intensity changes along its path through the atmosphere due to the balance between absorption and emission at each layer. Altogether, this approach not only deepens our understanding of GJ3470b but also contributes to the broader effort of characterizing and comparing sub-Neptune exoplanets across the galaxy.

2. Planetary system parameters

Below are the summarized stellar 1 and planetary 2 parameters of the GJ 3470 system, derived from multiple literature sources and databases, including ExoFOP-TESS, Gaia DR2, Kosiarek et al. 2019, Awiphan et al. 2016, and others found in the NASA Exoplanet Archive (2023).

Due to a number of interconnected features, GJ 3470 b is thought to be very favorable for detection. Frequent transits are made possible by its brief orbital period of about 3.3 days, which raises the possibility of seeing the planet as it passes in front of its host star. Furthermore, the photometric signal is further enhanced by the host star's small size, which helps to distinguish the transit. Since the planet has an inclination of almost 89 degrees, the orbit is almost edge-on from Earth's perspective, making the transits visible. All these features make this planet a very good candidate for studying its atmosphere using optical methods.

Table 1: Stellar Parameters of GJ 3470

Parameter	Value	Source
Spectral Type	M1.5	Awiphan et al. (2016)
$T_{\rm eff}$	3600 ± 100 K	Kosiarek et al. (2019)
$M_\star$	$0.498 \pm 0.02\, M_\odot$	Kosiarek et al. (2019)
$R_\star$	$0.500 \pm 0.015\, R_\odot$	Kosiarek et al. (2019)
$\log g$	4.74 ± 0.01	Kosiarek et al. (2019)
$\rho_\star$	$5.62 \pm 0.27\,\mathrm{g/cm^3}$	Kosiarek et al. (2019)
$\log L_\star/L_\odot$	-1.45 ± 0.09	Kosiarek et al. (2019)
[Fe/H]	0.20 ± 0.10 dex	Awiphan et al. (2016)
Age	$\sim 1.65 \pm 1.35$ Gyr	Awiphan et al. (2016)
Rotation Period	21.54 ± 0.49 days	Awiphan et al. (2016)

Table 2: Planetary Parameters of GJ 3470 b

Parameter	Value	Source
Orbital Period (P)	3.33665 ± 0.00001 days	Kokori et al. (2023)
Planet Radius (R_p)	$4.13 \pm 0.15\, R_\oplus$	Kokori et al. (2023)
Planet Mass (M_p)	$13.9 \pm 1.5\, M_\oplus$	Bonfils et al. (2012)
Planet Density (ρ_p)	$0.80 \pm 0.13\,\mathrm{g/cm^3}$	Bonfils et al. (2012)
Semi-major Axis (a)	0.0355 ± 0.0019 AU	Biddle et al. (2014)
Inclination (i)	$89.13 \pm 0.30°$	Awiphan et al. (2016)
Equilibrium Temp. ($T_{\rm eq}$)	595 ± 97 K	Kosiarek et al. (2019)
Eccentricity (e)	0.017 ± 0.014	Awiphan et al. (2016)

The JWST data collected from NASA archives for a transmission spectra looks as shown in the Figure 1: Here, on x axis, we have the central wavelength in microns and transit depth percentage on y axis.

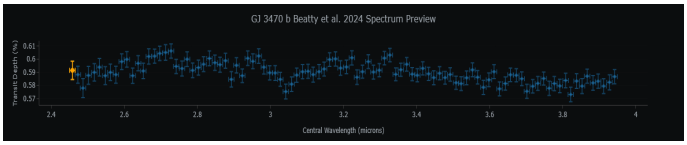


Fig. 1: Transmission spectrum of GJ3470b

3. Atmospheric study on GJ3470b

The estimations for the radius of GJ3470b is around 0.36-0.40 R_J and a mass of 0.039-0.043 M_J. Previous studies Beatty et al. (2024) have reported the presence of chemical species as water, methane, sulfur dioxide, and carbon dioxide in its atmosphere, and an equilibrium temperature of around $600K$. This makes GJ3470b one of the lowest-mass and coldest exoplanets known to show sulfur dioxide in its spectrum. GJ3470b is a transiting exoplanet, making it an easy choice to study the transmission spectrum observed by the James Webb Telescope.

Taurex gives us the freedom to play around with parameters and build a model for the exoplanet. Our task here is to study the knowledge of the atmosphere of the planet obtained by the telescopes and previous studies and use it to build a forward model for atmospheric retrieval.

3.0.1. Temperature

Taurex can work in bash environment as in Jupyter environment. For both, is necessary to create a .par file which contains the parameters (and their values) of the atmosphere. These parameters include temperature, radius, mass, chemical composition, and more. From this file Taurex creates a forward model and builds a synthetic spectra.

We set up the chemistry of the planet by filling it with gases like H_2, H_e and molecules as H_2O, CO_2, CH_4, and so on. Then we define the scattering and absorptions required to build the synthetic spectra. We also specify temperature and pressure profiles; this step is very crucial in modeling the spectra. There are various types of profile that Taurex provides us; we have explored a few of them, which will be explained further.

Once the spectrum is obtained on the basis of the parameters we provide, Taurex uses Bayesian inference to match this with the observed spectra taken from NASA archive.

The temperature profiles available in Taurex are the following ones:

1. Isothermal:
   - Simplest temperature profile. Assumes constant temperature throughout the atmosphere.
   - Uses only one temperature parameter to fit.
2. Guillot:
   - The temperature as a function of pressure in the Guillot (2010) profile is given by Guillot (2010):

$$T^4(P) = \frac{3T_{\rm int}^4}{4}\left(\frac{2}{3}+\tau\right)+\frac{3T_{\rm irr}^4}{4}\left[(1-\alpha)\left(\frac{2}{3}+\frac{1}{\gamma\sqrt{3}}+\frac{\gamma\tau}{\sqrt{3}}e^{-\gamma\tau}\right)+\alpha\left(\frac{2}{3}+\frac{\tau}{\gamma}\right)\right] \quad (1)$$

   where:
   - $T_{\rm int}$ is the internal (intrinsic) temperature of the planet
   - $T_{\rm irr}$ is the irradiation temperature from stellar flux
   - τ is the infrared optical depth at pressure P
   - $\gamma = \kappa_{\rm vis}/\kappa_{\rm IR}$ is the ratio of visible to infrared opacity
   - α is the fraction of incident stellar flux absorbed at high altitudes
   - It balances the effects of stellar irradiation, atmospheric opacities, and internal heat. Thus, requires five fitting parameters T_{irr}, κ_{irr}, κ_{v1}, κ_{v2}, α.
3. Npoint:
   - It is a generalized version of guillot where we can define temperatures at various heights in the atmosphere. Each temperature point has an associated pressure point.
   - The fitting parameters are $T_{surface}$, T_{top}, $P_{surface}$, P_{top}, $T_{point(n)}$, $P_{point(n)}$.
4. Rodgers:
   - Another T-P profile provided by Taurex used to approximate the planetary atmosphere. However, we did not incorporate this in our models.

3.0.2. Chemistry

Another important aspect in defining our model is the chemical composition of the atmosphere and the type of model can be described using variable chemistry type.

Before we get into the type of chemistry profiles available in Taurex, let us walk through the chemistry of a planet itself. Taurex computes the absorption of light in the atmosphere

of a planet by using molecular cross sections, which define how strongly a molecule absorbs radiation at each wavelength, these molecules can be find in Project (2025) which is an open database used for spectral characterization and simulation. Another physical process is the collision-induced absorption, which occurs when two molecules collide and temporarily absorb light even though they would not individually. It is important for molecules as $H_2 - H_2$ and $H_2 - He$, especially in hydrogen-dominated atmospheres like our target.

We used a free chemistry profile *Taurex* that allows us to define individual abundance profiles for each molecule. Molecules are either active or inactive, depending on what is available. If no cross sections are available, then the molecule is not actively absorbing Al-Refaie et al. (2021), Al-Refaie et al. (2022). The cross-sections of the molecules are available in Project (2025).

We fill the atmosphere for our forward model with hydrogen, helium and specify their ratio. Next, we go ahead and define the molecules of our choice along with a mixing ratio that specifies their abundance in the atmosphere.

Additionally, we can define the type of star that we will use. The simple one is a blackbody model, while a more complex and realistic one is the Phoenix star. The Phoenix model simulates a real star's atmosphere by solving the radiative transfer equation with detailed physics as compared to blackbody, which follows the Planck's radiation law. Further, for the planet, we can consider the radius and mass.

We used the results of previous studies as our prior for the forward model, as first try, we choose the following parameters.

```
[Chemistry]
chemistry_type = taurex
fill_gases = H2,He
ratio = 4.8962e-2

    [[H2O]]
    gas_type = constant
    mix_ratio=1.1185e-2

    [[CO]]
    gas_type = constant
    mix_ratio = 3.00739e-4

    [[SO2]]
    gas_type = constant
    mix_ratio = 1.11e-4

    [[CO2]]
    gas_type = constant
    mix_ratio = 3.00739e-4

    [[CH4]]
    gas_type = constant
    mix_ratio = 3.00739e-4

[Planet]
planet_type = simple
planet_mass = 0.043
planet_radius = 0.37
[Temperature]
profile_type = guillot
T_irr = 600
kappa_irr = 0.01
kappa_v1 = 0.002
kappa_v2 = 0.003
alpha = 0.3
```

3.0.3. Nested sampling

An efficient way of calculating the likelihood is to use the method of nested sampling. It works by sampling from the prior, the prior showcases the ignorance we have towards the problem, in the most basic case we start with a flat unconstrained prior. We proceed to sample points from this distribution (parameter space) and calculate the likelihood. We know from Baye's theorem that:

$$P(\theta|D) = \frac{L_\pi(\theta)}{E(D)}$$

Where E is the evidence and L is the likelihood for prior π. However, sampling from the entire prior can become inefficient, hence we try the method of constrained uniform sampling. Here, the region of sampling converges towards maximum likelihood with each iteration. This is what is used in Multinest algorithm Feroz et al. (2009). It constraints the parameter space in ellipsoids and then proceeds with the sampling. This sampling algorithm has been included in our models. It ultimately calculates the evidence $z = \int P(D|\theta)P(\theta)d\theta$ which is useful in estimating Baye's factor.

3.0.4. MPI

The forward modeling and retrieval involves the estimation of a lot of parameters in a wide parameter space. To do so, it generates thousands of model spectrum to compare with the observed data. This makes it computationally expensive and can take hours to run. For a faster process, we parallelize it using Message Passing Interface (MPI) Dalcín et al. (2005). It lets us run the same code on multiple CPUs of the system. Since each model evaluation is independent, MPI enables these to be done in parallel across many processors. This makes the process a lot faster and enables us to efficiently run various models.

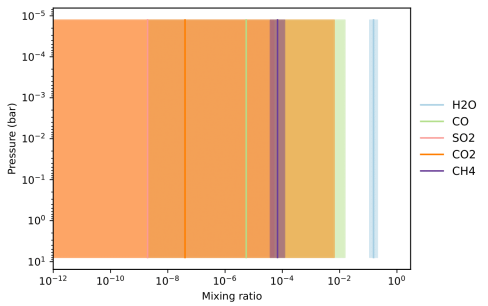
3.1. Retrieval

Keeping the basic physical properties of the planet and star same, we vary the chemistry of the models and run the retrievals. We have taken into consideration different molecules, scattering, absorptions, star type and temperature profiles.

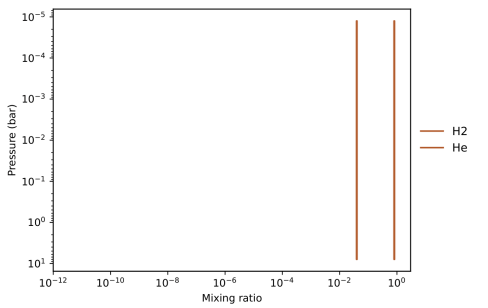
Model 1: Guillot, molecules: $H_2O, CO, SO_2, CO_2, CH_4$

The first outcome that we observe is the mixing ratio of the active and inactive chemical components, this depends on the availability of the cross sections, if they're absent, the molecule is considered to be inactive. From Figure 2a we can observe the fitting of the chemical molecules. For the species of H_2O and CH_4, we have a good fit but for SO_2, CO and CO_2 the variance is too large. This is represented in Figure 3 where the value for these molecules are not well defined. This may be because of the presence of more chemical substances that we are not

considering.



(a) Output of active mix-ratio



(b) Output of inactive mix-ratio

Fig. 2: Solution obtained after the retrieval for each molecule including the variance

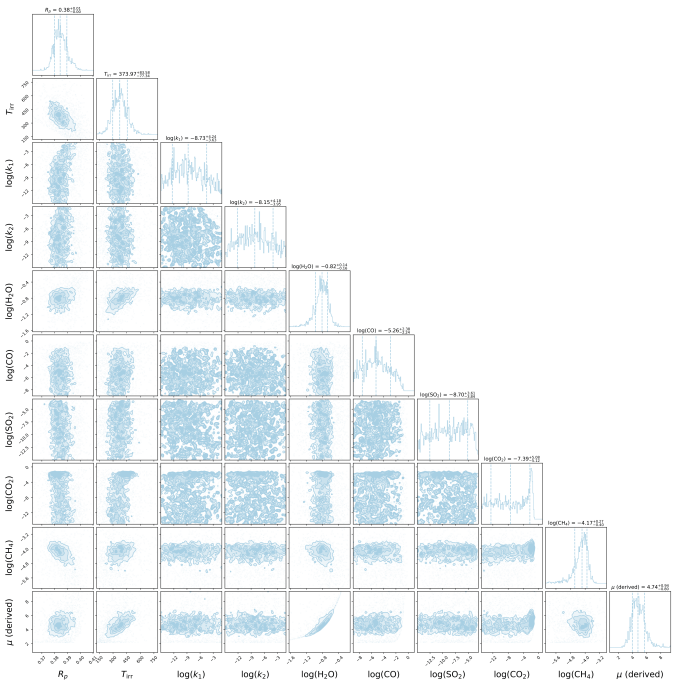
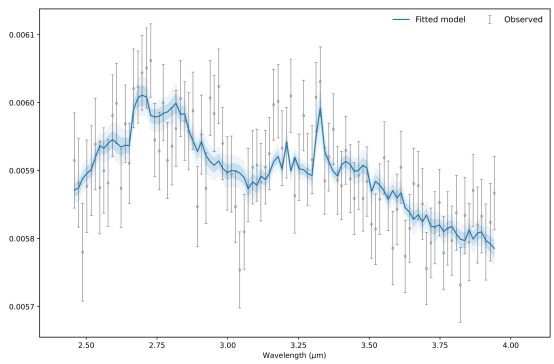


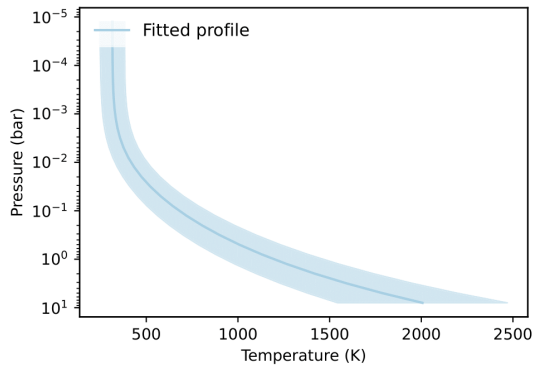
Fig. 3: Posterior distributions for each parameter

We can also observe that the equilibrium temperature and the radius of the planet are parameters that are fitted correctly. We observe the posterior spectrum obtained in Figure 4a matches well with the observed spectrum, showcasing regions of high peaks. In Figure 4b we observe the temperature profile. This shows that the planet is cold, as is verified from the posterior distribution.

It is important to note that for pressure lower than 10^0 bar, we do not have a contribution of the temperature because the region of absorption at that pressure is high so we cannot observe the planet's chemical and physical properties, this can be confirmed from Figure 5 from the optical depth where in the yellow region we have almost a null absorbance while in the dark zone the absorbance is high. This challenges the study of the planet at wavelengths of $2.0 - 12.0\mu m$ because the atmosphere absorbs all the incoming light, making it difficult to observe the internal components. In our case, we study the planet at a wavelength of $2.0 - 4.0\mu m$ with little or no information about the surface. An analogy can be made with an overexposed photograph; in this case, if the camera lens is not adjusted for the brightness, we will see only a white image which is noise.



(a) Forward Spectrum



(b) Temperature Profile

Fig. 4: In a) the final spectrum is shown, matching very well with the observed spectrum. On b) we observe how the temperature change with the atmosphere height.

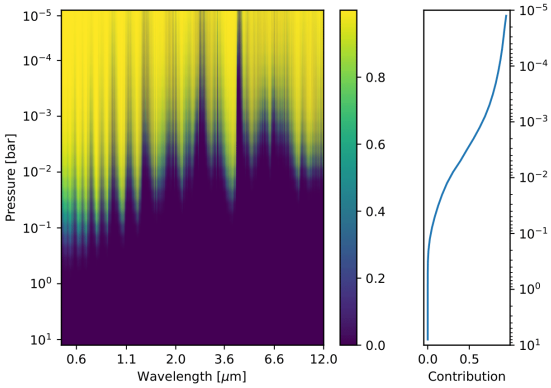
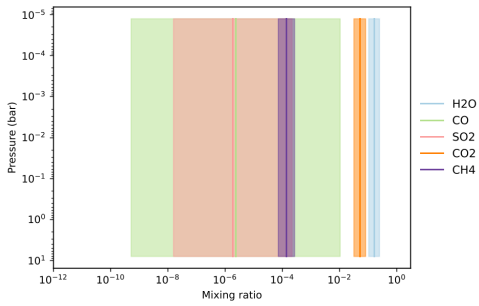
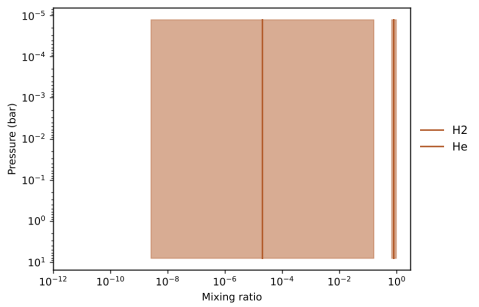


Fig. 5: Optical Depth of the planet. We can note that in pressure lower than 10^{-1} that all the incoming light is absorb

Model 2: Guillot, narrower bounds, H_e/H_2 ratio fitted. Knowing these distributions, we can run another model with narrower bounds to help find a better region in the parameter space. We also fit the He and H_2 ratio, which results in a variance in the He molecule as observed in Figure 6b. This means that the model couldn't properly fit the ratio $He/H2$ which can be confirmed through the next set of results in Figure 7.



(a) Output of active mix-ratio



(b) Output of inactive mix-ratio

Fig. 6: Solution obtained after the retrieval for each molecule including the variance for model 2

In the posterior, we see that more parameters have a better adjustment to the spectrum, as can be observed in 6a where the molecules are better fitted than in the past model. Also, for the posterior spectrum 7, we cannot observe a big change

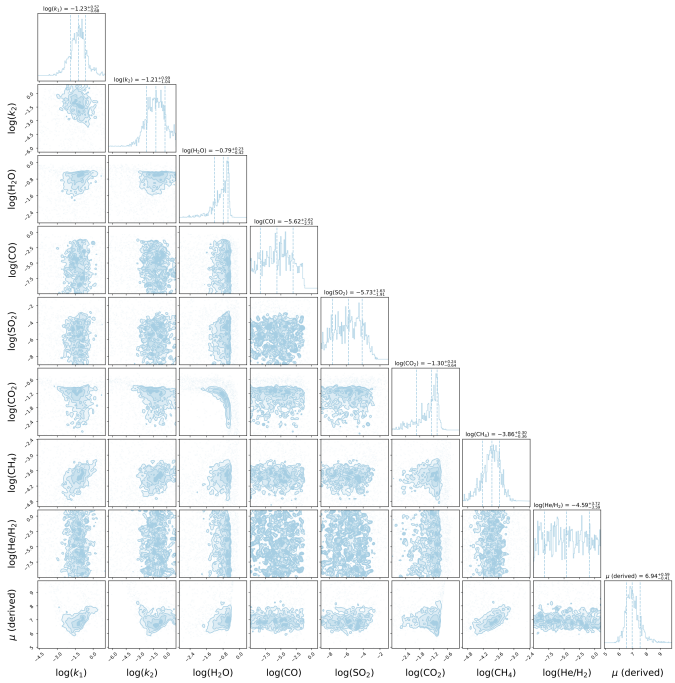


Fig. 7: Posterior distributions for each parameter for model 2

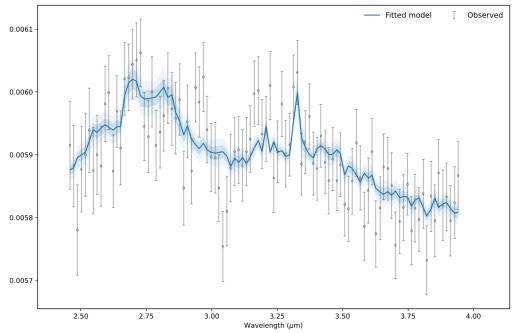
comparing visually the plots, but as we will see in the next section, we use a Bayesian approach to quantify them.

One very important result is the differences in the Temperature Profile, looking realistic, it aligns with the previous information from literature. This opens a new area of study to confirm if GJ3570b possesses a stratosphere. We observe how the temperature changes with the atmosphere length; this means that there are molecules that absorb the light and heat-up the atmosphere. From the spectrum contribution, Figure 10, is likely that CH_4 is one of these molecules, but we are constrained in the infrared regime. To conclude the existence of the stratosphere we need to study the UV regime to explore the upper atmosphere and find if other molecules are absorbing light, similar to the process observed on Earth.

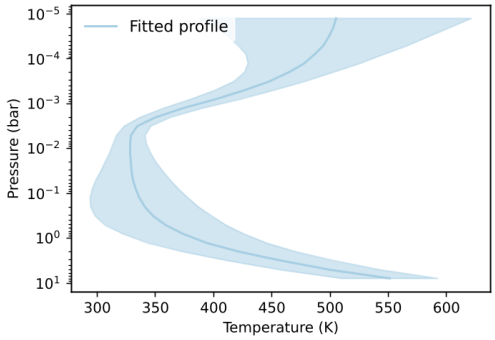
In Figure 10, in addition to the absorption of the molecules, we can observe the CIA (Collision-Induced Absorption) of the species He and H_2: the gases used to fill the atmosphere. This analysis gives us information about the interaction (collision) of $H_2 - He$ and $H_2 - H_2$. These interactions temporarily induce a dipole moment that allow them to interact with light. Incorporating CIA is really important to study the atmosphere because they are crucial for the depth length.

The last feature present in this graph is the Rayleigh of each molecule. This process indicates to us whether the molecule scatters the light. In this case, all the molecules absorb it, so the Rayleigh remains very close to zero.

A further aspect to study is the optical depth along with the altitude of the planet. This heatmap gives us information about the absorbance of the planet atmosphere. As we can note in



(a) Forward Spectrum Model 2



(b) Temperature Profile Model 2

Fig. 8: Comparative of the Forward spectrum a) and the Temperature Profile b) after fixing the knowing parameters. In b) we observe a stratosphere behavior

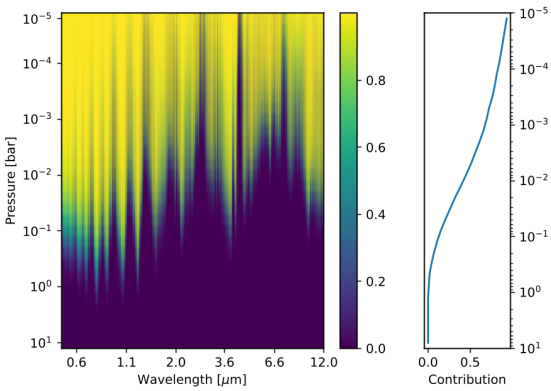


Fig. 9: Optical depth of the planet atmosphere for Model 2

Figure 9 the optical depth is very similar to the one obtained in the past model, but now we have more access to lower atmosphere length. What both plots represent is the absorbance region around 3.6μm, in this wavelength zone we have null access to information about the planet, from the spectrum contributions, Figure 10, we notice that in that wavelength region we have a peak in the CH_4 contribution, meaning that this molecule absorbs all the light incoming.

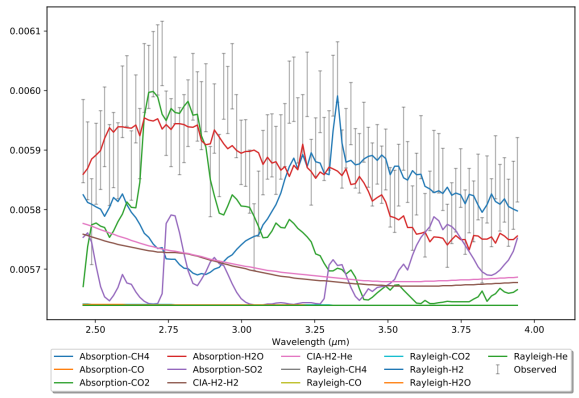
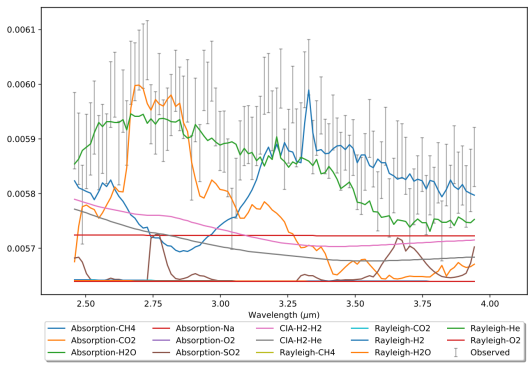


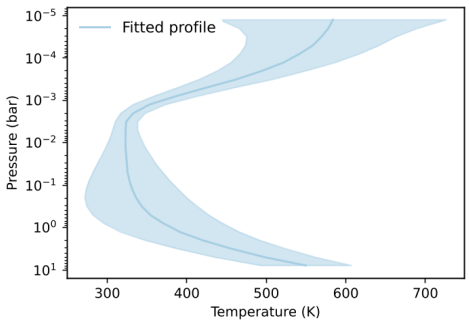
Fig. 10: Spectrum Contributions for Model 2

Model 3: Guillot, adding Na, O_2

Next, we compare our model with other chemical components and temperature models. As first example, we can try to search if more chemical molecules can be added to the atmosphere, in this case we add Na and O_2 leaving the other explored molecules with the same ratios. As a result, we infer that these molecules do not absorb light as we can observe in Figure 11a where the contribution of these gases is null.



(a) Spectrum Contribution Model 3



(b) Temperature Profile Model 3

Fig. 11: Solution obtained after the retrieval for each molecule including the variance for model 2

An important result from this model is the clear preference for the presence of a stratosphere in the planet's atmosphere, as illustrated in Figure 11b. An interesting feature in this plot is the Rayleight of O_2, indicating that this molecule could scatter the light in the infrared, but this does not confirm the existence of it in the planet. To confirm this, we need to study the atmosphere in a wide range of wavelengths.

Model 4: Isothermal, H_2O, CO_2, CH_4, CO

The models we have seen so far were based on the Guillot temperature profile. They were implemented for different molecules and ratios. Now we go ahead and compare them with isothermal temperature profile. These models have atmosphere made of H_2O, CO_2, CH_4 and CO, their abundance is shown in the figure 12. We see how the confidence interval for CO_2 is very large implying that the fit is not too well.

From the temperature profile in 13a that the constant temperature has been set around 513.5 K which is close to the value obtained from previous models. The yellow region in Figure 13b reaches the lowest pressures among all models, indicating this is the deepest we have probed into the planet's atmosphere as compared to the previous models.

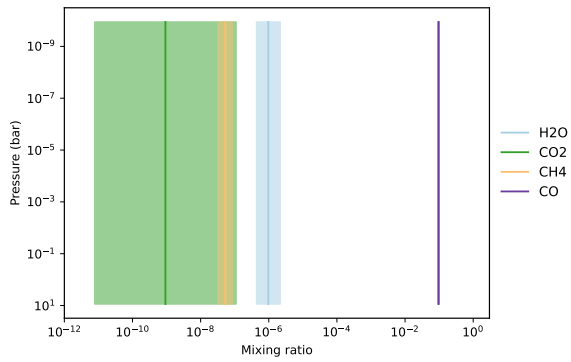
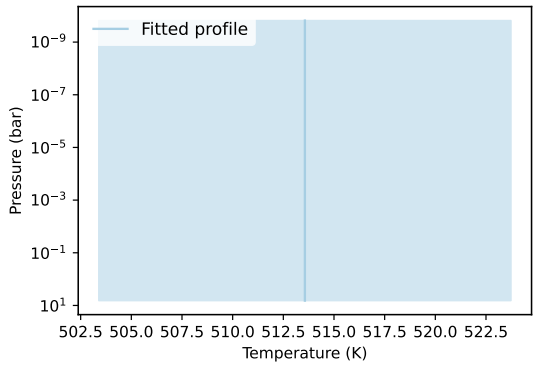


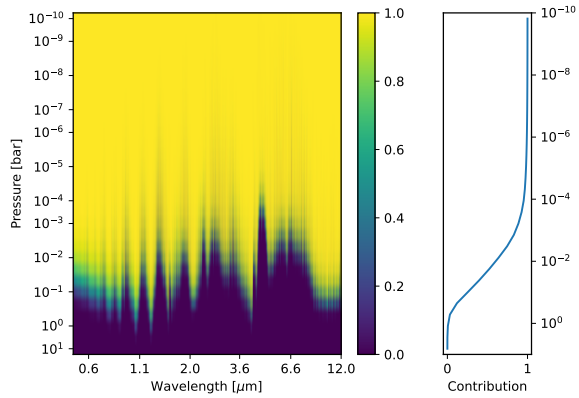
Fig. 12: Active components in isothermal model

We go ahead and study the posterior distributions in figure 14a, we observe how the posteriors for most of the parameters is well contained except for a few where the peak might be beyond the specified bounds.

Lastly, we inspect the individual contribution of the molecules in the transmission spectrum as observed in the figure 14 where the major peaks are due to absorption of water and methane. There is little contribution of CO_2 as well as CIA. The fitting matches the contribution of molecules as observed in previous models.



(a) Isothermal temperature profile



(b) Optical depth

Fig. 13: Temperature profile and optical depth for Model 4

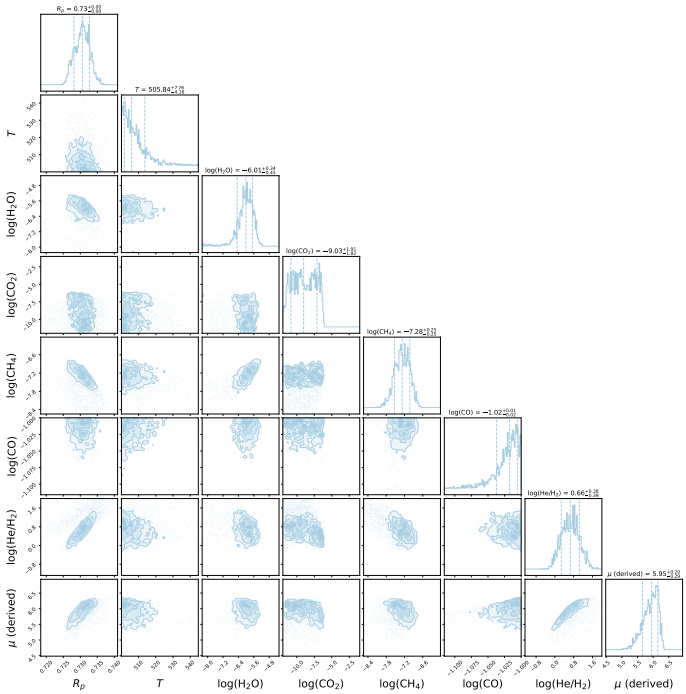
Model 5: Npoint

Moving on to the next temperature profile, we try fitting four temperature points using the Npoint method. The figure 15 shows how the temperature varies with pressure. We observe how in the middle to upper atmosphere there is thermal inversion i.e. temperature increases with decreasing pressure. This inversion is a marker for the presence of a stratosphere.

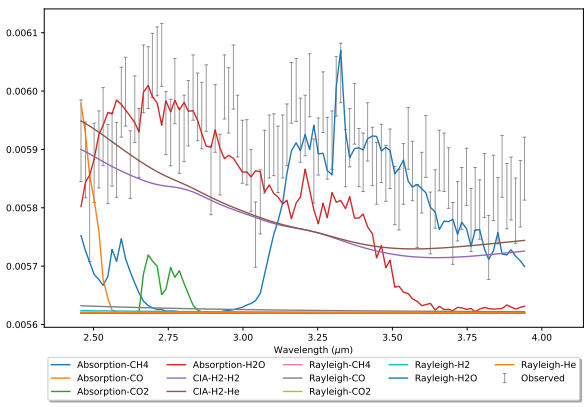
Under certain conditions the npoint profile becomes same as the Guillot. However, it will be interesting to try fitting more temperature and pressure points in our model. Due to the extra points being fitted here, the dimensionality of our parameter space has increased, making it computationally expensive to run. As before, the spectrum contribution in the figure 16b remains more or less the same, throughout all the models.

4. Model comparison

With more complex models, we need a strong and refined statistical analysis. For this we can use Bayesian methods for the comparative of models. As we have a lot of parameters to fit and limited resources, a solution to visualize how the change of



(a) Posteriors



(b) Spectrum contribution

Fig. 14: Posteriors and Spectrum Contribution for Model 5

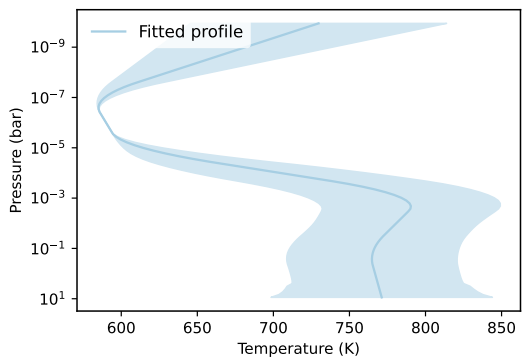
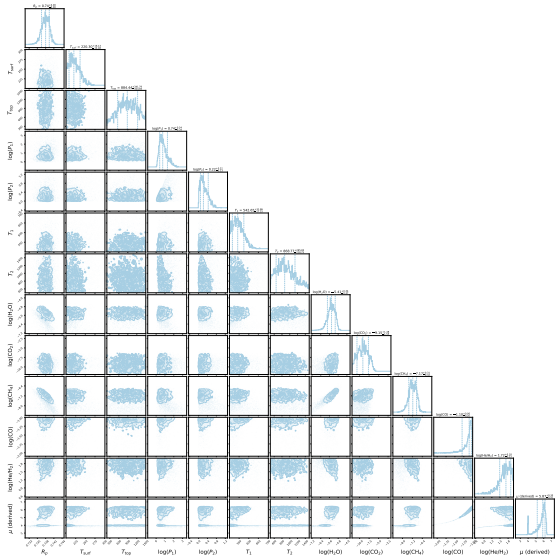
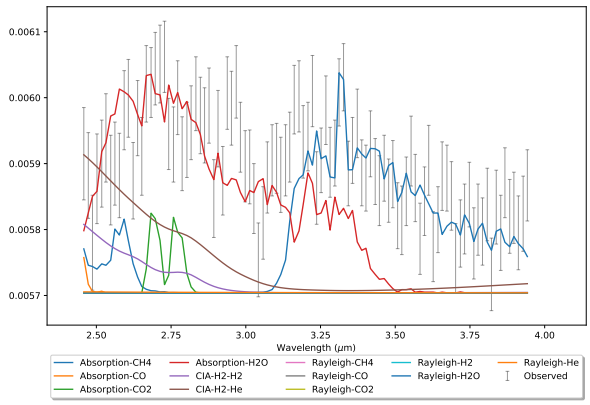


Fig. 15: Tp profile

parameters affect the posterior model is to run different models



(a) Posteriors



(b) Spectrum contribution

Fig. 16: Posteriors and Spectrum Contribution for Model 5

and compare them.

From the Bayes perspective, the comparison of models is dependent on the data, based on the Baye's evidence.

$$p(d|M) = \int_{\Omega_M} p(d|\theta, M)p(\theta|M)d\theta$$

Which is the average of the likelihood under the prior chosen. From the Baye's theorem the posterior is:

$$p(M|d) \propto p(M)p(d|M)$$

With this, two models can be compared as:

$$\frac{p(M_0|d)}{p(M_1|d)} = B_{01}\frac{p(M_0)}{p(M_1)}$$

Here, the Bayes factor is introduced as

$$B_{01} = \frac{p(d|M_0)}{p(d|M_1)}$$

Taking the logarithm

$$lnB_{01} = ln(p(d|M_0)) - ln(p(d|M_1))$$

Table 3: Bayes Factor Interpretation

$\lvert \ln B_{01} \rvert$	**Strength of Evidence**
< 1.0	Inconclusive
1.0	Weak evidence
2.5	Moderate evidence
5.0	Strong evidence

From empirical scale Trotta (2008) we have the following criteria shown in 3

Table 4: Bayes Factor for models

Model	**log evidence**
Model 1	835.24
Model 2	839.98
Model 3	841.196
Model 4	820.71
Model 5	828.35

From the table 4 we can see that the highest Baye factor is for model 3 after we narrowed the boundaries of the parameters and added more molecules. But because $|lnB_{01}| = 1.12$ the comparison is inconclusive.

Similarly to the first model, we obtain $ln(p(d|M_0) = 835.24$ for the second model, after fixing the parameters, we get $ln(p(d|M_1) = 839.98$ obtaining $lnB_{01} = 4.74$, which leads us to conclude that the model with the stratosphere (model 2) is better than the first model.

5. Conclusions

We started by studying how taurex works and in what capacity it helps us to understand the atmosphere of the planet. We begin by implementing various temperature profiles and proceeded to change the chemistry of the atmosphere. We noted that the GJ3470b has an atmosphere with high absorption of CH_4, CO_2 and H_2O, these absorption lines could very well fit the peaks of our observed data. Followed by little contribution of CIAs of $H_2 - H_2$ and $H_2 - He$.

We visualized the optical depth of the planet by looking at what wavelength can penetrate the atmosphere the deepest. The posterior distribution of each model gives us an idea about how the taurex is processing the parameters from the parameter space.

Since taurex offer a wide amount of options to customize our model and make it more realistic possible, including physics processes such as the Guillot temperature, consider clouds, phoenix stars, or personalize the chemistry of the planet. This liberty gives us a big space of features that will take more than the age of the universe to explore, and for this we need to use algorithms such as MultiNest and MPI to improve the searching on the parameter space and find the best results.

From the results obtained, future work will be to make the parameter space smaller and try to fit the $He/H2$ ratio better. Additionally, a study for different wavelengths in the atmosphere is needed. From the optical length, we can see that we have more access to the information of the planet around a wavelength of $0.6{-}2\mu m$. And, as we mentioned, for the confirmation of a stratosphere we need to analyze the components of the atmosphere in a UV regime and expand the study of GJ3470b spectra.

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