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RESEARCH PROJECTS IN THE THEORETICAL ASTROPHYSICS OF MODELING ATMOSPHERIC RADIATION ABSORPTION

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Contents

1 Abstract

An analysis of the sun's luminosity, earth's atmosphere, and earth's thermal equilibrium is carried out to illuminate the nature of the atmospheric effects of greenhouse gases. This model can be extended to atmospheres with different input parameters, namely from other solar and extra-solar planets and their stellar hosts. In this research, a simplified approach to a dynamic system is taken, this means that the model accounts for single spherical stars, circular planetary orbits, a uniform, well-mixed, and homogeneous planetary atmosphere, and thermodynamic equilibrium in all parts of the system. From these assumptions, a energy balance is derived between three components: Outer space, the planetary atmosphere, and the planet's effective temperature at the surface. The absorption of electromagnetic radiation in the atmosphere by three chemical species is then analyzed and presented.

Unified Astronomy Thesaurus Concepts: Radiative transfer (1335), Atmospheric effects (113), Atmospheric science (116), Planetary science (1255), Atmospheric extinction (114), Extinction (505)

2 Introduction

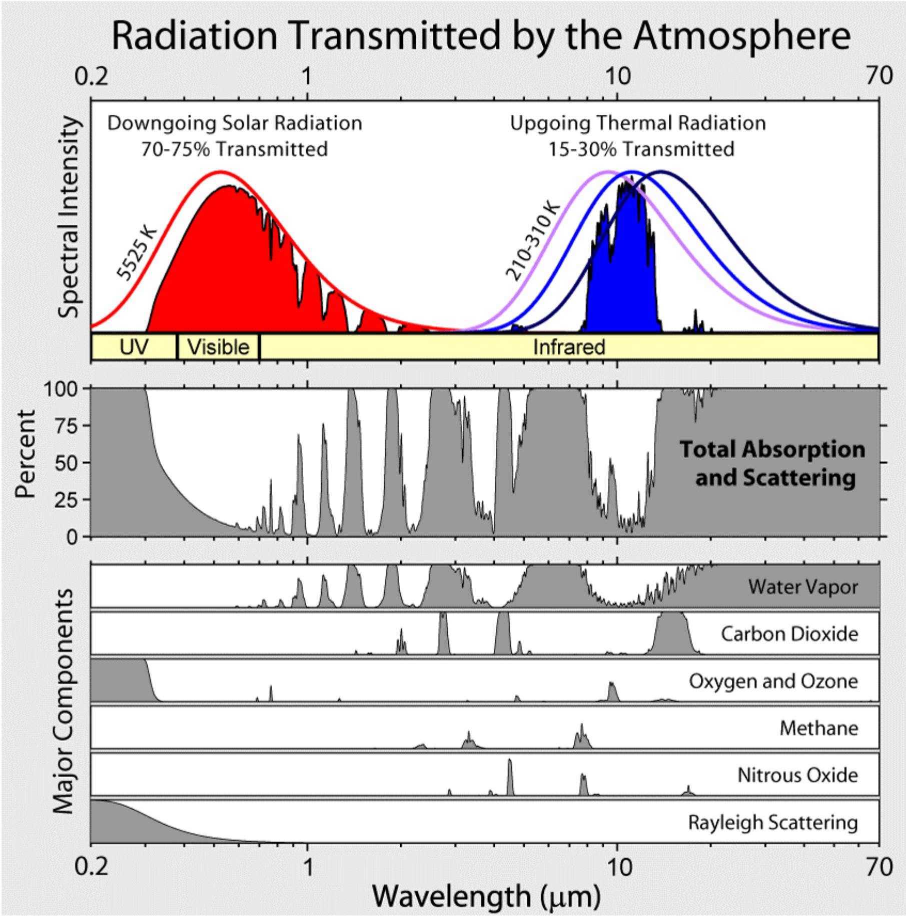
Radiative transfer is an essential component of many astronomical phenomena and theories. Heat passing through a vacuum is accomplished through these means and the vast majority of the warmth of our planet comes in this way from our sun. This report discusses how the fundamentals of radiative transfer can be used to model the flow of energy in a planetary atmosphere; both by preventing the absorbance of some, and allowing the re-absorbance of other, electromagnetic radiation re-emitted by the planet.

In the simplest of models, a planet has a negligible atmosphere and absorbs 100% of the radiative energy that reaches its surface from its nearby star(s). This makes the temperature of a planet to be higher than the near-absolute-zero of outer space, which in turn allows for the release of some of the planet's energy in its own form of black-body radiation. For the simplest of systems, the simplest of models might suffice; but for a greater understanding of how an atmosphere with various components and different possible concentrations this report looks to make a similar, but more robust model of atmospheric radiative dynamics on this planet that can then be applied to others.

This report considers atmospheres with properties similar to the earth, and then lays out the groundwork for generalizing them to other more exotic atmospheres. Humans have looked up the sky since time immemorial, but the development of tools and techniques to see further, fainter, and sometimes unfathomable objects is only hundreds of years old. As technology improved and our ability to detect non-visible light developed, astronomers discovered that either the universe was filled with certain wavebands of light and not others, or more likely that our earthly atmosphere blocked out the transfer of certain wavebands of light. Again, as technology improved and access to the highest layers of the atmosphere and space-based satellites and telescopes came on-line we discovered the rest of the basis for what could be called Modern Astronomy. We have been capable of determining the wavebands that are the windows in which light can pass through the atmosphere for many years; these are seen in figure 1, which was used in the project prompt at the start of the semester [1], and we will soon be aiming to apply similar techniques to the atmospheres of distant planets [2].

After setting up a system with three components: A planet, its atmosphere, and the radiance in outer space, which includes the luminosity of a nearby star, this report analyzes the behavior that is characteristic of this system. This is accomplished by examining parameters that allow for blocking, scattering, and reabsorbing of electromagnetic radiation based on the optical depth of various materials within an atmosphere. The data on water, methane, and carbon dioxide's cross-sectional area of absorption at various wavelengths was obtained from the ExoMol database [3][4]. Though these measurements were made here on earth, they can prove to be useful for other

Figure 1: Research Project Prompt Figure [1]



atmospheres if the size, density profile, and concentrations of the molecules in another atmosphere are known.

With an energy balance and knowledge of the several near-constants like, the luminosity of the sun, the distance between the sun and earth, height of the atmosphere, concentrations of light-absorbing molecules in the atmosphere, this paper shows how a quantity like the amount of light that will pass through an atmosphere unhindered (and thus the amount that will be absorbed and re-emitted) can be modeled from first principles.

Complexities in this research arose and gave rise to several considerations that are partially in this paper, and partially left for future research projects to pick up where this one leaves off. Time is always the limiting factor in work, but having a direction of where to go with that time is generally of great importance, and we are not left without guidance here.

The rest of this report is organized as follows: Section 3 describes idealized black-body radiation and data that relates to the sun and earth's non-ideal radiation absorption. In Section 4 we present and describe an energy balance over a space-atmosphere-planet system, while in section 5 we look at some of the parameters needed to model a planetary atmosphere. A discussion of the results is found in section 6, this includes the many possible directions that would be perused in future research. Lastly, we end with a summary conclusion of the report, acknowledgements, references, and an appendix which contains technical details on ExoMol and most of the content of my python script used to make the plots and calculations.

3 Black-body radiation

The project's descriptive prompt contained figure 1. We can see that the sun and earth are modeled as black-body radiators with various wavelengths of light being reflected, absorbed, and scattered by the earth's atmosphere—narrow line width patterns in the sun's radiation in-coming transmission through the atmosphere and broad width patterns in the earth's radiation out-going through the same atmosphere. Black-body radiation is well-known and described mathematically as,

$$B = \frac{2hc^2}{\lambda^5(e^{hc/\lambda kT} - 1)}$$

These deviations from smooth and idealized Planckian radiation curves are primarily caused by the absorption of electromagnetic energy of certain wavelengths by various chemical species in the atmosphere. Now with a (approximated constant) temperature of the earth, a black-body radiation curve was drawn for electromagnetic radiation emanating from the earth. This as well as the sun's distribution can be seen in figure 2.

Instead of assuming the measured average temperature on earth (14°C or 287 K) from literature [5]. This project used a simple model of planetary temperature [5]:

$$T_{eq} = \left(\frac{L_s(1{-}A_B)}{16\pi\sigma}\right)^{1/4} \frac{1}{\sqrt{d_p}}$$

Where A_B is the albedo of the planet and ranges between 0 and 1. In this project it is assumed to be 0 for the earth, and the equation simplifies to:

$$T_{eq} = \left(\frac{L_s}{16\pi\sigma}\right)^{1/4} \frac{1}{\sqrt{d_p}}$$

Plugging the constants from the table below into L_s and d_p yields a temperature of the earth at approximately 279 K. There is strong agreement between the simplified theory and the measured value in the literature. Though, it should be noted that any non-zero value of albedo will cause a calculated value that will be colder and more inaccurate with respect to the literature value than what has been assumed. This could possibly be offset in a more robust model by heat transfer from the inner parts of the earth to the surface.

3.1 Data Acquisition

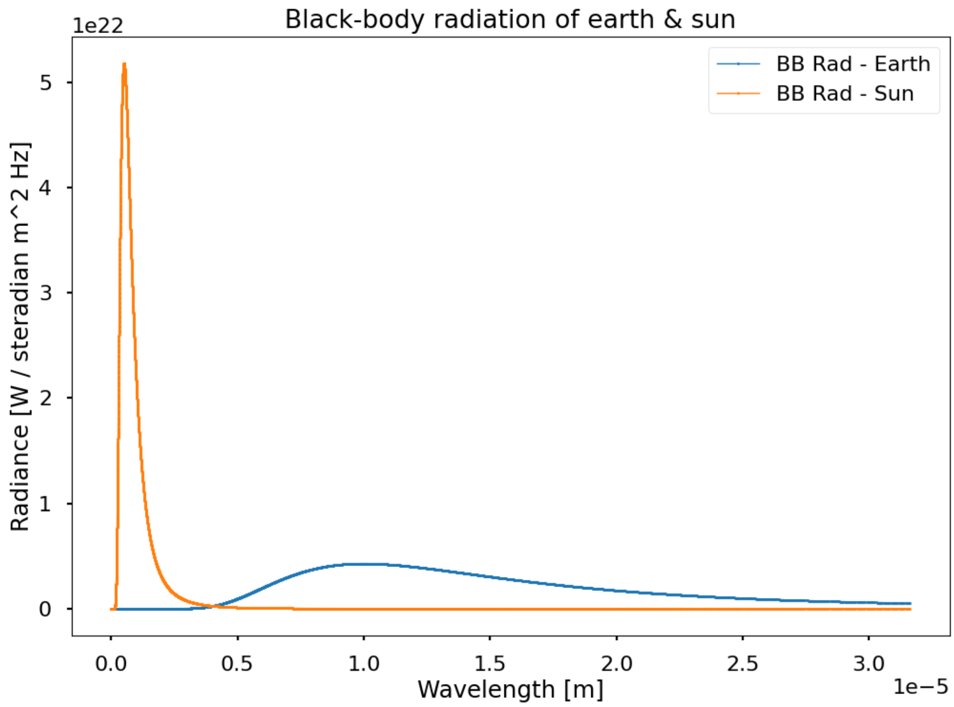
In order to understand the effect of greenhouse gases, I obtained data from the ExoMol database website [3][4] for the cross-sectional areas of three known greenhouse gas chemical species: Methane (CH_4), carbon dioxide (CO_2), and water vapor (H_2O). An example is seen in figure 3.

The data obtained was verified visually in simple plots showing the size of cross-sections over a range of frequencies; this is partially seen in figure 3 and the logarithmic image in figure 4. Figure 3 is quite deceptive in that it falsely conveys the idea that all of the cross sections are rapidly approaching zero and all will behave similarly at the low values in between peaks and towards higher frequencies than the few and prominent peaks. The same information, which plotted in on a logarithmic axis in figure 4 shows how each chemical species is remarkably unique in where its local maxima and minima are found as well as the variance between them. This data proved useful in this project; the inquiry into and acquisition of it from this database was deemed successful. Like many other aspects of astronomy, this project deals with vast differences in orders of magnitudes in data. With the measurements in hand, a model which could be compared to this data was derived from the law of conservation of energy.

4 Energy Balance

When considering questions on the nature of radiative transfer in a complex (3 component system), it is often wise to perform an energy balance. This was accomplished using the diagram in figure

Figure 2: Black-body radiation from an ideal sun and earth



5. The conservation of energy states that,

$$\frac{dE}{dt} = E_{in} - E_{out} \; + \; E_{gen} - E_{cons}$$

In the areas of space, the atmosphere, and the earth, nuclear reactions are very unlikely and, I assumed

$$E_{gen} \; = \; E_{cons} \; = \; 0$$

Additionally, thermodynamic equilibrium is assumed and,

$$\frac{dE}{dt} = 0$$

Now applying this conservation law to the area encapsulating each of the three components (space, atmosphere, and earth) in the system yields this set of equations,

$$E_{AS} \; + \; E_{ES} - E_{SA} - E_{SE} \; = \; 0$$

$$E_{SA} \; + \; E_{EA} - E_{AS} - E_{AE} \; = \; 0$$

$$E_{SE} \; + \; E_{AE} - E_{EA} - E_{ES} \; = \; 0$$

Where the subscripts indicate where the energy transfer is coming from and going to (i.e. E_{AS} is the amount of energy that moves from the Atmosphere to (outer) Space). Of great interest in this project are the fractions of energy that pass through the atmosphere unhindered from space and from the earth. Therefore I define these ratios as,

$$f_s = \frac{E_{SE}}{E_{SE} + E_{SA}} = \frac{E_{SE}}{E_{sun}} = \frac{E_{SE}}{E_S}$$

$$f_e = \frac{E_{ES}}{E_{ES} + E_{EA}} = \frac{E_{ES}}{E_{earth}} = \frac{E_{ES}}{E_E}$$

Figure 3: Cross Sections of Selected Chemical Species

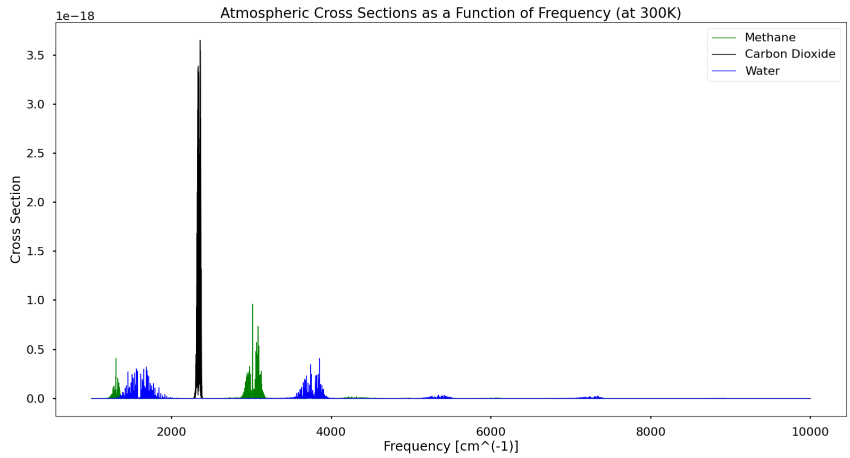
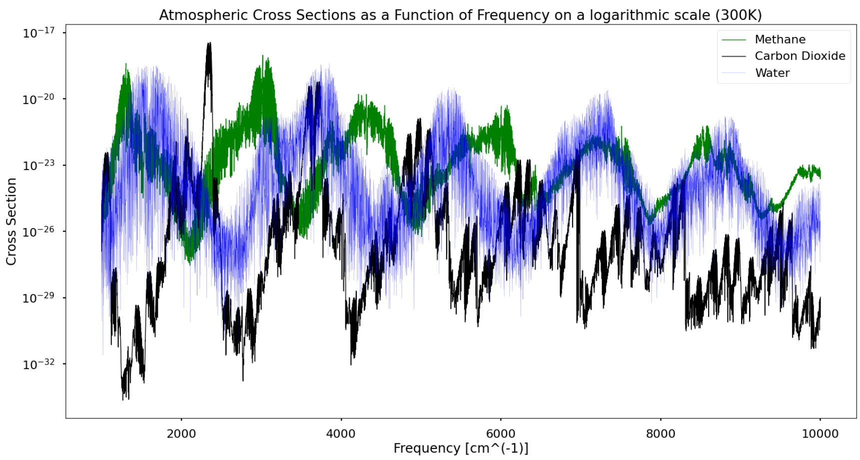


Figure 4: Cross Sections of Selected Chemical Species - Log



The general setup allows for a complete perspective of the model. But the generalized rigor is not essential for the particular topics of this report. Because thermodynamic equilibrium is asserted (or mathematically, $E_i = B_i$), the specific intensity of the incoming light will exhibit behavior seen reproduced by radiative transfer equations, namely they decay exponentially with the optical depth, so the general

$$dE_\nu = I_\nu d\nu$$

becomes the more specific as,

$$I_{SE} = I_S e^{-\tau}$$

where,

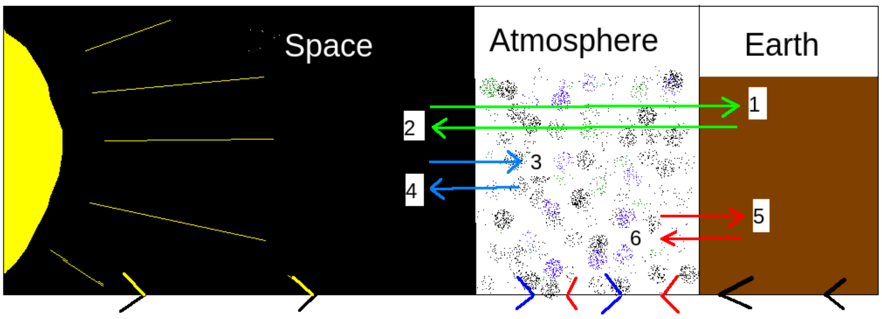
$$I_S = I_{SA} + I_{SE}$$

Using,

$$E_S(1\text{–}f) = B_S(1\text{–}f) = B_{SE} = E_{SE}$$

$$(1\text{–}f) = \frac{B_{SE}}{B_S} = \frac{\int_{\nu_0}^{\nu} I_{\nu,SE}\, d\nu}{\int_{\nu_0}^{\nu} I_{\nu,S}\, d\nu}$$

Figure 5: Energy Balance Diagram



The fraction f is obtained as,

$$f = 1 - \frac{\int_{\nu_0}^{\nu} I_S e^{-\tau}\, d\nu}{\int_{\nu_0}^{\nu} I_S\, d\nu}$$

where,

$$I_S = B_S = \frac{2h\nu^3}{c^2(e^{\frac{h\nu}{kT}} - 1)}$$

substitution, factoring constants, and cancellations yield,

$$f = 1 - \frac{\int_{\nu_0}^{\nu} \frac{\nu^3 e^{-\tau}}{e^{h\nu/kT} - 1}\, d\nu}{\int_{\nu_0}^{\nu} \frac{\nu^3}{e^{h\nu/kT} - 1}\, d\nu}$$

This formula will be used in the next section. The limits of this integration can be difficult to determine for hot or closely-orbiting planets but if the black-body radiation from the star is already sufficiently small at the frequencies that a colder planet's black-body radiation starts to rise at, than this absolute minimum in the sum of the two function is an ideal place to stop one integration and start the second. Before any integration over a frequency, we must examine the nature of τ, the optical depth for the absorbing chemical species in the atmosphere.

5 Dynamics in the Earth's Atmosphere

In order to probe the effect that these chemical species have on any planetary atmosphere, we shall see if they can predict the nature of this atmosphere first. In considering the our unique home, we first look at the radiative power of the sun, the distance to, and the size of earth. By using several known constants seen in the table below. An idealized black-body radiation distribution of the sun is obtained. This line of research made use of several approximations and simplifications. I clearly state them this this section of the report, their inherent inaccuracies and limitations are presented in the discussion of the report, and the opportunities for future research largely discusses how using more realistic and complex assumptions would be a worthwhile endeavor if allocated additional time.

Parameter List		
effective temperature, sun	T_{eff}	$5778K$
radius of the sun	R_s	$6.9634 \cdot 10^8\ m$
distance between sun & earth	d_{se}	$1.485 \cdot 10^{11}\ m$
radius of the earth	R_e	$6.371 \cdot 10^6\ m$
luminosity of the sun	L_s	$3.828 \cdot 10^{26}\ W$
ratio of scattered light return	X	1/2
temperature of the earth	T_e	290 K
number density of air	$\rho_{num,air}$	$\frac{10^{25}}{m^{-3}}$(molecules)
height of atmosphere	h_{atm}	17000 m
concentration of CO2	c_{CO2}	415 ppm
concentration of CH4	c_{CH4}	400 ppm
concentration of H2O	c_{H2O}	1.87 ppm

Because radiative transfer can be markedly different between atmospheric satellites like the earth and non-atmospheric satellites like the moon, this paper aims to model aggregate aspects of atmospheric absorption.

The key parameter that arises in the radiative transfer through a medium is the optical depth. In much in the same way that most people are familiar with fog inhibiting our visual perspective, so too can the radiative power from the sun be blocked by a "fog" which is any material with a large optical depth. This optical depth can be thought of in terms of probability: every photon from the sun that reaches the atmosphere has a speed (that of light) and a direction; if the direction is such that its passage through the air to the ground is without disturbance from the atmosphere then the atmosphere is transparent. If we consider 100 photons, some will pass without interaction, but some will also encounter a molecule that absorbs and then re-emits the photon, which we assume in this paper will be done, in a random direction. The optical depth is then how many of these 100 photons get through without atmospheric interference. Intuitively, atmospheres with a large optical depth are going to have large cross-sectional areas and high densities. Mathematically, this is represented by [7],

$$\tau = optical\ depth = \sigma N$$

where,

$$\sigma = cross - sectional\ area\ (obtained\ from\ ExoMol)$$

$$N = column\ number\ density$$

This column number density is valid for each chemical species in the air and is obtained from,

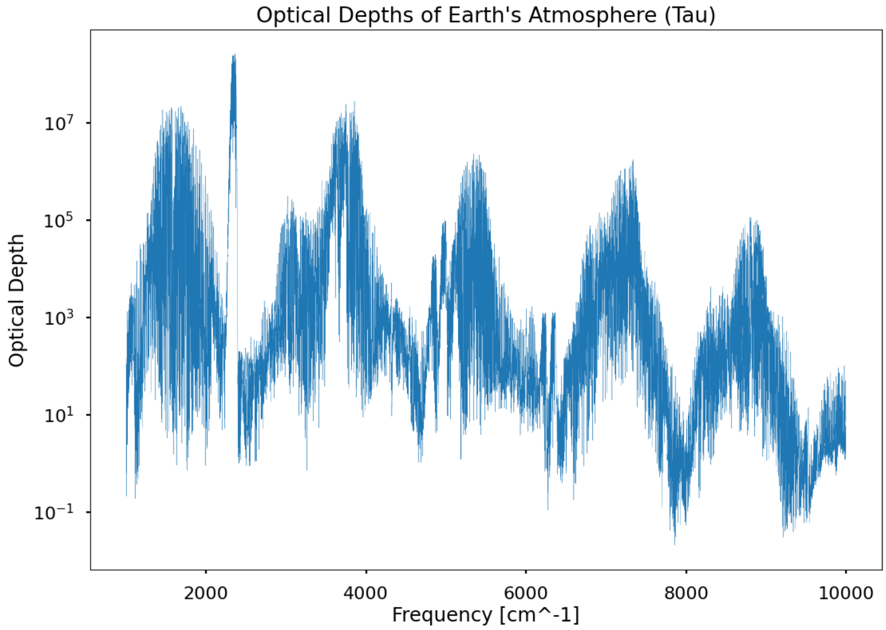
$$N = \sum_{i=1}^{m} N_i$$

$$N_i = c_i \rho_{air,number} h_{atm}$$

A validation for, and sight of greater interest than, this calculated fraction is the optical depth in the atmosphere at various frequencies, which is shown in figure 6. He were can see the effect of the cross sectional areas from the first part of this report.

In the many needle plummets down below an optical depth of one and in the fewer wide wave-like troughs that reside below an optical depth of one, we find the "windows or opaque regions" that allow for incoming electromagnetic radiation to completely pass through the atmosphere unhindered. These are the wavebands that some of the UV, visible, and IR astronomers covet dearly for the opportunity to make observations from the ground; they are the same as the wavebands that make for novel and intrepid space missions as they show a world of light and the objects that emit such, which is entirely invisible here from the surface of the earth.

Figure 6: Optical Depth - Original



Though the optical depth is going to be a function of cross-section and frequency, with the assumptions made above, the column number density of each chemical species is constant. If this project had an industrial or monetary aim, then regret would have arisen due to the weak agreement between the results of the model and the established data given in the project prompt (figure 1). Thankfully, the purpose of this project has been believed to be to learn and discover some of realistic nature of doing research on theoretical astrophysics. In this regard, much head-scratching and discussions with my mentor led to new insights both on atmospheric radiative transfer, and in the methodical approach to complex phenomena that characterizes good science. The initial results can be seen in figure 6. These large optical depths (from 0.1 to 10^7) are going to cause enormous extinction and it is as if the atmosphere of the planet is a perfect absorber much like the surface of a perfectly non-reflecting planet itself. This is easily seen in figures 7 and 8, which I have simply described as a messy slew of absorption lines that are dispersed over all the wavelengths of interest.

Calculating the integral in the energy balance analysis for the "f factors" predicts that a fraction of 0.81863 or 82% of the radiation of the sun is absorbed by the atmosphere and 18% reaches the surface of the earth unaffected. The relative weights of the species were: carbon dioxide's f factor has a value of: 9.45%, methane's f factor has a value of: 42.3%, water's f factor has a value of: 71.0%. This is inaccurate to observations of earth's atmosphere.

In these initial results, water vapor posed a particularly difficult problem. No chemical species holds a monopoly on the optical depth of radiation for all frequencies, but the peaks of water were the highest of all, and more importantly the troughs of water were significantly higher than the other two species of interest; this caused almost all frequencies to never transmit more than a few fractions of a percent of the light incoming from the sun.

I obtained poor results from the created model, but a closer inspection does show that the results might track changes in frequency and differences in chemical species well. From this observation an investigation of the absolute error between this model and the original project prompt was launched. If one parameter, a small constant on the order of 10^{-4} was introduced, in the column number density equation (for all species), then the results obtained show large agreement with the literature values.

Figure 7: Raditative Transfer - Original

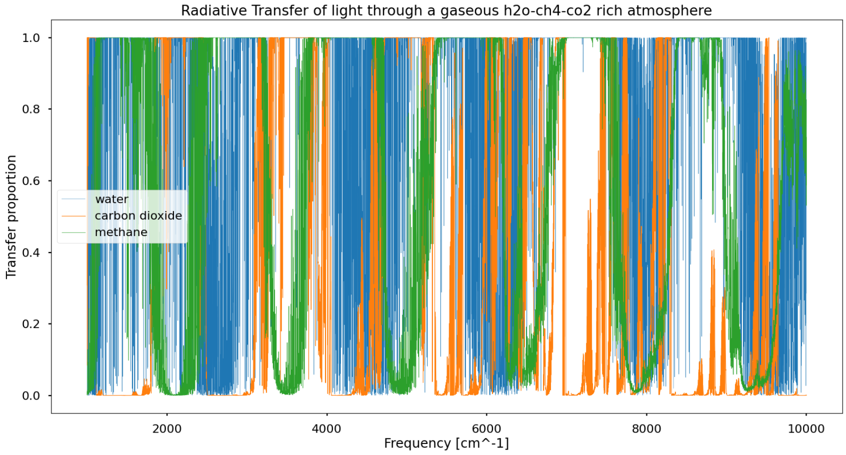
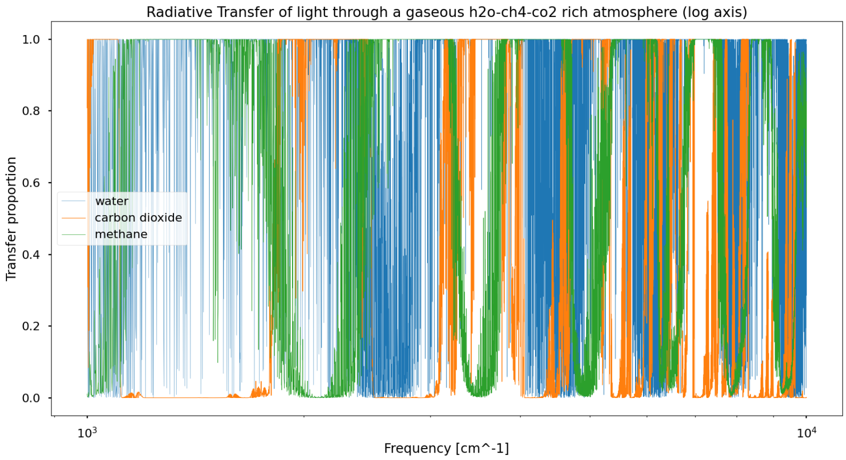


Figure 8: Raditative Transfer with Logarithmic Axis - Original



6 Discussion

By creating a model of a simple atmosphere, using real data of gaseous molecular cross sections, and then comparing the combination of the two to the measured parameters of the earth's atmosphere we can get a baseline for the usefulness of this model to other atmospheres (and this atmosphere under different circumstances and times).

6.1 Empirical Modification for Parameter Analysis & Fitting Deviations

The results obtained were unrealistic from the known nature of the earth's atmosphere. After many considerations, evaluations, and estimations, it was found that by introducing a constant of 10^{-4} into the calculations for column number density, the results matched to a high degree with the optical depth data over the frequencies of interest. So now the column number density is given by,

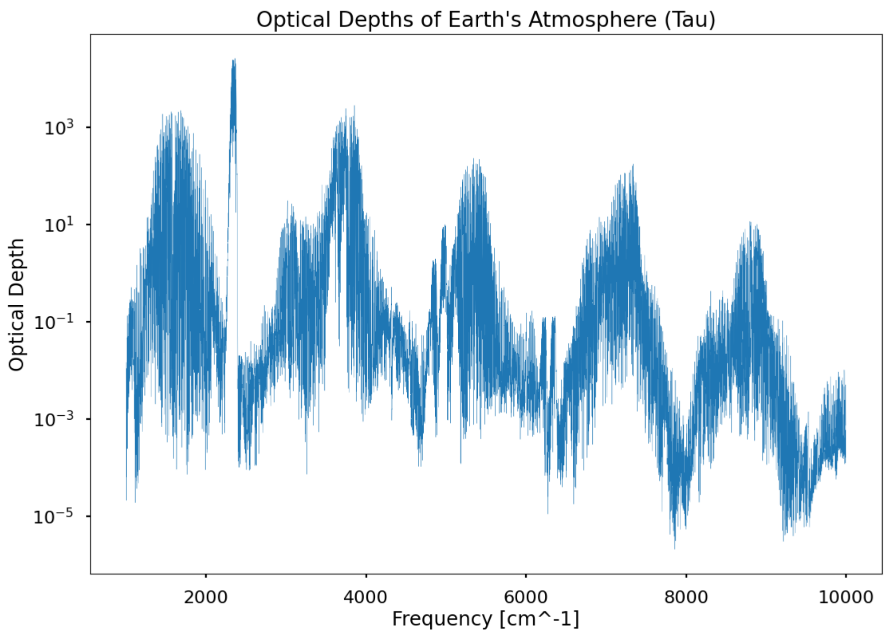
$$N_i = 10^{-4} \cdot c_i \rho_{air,number} h_{atm}$$

In the adjusted model with a factor of 10^{-4} in the calculations this fraction becomes 0.07577 or 7.6% of the light that reaches the atmosphere will get absorbed and 92.4% will pass through to reach the surface of the earth. Additionally, the relative weights of the species were more realistically small: carbon dioxide's f factor has a value of 0.00324%, methane's f factor has a value of

0.0302%, water's f factor has a value of 7.55%. Water still had the strongest effect, but it did not dominate the entire domain of investigated wavelengths.

In figure 9 the frequencies of light which varied optical depth block and allow passage of incoming and outgoing light are obtained and appear similar to the ones in the literature. Figures 10 and 11 contain the predicted atmospheric absorbance and qualitatively it matches the second figure decently well. This indicates that this model is likely capturing the changes in optical depth as frequencies change. Getting the model to predict the correct order of magnitude for a column number density in the earth's atmosphere has not worked and will be discussed more in future works. The 10^{-4} constant could be caused by a multitude of possibilities. One suggests that the in converting the complex and dynamic atmosphere with gradients in temperature, pressure, concentration, and radiative exposure (night & day) into a simple homogeneous thick hollow shell around the earth estimating average is significantly different from the actual phenomena. For example, if the height of the atmosphere is 17 000 m, and the concentration of water that is obtained around the world's surface to estimate the amount of water in the entire atmosphere, then we might find orders of magnitude difference between the amount of water that calculated in the upper atmosphere and what is down lower. This might be intuitive to frequent-fliers who enjoy window seats as one might have seen clouds below the window more often than above it. Many other possible sources of error could arise from these assumptions like interrelated phenomena, convection, and non-thermodynamic equilibrium. Pursuing better, more accurate models will be discussed in the future works section.

Figure 9: Optical Depth - Adjusted



Though the results obtained in this project were not derived from robust enough assumptions and initially lacked accuracy in their agreement to the earth's observed phenomena, the introduction of a simple constant in the calculation of the column number density of any chemical species made the model, which was tracking changes in wavelengths well already, turn into a model which mimicked the initial investigation's atmospheric prompt remarkably well.

Figure 10: Radiative Transfer - Adjusted

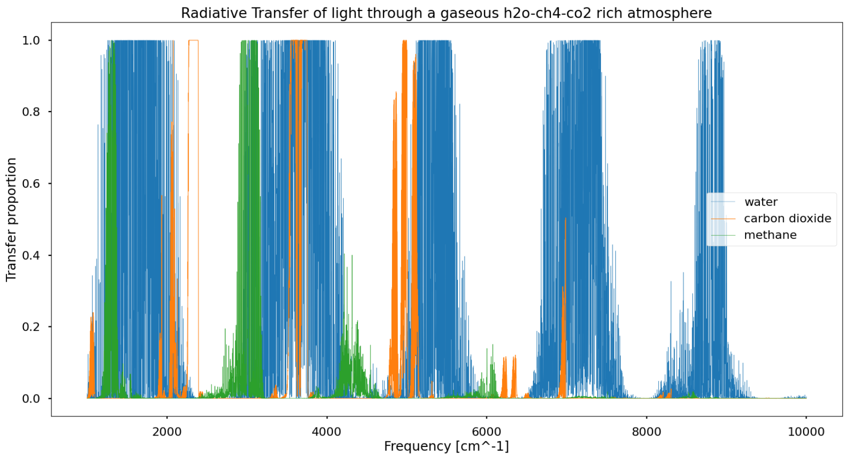
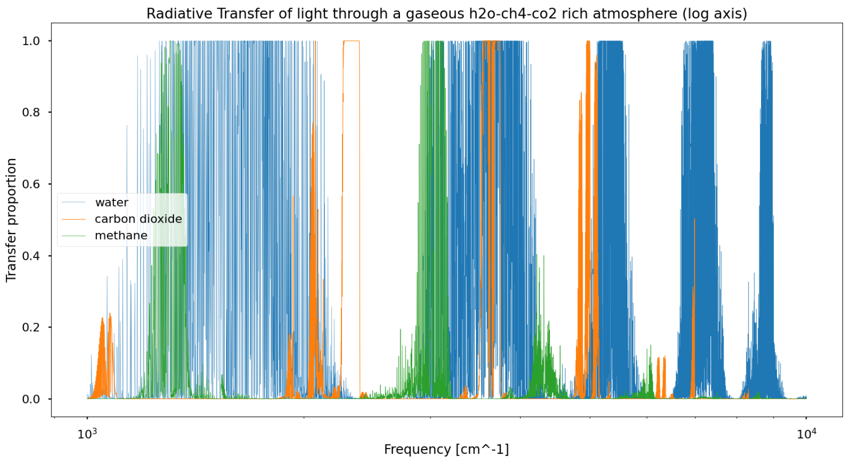


Figure 11: Radiative Transfer with Logarithmic Axis - Adjusted



6.2 Future Work

As with most scientific research, this project is not a complete treatise on the nature of a subset of phenomena. As is seen in the abstract and introduction, numerous assumptions were made in the derivation of the energy balance around the space-atmosphere-planetary system, and future investigations will undoubtedly provide for a methodical analysis of each of the assumptions made and determination of their relevancy compared to the analyzed parameters.

One of the most relevant, practical, and scientific steps to take next with this line of scientific research is in the possible expansion of the habitable zones of exoplanets. It is easy and intuitive to imagine life on another planet living in, on, or around liquid water, in much the same way that life on earth does. Though it is worth investigating concepts in Astrobiology and discover possible mechanisms for chemical and biological complexity to thrive in an environment devoid of water, that is beyond the scope of this paper; if we keep to a more classical (or perhaps antiquated) perspective, life needs liquid water. This water can be found in distances that form a thick shell or sphere around a star. Farther distances yield ice and closer distances yield steam, but in between can foster temperatures between 0° and 100° Celsius (with slight added variance that arises from water's colligative properties and the atmospheric pressure put on it). This habitable zone is typically calculated from the most simple assumptions possible: black-body radiation of a star and pure absorption of its planet. This next step in the creation of a superior, more accurate and sophisticated model is to consider the atmospheric absorption and re-emission onto the planet's surface in order to account for potential greenhouse effects. This then has the potential to expand the habitable zone around stars into regions that before planets would have been thought to be too cold to foster liquid water and advanced lifeforms. Perhaps, if the re-emitted light can keep the ice from forming than life might arise in the places we would have overlooked without this improved model.

A better model of the earth's atmosphere can be developed as well. This project made the very large assumption that the air on the streets of Leuven on a hot summer day is the same in temperature, chemical composition, and density as the air 15km above the poles on a cold winter night. A homogeneous and gradient-less atmosphere that abruptly stops at 17km is not realistic and can be improved. A cursory examination of the mathematics and parameters needed to model an atmosphere with temperature, density, and composition gradients suggested that the amount of time necessary for such an endeavor would be more than triple what was dedicated to this task.

A small improvement that would be accomplished in working more on this project would be to find values of albedo for earth and if necessary turn these constants into time-dependent functions that capture the asymmetric character of the earth's lands and oceans. Other planets albedo would also be helpful in determining how robust we could make this model, though it might take earnest space missions to get more than a constant approximation of albedo of other planets.

7 Conclusion

This project analyzed simple models of radiative transfer from stars to their planets and developed a complex model with multiple simplifying assumptions of an atmosphere as a intermediate between stellar radiation and planetary warmth. Use of professional databases like ExoMol allowed for model atmosphere development. Known parameters of the earth where used for comparison between the generated model and the observed natural world. The results of the model show that making assumptions can easily lead to incorrect predictions by multiple orders of magnitude; nevertheless, the insertion of a simple constant in the calculations of a column number density showed that the model had value in tracking the changes of absorbance in earth's atmosphere as a function of cross section, and thus frequency. Many improvement and side avenues of research are available to myself or other researchers who wish spend their time on such, but despite the open-ended nature of this project vast quantities of knowledge and experience were obtained in the diligent work that has gone into this project.

8 Acknowledgments

A special thanks to my adviser Sven Kiefer for making explanations of intermediate ideas simple to someone who struggles with these concepts every day. His tireless patience and enduring wisdom have helped illuminate great swaths of the field of atmospheric radiative transfer and chemistry, as well as the scientific approach to model such complex phenomena. Any and all mistakes in this report are my own.

9 References

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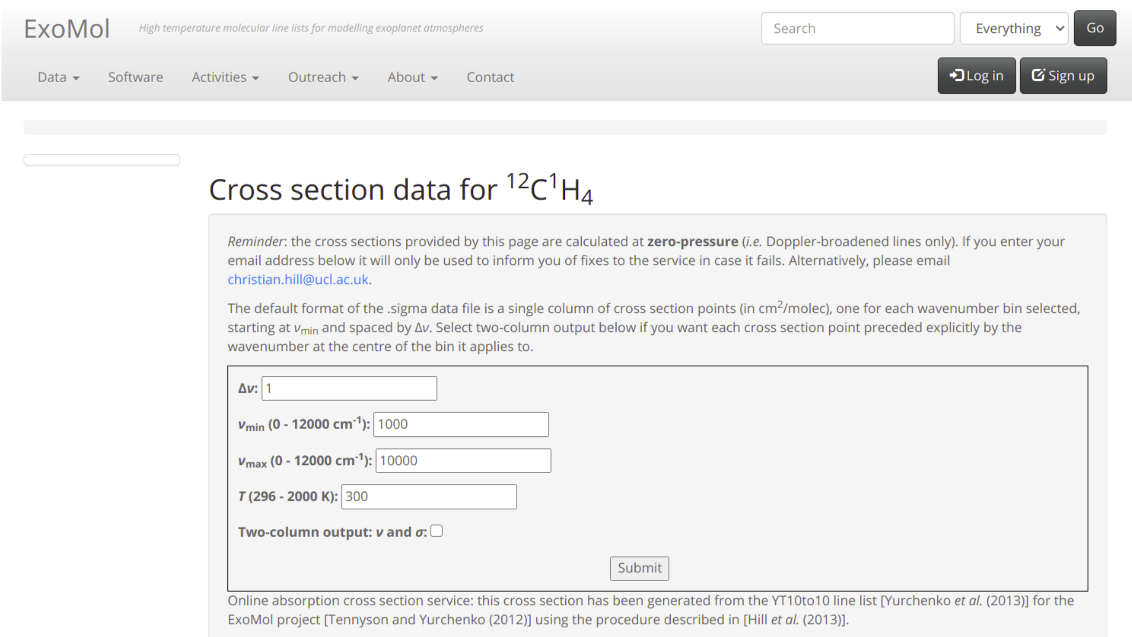
10 Appendix: ExoMol's Data Acquisition

Figure 12: ExoMol, for the Acquisition of Cross-Section Data



11 Appendix: Code and Calculations

Herein are my condensed calculations and python code written for this project:

```
# Theoretical Astrophysics - Research Projects - Greenhouse gases of exoplanetary atmospheres

import pandas as pd
import numpy as np
from matplotlib import pyplot as plt
plt.style.use('seaborn-poster')

### Constants in SI units ###
h = 6.62607015*(10**-34)
c = 299792458
k = 1.380649*(10**-23)          # boltzmann
sigma = 5.670374419*(10**-8)    # stephan-boltzmann
SBc = 5.67*(10**-8)
Tsun = 5770 # K
Lsun = 3.828*(10**26) # watts       # BB Rad of the sun
Re = 6.371*(10**6)    # meters
Rau = 1.485*(10**11)  # meters
Rsun = 696340000 # meters
X = 1/2 # The ratio of (black body) radiation going into the Earth (not outer space?)
########################
### ExoMol Data Entry ###
########################
# Define dataframe and arrays of methane from ExoMol csv file.
ch4 = pd.read_csv("/home/Documents/Research Proj - Theo Astro - Greenhouse Gases Exoplanet Atmosphere/CrossSection_ch4.csv")
ch4_nu = ch4["frequency"] # in the units of cm^-1
ch4_xsec = ch4["cross_section"]
# Define dataframe and arrays of carbon dioxide from ExoMol csv file.
co2 = pd.read_csv("/home/Documents/Research Proj - Theo Astro - Greenhouse Gases Exoplanet Atmosphere/CrossSection_co2.csv")
co2_nu = co2["frequency"]       # this is in cm^-1
nuExM = co2_nu
co2_xsec = co2["cross_section"] # this is unitless, it's like a %
# Define dataframe and arrays of water vapor from ExoMol csv file.
h2o = pd.read_csv("/home/Documents/Research Proj - Theo Astro - Greenhouse Gases Exoplanet Atmosphere/CrossSection_h2o.csv")
h2o_nu = h2o["frequency"]
h2o_xsec = h2o["cross_section"]
# Graph all 3 cross-sections wrt frequency on one plot
plt.plot(ch4_nu, ch4_xsec, linewidth=1, color='g', label='Methane')
plt.plot(co2_nu, co2_xsec, linewidth=1, color='k', label='Carbon Dioxide')
plt.plot(h2o_nu, h2o_xsec, linewidth=1, color='b', label='Water')
plt.title('Atmospheric Cross Sections as a Function of Frequency (at 300K)')
plt.xlabel('Frequency [cm^(-1)]')
plt.ylabel('Cross Section')
#plt.xlim(900, 4600) # use the zoom in on this linear graph, and then don't zoom in for a ylog graph
plt.legend()
plt.show()
plt.plot(ch4_nu, ch4_xsec, linewidth=1, color='g', label='Methane')
plt.plot(co2_nu, co2_xsec, linewidth=1, color='k', label='Carbon Dioxide')
plt.plot(h2o_nu, h2o_xsec, linewidth=0.15, color='b', label='Water')
plt.title('Atmospheric Cross Sections as a Function of Frequency on a logarithmic scale (300K)')
plt.xlabel('Frequency [cm^(-1)]')
plt.ylabel('Cross Section')
plt.yscale('log')
plt.legend()
plt.show()
############################################
### Convert frequencies to SI wavelengths ###
############################################
cm_to_hz = 29979245800 # 1 cm^-1 is many many Hz
si_ch4_nu = ch4_nu * cm_to_hz #and for other species
ch4_wavelen = c/si_ch4_nu #and for other species
###########################
### Black-body radiation ###
###########################
#nu = np.linspace(10,2000000000000000,num = 100)
wavelen = np.logspace(-10, -4.5, num=len(ch4_nu))   # np.linspace(10**-10,3*10**-4, num=len(ch4_nu)) # in um
nu = c/wavelen                              # nu = np.array([100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 10000, ...])
T = 290 # Temp of Earth                     # this might be unrealistically low
B_nonArea = ( 2*h*(c**2) ) / ( (wavelen**5)*(np.exp((h*c)/(wavelen*k*T)) - 1 ) )
B = B_nonArea * 4*np.pi*Re**2               #B = (2*h*(nu**3))/((c**2)*(np.exp((h*nu)/(k*T))-1)) #undo the np commands
#B = (2*h*(np.power(nu,3)))/((c**2)*(np.exp((np.multiply(h,nu))/(k*T))-1)) #undo the np commands, just input with np arrays
Tsun = 5778 # Temp of sun
Bsun = (2*h*(c**2))/((wavelen**5)*(np.exp((h*c)/(wavelen*k*Tsun))-1)) #Bsun = (2*h*(nu**3))/((c**2)*(np.exp((h*nu)/(k*Tsun))-1))

Normalizer = ((Re/(2*Rau))**2)*0.7 #no L_sun!
Asun = 4*np.pi*Rsun**2
Bsun_Normalized = Bsun*Normalizer*Asun
plt.plot(wavelen, B, marker='.', markersize=4, linewidth=1, label='BB Rad - Earth')
```

```
plt.plot(wavelen, Bsun_Normalized, marker='.', markersize=4, linewidth=1, label='BB Rad - Sun')
ymax = np.array(10**32, dtype=float) # USE THIS DTYPE SO THAT THE GRAPH DOESN'T "ERROR AT INFINITY"
#plt.ylim(10**-34, ymax)
plt.title('Black-body radiation of earth & sun')
plt.xlabel('Wavelength [m]')
plt.ylabel('Radiance [W / steradian m^2 Hz]')
plt.legend()
plt.show()

# Blackbody Radiation From Outer Space Into Earth's Atmosphere = Bos
# Blackbody Radiation From the Earth Into Earth's Atmosphere = Be
# Blackbody Radiation From the Earth's Atmosphere Into both the Earth and Outer Space = Batm
Bos = Lsun*((Re/Rau)**2)
Be = Bos
Batm = Be/X

T_text = (1/np.sqrt(Rau))*(Lsun/(16*np.pi*SBc))**(1/4)
T = (Lsun/(4*np.pi*SBc*(Rau**2)))**(1/4)
#########################################################
### Combine cross-sections and column number densities ###
### Plot the integrand of the f factor equations       ###
#########################################################
NumberDensityAir = 1*10**25 # molecules air/m^3 from literature # or calculate with IG law ~P/RT = (10^5 * 6*10^23)/(8.3*270)
HeightAir = 17000 # m (this could be between 17,000 m and 500,000 m. Maybe 200000 is best)
# make this factor smaller and small water larger and large to get ratios to balance
TwickingFactor = 0.0001 #1
co2_concen = 415/1000000 # parts co2 / 1Mil parts air
co2_N = co2_concen*NumberDensityAir*HeightAir*TwickingFactor # column number density [=] partsco2*molcair*m/partsair*m^3[=]molcco2/m^2
h2o_concen = 400/1000000 # 4000 was originally used, but this seems to be a good estimate for sea-level only
h2o_N = h2o_concen*NumberDensityAir*HeightAir*TwickingFactor
ch4_concen = 1.87/1000000
ch4_N = ch4_concen*NumberDensityAir*HeightAir*TwickingFactor

co2_tau = np.array(co2_xsec*co2_N)
h2o_tau = np.array(h2o_xsec*h2o_N)
ch4_tau = np.array(ch4_xsec*ch4_N)

tau = co2_tau + h2o_tau + ch4_tau #, dtype=float) # optical depth = sum of the products of cross sections and column number densities

plt.plot(nuExM, tau, linewidth=0.25)
plt.xlabel('Frequency [cm^-1]')
plt.ylabel('Optical Depth')
plt.yscale('log')
plt.title('Optical Depths of Earth\'s Atmosphere (Tau)')
plt.show()
# Plot 1 - e^-tau's
plt.plot(nuExM, 1-np.exp(-1*h2o_tau), linewidth=0.35, label='water')
plt.plot(nuExM, 1-np.exp(-1*co2_tau), linewidth=0.75, label='carbon dioxide')
plt.plot(nuExM, 1-np.exp(-1*ch4_tau), linewidth=0.5, label='methane')
plt.xscale('log')
plt.legend()
plt.title('Radiative Transfer of light through a gaseous h2o-ch4-co2 rich atmosphere (log axis)')
plt.xlabel('Frequency [cm^-1]')
plt.ylabel('Transfer proportion')
plt.show()
plt.plot(nuExM, 1-np.exp(-1*h2o_tau), linewidth=0.35, label='water')
plt.plot(nuExM, 1-np.exp(-1*co2_tau), linewidth=0.75, label='carbon dioxide')
plt.plot(nuExM, 1-np.exp(-1*ch4_tau), linewidth=0.5, label='methane')
plt.legend()
plt.title('Radiative Transfer of light through a gaseous h2o-ch4-co2 rich atmosphere')
plt.xlabel('Frequency [cm^-1]')
plt.ylabel('Transfer proportion')
plt.show()

nuExoMol_InverseCM = co2_nu # this is the same for each chemical, beucase they were all obtained from ExoMol in the same way
nuExoMol = nuExoMol_InverseCM*(29979245800) # this is in SI units
RadTrans = np.array( (nuExoMol**3) * np.exp(-1*tau) / (np.exp(h*nuExoMol/(k*Tsun)) - 1 ) ) # Should this be Tsun or Tearth (T)?
# RadTrans_test = 10**200 * (nuExoMol**3) * np.exp(-1*tau) / (np.exp(h*nuExoMol/(k*Tsun)) - 1 ) This still makes y always = 0
plt.plot(nuExoMol, RadTrans, linewidth=0.3)
plt.title('Radiative Transfer: Absorption Through a Simple Atmosphere')
plt.xlabel('frequency [Hz?]')
plt.ylabel('absorbance')
plt.show()
###########################
### Calculate f factors ###
###########################
co2_numerator = ( (np.exp(-co2_xsec*co2_N)*(nu**3)) / (np.exp( (h*nu)/(k*T) ) - 1) )
h20_numerator = ( (np.exp(-h2o_xsec*h2o_N)*(nu**3)) / (np.exp( (h*nu)/(k*T) ) - 1) )
ch4_numerator = ( (np.exp(-ch4_xsec*ch4_N)*(nu**3)) / (np.exp( (h*nu)/(k*T) ) - 1) )
numerator = (np.exp(-tau)*(nu**3)) / (np.exp( (h*nu)/(k*T) ) - 1)
denominator = (nu**3) / (np.exp( (h*nu)/(k*T) ) - 1) # same for all species of chemicals
xsun = np.linspace(0,2.18*10**-6,num=100)           # Make the num=number very large for accuracy at the end
xearth = np.linspace(2.18*10**-6,10**3,num=100)
co2_f = 1 - ( (np.trapz(co2_numerator, x=nu, dx=0.1, axis=-1)) / (np.trapz(denominator, x=nu, dx=1.0, axis=-1) ) )
h2o_f = 1 - ( (np.trapz(h20_numerator, x=nu, dx=0.1, axis=-1)) / (np.trapz(denominator, x=nu, dx=1.0, axis=-1) ) )
ch4_f = 1 - ( (np.trapz(ch4_numerator, x=nu, dx=0.1, axis=-1)) / (np.trapz(denominator, x=nu, dx=1.0, axis=-1) ) )
f     = 1 - ( (np.trapz(numerator, x=nu, dx=0.1, axis=-1)) / (np.trapz(denominator, x=nu, dx=1.0, axis=-1) ) )# can I merge them all?
co2_absorbance = co2_f*B
```