# Estimation of atmospheric IR absorption

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# Abstract

In this work, we present a program to numerical integrate the atmospheric absorption due to carbon dioxide and water vapour of infrared photons by the atmosphere. We also investigate the effect of water evaporation on climate sensitivity. We present a prediction of increase temperature from doubling $CO_2$ of just under a fifth of a degree.



# Keywords

Global Warming, Carbon Dioxide, Water Vapour, Climate Sensitivity, Rainfall


# Introduction

w In recent years, the hypothesis that human released carbon dioxide will warm planet earth has become an huge issue. There is naturally a large body of work in it. The UN has summarized these in annual reports [23]. However very few of the calculation tools for the issue are released as open source. In this work we present a program and it results to numerical integrate carbon dioxide and water vapour absorption over frequency, latitude and height, producing a percentage absorption amount for the two green house gases. In order works, with less computer time, transmission of in the middle atmosphere was performed using precomputed tables [22]. We however compute it directly. Any such calculation requires temperature and pressure to be given at each height and latitude in the atmosphere [21], we calculate this to 25Km high, using [8] Lente at al approximation.

# Input Absorption Lines

Spectra absorption lines for many molecules are available on the HITRAN database online [5]. We are interest in the strongest lines for absorption by the molecules with the most common isotopes from the ground state, since it is the ground state is far more common than the higher levels. We download the HITRAN frequency, upper and lower quantum states, with the Einstein $A$ Coefficient that gives the absorption strength of the lines. Using the line intensity $S$, from HITRAN we order the lines from strongest to weakest, and select those starting at ground strength. We find 3 lines for carbon dioxide and 4 for water, and present them in the table below. For the line to ground state we find the upper level multiplicity is 3, that is the undegenerate ground state, can be stimulated to one of three degenerate upper levels.

Where the wave number $\tilde{\nu}$ is the frequency divided by the speed of light $c$

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} \tag{1}$$

Table 1: The most prominent absorption lines from ground state

| Molecule | Wave-number ($cm^-1$) | Einstein Coefficient $A$ | upper state | line v |
|---|---|---|---|---|
| $CO_2$ | 2349.91 | 140.7 | $v_1 = 0$,$v_2 = 0$, $i_2 = 1$, $v_3 = 1$, $J = 1$, $r = 1$ | |
| $CO_2$ | 686.16 | 1.023 | $v_1 = 0$,$v_2 = 1$, $i_2 = 1$, $J = 1$, $r = 1$ | |
| $CO_2$ | 3716.56 | 5.9031 | $v_1 = 1$,$v_2 = 1$, $i_2 = 0$, $J = 1$, $r = 1$ | |
| $H_2O$ | 1634.96 | 7.599 | $v_1 = 0$, $v_2 = 1$, $v_3 = 0$, $J = 1$, $K_a = 1$, $K_c = 1$ | |
| $H_2O$ | 3693.29 | 1.031 | $v_1 = 1$, $v_2 = 0$, $v_3 = 0$, $J = 1$, $K_a = 1$, $K_c = 1$ | |
| $H_2O$ | 3196.09 | 0.1982 | $v_1 = 0$, $v_2 = 2$, $v_3 = 0$, $J = 1$, $K_a = 1$, $K_c = 1$ | |
| $H_2O$ | 3779.49 | 28.98 | $v_1 = 0$, $v_2 = 1$, $v_3 = 0$, $J = 1$, $K_a = 1$, $K_c = 1$ | |

# Required Equations

The Intensity of radiation in the presence of an absorber is, [2]

$$I = I_0 e^{-N\alpha L} \tag{2}$$

Where N is number density of the absorbing molecule, L the length of the absorbing region, and $\alpha$ the cross section of absorption. Tokmakoff also gives for a single spectral line,

$$\alpha = \frac{h\nu}{c} B_1 2 \tag{3}$$

Where $\nu$ is the frequency, and $B$ is the Einstein $B$ coefficient. HITRAN gives us the Einstein $A$ coefficient, which is related to $B$ (at equilibrium) by [6]

$$A_2 1 = \frac{8\pi h\nu^3}{c^3} B_2 1 \tag{4}$$

and

$$B_{12} = \frac{g_u}{g_l} B_{21} \tag{5}$$

The ratio of lower to upper transition to the upper to lower transition is the ratio of the number of quantum states in the upper and lower states. So

$$\alpha(\nu)\Delta_\nu = \frac{c^2}{8\pi\nu^2} g_u A_2 1 \tag{6}$$

Of course we need the spectral lines for each absorber, labelled $M$, so

$$I = I_0 e^{-L\left(\sum_M N_m \ \sum_\nu \frac{c^2}{8\pi\Delta_\nu \nu^3}\right)} \tag{7}$$

The input intensity is the Planck Radiation Law of EM emission from a surface at temperature T, [3]

$$I_0(\nu) = \frac{8\pi h\nu^5}{c^4} \frac{1}{e^{\frac{-h\nu}{kT}}} - 1 \tag{8}$$

The width of the spectra line is commonly approximated as a Lorentzian, due to Natural and Collisional broadening. [4] In fact the Lorenz shape estimate

Table 2: Reconstructed 1961-1990 Average Surface Air Temperature By Latitude

| Latitude | Temperature Celsius |
|---|---|
| -90 | -20 |
| -80 | -15 |
| -70 | -8 |
| -60 | -1 |
| -50 | 10 |
| -40 | 16 |
| -30 | 20 |
| -20 | 24 |
| -10 | 26 |
| 0 | 27 |
| 10 | 27 |
| 20 | 25 |
| 30 | 20 |
| 40 | 17 |
| 50 | 7 |
| 60 | -1 |
| 70 | -8 |
| 80 | -15 |
| 90 | -17 |

the tail of absorption, and is often cut off at the edges, but we will not do that here. In HITRAN [5] units, we lose the factor of $4\pi^2$ and the line width is proportional to the pressure $P$, $\Gamma = P\gamma$, of the line width in table 1.

$$\phi(\nu) = \frac{1}{\pi} \frac{\Gamma}{(\nu - \nu_0)^2 + \Gamma^2} \tag{9}$$

Then $\Delta_\nu$ can be approximately the line width $\Gamma$
HITRAN [5] approximates the line width $\Gamma$ for air to

$$\Gamma(p, T) = \left(\frac{T_{ref}}{T}\right)^{n_a ir} \gamma_{air} p \tag{10}$$

So now we have the absorption equation for surface temperature $T$ and Pressure $P$ at each height, so need a model of earths surface temperature at latitude $\theta$, and atmospheric pressure at height $h$, to complete our input equations. To begin with we will average the temperature over day and night, we need a rough input function of latitude that provides an average surface air temperature, we find this Fuelner at al [7], as graph Fig 5, we copy the data for Observations from 1961-1990 which we approximate place the data points for each 10 degree latitude in the table below. We will then interpolate between the given points to provide a programmatic function to give a value for any latitude.

Given the Pressure $P_0$ and Temperature $T_0$ at the Earths surface we can find the temperature, $T(h)$ and pressure a $P(h)$ a height $h$, using a Barometric formula, we use Lente and Osz's formulae [8]

$$P(h) = \left( P_0^{\frac{1}{\nu+1}} - \frac{Mg_0 R_E P_0^{\frac{1}{\nu+1}} h}{(v+1)RT_0(R_E+h)} \right)^{\nu+1} \tag{11}$$

and

$$T(h) = T_0 \left( 1 - \frac{Mg_0 R_E h}{(\nu+1)RT_0(R_E+h)} \right) \tag{12}$$

where $R$ is the gas constant, $R_E$ is the radius of the Earth, $m$ is the mass density of air $M = mN_A$ is the molar mass of air. $N_A$ is Avogadro's constant, $g$ is acceleration due to gravity at the surface, $K$ is Boltzmann's constant, $v$ is the number of degree of freedom of the average molecule in air $\nu \approx 5/2$, and $m$ is mass density of air. The formula works to about $30Km$, which is around 4 e-folds of exponentially growth, as the scale height of air pressure is around $7Km$.

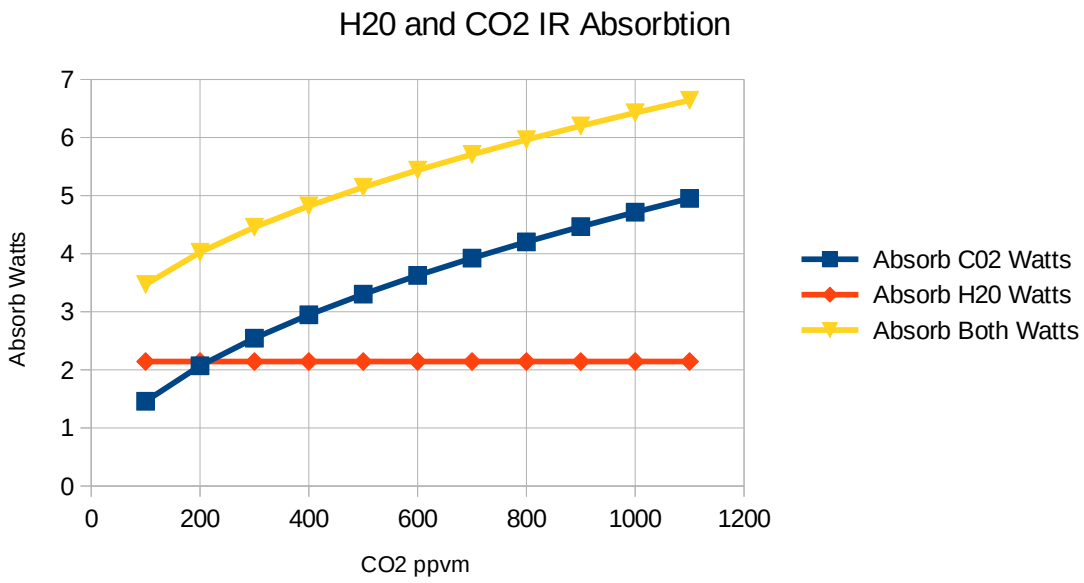
For pressure we just take the average surface pressure a earth surface. The above equations are enough for CO2 but for water, we need the humidity in the atmosphere. We assume constant relative humanity the August Roche Magnus equation [9].

$$P_{h20} = 0.61094 exp \left( \frac{17.625}{T + 243.04} \right) \tag{13}$$

With T in Kelvin. Then the idea gas law will give the density of water vapour.

## Results of absorption integration

We release the source code of our calculation at GitHub [10]. We step in 10 meter intervals to 25km, frequencies between $10^{11}$ and $3 * 10^{15}$ in steps of $10^5$, and a hundred steps in latitude, integrating triply using Simpsons law. We use C02 concentrations from 100 to 1200 and plot the graph of individual and combined contributions from the two gases. It takes around 6 hours on typical modern PC. We find that $CO_2$ matches similar results, but $H_20$ is some six time lower than modern estimates of water which is considered to the primary green house gases at 60% of the total absorption. Green, Newman et al [11], state the individual lines from HITRAN do not well fit the absorption for water vapour, instead a sum of long tails of weaker lines, makes up most of the absorption, and "however, there is no universally accepted underlying physical model for the source of the continuum absorption." Also see P. Varanasi [20] for more on the water vapour absorption. In our results we find that doubling $CO_2$ from $400ppvm$ to $800ppvm$ increases total absorption by $1.1Wm^{-2}$, one point one, Watts per square meter. The change for $CO_2$ only is $1.2Wm^{-2}$. See the figure.


H20 and CO2 IR Absorbtion
Absorb Watts
0
1
2
3
4
5
6
7
0
200
400
600
800
1000
1200
CO2 ppvm
Absorb C02 Watts
Absorb H20 Watts
Absorb Both Watts

## Climate Sensitivity and Rainfall

The usual model of climate sensitivity is to use the Stefan Boltzmann equation to assume the increase in heat absorption all goes into the the heat balance between incoming and outgoing radiation [12]

$$\Delta F_{2xCO_2} = \frac{dF}{dT}\Delta T_{2xCO_2} = 4\sigma T^3 \Delta T_{2xCO_2} \tag{14}$$

However we see an additional heat loss mechanism evaporation. At present an average rainfall of 39 inch lands upon the earth surface annually [13]. But rainfall increases 7% for each degree warmer it gets [14]. Using the mean temperature of 17.5, and the usual heat of vaporization of water, we multiply the volume of water falling per square meter, $970kg$, by the specific heat of water times the average 82.5 degree heating plus the heat of vaporization, gets $2.526GJ$ per year, or 80.11 Watts per square meter, we call $E_{evap}$. Adding the increase in rainfall to the energy balance derivative equation gives.

$$\Delta T_{2xCO_2} = \frac{\Delta F}{4\sigma T^3 + 0.07 * E_{evap} exp(T - 17.5) * 0.07)} \tag{15}$$

For our 1.1 Watts of additional $CO_2$ absorption from doubling $CO_2$, we get a warming of just $.17C$. This five times lower than the [12] Climate sensitivity in Wikipedia, and we thus find it would make little difference to the modern world to continue Carbon emissions at current levels.

## Conclusions

We have performed an ab inito calculation of $CO_2$ and $H_2O$ absorption of Infrared radiation from the earth Surface, we begin from the absorption lines listed at HITRAN, for $CO_2$ our figures for doubling, $1.2Wm^-2$ are lower than some other studies, for example The ACS [15] claims $3.5Wm^-2$ an CO2 going from $280ppmv$ to $560ppmv$, which from our graph would be around $1.5Wm^{-2}$. [15] does not not list a citation or provider the code for there claim which is slightly over double ours. However our figure for $400ppmv$ $CO_2$ of $2.9Wm^{-2}$ is actually one Watt higher than Richard Tuckett claims in the Encyclopedia of Analytical Science [17], so we are not outside the range provided by the literature. Our figures for water Vapour $2.1Wm^{-2}$ are dramatically lower than Claimed in the literature. This may be because, Green, Newman et al [11], state the individual lines from HITRAN do not well fit the absorption for water vapour, but rather a sum of long tails from smaller water vapour lines, produce most of the absorption. Also see P. Varanasi [20] for more on the water vapour absorption.

To understand the temperature increase from adding $CO_2$ to that atmosphere, a calculation of Climate Sensitivity is needed. Most formulations of Climate Sensitivity e.g. ACS [16], purely use the Boltzmann equation, we also

use that, but we also consider the increase in cooling due to additionally rainfall. We find that a the quoted 7% increase in rainfall per degree warming [13] decreases sensitivity by a factor of about 5.5, so our prediction of temperature increase for doubling $CO_2$ is as little as .17 degrees. Any increase in temperature causes additional humidity itself increase $H_2O$ absorption of IR [19]. If however the heat is reduced by rainfall, there will be far less extra absorption by water vapour. So while the water vapour feedback model, predicts, an unphysical thermal runaway. Our model including rainfall, predicts that temperature increases are capped by the increase in rainfall, and will not thermally runaway,

Since Global Governments are planning trillions of dollars of spending on reducing $CO_2$, it is crucial that all factors are well computed and taken into account. Our work seems to support a more tolerant approach to carbon emissions, due to both the lower raw $CO_2$ absorption, and reduced climate sensitivity.

# Bibliography


[1] Prof A. Mourya, Engineering Physics, Lecture Notes, https://sites.google.com/site/puenggphysics/home/unit-i/relation-between-einstein-s-a-and-b-coefficient (2015)

[2] Tokmakoff, Absolute Cross Sections, Lecture Notes, http://home.uchicago.edu/~tokmakoff/TDQMS/Notes/4.3._Abs_Cross-Sec_2-12-08.pdf

[3] Britannica, T. Editors of Encyclopaedia (Invalid Date). Planck's radiation law. Encyclopedia Britannica. https://www.britannica.com/science/Plancks-radiation-law

[4] Kenneth Wood,University of St Andrews , Nebulae, Lecture 8, Line Widths http://www-star.st-and.ac.uk/~kw25/teaching/nebulae/lecture08_linewidths.pdf

[5] HITRAN Definitions and Units https://hitran.org/docs/definitions-and-units/

[6] Einstein A-coefficients and statistical weights for molecular absorption transitions in the HITRAN database, Marie Simeckova, David Jacquemarta, Laurence S. Rothmana, Robert R. Gamacheb, Aaron Goldmanc. https://lweb.cfa.harvard.edu/atmosphere/publications/2006-EinsteinA-JQSRT-98.pdf

[7] G. Feulner, S. Rahmstorf, A. Levermann, S. Volkwardt, On the Origin of Surface Air Temperature Difference between Hemispheres in the Earth's Present-Day Climate, pg 7136-7130 Vol 26 Journal of Climate (2013)

[8] Lente, G., Ősz, K. Barometric formulas: various derivations and comparisons to environmentally relevant observations. ChemTexts 6, 13 (2020). https://doi.org/10.1007/s40828-020-0111-6

[9] https://en.wikipedia.org/wiki/Vapour_pressure_of_water

[10] https://github.com/badams77-cpu/agw

[11] Recent advances in measurement of the water vapour continuum in the far-infrared spectral region Paul D. Green , Stuart M. Newman , Ralph J. Beeby , Jonathan E. Murray , Juliet C. Pickering and John E. Harries June 2012 https://doi.org/10.1098/rsta.2011.0263

[12] https://en.wikipedia.org/wiki/Climate_sensitivity

[13] https://en.wikipedia.org/wiki/Earth_rainfall_climatology

[14] https://phys.org/news/2018-05-higher-temperature-heavier.html

[15] https://www.acs.org/content/acs/en/climatescience/atmosphericwarming/radiativeforcing.html

[16] https://www.acs.org/content/acs/en/climatescience/atmosphericwarming/climatsensitivity.html

[17] Richard Tuckett, in Encyclopedia of Analytical Science (Third Edition), 2019 /urlhttps://www.sciencedirect.com/topics/chemistry/greenhouse-gas

[18] "It's Water Vapor, Not the CO2". American Chemical Society. https://www.acs.org/content/acs/en/climatescience/climatesciencenarratives/its-water-vapor-not-the-co2.html

[19] "Water vapour confirmed as Major Player in climate change" https://www.nasa.gov/topics/earth/features/vapor_warming.html

[20] Varanasi P. Infrared absorption by water vapour in the atmospheric window. In Modelling of the Atmosphere 1998 Aug 24 (Vol. 998, pp 213-230). Internation Society for Optics and Photonics. https://doi.org/10.1117/12.975629

[21] Rosenfeld J.E. A simple parametrization of ozone infrared absorption for atmospheric heating rate calculations. Journal of Geophysical Research. Atmospheres. 1991 May 20; 96(D5):9065-74.

[22] Ming-Dah Chou, David P. Kratz and William Ridgway Journal of Climate Vol. 4, No. 4 (April 1991), pp. 424-437 (14 pages) Published By: American Meteorological Society Journal of Climate https://www.jstor.org/stable/26196300

[23] United Nations, Climate Reports https://www.un.org/en/climatechange/reports