Simple Radiative Transport

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Contents

1. Introduction

Climate change, its causes, and possible remedies are in public focus. There is a consensus on the human made climate change amoung a vast majority of climate scientist. Yet there are still people who promote the idea that there is no climate change or if there is climate change that the causes are natural and not man made und thus can not be influenced by humans.

As a small contribution to the ongoing discussions in the public realm the objective of this report is to define and implement a very basic model of the earth's atmosphere and determine the amount of infrared radiation that is absorbed in the $15\mu m$ absorption band of CO_2. The results of this simple model are only meant to show the effect of CO_2 under quite simplifying assumptions and are by no means a replacement for the many excellent research made in this field.

The model is described below and the source code is made available so that everybody interested can check the results. If the author has made a mistake, be it in the model definition or the computational code, he would be very appreciative for any hint.

2. Model Description

The key assumptions of the simple atmosphere model are:

- The atmosphere consists mostly of molecules that don't interact with infrared radiation in the $15\mu m$ range

- Only CO_2 is absorbing and emitting infrared radiation

- The temperature and pressure of the atmosphere is assumed to be fixed, thus there is no self consistency between absorption and temperature

- Only upward traveling radiation is considered

- The main result is the difference in infrared radiation at the top of the atmosphere (TOA) at $70km$ escaping to free space

- Scattering will be neglected

- The atmospheric gas is in local thermodynamic equilibrium so that all energy levels are occupied according to the Boltzmann factor

- All spectroscopic data of CO_2 are taken from the HITRAN data base.

2.1. Radiation Transport Equation

The radiation transport equation reads:

$$\frac{dI_\lambda}{ds} = -\kappa_\lambda I_\lambda + \epsilon_\lambda \tag{1}$$

with:

$$I_\lambda : \left[\frac{W}{m^2 \ sr \ m} \right]$$

$$\epsilon_\lambda : \left[\frac{W}{m^3 \ sr \ m} \right]$$

$$\kappa_\lambda : \left[\frac{1}{m} \right]$$

The spontaneous emission ϵ_λ is given by:

$$\epsilon_\lambda = \frac{1}{4\pi} \frac{hc}{\lambda} N_u A_{ul} f(\lambda) \frac{\lambda^2}{c} \tag{2}$$

A_{ul} ist the Einstein coefficient of spontaneous emission from upper to lower energy state, N_u the density of the upper state and $f(\lambda)$ is the line shape. The absorption coefficient κ_λ is given by:

$$\kappa_\lambda = \frac{h}{\lambda} \left(B_{lu} N_l - B_{ul} N_u \right) f(\lambda) \frac{\lambda^2}{c} \tag{3}$$

with the Einstein coefficients of absorption and stimulated emission:

$$B_{ul} = \frac{1}{8\pi} \frac{\lambda^3}{h} A_{ul} \quad , \quad \left[\frac{m^3}{Js^2} \right] \tag{4}$$

$$B_{lu} = \frac{g_u}{g_l} B_{ul} \tag{5}$$

The densities of the upper and lower states are given by the Boltzmann distribution at local temperature T:

$$N_u = N \frac{g_u}{Q(T)} \exp\left(-\frac{E_u}{k_B T} \right) \tag{6}$$

$$N_l = N \frac{g_l}{Q(T)} \exp\left(-\frac{E_l}{k_B T} \right) \tag{7}$$

g_u and g_l are the degeneracies of the upper and lower level respectively and Q(T) is the partition function.

2.2. Line Shapes

The main line broadening mechanisms in gases are natural line broadening, Doppler broadening and pressure broadening. Natural line broadening can be neglected. Pressure broadening is dominant in the denser parts of the atmosphere whereas Doppler broadening only becomes the dominant broadening mechanism in higher diluted regions of the atmosphere.

2.2.1. Doppler Broadening

Doppler broadened line shapes are given by a Gaussian function:

$$f_G(\lambda) = \sqrt{\frac{\ln 2}{\pi \Delta \lambda^2}} \exp \left(-\frac{\ln 2}{\Delta \lambda^2} (\lambda - \lambda_0)^2 \right) \tag{8}$$

$$\int_{-\infty}^{\infty} f_G(\lambda) d\lambda = 1 \tag{9}$$

with the half width at half maximum (HWHM) line width:

$$\frac{\Delta \lambda}{\lambda} = \frac{v}{c} = \frac{1}{c} \sqrt{\frac{2 k_B T}{m}} \tag{10}$$

Doppler broadening is determined by the temperature and the mass of the particles.

2.2.2. Pressure Broadening

Pressure broadening is caused by the collisions between molecules, in the present model between N_2 and O_2 with CO_2. The main determining factors are the concentration of the collision partners and the collision frequency. The line shapes are given by a Lorentz function:

$$f_L(\lambda) = \frac{1}{\pi} \frac{\Delta \lambda}{(\lambda - \lambda_0)^2 + \Delta \lambda^2} \tag{11}$$

$$\int_{-\infty}^{\infty} f_L(\lambda) d\lambda = 1 \tag{12}$$

Contrary to the Gaussian line shapes of Doppler broadening Lorentz functions have a much wider extend. In order to keep computation times low the Lorentz functions have to be cut at a point. To estimate the introduced error the normalized Lorentz function is integrated from $-x_p$ to x_p:

$$F(x_p) = \frac{1}{\pi} \int_{-x_p}^{x_p} \frac{1}{1 + x^2} dx = \frac{1}{\pi} \left(\arctan(x_p) - \arctan(-x_p) \right) \tag{13}$$

$F(x_p) = 0.9$ at $x_p \approx 6.3$, 0.97 at $x_p = 20$ and 0.99 at $x_p = 40$. In the absorption computations the limit is set at $20 \Delta \lambda$ so that approximately 3% of the radiation power is missing. To compensate for this a background of 3% of a moving average will be added.

2.3. Integration of the Radiation Transfer Equation

The intensity in Equation 1 is integrated along a path from the earth surface to the TOA (top of atmosphere) which is assumed to be at a height of $70 km$. Assuming constant κ and ϵ in Equation 1 the solution is given by:

$$I(s) = I(s_0) \exp(-\kappa(s - s_0)) + \frac{\epsilon}{\kappa} \left(1 - \exp(-\kappa(s - s_0)) \right) \tag{14}$$
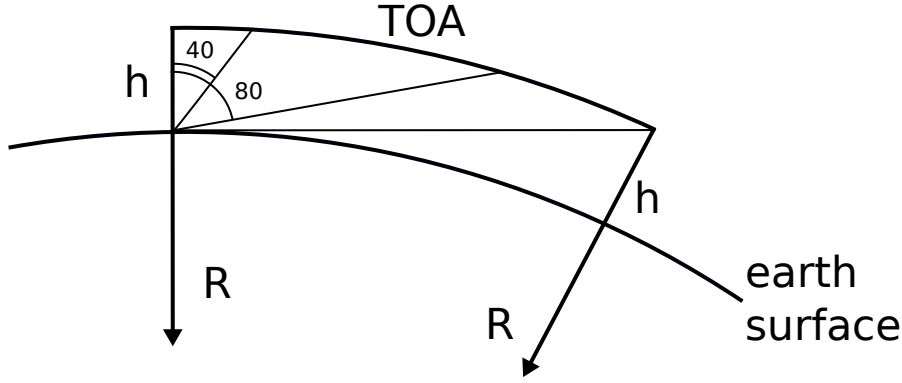
Figure 1: "Geometry of earth and atmosphere"

Because κ and ϵ are not constant along the path from earths surface to TOA the integration is subdivided into many steps. At each step κ and ϵ are calculated using local values of temperature and density.

In order to compute the total irradiance emanating from an area element of the surface to TOA the integration has to be done over the half sphere:

$$F(\theta) = \int_0^{2\pi} \int_0^{\pi/2} I(\theta)\sin(\theta)\cos(\theta)d\theta d\phi \tag{15}$$

$$= 2\pi \int_0^{\theta} I(\theta)\sin(\theta)\cos(\theta)d\theta \tag{16}$$

The intensity $I(\theta)$ is computed at 0° and two further angles (in the computations 40° and 80° are chosen), the intermediate values are interpolated by a cubic polynomial (Chapter B). After determining the polynomial coefficients:

$$a_2 = \frac{(F_1 - F_0)\theta_2^3 - (F_2 - F_0)\theta_1^3}{\theta_1^2\theta_2^3 - \theta_1^3\theta_2^2} \tag{17}$$

$$a_3 = \frac{(F_2 - F_0)\theta_1^2 - (F_1 - F_0)\theta_2^2}{\theta_1^2\theta_2^3 - \theta_1^3\theta_2^2} \tag{18}$$

the integral is given by:

$$F(\theta) = 2\pi \int_0^{\theta} \left(a_0 + a_2\theta^2 + a_3\theta^3\right)\sin(\theta)\cos(\theta)d\theta d\phi \tag{19}$$

The contributions of the different polynomial orders assuming constant $I(\theta)$ are:

$$\int_0^\theta \sin(\theta)\cos(\theta)d\theta = 0.5$$

$$\int_0^\theta \theta^2 \sin(\theta)\cos(\theta)d\theta = 0.37$$

$$\int_0^\theta \theta^3 \sin(\theta)\cos(\theta)d\theta = 0.38$$

2.4. The HITRAN Data

The spectroscopic CO_2 data where taken from the HITRAN database ([2]). The standard HITRAN data files use a fixed size format and include data that are not used in the present report. HITRAN allows to define ones own format and data output. For easier handling the entries are separated by commas. The data rows are composed of:

1. Molecule ID, for CO_2 this is 2

2. Isotopologue ID, for CO_2 $1-9$

3. The transition wavenumber ν $[cm^{-1}]$

4. The line strength multiplied by isotopologue abundance S, $[cm^{-1}/(molec\ cm^{-2}]$

5. Einstein coefficient of spontaneous emission A $[s^{-1}]$

6. Pressure line broadening coefficient by collisions with air molecules γ_{air} $[cm^{-1}atm^{-1}]$

7. pressure line broadening coefficient by collisions with CO_2 molecules γ_{self} $[cm^{-1}atm^{-1}]$

8. Energy of the lower state $E"$ $[cm^{-1}]$

9. Temperature exponent n_{air} for the air broadened HWHM

10. Pressure shift induced by air δ_{air}, referred to $p = 1atm$ $[cm^{-1}atm^{-1}]$

11. Upper state degeneracy g'

12. Lower state degeneracy $g"$

In the present report wavelength λ $[m]$ and energy $[J]$ is used, whereas HITRAN uses wavenumber $[cm^{-1}]$. The transition from wavelength to wavenumber has to be done

carefully.

$$\lambda_{ul} \leftarrow \frac{10^{-2}}{\nu} \qquad\qquad [m]$$

$$\Delta E_{ul} \leftarrow \frac{hc}{\lambda_{ul}} \qquad\qquad [J]$$

$$E_l \leftarrow hc\frac{E''}{10^{-2}} \qquad\qquad [J]$$

$$E_u \leftarrow E_l + \Delta E_u l \qquad\qquad [J]$$

$$\gamma_a \leftarrow \frac{\gamma_{air}}{10^{-2}}10^{-5} \qquad\qquad \left[\frac{1}{m\ Pa}\right]$$

$$\gamma_s \leftarrow \frac{\gamma_{self}}{10^{-2}}10^{-5} \qquad\qquad \left[\frac{1}{m\ Pa}\right]$$

$$\delta_a \leftarrow \frac{\delta_{air}}{10^{-2}}10^{-5}$$

The HWHM Doppler line broadening is given by:

$$\alpha_D(T) = \frac{\nu_{ij}}{c}\sqrt{\frac{2N_A kT \ln 2}{M}}$$

The temperature and pressure dependence of pressure broadened line width and pressure shift are defined by HITRAN as follows [1]:

$$\gamma(p,T) = \left(\frac{T_{ref}}{T}\right)^{n_{air}}\left(\gamma_{air}(p_{ref},T_{ref})(p - p_{self}) + \gamma_{self}(p_{ref},T_{ref})p_{self}\right)$$

$$\nu_{ij}^* = \nu_{ij}\delta(p_{ref})p$$

Temperature dependent partition functions can be found at [3].

2.5. Computational Details

The wavelength dependent intensity and the absorption and emission coefficients are discretized between $13\mu m$ and $17\mu m$. The wavelength resolution used is $10^{-11}m$. In order to check if this resolution is sufficient computations with $10^{-12}m$ were performed but showed only very small differences compared to the coarser resolution.

The initial intensity is given by the Planck function at $288K$:

$$I_\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1} \qquad\qquad (20)$$

The absorption and emission coefficients are the sums of all contributing lines:

$$\kappa(\lambda_j) = \sum_i \kappa_i f_i(\lambda_j - \lambda_i)$$

$$\epsilon(\lambda_j) = \sum_i \epsilon_i f_i(\lambda_j - \lambda_i)$$

The sums are over all transition lines included. j is the wavelength index of the descretized wavelength.

3. Results

In the following some results are presented.
Figure 2 shows the intensity as a function of the wavelength at TOA computed by the above described model excluding emission.
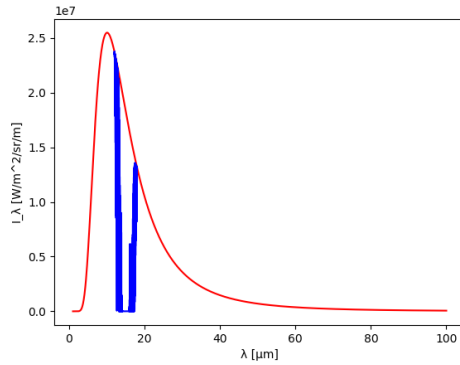

Figure 2: Intensity at the TOA without emission.

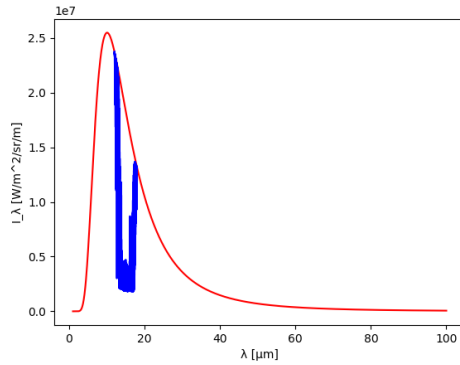Figure 3 shows the intensity versus wavelength at TOA including emission.

Figure 3: Intensity at the TOA including emission.

Figure 4 shows the difference of the intensity integrated from $13\mu m$ to $17\mu m$ as a function of the height above earths surface at $400 ppm$ and $800 ppm$ CO_2 respectively.
Figure 5 and Figure 6 show the wavelength dependent absorption and emission coefficients.
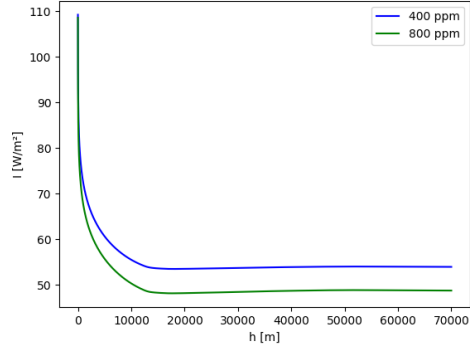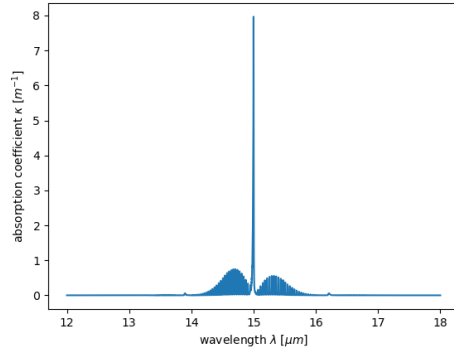
Figure 4: Intensity vs. height.

Figure 5: Absorption coefficient

Figure 7 shows the intensity over the wavelength at TOA for $400ppm$ and $800ppm$ CO_2 respectively.

In the following table intensity difference values between $400ppm$ and $800ppm$ CO_2.

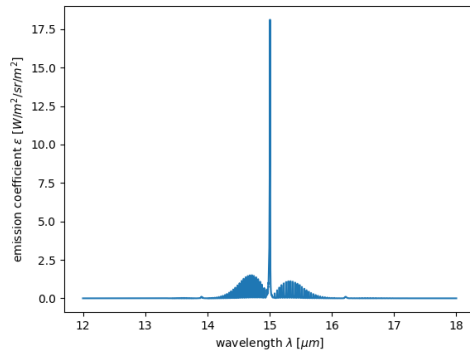| $I(400bpm) - I(800bpm)$ $[W/m^2]$	including emission	number of isotopes
14.8	yes	12
15.3	yes	1
17.4	no	1
12.1	yes	1

Figure 6: Emission coefficient
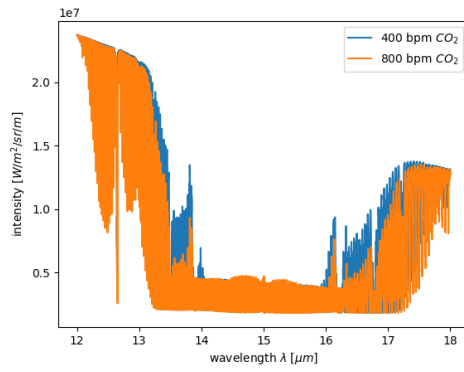
Figure 7: Intensity at TOA

4. Bibliography

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

[2] HITRAN. *Main Page*. URL: https://hitran.org/.

[3] HITRAN. *Partition Functions*. URL: https://hitran.org/docs/iso-meta/.

A. Integration of the Radiation Transfer Equation

The radiation transfer equation Equation 1 is of the form:

$$\frac{dy}{dx} = -ay + b \tag{21}$$

If a and b are constant the solution can be written as:

$$y(x) = c(x)\exp(-ax) \tag{22}$$

Inserting into Equation 21 yields:

$$\frac{dy}{dx} = \frac{dc(x)}{dx}\exp(-ax) - ac(x)\exp(-ax) = -ac(x)\exp(-ax) + b \tag{23}$$

and further:

$$\frac{dc(x)}{dx} = b\exp(ax) \tag{24}$$

This can be integrated:

$$dc(x) = b\exp(ax)dx \tag{25}$$

$$\int_{c_0}^{c} dc(x) = b\int_{0}^{x}\exp(ax)dx \tag{26}$$

$$c - c_0 = \frac{b}{a}\left(\exp(ax) - 1\right) \tag{27}$$

And finally:

$$y(x) = y(0)\exp(-ax) + \frac{b}{a}\left(1 - \exp(-ax)\right) \tag{28}$$

B. Cubic Polynomial Interpolation

$$y(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 \tag{29}$$

With $a_0 = y(0)$ and $\dfrac{dy(0)}{dx} = 0$ it follows that $a_1 = 0$. The coefficients a_2 and a_3 are determined by the linear system:

$$y(x_1) = y(0) + a_2 x_1^2 + a_3 x_1^3 \tag{30}$$
$$y(x_2) = y(0) + a_2 x_2^2 + a_3 x_2^3 \tag{31}$$

which can be written as matrix equation:

$$x \begin{pmatrix} x_1^2 & x_1^3 \\ x_2^2 & x_2^3 \end{pmatrix} \begin{pmatrix} a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} y(x_1) - y(0) \\ y(x_2) - y(0) \end{pmatrix} \tag{32}$$

Using Cramer's rule the solution is given by:

$$a_2 = \frac{(y(x_1) - y(0))x_2^3 - (y(x_2) - y(0))x_1^3}{x_1^2 x_2^3 - x_1^3 x_2^2} \tag{33}$$

$$a_3 = \frac{(y(x_2) - y(0))x_1^2 - (y(x_1) - y(0))x_2^2}{x_1^2 x_2^3 - x_1^3 x_2^2} \tag{34}$$

C. Line Shapes

C.1. Gaussian Lineshape

$$\frac{\Delta\lambda}{\lambda} = \frac{v}{c} = \frac{1}{c}\sqrt{\frac{2k_BT}{m}} \tag{35}$$

$$\exp(-ax_h^2) = \frac{1}{2} \tag{36}$$

$$-ax_h^2 = \ln\frac{1}{2} \tag{37}$$

$$a = \frac{\ln 2}{x_h^2} \tag{38}$$

$$x_h = x_{hwhm} = \Delta\lambda \tag{39}$$

$$a = \frac{\ln 2}{\Delta\lambda^2} \tag{40}$$

$$\int \exp\left(-\frac{\ln 2}{\Delta\lambda^2}x^2\right)dx = \sqrt{\frac{\pi}{a}} \tag{41}$$

$$\sqrt{\frac{a}{\pi}}\int \exp\left(-\frac{\ln 2}{\Delta\lambda^2}x^2\right)dx = 1 \tag{42}$$

$$\sqrt{\frac{\frac{\ln 2}{\Delta\lambda^2}}{\pi}}\int \exp\left(-\frac{\ln 2}{\Delta\lambda^2}x^2\right)dx = 1 \tag{43}$$

$$\Delta\lambda = \frac{1}{c}\sqrt{\frac{2k_BT}{m}}\lambda \tag{44}$$

$$\sqrt{\frac{\ln 2}{\pi\Delta\lambda^2}}\int \exp\left(-\frac{\ln 2}{\Delta\lambda^2}(\lambda-\lambda_0)^2\right)dx = 1 \tag{45}$$

C.2. Lorentz Lineshape

$$L(\nu) = \frac{a^2}{(\nu - \nu_0)^2 + a^2} \tag{46}$$

$$L(\nu_0) = 1 \tag{47}$$

$$L(\nu_h) = 1/2 = \frac{a^2}{(\nu_h - \nu_0)^2 + a^2} \tag{48}$$

$$(\nu_h - \nu_0)^2 + a^2 = 2a^2 \tag{49}$$

$$(\nu_h - \nu_0) = \Delta\nu = a \tag{50}$$

$$L(\nu) = \frac{\Delta\nu^2}{(\nu - \nu_0)^2 + \Delta\nu^2} \tag{51}$$

$$L(\lambda) = \frac{b^2}{c^2(1/\lambda - 1/\lambda_0)^2 + b^2} \tag{52}$$

$$L(\lambda) = \frac{b^2}{c^2 \left(\dfrac{\lambda - \lambda_0}{\lambda\lambda_0} \right)^2 + b^2} \tag{53}$$

$$L(\lambda) = \frac{b^2 \lambda^2 \lambda_0^2}{c^2} \frac{1}{(\lambda - \lambda_0)^2 + \lambda^2 \lambda_0^2 b^2/c^2} \tag{54}$$

$$L(\lambda_0) = 1 \tag{55}$$

$$L(\lambda_h) = \frac{1}{2} = \frac{b^2 \lambda_h^2 \lambda_0^2}{c^2} \frac{1}{(\lambda_h - \lambda_0)^2 + \lambda_h^2 \lambda_0^2 b^2/c^2} \tag{56}$$

$$2\frac{b^2\lambda_h^2\lambda_0^2}{c^2} = (\lambda_h - \lambda_0)^2 + \lambda_h^2\lambda_0^2 b^2/c^2 \tag{57}$$

$$\frac{b^2\lambda_h^2\lambda_0^2}{c^2} = (\lambda_h - \lambda_0)^2 \tag{58}$$

$$\frac{b^2}{c^2} = (\lambda_h - \lambda_0)^2 \frac{1}{\lambda_h^2\lambda_0^2} \tag{59}$$

$$L = (\lambda_h - \lambda_0)^2 \frac{1}{(\lambda - \lambda_0)^2 + (\lambda_h - \lambda_0)^2} \tag{60}$$

$$\Delta\lambda_{hwhm} = \lambda - \lambda_0 \tag{61}$$

$$L = \frac{\Delta\lambda^2}{(\lambda - \lambda_0)^2 + \Delta\lambda^2} \tag{62}$$

$$\int_{-\infty}^{-\infty} \frac{1}{1+x^2} dx = \arctan(\infty) - \arctan(-\infty) = \pi \tag{63}$$

$$x = \frac{(\lambda - \lambda_0)}{\Delta\lambda} \tag{64}$$

$$dx = \frac{1}{\Delta\lambda} d\lambda \tag{65}$$

$$L = \frac{\frac{1}{\pi}\Delta\lambda}{(\lambda - \lambda_0)^2 + \Delta\lambda^2} \tag{66}$$

$$L = \frac{1}{\pi}\frac{\Delta\lambda}{(\lambda - \lambda_0)^2 + \Delta\lambda^2} \tag{67}$$

$$\int \frac{1}{\pi}\frac{\Delta\lambda}{(\lambda - \lambda_0)^2 + \Delta\lambda^2} d\lambda = 1 \tag{68}$$

$$\int \frac{1}{\pi}\frac{\Delta\lambda}{(\lambda - \lambda_0)^2 + \Delta\lambda^2} d\lambda = 1 \tag{69}$$

D. Derivation of the Radiation Transfer Equation

D.1. Radiation Transfer Equation in Frequency Space

The radiation transfer equation is given by:

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \epsilon_\nu \tag{70}$$

$$I_\nu : \left[\frac{W}{m^2 \; sr \; Hz}\right] \tag{71}$$

$$\epsilon_\nu : \left[\frac{W}{m^3 \; sr \; Hz}\right] \tag{72}$$

$$\kappa_\nu : \left[\frac{1}{m}\right] \tag{73}$$

The spontaneous emission is given by:

$$\epsilon_\nu = \frac{1}{4\pi} h\nu N_u A_{ul} f(\nu) \quad , \quad \left[\frac{W}{m^3 srHz}\right] \tag{74}$$

With the line shape $f(\nu)$ function which is normalized according to:

$$\int f(\nu)d\nu = 1 \tag{75}$$

D.1.1. Thermodynamic Equilibrium

In total thermodynamic equilibrium it holds:

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \epsilon_\nu = 0 \tag{76}$$

The radiation density in thermodynamical equilibrium is given by the Planck function:

$$u_\nu = \frac{4\pi}{c^3} \frac{2h\nu^3}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \quad , \quad \left[\frac{J}{m^3 Hz}\right] \tag{77}$$

The intensity is given by:

$$I_\nu = \frac{u_\nu}{4\pi} c \tag{78}$$

which yields:

$$I_\nu = \frac{2h\nu^3}{c^2} \frac{1}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \quad , \quad \left[\frac{W}{m^2 srHz}\right] \tag{79}$$

The absorption coefficient κ then is given by.

$$\kappa_\nu = \frac{1}{4\pi} h\nu N_u A_{ul} f(\nu) \; \left(\exp\left(\frac{h\nu}{k_B T}\right) - 1 \right) \frac{c^2}{2h\nu^3} \quad , \quad \left[\frac{1}{m}\right] \tag{80}$$

$$\kappa_\nu = \frac{1}{8\pi} \frac{c^2}{\nu^2} N_u A_{ul} \left(\exp\left(\frac{h\nu}{k_B T}\right) - 1 \right) f(\nu) \quad , \quad \left[\frac{1}{m}\right] \tag{81}$$

$$\kappa_\nu = \frac{h\nu}{c} \left(N_l B_{lu} - N_u B_{ul} \right) f(\nu) \tag{82}$$

$$\kappa_\nu = \frac{h\nu}{c} N \left(g_l \exp\left(-\frac{E_l}{k_B T}\right) B_{lu} - g_u \exp\left(-\frac{E_u}{k_B T}\right) B_{ul} \right) f(\nu) \tag{83}$$

$$\kappa_\nu = \frac{h\nu}{c} N \exp\left(-\frac{E_u}{k_B T}\right) \left(\exp\left(-\frac{(E_u - E_l)}{k_B T}\right) g_l B_{lu} - g_u B_{ul} \right) f(\nu) \tag{84}$$

$$g_l B_{lu} = g_u B_{ul} \tag{85}$$

$$\kappa_\nu = \frac{h\nu}{c} N g_u B_{ul} \exp\left(-\frac{E_u}{k_B T}\right) \left(\exp\left(-\frac{h\nu}{k_B T}\right) - 1 \right) f(\nu) \tag{86}$$

$$\kappa_\nu = \frac{h\nu}{c} B_{ul} N_u \left(\exp\left(-\frac{h\nu}{k_B T}\right) - 1 \right) f(\nu) \quad , \quad \left[\frac{1}{m}\right] \tag{87}$$

$$\frac{h\nu}{c} B_{ul} N_u = \frac{1}{8\pi} \frac{c^2}{\nu^2} N_u A_{ul} \tag{88}$$

$$B_{ul} = \frac{1}{8\pi} \frac{c^3}{h\nu^3} A_{ul} \quad , \quad \left[\frac{m^3}{Js^2}\right] \tag{89}$$

D.2. Radiation Transfer Equation in Wavelength Space

$$I_\lambda = \frac{2\pi hc^2}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1} \tag{90}$$

$$I = \int I_\lambda d\lambda \tag{91}$$

$$I_\nu d\nu = I_\lambda d\lambda \tag{92}$$

$$\nu = \frac{c}{\lambda} \tag{93}$$

$$d\nu = -\frac{c}{\lambda^2} d\lambda \tag{94}$$

$$I_\nu \frac{c}{\lambda^2} d\lambda = I_\lambda d\lambda \tag{95}$$

$$I_\nu \frac{c}{\lambda^2} = I_\lambda \tag{96}$$

$$I_\nu = I_\lambda \frac{\lambda^2}{c} \tag{97}$$

$$\frac{dI_\lambda}{ds} = -\kappa_\lambda I_\lambda + \epsilon_\lambda \tag{98}$$

$$\kappa_\lambda = \frac{h}{\lambda_0} \left(N_l B_{lu} - N_u B_{ul}\right) f(\lambda) \frac{\lambda^2}{c} \tag{99}$$

$$\kappa_\lambda = \frac{h\lambda}{c} \left(N_l B_{lu} - N_u B_{ul}\right) f(\lambda) \quad , \quad \left[\frac{1}{m}\right] \tag{100}$$

$$\epsilon_\nu f(\nu) d\nu = \epsilon_\lambda f(\lambda) d\lambda \tag{101}$$

$$f(\nu) d\nu = f(\lambda) d\lambda \tag{102}$$

$$\epsilon_\nu = \epsilon_\lambda \tag{103}$$

$$\epsilon_\lambda = \frac{1}{4\pi} \frac{hc}{\lambda} N_u A_{ul} f(\lambda) \quad , \quad \left[\frac{W}{m^3 sr \ m}\right] \tag{104}$$

$$\int f_\lambda d\lambda = 1 \tag{105}$$

$$B_{ul} = A_{ul}\frac{\lambda^3}{8\pi h} \quad , \quad \left[\frac{m^3}{Js^2}\right] \tag{106}$$

$$B_{lu} = \frac{g_u}{g_l}B_{ul} \tag{107}$$

$$< \epsilon > = \int \epsilon_\lambda(\lambda)d\lambda \tag{108}$$

$$< \kappa > = \frac{\int \kappa_\lambda(\lambda)I_\lambda(\lambda)d\lambda}{\int I_\lambda(\lambda)d\lambda} \tag{109}$$

In thermal equilibrium the intensity is constant:

$$\frac{dI_\lambda}{ds} = -\kappa_\lambda I_\lambda + \epsilon_\lambda = 0 \tag{110}$$

$$\kappa_\lambda = \frac{\epsilon_\lambda}{I_\lambda} \tag{111}$$

and the intensity is given by Planck's formula:

$$I_\lambda = \frac{2hc^2}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1} \tag{112}$$

With this the net absorption coefficient κ_λ is:

$$\kappa_\lambda = \frac{\frac{1}{4\pi}\frac{hc}{\lambda}N_u A_{ul} f(\lambda)}{\frac{2hc^2}{\lambda^5}\frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1}} = \frac{\lambda^4}{8\pi c}A_{ul}N_u\left(\exp\left(\frac{hc}{\lambda k_B T}\right) - 1\right)f(\lambda) \tag{113}$$

The densities of upper and lower state are given by:

$$N_u = N\frac{g_u}{Q(T)}\exp\left(-\frac{E_u}{k_B T}\right) \tag{114}$$

$$N_l = N\frac{g_l}{Q(T)}\exp\left(-\frac{E_l}{k_B T}\right) \tag{115}$$

which yields:

$$\kappa_\lambda = \frac{\lambda^4}{8\pi c}A_{ul}N\frac{g_u}{Q(T)}\left(\exp\left(-\frac{E_l}{\lambda k_B T}\right) - \exp\left(-\frac{E_u}{\lambda k_B T}\right)\right)f(\lambda) \tag{116}$$

With:

$$B_{ul} = \frac{1}{8\pi} \frac{\lambda^3}{h} A_{ul} \quad , \quad \left[\frac{m^3}{Js^2}\right] \tag{117}$$

$$B_{lu} = \frac{g_u}{g_l} B_{ul} \tag{118}$$

this becomes

$$\kappa_\lambda = \frac{h\lambda}{c} \left(B_{ul} N \frac{g_u}{Q(T)} \exp\left(-\frac{E_l}{\lambda k_B T}\right) - B_{lu} N \frac{g_l}{Q(T)} \exp\left(-\frac{E_u}{\lambda k_B T}\right) \right) f(\lambda) \tag{119}$$

and:

$$\kappa_\lambda = \frac{h\lambda}{c} \left(B_{lu} N_l - B_{ul} N_u \right) f(\lambda) \tag{120}$$

E. Coments on the Article Reinhart

E.1. Difference between the Radiation Transfer Equation and Reinhart Equation (9)

E.1.1. Radiation Transfer Equation

The radiation transfer equation excluding emission reads:

$$\frac{dI(\lambda, s)}{ds} = -I(\lambda, s) \sum_i \kappa_i f_i(\lambda) \tag{121}$$

Integration along the propagation path yields:

$$\frac{I(\lambda, s)}{I(\lambda, s = 0)} = \left(1 - \exp\left(-\sum_i \kappa_i f_i(\lambda) s \right) \right) \tag{122}$$

Integration over a wavelength interval yields:

$$\frac{I_{abs}}{I_0} = \int_{\Delta\lambda} \left(1 - \exp\left(-\sum_i \kappa_i f_i(\lambda) s \right) \right) d\lambda \tag{123}$$

E.1.2. Wavelengths Average Absorption

Integrating Equation 121 over a wavelength interval:

$$\frac{d}{ds} \int_{\Delta\lambda} I(\lambda, s) d\lambda = -\sum_i \int_{\Delta\lambda} I(\lambda, s) \kappa_i f_i(\lambda) d\lambda \tag{124}$$

Assuming that the intensity is constant within the integration interval:

$$\frac{dI(s)}{ds} = -\frac{I}{\Delta\lambda} \sum_i \kappa_i \int_{\Delta\lambda} f_i(\lambda) d\lambda \tag{125}$$

$$= -\frac{I}{\Delta\lambda} \sum_i \kappa_i(\lambda_i) \tag{126}$$

Integrating along the propagation path:

$$\frac{dI(s)}{I(s)} = -\frac{1}{\Delta\lambda} \sum_i \kappa_i ds \tag{127}$$

yields:

$$\ln \frac{I(s)}{I(0)} = -\frac{1}{\Delta\lambda} \int_0^s \sum_i \kappa_i ds \tag{128}$$

and finally:

$$\frac{I_{abs}}{I_0} = 1 - \exp\left(-\frac{1}{\Delta\lambda}\int_0^s \sum_i \kappa_i ds\right) \tag{129}$$

Equation 123 and Equation 129 result in different values. This is because the assumption of constant intensity is in general not valid and that spectrally overlapping lines cannot be treated separatly. In the following section a simple is employed to demonstrate this.

E.1.3. Simple Model

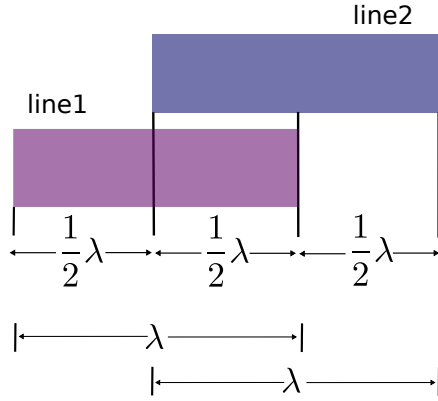Two partially overlapping lines with rectangle shaped line shapes:

Figure 8: Two overlapping lines with rectangle line shape functions

Reinhart:

$$\Delta J_1 = (1 - \exp(-\kappa_1 z))\,\Delta\lambda \tag{130}$$
$$\Delta J_2 = (1 - \exp(-\kappa_2 z))\,\Delta\lambda \tag{131}$$

$$A = \frac{\Delta J_1 + \Delta J_2}{\Delta\lambda} = (1 - \exp(-\kappa_1 z)) + (1 - \exp(-\kappa_2 z)) \tag{132}$$

Radiation transfer solution :

$$\Delta I_1 = (1 - \exp(-\kappa_1 z))\frac{\Delta\lambda}{2} \tag{133}$$
$$\Delta I_2 = (1 - \exp(-\kappa_2 z))\frac{\Delta\lambda}{2} \tag{134}$$
$$\Delta I_{12} = (1 - \exp(-\kappa_1 z - \kappa_2 z))\frac{\Delta\lambda}{2} \tag{135}$$

$$B = \frac{\Delta I_1 + \Delta I_2 + \Delta I_{12}}{I_0 \Delta \lambda} = \frac{1}{2} \left(1 - \exp(-\kappa_1 z) \right) + \tag{136}$$

$$\frac{1}{2} \left(1 - \exp(-\kappa_2 z) \right) + \tag{137}$$

$$\frac{1}{2} \left(1 - \exp(-\kappa_1 z - \kappa_2 z) \right) \tag{138}$$

The difference is:

$$2(A - B) = (1 - \exp(-\kappa_1 z)) + (1 - \exp(-\kappa_2 z)) - (1 - \exp(-\kappa_1 z - \kappa_2 z) \tag{139}$$

$$= 1 + \exp(-\kappa_1 z - \kappa_2 z) - \exp(-\kappa_1 z) - \exp(-\kappa_2 z) \tag{140}$$

In case of $\kappa_1 \gg 1$ and $\kappa_2 \gg 1$ this yields:

$$(\Delta J_1 + \Delta J_2) - (\Delta I_1 + \Delta I_2 + \Delta I_{12}) = I_0 \frac{\Delta \lambda}{2} \tag{141}$$

That means the absorption of the overlapping region is counted twice.