

SARM: Simple Atmospheric Radiation Transfer Model

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1. Introduction

SARM is a model for the radiative transfer of IR radiation from the earth’s surface to the top of the atmosphere (TOA) in which only CO₂ interacts with the radiation. It is by no means an accurate model of radiative transport in the atmosphere with its multitude of climate-active gases, clouds, aerosols etc. The current model is only intended to provide some basic insights into the absorption and emission processes of infrared radiation on its way from the earth’s surface to TAO. The wavelength range is limited to $(13 - 17) \mu m$. Temperature and pressure of the atmosphere are functions of altitude. However, they are not self-consistently calculated in the frame of the model but are assumed to be given.

2. Model Description

The key assumptions of **SARM** are:

- The only species interacting with infrared radiation in the $15\mu m$ range is CO_2
- The temperature and pressure profiles of the atmosphere are prescribed, thus there is no self consistency between absorption, emission and temperature
- Only upward traveling radiation is considered, the model is 1-dimensional
- The main result is the difference in the power of infrared radiation at the top of the atmosphere (TOA) at 70 km at different CO_2 concentrations.
- Scattering at aerosols, droplets etc. will be neglected
- The atmospheric gas is in local thermodynamic equilibrium so that all energy levels are occupied according to the Boltzmann factor
- All CO_2 spectroscopic data are taken from the HITRAN data base.

2.1. Radiation Transport Equation

The radiation transport equation reads:

$$\frac{dI(\lambda)}{dz} = -\kappa(\lambda)I(\lambda) + \epsilon(\lambda) \quad (1)$$

with the spectral intensity:

$$I(\lambda) : \left[\frac{W}{m^2 \text{ sr } m} \right]$$

the absorption coefficient:

$$\kappa(\lambda) : \left[\frac{1}{m} \right]$$

and the emission coefficient:

$$\epsilon(\lambda) : \left[\frac{W}{m^3 \text{ sr } m} \right]$$

The absorption and emission coefficients are given by the sums over all line coefficients:

$$\begin{aligned} \epsilon(\lambda) &= \sum_j \epsilon_j(\lambda) \\ \kappa(\lambda) &= \sum_j \kappa_j(\lambda) \end{aligned}$$

The emission coefficient $\epsilon_j(\lambda)$ due to spontaneous emission from the upper level u to the lower level l is given by:

$$\epsilon_j(\lambda) = \frac{1}{4\pi} \frac{hc}{\lambda} N_{u,j} A_{ul,j} f_j(\lambda) \frac{\lambda^2}{c} \quad (2)$$

$A_{ul,j}$ is the Einstein coefficient of spontaneous emission from upper to lower energy state, $N_{u,j}$ the density of the upper state and $f_j(\lambda)$ is the line shape. The absorption coefficient $\kappa_j(\lambda)$ of this transition is given by:

$$\kappa_j(\lambda) = \frac{h}{\lambda} (B_{lu,j}N_{l,j} - B_{ul,j}N_{u,j}) f_j(\lambda) \frac{\lambda^2}{c} \quad (3)$$

with the Einstein coefficients of absorption and stimulated emission:

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

$$B_{lu,j} = \frac{g_u}{g_l} B_{ul,j} \quad (5)$$

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

$$N_{u,j} = N \frac{g_{u,j}}{Q(T)} \exp\left(-\frac{E_{u,j}}{k_B T}\right) \quad (6)$$

$$N_{l,j} = N \frac{g_{l,j}}{Q(T)} \exp\left(-\frac{E_{l,j}}{k_B T}\right) \quad (7)$$

$g_{u,j}$ and $g_{l,j}$ are the degeneracies of the upper and lower level respectively and $Q(T)$ is the partition function of the CO₂ isotope of line j .

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:

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

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

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

$$\frac{\Delta \lambda}{\lambda} = \frac{v}{c} = \frac{1}{c} \sqrt{\frac{2k_B T}{M}} \quad (10)$$

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

2.2.2. Pressure Broadening

Pressure broadening is caused by the collisions between molecules, in the present model mainly between N₂ and O₂ with CO₂. The main determining factors are the concentration of the collision partners

and the collision frequency. The line shapes are given by a Lorentz function:

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

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

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 :

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

$F(x_p) = 0.9$ 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 is being added.

2.2.3. Voigt Profile

Pressure and Doppler broadening occur simultaneously, the line shape is a convolution of Lorentz and Gauss functions which is called Voigt profile. For the sake of performance the Voigt profile is approximate by a linear interpolation of Lorentz and Gauss shapes:

$$f(\lambda, \lambda_0) = \begin{cases} f_L(\lambda, \lambda_0) & v > 1 \\ v f_L(\lambda, \lambda_0) + (1-v) f_G(\lambda, \lambda_0) & \text{otherwise} \end{cases} \quad (14)$$

with:

$$a = \frac{\Delta\lambda_L}{\Delta\lambda_G \lambda_0}$$

$$v = \max(0.0, 1.36606 a - 0.47719 a^2 + 0.11116 a^3)$$

2.3. Integration of the Radiation Transfer Equation

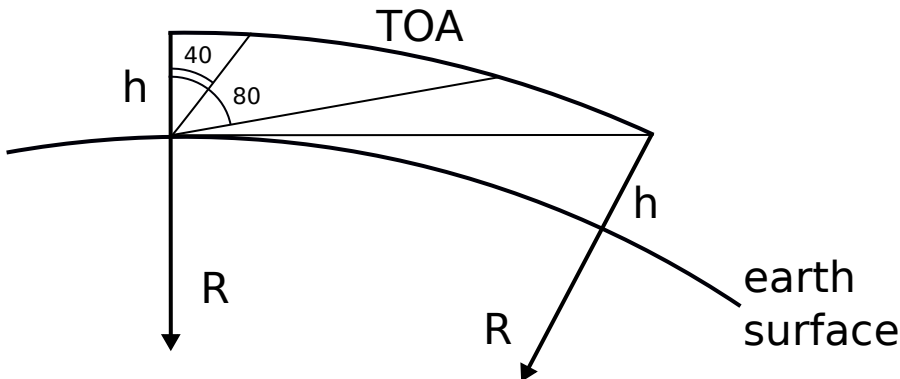


Figure 1: Geometry of earth and atmosphere

The intensity in Eq.(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 Eq.(1) the solution

is given by:

$$I(\lambda, z) = I(\lambda, z_0) \exp(-\kappa(\lambda)(z - z_0)) + \frac{\epsilon(\lambda)}{\kappa(\lambda)} (1 - \exp(-\kappa(\lambda)(z - z_0))) \quad (15)$$

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 (Fig.(1)):

$$F = \int_0^{2\pi} \int_0^{\pi/2} I(\theta) \sin(\theta) \cos(\theta) d\theta d\phi \quad (16)$$

$$= 2\pi \int_0^{\pi/2} I(\theta) \sin(\theta) \cos(\theta) d\theta \quad (17)$$

The intensity $I(\theta)$ is computed at $\theta_1 = 0^\circ, \theta_2 = 40^\circ, \theta_3 = 40^\circ$. The intermediate values are interpolated by a cubic polynomial (see Chapter B):

$$I(\theta) = I(\theta = 0) + a_2\theta_2^2 + a_3\theta_3^3 \quad (18)$$

The term linear in θ is zero because of $\frac{dI(\theta)}{d\theta}|_{(\theta=\theta_1)} = 0$.

The polynomial coefficients can be determined analytically:

$$a_2 = \frac{(I(\theta_2) - I(\theta_1))\theta_3^3 - (I(\theta_3) - I(\theta_1))\theta_2^3}{\theta_1^2\theta_2^3 - \theta_1^3\theta_2^2} \quad (19)$$

$$a_3 = \frac{(I(\theta_3) - I(\theta_1))\theta_2^2 - (I(\theta_2) - I(\theta_1))\theta_3^2}{\theta_1^2\theta_2^3 - \theta_1^3\theta_2^2} \quad (20)$$

With this the integral is given by:

$$F = 2\pi \int_0^{\pi/2} (I(0) + a_2\theta^2 + a_3\theta^3) \sin(\theta) \cos(\theta) d\theta \quad (21)$$

The contributions of the different polynomial orders assuming $I(\theta) = 1$ are:

$$\begin{aligned} \int_0^{\pi/2} \sin(\theta) \cos(\theta) d\theta &= 0.5 \\ \int_0^{\pi/2} \theta^2 \sin(\theta) \cos(\theta) d\theta &= 0.37 \\ \int_0^{\pi/2} \theta^3 \sin(\theta) \cos(\theta) d\theta &= 0.38 \end{aligned}$$

2.4. The HITRAN Data

The spectroscopic CO₂ data were taken from the HITRAN database (HITRAN n.d.(b)). The standard HITRAN data files use a fixed size format and include data that are not used in the present model. HITRAN allows to define one's own format and data output. For easier handling the entries

are separated by commas. The data rows are composed of:

1. Molecule ID, for CO₂ this is 2
2. Isotopologue ID, for CO₂ 1 – 9
3. The transition wavenumber ν [cm^{-1}]
4. The line strength multiplied by isotopologue abundance S , [$cm^{-1}/(mole\ cm^{-2})$]
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 CO₂ molecules γ_{self} [$cm^{-1}atm^{-1}$]
8. Energy of the lower state E_l [cm^{-1}]
9. Temperature exponent n_{air} for the air broadened HWHM
10. Pressure shift induced by air (pressure) δ_{air} , referred to $p = 1\ atm$ [$cm^{-1}atm^{-1}$]
11. Upper state degeneracy g_u
12. Lower state degeneracy g_l

In the present report wavelength unit is meter and energy unit is Joule, whereas HITRAN uses wavenumber [cm^{-1}]. The transition from wavelength to wavenumber has to be done carefully.

$$\begin{aligned}
\lambda_{ul} &\leftarrow \frac{10^{-2}}{\nu} & [m] \\
\Delta E_{ul} &\leftarrow \frac{hc}{\lambda_{ul}} & [J] \\
E_l &\leftarrow hc \frac{E_l}{10^{-2}} & [J] \\
E_u &\leftarrow E_l + \Delta E_{ul} & [J] \\
\gamma_a &\leftarrow \frac{\gamma_{air}}{10^{-2}} 10^{-5} & \left[\frac{1}{m\ Pa} \right] \\
\gamma_s &\leftarrow \frac{\gamma_{self}}{10^{-2}} 10^{-5} & \left[\frac{1}{m\ Pa} \right] \\
\delta_a &\leftarrow \frac{\delta_{air}}{10^{-2}} 10^{-5} &
\end{aligned}$$

The Gauss profile is given as:

$$g_G(\nu; \nu_{ij}, T) = \sqrt{\frac{\ln 2}{\pi \alpha_D^2}} \exp\left(-\frac{(\nu - \nu_{ij})^2}{\alpha_D^2}\right)$$

with the HWHM Doppler line broadening:

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

N_A is the Avogadro constant and M_{mole} is the molar mass of the isotopologue.

The Lorentz profile is given by HITRAN as HITRAN n.d.(a):

$$g_G(\nu; \nu_{ij}, T) \frac{1}{\pi} \frac{\gamma(p, T)}{\gamma(p, T)^2 + [\nu - (\nu_{ij} + \delta(p_{ref}))^2]}$$

with the temperature and pressure dependence of pressure broadened line width and pressure shift:

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

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

Temperature dependent partition functions for CO₂ can be found at HITRAN n.d.(c).

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 $288K$:

$$I_\lambda = \frac{2\pi hc^2}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1} \quad (22)$$

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

$$\kappa(\lambda_i) = \sum_j \kappa_j f_j(\lambda_i - \lambda_j)$$

$$\epsilon(\lambda_i) = \sum_j \epsilon_j f_j(\lambda_i - \lambda_j)$$

i is the wavelength index of the discretized wavelength and j is the line index.

3. Results

In the following some results are presented.

In the following table intensity difference values between $400ppm$ and $800ppm$ CO₂.

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

References

- HITRAN (n.d.[a]). *Definitions and Units*. URL: <https://hitran.org/docs/definitions-and-units/>.
- (n.d.[b]). *Main Page*. URL: <https://hitran.org/>.
- (n.d.[c]). *Partition Functions*. URL: <https://hitran.org/docs/iso-meta/>.

A. Integration of the Radiation Transfer Equation

The radiation transfer equation Eq.(1) is of the form:

$$\frac{dy}{dx} = -ay + b \quad (23)$$

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

$$y(x) = c(x) \exp(-ax) \quad (24)$$

Inserting into Eq.(23) yields:

$$\frac{dy}{dx} = \frac{dc(x)}{dx} \exp(-ax) - ac(x) \exp(-ax) = -ac(x) \exp(-ax) + b \quad (25)$$

and further:

$$\frac{dc(x)}{dx} = b \exp(ax) \quad (26)$$

This can be integrated:

$$dc(x) = b \exp(ax) dx \quad (27)$$

$$\int_{c_0}^c dc(x) = b \int_0^x \exp(ax) dx \quad (28)$$

$$c - c_0 = \frac{b}{a} (\exp(ax) - 1) \quad (29)$$

And finally:

$$y(x) = y(0) \exp(-ax) + \frac{b}{a} (1 - \exp(-ax)) \quad (30)$$

B. Cubic Polynomial Interpolation

$$y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 \quad (31)$$

With $a_0 = y(x_1)$ and $\frac{dy(x_1=0)}{dx} = 0$ it follows that $a_1 = 0$. The coefficients a_2 and a_3 are determined

by the linear system:

$$y(x_2) = y(x_1) + a_2x_2^2 + a_3x_2^3 \quad (32)$$

$$y(x_3) = y(x_1) + a_2x_3^2 + a_3x_3^3 \quad (33)$$

which can be written as matrix equation:

$$\begin{pmatrix} x_2^2 & x_2^3 \\ x_3^2 & x_3^3 \end{pmatrix} \begin{pmatrix} a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} y(x_2) - y(x_1) \\ y(x_3) - y(x_1) \end{pmatrix} \quad (34)$$

Using Cramer's rule the solution is given by:

$$a_2 = \frac{(y(x_2) - y(x_1))x_3^3 - (y(x_3) - y(x_1))x_2^3}{x_2^2x_3^3 - x_3^2x_2^3} \quad (35)$$

$$a_3 = \frac{(y(x_3) - y(x_1))x_2^2 - (y(x_2) - y(x_1))x_3^2}{x_2^2x_3^3 - x_3^2x_2^3} \quad (36)$$