

ARTS Theory

edited by

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Chapter 1

Theoretical formalism

In this section, a theoretical framework of the forward model is presented. The presentation follows *Rodgers [1990]*, but some extensions are made, for example, the distinction between the atmospheric and sensor parts of the forward model is also discussed. After this chapter was written, C.D. Rodgers published a textbook [*Rodgers, 2000*] presenting the formalism in more detail than *Rodgers [1990]*.

1.1 The forward model

The radiative intensity, I , at a point in the atmosphere, r , for frequency ν and traversing in the direction, ψ , depends on a variety of physical processes and continuous variables such as the temperature profile, T :

$$I = F(\nu, r, \psi, T, \dots) \quad (1.1)$$

To detect the spectral radiation some kind of sensor, having a finite spatial and frequency resolution, is needed, and the observed spectrum becomes a vector, \mathbf{y} , instead of a continuous function. The atmospheric radiative transfer is simulated by a computer model using a limited number of parameters as input (that is, a discrete model), and the forward model, \mathcal{F} , used in practice can be expressed as

$$\mathbf{y} = \mathcal{F}(\mathbf{x}_{\mathcal{F}}, \mathbf{b}_{\mathcal{F}}) + \varepsilon(\mathbf{x}_{\varepsilon}, \mathbf{b}_{\varepsilon}) \quad (1.2)$$

where $\mathbf{x}_{\mathcal{F}}$, $\mathbf{b}_{\mathcal{F}}$, \mathbf{x}_{ε} and \mathbf{b}_{ε} together give a total description of both the atmospheric and sensor states, and ε is the measurement errors. The parameters are divided in such way that \mathbf{x} , the state vector, contains the parameters to be retrieved, and the remainder is given by \mathbf{b} , the model parameter vector. The total state vector is

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_{\mathcal{F}} \\ \mathbf{x}_{\varepsilon} \end{bmatrix} \quad (1.3)$$

History

110610 Outdated information was removed (Patrick Eriksson).

000306 Written by Patrick Eriksson, partly based on *Eriksson [1999]* and *Eriksson et al. [2002]*.

and the total model parameter vector is

$$\mathbf{b} = \begin{bmatrix} \mathbf{b}_{\mathcal{F}} \\ \mathbf{b}_{\varepsilon} \end{bmatrix} \quad (1.4)$$

The actual forward model consists of either empirically determined relationships, or numerical counterparts of the physical relationships needed to describe the radiative transfer and sensor effects. The forward model described here is mainly of the latter type, but some parts are more based on empirical investigations, such as the parameterisations of continuum absorption.

Both for the theoretical formalism and the practical implementation, it is suitable to make a separation of the forward model into two main sections, a first part describing the atmospheric radiative transfer for pencil beam (infinite spatial resolution) monochromatic (infinite frequency resolution) signals,

$$\mathbf{i} = \mathcal{F}_r(\mathbf{x}_r, \mathbf{b}_r) \quad (1.5)$$

and a second part modelling sensor characteristics,

$$\mathbf{y} = \mathcal{F}_s(\mathbf{i}, \mathbf{x}_s, \mathbf{b}_s) + \varepsilon(\mathbf{x}_{\varepsilon}, \mathbf{b}_{\varepsilon}) \quad (1.6)$$

where \mathbf{i} is the vector holding the spectral values for the considered set of frequencies and viewing angles ($\mathbf{i}^i = I(\nu^i, \psi^i, \dots)$, where i is the vector index), and $\mathbf{x}_{\mathcal{F}}$ and $\mathbf{b}_{\mathcal{F}}$ are separated correspondingly, that is, $\mathbf{x}_{\mathcal{F}}^T = [\mathbf{x}_r^T, \mathbf{x}_s^T]$ and $\mathbf{b}_{\mathcal{F}}^T = [\mathbf{b}_r^T, \mathbf{b}_s^T]$. The vectors \mathbf{x} and \mathbf{b} can now be expressed as

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_s \\ \mathbf{x}_{\varepsilon} \end{bmatrix} \quad (1.7)$$

and

$$\mathbf{b} = \begin{bmatrix} \mathbf{b}_r \\ \mathbf{b}_s \\ \mathbf{b}_{\varepsilon} \end{bmatrix}, \quad (1.8)$$

respectively. The subscripts of \mathbf{x} and \mathbf{b} are below omitted as the distinction should be clear by the context.

1.2 The sensor transfer matrix

The modelling of the different sensor parts can be described by a number of analytical expressions that together makes the basis for the sensor model. These expressions are throughout linear operations and it possible, as suggested in *Eriksson et al. [2002]*, to implement the sensor model as a straightforward matrix multiplication:

$$\mathbf{y} = \mathbf{H}\mathbf{i} + \varepsilon \quad (1.9)$$

where \mathbf{H} is here denoted as the sensor transfer matrix. Expressions to determine \mathbf{H} are given by *Eriksson et al. [2006]*.

The matrix \mathbf{H} can further incorporate effects of a data reduction and the total transfer matrix is then

$$\mathbf{H} = \mathbf{H}_d \mathbf{H}_s \quad (1.10)$$

as

$$\mathbf{y} = \mathbf{H}_d \mathbf{y}' = \mathbf{H}_d (\mathbf{H}_s \mathbf{i} + \boldsymbol{\varepsilon}') = \mathbf{H} \mathbf{i} + \boldsymbol{\varepsilon} \quad (1.11)$$

where \mathbf{H}_d is the data reduction matrix, \mathbf{H}_s the sensor matrix, and \mathbf{y}' and $\boldsymbol{\varepsilon}'$ are the measurement vector and the measurement errors, respectively, before data reduction.

1.3 Weighting functions

1.3.1 Basics

A weighting function is the partial derivative of the spectrum vector \mathbf{y} with respect to some variable used by the forward model. As the input of the forward model is divided between \mathbf{x} or \mathbf{b} , the weighting functions are divided correspondingly between two matrices, the state weighting function matrix

$$\mathbf{K}_x = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \quad (1.12)$$

and the model parameter weighting function matrix

$$\mathbf{K}_b = \frac{\partial \mathbf{y}}{\partial \mathbf{b}} \quad (1.13)$$

For the practical calculations of the weighting functions, it is important to note that the atmospheric and sensor parts can be separated. For example, if \mathbf{x} only hold atmospheric and spectroscopic variables, \mathbf{K}_x can be expressed as

$$\mathbf{K}_x = \frac{\partial \mathbf{y}}{\partial \mathbf{i}} \frac{\partial \mathbf{i}}{\partial \mathbf{x}} = \mathbf{H} \frac{\partial \mathbf{i}}{\partial \mathbf{x}} \quad (1.14)$$

This equation shows that the new parts needed to calculate atmospheric weighting functions, are functions giving $\partial \mathbf{i} / \partial \mathbf{x}$ where \mathbf{x} can represent the vertical profile of a species, atmospheric temperatures, spectroscopic data etc.

1.3.2 Transformation between vector spaces

It could be of interest to transform a weighting function matrix from one vector space to another¹. The new vector, \mathbf{x}' , is here assumed to be of length n ($\mathbf{x}' \in \mathbf{R}^{n \times 1}$), while the original vector, \mathbf{x} is of length p ($\mathbf{x} \in \mathbf{R}^{p \times 1}$). The relationship between the two vector spaces is described by a transformation matrix \mathbf{B} :

$$\mathbf{x} = \mathbf{B} \mathbf{x}' \quad (1.15)$$

where $\mathbf{B} \in \mathbf{R}^{p \times n}$. For example, if \mathbf{x}' is assumed to be piecewise linear, then the columns of \mathbf{B} contain tenth functions, that is, a function that are 1 at the point of interest and decreases

¹This subject is also discussed in *Rodgers [2000]*, published after writing this.

linearly down to zero at the neighbouring points. The matrix can also hold a reduced set of eigenvectors.

The weighting function matrix corresponding to \mathbf{x}' is

$$\mathbf{K}_{\mathbf{x}'} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}'} \quad (1.16)$$

This matrix is related to the weighting function matrix of \mathbf{x} (Eq. 1.12) as

$$\mathbf{K}_{\mathbf{x}'} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{x}'} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \mathbf{B} = \mathbf{K}_{\mathbf{x}} \mathbf{B} \quad (1.17)$$

Note that

$$\mathbf{K}_{\mathbf{x}'\mathbf{x}'} = \mathbf{K}_{\mathbf{x}} \mathbf{B} \mathbf{x}' = \mathbf{K}_{\mathbf{x}} \mathbf{x} \quad (1.18)$$

However, it should be noted that this relationship only holds for those \mathbf{x} that can be represented perfectly by some \mathbf{x}' (or vice versa), that is, $\mathbf{x} = \mathbf{B}\mathbf{x}'$, and not for all combinations of \mathbf{x} and \mathbf{x}' .

If \mathbf{x}' is the vector to be retrieved, we have that [Rodgers, 1990]

$$\hat{\mathbf{x}}' = \mathcal{I}(\mathbf{y}, \mathbf{c}) = \mathcal{T}(\mathbf{x}, \mathbf{b}, \mathbf{c}) \quad (1.19)$$

where \mathcal{I} and \mathcal{T} are the inverse and transfer model, respectively.

The contribution function matrix is accordingly

$$\mathbf{D}_{\mathbf{y}} = \frac{\partial \hat{\mathbf{x}}'}{\partial \mathbf{y}} \quad (1.20)$$

that is, $\mathbf{D}_{\mathbf{y}}$ corresponds to $\mathbf{K}_{\mathbf{x}'}$, not $\mathbf{K}_{\mathbf{x}}$.

We have now two possible averaging kernel matrices

$$\mathbf{A}_{\mathbf{x}} = \frac{\partial \hat{\mathbf{x}}'}{\partial \mathbf{x}} = \frac{\partial \hat{\mathbf{x}}'}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \mathbf{D}_{\mathbf{y}} \mathbf{K}_{\mathbf{x}} \quad (1.21)$$

$$\mathbf{A}_{\mathbf{x}'} = \frac{\partial \hat{\mathbf{x}}'}{\partial \mathbf{x}'} = \frac{\partial \hat{\mathbf{x}}'}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{x}'} = \mathbf{D}_{\mathbf{y}} \mathbf{K}_{\mathbf{x}'} = \mathbf{A}_{\mathbf{x}} \mathbf{B} \quad (1.22)$$

where $\mathbf{A}_{\mathbf{x}} \in \mathbf{R}^{p \times n}$ and $\mathbf{A}_{\mathbf{x}'} \in \mathbf{R}^{p \times p}$, that is, only $\mathbf{A}_{\mathbf{x}'}$ is square. If $p > n$, $\mathbf{A}_{\mathbf{x}}$ gives more detailed information about the shape of the averaging kernels than the standard matrix ($\mathbf{A}_{\mathbf{x}'}$). If the retrieval grid used is coarse, it could be the case that $\mathbf{A}_{\mathbf{x}'}$ will not resolve all the oscillations of the averaging kernels, as shown in Eriksson [1999, Figure 11].

Chapter 2

Gas absorption

This chapter contains theoretical background and scientific details for gas absorption calculations in ARTS. A more practical overview, with focus on how to set up calculations, is given in *ARTS User Guide*, Chapter 4.

Gas absorption generally consists of a superposition of spectral lines and continua. Depending on the gas species, the continua either have a real physical meaning, or they are more or less empirical corrections for deficits in the explicit line-by-line calculation. In the latter case the magnitude of the continuum term will depend strongly on the exact setup of the line-by-line calculation. Combining continua and line-by-line calculation therefore requires expertise.

This chapter is structured in three main parts: Line absorption, continuum absorption, and complete absorption models. It should be noted that the three topics are tightly related. In particular, complete absorption models will normally include a line part and a continuum part. Some absorption models, notably those by Rosenkranz and Liebe will show up under both continua and complete absorption models. The continuum section then treats specifically the continuum parameterization of these model, the complete absorption model section puts more focus on the line part and the model as a whole.

2.1 Line absorption

2.1.1 Background

We will introduce here the main concepts concerning line absorption. The aim is to give some overview and show some key equations, not to give a full treatment of the theory. To really understand line absorption, you should refer to one of the cited books, or some other book on spectroscopy.

History

- 2011-07-05 Revised for ARTS2 by Stefan Buehler.
- 2001-11-21 Continuum absorption part written, Thomas Kuhn.
- 2001-10-05 Line absorption part written, Nikolay Koulev.

Basic expressions

An absorption line is described by the corresponding absorption coefficient as a function of frequency $\alpha(\nu)$, which can be written as [Goody and Yung, 1989]:

$$\alpha(\nu) = nS(T)F(\nu) \quad (2.1)$$

where $S(T)$ is called the line strength, T is the temperature, $F(\nu)$ is called the line shape function, and n is the number density of the absorber. The line shape function is normalized as:

$$\int F(\nu)d\nu = 1 \quad (2.2)$$

The values of $S(T)$ at reference temperature T_0 are contained in spectroscopic databases (more on this below). The conversion to different temperatures is done by

$$S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \frac{e^{-E_f/(kT)} - e^{-E_i/(kT)}}{e^{-E_f/(kT_0)} - e^{-E_i/(kT_0)}} \quad (2.3)$$

given the energies E_f and E_i of the two levels between which the transition occurs as well as the partition function $Q(T)$ [Rothman et al., 1998]. The databases contain the lower state energy E_l tabulated along with the S and the transition frequency ν , so that the upper state energy can be computed by $E_u = E_l + h\nu$. Partition functions for all molecular species are also available along with spectroscopic databases, either in the form of tabulated values for a set temperatures, or in the form of FORTRAN routines. One can obtain the total absorption coefficient by adding the absorption of all spectral lines of all molecular species.

The problem of describing the line shape function is discussed in the following subsection. Then another subsection discusses partition functions and their calculation.

Line shape functions

So far, there exists no complete analytical function that accurately describes the line shape in all atmospheric conditions and for all frequencies. But for most cases very accurate approximations are available. Which approximation is appropriate depends mostly on the atmospheric pressure, and on whether the frequencies of interest are close to the line center, or far out in the line wing.

There are three phenomena which contribute to the line shape. These are, in increasing order of importance, the finite lifetime of an excited state in an isolated molecule, the thermal movement of the gas molecules, and their collisions with each other. They result in corresponding effects to the line shape: natural broadening, Doppler, and pressure broadening. Of these, the first one is completely negligible compared to the other two for typical atmospheric conditions. Nevertheless, we will pay a special attention to the natural broadening because its implications are of a conceptual importance for the broadening processes.

The spectral line shape can be derived in the case of natural broadening from basic physical considerations and a well-known Fourier transform theorem from the time to the frequency domain [Thorne et al., 1999]. If we consider classically the spontaneous decay of the excited state of a two-level system in the absence of external radiation, then the population n of the upper level decreases according to

$$\frac{dn(t)}{dt} = -An(t) \quad (2.4)$$

where A is Einstein A coefficient. This equation can also be interpreted as the rate of the spontaneously emitted photons because of decay. The integral form of this relation is

$$n(t) = n(0) e^{-At} = n(0)e^{-t/\tau} \quad (2.5)$$

where τ is the mean lifetime of the excited state. Thus, the number of spontaneously emitted photons and in this way the flux of the emitted radiation then will be proportional to n . Therefore we can write for the flux L that

$$L(t) = L(0) e^{-t/\tau} = L(0) e^{-\gamma t} \quad (2.6)$$

By the afore mentioned theorem, multiplying in the time domain by $e^{-\gamma t}$ is equivalent to convolving in the frequency domain with a function $1/[\nu^2 - (\gamma/4\pi)^2]$. Accordingly, the line profile of a spectral line at frequency ν_0 as a normalized line shape function will be, as defined in *Thorne et al.* [1999],

$$F(\nu) = \frac{1}{\pi} \frac{\gamma/4\pi}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \quad (2.7)$$

This gives a bell-shaped profile and the function itself is called Lorentzian. The dependence on the position of the line is apparent through ν_0 , that is why some authors prefer to denote the function by $F(\nu, \nu_0)$. The result is important because of two major reasons. Firstly, without the natural broadening the line would be the delta function $\delta(\nu - \nu_0)$, as pointed out in *Bernath* [1995]. So the spontaneous decay of the excited state is responsible for the finite width and the certain shape of the line shape function. Secondly, the Lorentzian type of function comes significantly into play when explaining some of the other broadening effects or the complete picture of the broadened line [*Thorne et al.*, 1999].

The second effect, Doppler broadening, is important for the upper stratosphere and mesosphere for microwave frequencies. The line shape follows the velocity distribution of the particles. Under the conditions of thermodynamic equilibrium, we have a probability distribution for the relative velocity u between the gas molecule and the observer of Maxwell type

$$p(u) = \sqrt{\frac{m}{2\pi kT}} \exp \left[-\frac{mu^2}{2kT} \right] \quad (2.8)$$

where m is the mass of the molecule. Using then the formula for the Doppler shift for the non-relativistic region $\nu - \nu_0 = \nu_0 u / c$, one can easily derive the line shape function [*Bernath*, 1995],

$$F_D(\nu) = \frac{1}{\gamma_D \sqrt{\pi}} \exp \left[-\left(\frac{\nu - \nu_0}{\gamma_D} \right)^2 \right] \quad (2.9)$$

where the quantity γ_D is called Doppler line width and equals

$$\gamma_D = \frac{\nu}{c} \sqrt{\frac{2kT}{m}} \quad (2.10)$$

In contrast to the line shape function for the natural broadening, the Doppler broadening leads to a Gaussian line shape function $F(\nu)$. The Doppler line width γ_D is so defined that

it is equal to the half width at half of the maximum (HWWM) of the line shape function. A similar notation is used for all other width parameters γ_{xy} below.

The third broadening mechanism is pressure broadening. It is the most complicated broadening mechanism, and still subject to theoretical and experimental research. So far, there is no way to derive the exact shape of a pressure-broadened line from first principles, at least not for the far wing region. The various approximations, which are therefore used, are immanently limited to the certain line regions they deal with. The most popular among these approximations is the *impact approximation* which postulates that the duration of the collisions of the gas particles is very small compared to the average time between the collisions. Due to the Fourier-pair relationship between time and frequency, the line shape that follows from the impact approximation can only be expected to be accurate near the line center, not in the far wings of the line.

Lorentz was the first to achieve a result exploiting the impact approximation, the Lorentz line shape function:

$$F_L(\nu) = \frac{\gamma_L}{\pi} \frac{1}{(\nu - \nu_0)^2 + \gamma_L^2} \quad (2.11)$$

where γ_L is the Lorentz line width [*Thorne et al., 1999*]. As one can see, the result Eq. 2.11 is pretty similar to Eq. 2.7 but the specific line parameters γ and γ_L make them differ significantly in the corresponding frequency regions of interest. For atmospheric pressures γ_L is much greater and because of that, of experimental significance in contrast to γ .

Elaborating the model of Lorentz, van Vleck and Weisskopf made a correction to it [*Van Vleck and Weisskopf, 1945*], particularly for the microwave region:

$$F_{VW}(\nu) = \left(\frac{\nu}{\nu_0}\right)^2 \frac{\gamma_L}{\pi} \left[\frac{1}{(\nu - \nu_0)^2 + \gamma_L^2} + \frac{1}{(\nu + \nu_0)^2 + \gamma_L^2} \right] \quad (2.12)$$

which can be reduced to a Lorentzian for $(\nu - \nu_0) \ll \nu_0$ and $0 \ll \nu_0$. Except for the additional factor $(\nu/\nu_0)^2$, F_{VW} can be regarded as the sum of two F_L lines, one with its center frequency at ν_0 , the other at $-\nu_0$.

The van Vleck and Huber lineshape [*Van Vleck and Huber, 1977*] is similar to Eq. 2.12, except for the factor $(\nu/\nu_0)^2$ which is replaced by $(\nu * \tanh(h * \nu / (2kT))) / (\nu_0 * \tanh(h * \nu_0 / (2kT)))$, with k the Boltzmann constant, h the Planck constant, and T the atmospheric temperature (the denominator is actually a consequence of the line strength definition in the spectroscopic catalogs). The lineshape Eq. 2.12 with this factor can be used for the entire frequency range, since the microwave approximation: $\tanh(x) = x$, that leads to the factor $(\nu/\nu_0)^2$, is not made.

The combined picture of a simultaneously Doppler and pressure broadened line is the next step of the approximations development. The line shape function has to be approximated in this case by the Voigt line shape function

$$F_{Voigt}(\nu, \nu_0) = \int F_L(\nu, \nu') F_D(\nu', \nu_0) d\nu' \quad (2.13)$$

though there's no strict justification for its use - the two processes are assumed to act independently, which in reality is not the fact. Regardless of this flaw, it is the only way up to now to model the combination of the broadening processes. The integral in Eq. 2.13 can not be computed analytically, so certain approximation algorithms must be used.

Another possibility would be the combination of the last two equations Eq. 2.12 and Eq. 2.13. The respective result then will be

$$F_S = \left(\frac{\nu}{\nu_0}\right)^2 [F_{Voigt}(\nu, \nu_0) + F_{Voigt}(\nu, -\nu_0)] \quad (2.14)$$

The advantage of such a model is that it behaves like a van Vleck-Weisskopf line shape function in the high pressure limit and like a Voigt one in the low pressure limit. There is one important caveat to the equation Eq. 2.14: it has to be made sure that the algorithm that is used to compute the Voigt function really produces a Lorentz line in the high pressure limit. Another point of significance is the demand that the model yields meaningful results far from the line center, since the line center from the “mirror” line at $-\nu_0$ is situated approximately $2\nu_0$ away from the frequency ν_0 of computation. We explicitly verified that the algorithms of *Drayson* [1976], *Oliveiro and Longbothum* [1977], and *Kuntz and Höpfner* [1999] satisfy both requirements, while this was found to be not true for some other algorithms commonly used for Voigt-shape computation. In particular, it is not true for the Hui-Armstrong-Wray Formula, as defined in *Hui et al.* [1978] and in Equation 2.60 of *Rosenkranz* [1993]. Provided the condition above is fulfilled, the F_S line shape gives a smooth transition from high tropospheric pressures to low stratospheric ones, and should be valid near the line centers throughout the microwave region. With a Van Vleck / Huber forefactor instead of the Van Vleck / Weisskopf forefactor, it should be valid throughout the thermal infrared spectral range, but there the mirror line at negative frequency is negligible anyway, because it is so far away.

Partition functions

Partition functions are needed to compute the temperature dependence of line intensities (Equation 2.3 on page 6). They are related to the molecular energy states and their statistical distribution during the radiation process.

In any case of spectroscopic interest the free molecules of a gas are not optically thick at all frequencies, so the radiation energy is not represented by blackbody radiation. The most common assumption made, which is sufficient in the case of tropospheric and low stratospheric research, is the *local thermodynamic equilibrium* or *LTE*. According to it, it's possible to find a common temperature, which may vary from place to place, that fits the Boltzmann energy population distribution and the Maxwell velocities distribution. This practically means, that under *LTE* the collisional processes must be of greater importance than radiative ones. In other words, an excited state must have a higher probability of de-excitation by collision than by spontaneous radiation. This is the important factor which makes natural broadening differ quantitatively so much from the pressure (collisional) one, though both are described qualitatively almost identically by Lorentzian line shape functions.

According to the Maxwell-Boltzmann distribution law, in *LTE* the total number of gas particles N_n in a state E_n is given by

$$N_n = N_0 \frac{g_n}{g_0} e^{-E_n/kT} \quad (2.15)$$

where N_0 is particle number in the ground state, and g_n, g_0 are the statistical weights (degeneracies) of the n -state and the ground state [*Gordy and Cook*, 1970]. Thus the total

particle number N is given by

$$N = \frac{N_0}{g_0} \sum_{n=0}^{\infty} g_n e^{-E_n/kT} = \frac{N_0}{g_0} Q(T) \quad (2.16)$$

The quantity $Q(T)$ is the *partition function* of the gas, which generally speaking describes the energy states distribution of the gas particles.

The partition function for a perfect gas molecule can be represented by the product of the *translational* and the *internal* partition functions, as defined in *Herzberg* [1945],

$$Q = Q_{tr} Q_{int} \quad (2.17)$$

bearing in mind that the respective energies, translational and internal, are independent of each other. The first quantity Q_{tr} accounts for the distribution of the translational energy of the gas particles - it takes into account that the translational velocities of the particles fulfill the Maxwell distribution. The quantity, however, which we are interested in in (3.3) is the *internal* partition function (or the *total internal partition function* because the transitions between the discrete internal energy states are responsible for the absorption or emittance of radiation. Accordingly Q_{int} describes the distribution of energy among the internal energy states of the gas particles.

The internal partition function for free gaseous molecules is a function of the electronic, the vibrational, the rotational, and the nuclear spin states. An approximation is used in *Gordy and Cook* [1970] in order to display the individual contributions explicitly

$$Q_{int} = Q_e Q_v Q_r Q_n \quad (2.18)$$

and thus the interaction between these various states is neglected. For practically all polyatomic molecules the excited electronic states are entirely negligible to those of the ground states, i.e. $Q_e = 1$. Only for the very few polyatomic molecules with a multiplet ground state (NO_2 , ClO_2 , and free radicals) the electronic contribution has to be considered.

If we neglect the anharmonicities, the vibrational partition function, with vibrational energy levels measured with respect to the ground state for the *harmonic oscillator*, is according to *Herzberg* [1945]

$$Q_v = \left(\sum_{\nu_1} e^{-\nu_1 h \omega_1 / kT} \right) \left(\sum_{\nu_2} e^{-\nu_2 h \omega_2 / kT} \right) \dots \quad (2.19)$$

where ν_1, ν_2, \dots , the vibrational quantum numbers, can each have the values 0,1,2,... and $\omega_1, \omega_2, \dots$ are the frequencies of the fundamental modes of vibration. The summation is taken over all values of ν_1, ν_2, \dots , and each fundamental mode is counted separately. This result is valid for non-degenerate vibrations. If we use the simple expression for geometric progression

$$\sum_{\nu_i} e^{-\nu_i h \omega_i / kT} = \frac{1}{1 - e^{h \omega_i / kT}} \quad (2.20)$$

and the degeneracies d_1, d_2, \dots of the fundamental modes, we get finally for the vibrational partition function

$$Q_v = \left(1 - e^{h \omega_1 / kT} \right)^{-d_1} \left(1 - e^{h \omega_2 / kT} \right)^{-d_2} \dots \quad (2.21)$$

The rotational partition function looks differently for the different symmetry types of molecules. For diatomic and linear polyatomic molecules with no center of symmetry the corresponding expression is, as defined in *Gordy and Cook* [1970]

$$\begin{aligned} Q_r &= \sum_{J=0}^{\infty} (2J+1) e^{-hBJ(J+1)/kT} \\ &= \frac{kT}{hB} + \frac{1}{3} + \frac{1}{15} \frac{hB}{kT} + \frac{4}{315} \left(\frac{hB}{kT} \right)^2 + \dots \\ &\cong \frac{kT}{hB} \end{aligned} \quad (2.22)$$

For *rigid symmetric*-, *asymmetric*-, and *spherical* top molecules there are also other factors to be taken into consideration, such as the spatial structure of the molecules, nuclear spin, inversion and internal rotation. The general expression in the case of a *rigid symmetric*- top molecule according to *Herzberg* [1945] is

$$Q_r = \frac{1}{\sigma} \sum_{J=0}^{\infty} \sum_{K=-J}^J (2J+1) e^{-h[BJ(J+1)+(A-B)K^2]/kT} \quad (2.23)$$

where σ is a measure of the degree of symmetry. The usual symmetric top has C_3 or $C_{3\nu}$ symmetry, therefore $\sigma = 3$. To a good approximation, the summation above can be expressed as in *Gordy and Cook* [1970]

$$Q_r = \frac{1}{\sigma} \left[\left(\frac{\pi}{B^2 A} \right) \left(\frac{kT}{h} \right)^3 \right]^{1/2} = \frac{5.34 \times 10^6}{\sigma} \left(\frac{T^3}{B^2 A} \right)^{1/2} \quad (2.24)$$

For an *asymmetric* top the formula would then be

$$Q_r = \frac{5.34 \times 10^6}{\sigma} \left(\frac{T^3}{ABC} \right)^{1/2} \quad (2.25)$$

and for a *spherical* top, using the current notation of *Gordy and Cook* [1970] in the respective expression in *Herzberg* [1945],

$$Q_r = \frac{5.34 \times 10^6}{\sigma} \left(\frac{T^3}{A^3} \right)^{1/2} \quad (2.26)$$

2.1.2 Spectral-line-specific data and line catalogues

ARTS has an internal representation of spectral line data that maps naturally to a native catalogue format, which we will discuss below. But ARTS can read also several other catalogue formats, in particular HITRAN and JPL format. If these other catalogues are used, line data are converted to the internal representation during reading. In other words, all unit conversions are done by the reading routines.

The ARTS internal spectral line data files contain an XML header and footer, and between them one entry for each spectral line. Each entry starts with with an '@' character. It then contains the different line parameters, separated by one or more blank characters. Scientific notation is allowed, e.g. 501.12345e9.

In contrast to other catalogues that are optimized for processing with programs written in the FORTRAN language, ARTS does not use fixed column widths. The advantage of this is that the precision of the parameters is not limited by the format.

The first column of each entry contains the species and isotope, following the naming scheme described below. Note that the intensity is per molecule, i.e., it does not contain the isotopic ratio. This is similar to JPL, but different to HITRAN. The line format is:

Col	Variable	Label	Unit
0	'@'	ENTRY	-
1	name	NAME	-
2	center frequency	F	Hz
3	pressure shift of F	PSF	Hz/Pa
4	line intensity per molecule	I0	m ² /Hz
5	reference temp. for I0	T_I0	K
6	lower state energy	ELOW	J
7	air broadened width	AGAM	Hz/Pa
8	self broadened width	SGAM	Hz/Pa
9	AGAM temp. exponent	NAIR	-
10	SGAM temp. exponent	NSELF	-
11	ref. temp. for AGAM, SGAM	T_GAM	K
12	number of aux. parameters	N_AUX	-
13	auxiliary parameter	AUX1	-
14	...		
15	error for F	DF	Hz
16	error for I0	DI0	%
17	error for AGAM	DAGAM	%
18	error for SGAM	DSGAM	%
19	error for NAIR	DNAIR	%
20	error for NSELF	DNSELF	%
21	error for PSF	DPSF	%

The parameters 0-12 must be present, the others can be missing, since they are not needed for the calculation. For the error fields (15-21), a -1 means that no value exists.

Some species may need special parameters that are not needed by other species (for example overlap coefficients for O₂). In the case of oxygen two parameters are sufficient to describe the overlap, but other species, e.g., methane, may need more coefficients. The default for N_AUX is zero. In that case, no further AUX fields are present.

2.1.3 Species-specific data

A line absorption species in ARTS is a particular isotopologue of a particular molecule. Quantities such as the molecular mass and the isotopic ratio are specific and constant for each species. Here is a list of all species-specific information that is needed:

- Molecule name
- Isotope name

- Isotopic ratio
- Molecular mass
- Corresponding tag in different catalogues (MYTRAN, HITRAN, JPL)
- Partition function data

These data are currently stored in two source code files, `species_data.cc` and `partition_function_data.cc`. It is planned to change this in the not too far future, at least for the isotopic ratios, in order to allow calculations for other planets. The data will then be read from include files instead.

Buehler et al. [2005] contains an explicit list of species that were implemented at the time of writing and their data. We do not have such a list here, because it is too hard to maintain. Currently, the best is to look directly in file `species_data.cc`. The different data sources are also documented there.

Partition function data

ARTS uses third order polynomials to approximate partition functions, so four polynomial coefficients have to be stored for each isotopic species. These data can be found in file `partition_function_data.cc`. The file also contains documentation, including the source of the data for the different species.

The consistency of partition function data from different sources, and the impact of partition function errors on sub-millimeter wave limb sounder retrievals, was studied in detail in *Verdes et al. [2005]*. The partition function data collection in ARTS is based on that study.

The data are from three different sources:

TIPS_2003: Default.

JPL: Only Species (including individual isotopes) not covered by TIPS_2003.

Agnes Perrin: Personal communication, only species BrO.

In most cases, we calculated the coefficients using TIPS_2003, provided by B. Gamache. The program was obtained from the ‘Software and Data’ section of the web page http://faculty.uml.edu/robert_gamache/. It includes the data for all molecular species found in the 2000 HITRAN database.

The coefficients for the few species which are not covered in TIPS_2003 were calculated from JPL values. The JPL catalogue has a different way to calculate the partition function, it gives the partition function at specific temperatures: 300, 225, 150, 75, 37.5, 18.75, 9.375 K and an interpolation scheme is given for values inbetween. The partition functions are proportional to temperature $T^{1.5}$ for non-linear molecules (degrees of freedom: 3) and proportional to T for linear molecules (degrees of freedom 2).

The partition function data for BrO were provided by Agnes Perrin, Orsay, France.

2.2 Continuum absorption

As pointed out above, some molecules show beside the resonant line absorption also non-resonant continuum absorption. The main qualitative difference is the smooth dependence on frequency of the non-resonant absorption part in contrast to the resonant absorption part who shows strong local maxima and minima.

The implemented continuum absorption modules are connected with water vapor (H_2O), oxygen (O_2), nitrogen (N_2), and carbon dioxide (CO_2). Since these molecules have various permanent electric or magnetic multipoles, the physical explanations for the continuum absorption is different for each of these molecules.

Water Vapor has a strong electric dipole moment and posses therefore a wealth of rotational transitions in the microwave up to the submillimeter range. One explanation for the H_2O -continuum absorption is the inadequate formulation of the far wings of a spectral line, since the usually employed *Van Vleck and Weisskopf* [1945] line shape is according to its derivation only valid in the near wing zone. Other explanations are (see *Rosenkranz* [1993] for details) far wing contribution from far-infrared water vapor lines, collision induced absorption (CIA), and water polymer absorption. At present one can not definitively decide which of these possibilities is the correct one, probably all of them play a more or less important role, depending on the frequency range.

Oxygen is special, because it has no permanent electric dipole moment, but a permanent magnetic dipole moment. The aligned spins of the two valence electrons gives a $^3\Sigma$ ground state of molecular oxygen. Due to the selection rules for magnetic dipole transitions, transitions with resonance frequency equal to zero are allowed. Such transitions have a characteristic Debye line shape function.

The homonuclear nitrogen molecule has in lowest order an electric quadrupole moment of modest magnitude. For the frequency range below 1 THz the collision induced rotation absorption band [*Goody and Yung*, 1989] is of most importance. The band center is around 3 THz and at 1 THz the band strength is approximately 1/6 of the maximum value (see Figure 5.2 of *Goody and Yung* [1989]). The electric field of the quadrupole moment of one molecule induces a dipole moment in the second molecule. This allows rotational transitions according to the electric quadrupole selection rules, $|\Delta J| = 0, 2$ (see *Rosenkranz* [1993] for details).

In a similar way, carbon dioxide also exhibits a collision induced absorption band (maximum around 1.5 THz, Figure 5.10 of *Goody and Yung* [1989]). Characteristic for collision induced absorption is the dependency on the square of the molecular density.

2.2.1 Water vapor continuum models

As shown by *Liebe and Layton* [1987], *Rosenkranz* [1998], and *Ma and Tipping* [1990], the water vapor continuum absorption can be well described by

$$\alpha_c = \nu^2 \cdot \Theta^3 \cdot (C_{\text{H}_2\text{O}}^0 \cdot P_{\text{H}_2\text{O}}^2 \cdot \Theta^{\text{ns}} + C_{\text{d}}^0 \cdot P_{\text{H}_2\text{O}} \cdot P_{\text{d}} \cdot \Theta^{\text{nf}}) \quad (2.27)$$

where the microwave approximation ($h\nu \ll k_B T$) of the radiation field term is already applied. The adjustment of Eq. 2.27 to the data is performed through the parameter set $C_{\text{H}_2\text{O}}^0$, n_s , C_{d}^0 , and n_f . Table 2.1 gives some commonly used continuum parameter sets.

model	$C_{\text{H}_2\text{O}}^{\text{O}}$ [$\frac{\text{dB/km}}{\text{hPa}^2 \cdot \text{GHz}^2}$]	n_s [1]	C_d^{O} [$\frac{\text{dB/km}}{\text{hPa}^2 \cdot \text{GHz}^2}$]	n_d [1]	ref.
MPM87	$6.50 \cdot 10^{-8}$	7.5	$0.206 \cdot 10^{-8}$	0.0	<i>Liebe and Layton [1987]</i>
MPM89	$6.50 \cdot 10^{-8}$	7.3	$0.206 \cdot 10^{-8}$	0.0	<i>Liebe [1989]</i>
CP98	$8.04 \cdot 10^{-8}$	7.5	$0.254 \cdot 10^{-8}$	0.0	<i>Cruz Pol et al. [1998]</i>
PWR98	$7.80 \cdot 10^{-8}$	4.5	$0.236 \cdot 10^{-8}$	0.0	<i>Rosenkranz [1998]</i>
MPM93*	$7.73 \cdot 10^{-8}$	4.55	$0.253 \cdot 10^{-8}$	1.55	<i>Liebe et al. [1993]</i>

Table 2.1: Values of commonly used continuum parameter sets. The last line (MPM93*) represents an approximation of the pseudo-line continuum of MPM93 in the form of Eq. 2.27.

The MPM93 continuum parameterization

In the MPM93 model [*Liebe et al., 1993*], the water vapor continuum is treated as a pseudo-line located in the far infrared around 2 THz. The pseudo-line continuum has therefore not four but seven parameters, the pseudo-line center frequency (ν^*) and the six pseudo-line parameters (b_1^*, \dots, b_6^*):

$$\alpha_c^{\text{MPM93}} = 0.1820 \cdot \frac{b_1^*}{\nu^*} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{3.5} \cdot \exp(b_2^* \cdot (1 - \Theta)) \cdot \nu^2 \cdot F_c(\nu, \nu_k) \quad (2.28)$$

$$F_c(\nu, \nu_k) = \left[\frac{\gamma_c}{(\nu^* + \nu)^2 + \gamma_c^2} + \frac{\gamma_c}{(\nu^* - \nu)^2 + \gamma_c^2} \right] \quad (2.29)$$

$$\gamma_c = b_3^* \cdot (b_4^* \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{b_6^*} + P_d \cdot \Theta^{b_5^*}) \quad (2.30)$$

Table 2.2 lists the values of this continuum parameter set. It is remarkable that all these parameters are much larger compared to the physical water vapor line parameters of the same model. The only exception is b_2^* , the parameter which governs the exponential temperature behavior of the line strength. The magnitude of the pseudo-line width is shown for four

ν^* [GHz]	b_1^* [$\frac{\text{kHz}}{\text{hPa}}$]	b_2^* [1]	b_3^* [$\frac{\text{MHz}}{\text{hPa}}$]	b_4^* [1]	b_5^* [1]	b_6^* [1]
1780.000	2230.000	0.952	17.620	30.50	2.00	5.00

Table 2.2: List of the MPM93 pseudo-line water vapor continuum parameters.

different cases in Table 2.3.

This change of continuum parameterization makes it difficult to compare MPM93 with the models which use Eq. (2.27). However, with respect to microwave frequencies, the line shape function, $F_c(\nu)$, can be approximated since the magnitude of the pseudo-line width is much smaller compared to the distance between microwave frequencies and ν^* , as shown for four different cases in Table 2.3:

$$F_c(\nu, \nu_k) \approx 2 \cdot \frac{\gamma_c}{\nu_c^2} \quad (2.31)$$

	contribution		total
	H ₂ O–H ₂ O	H ₂ O–air	
$\gamma_c(200\text{ K})$	40.8 GHz	80.4 GHz	121.2 GHz
$\gamma_c(300\text{ K})$	5.4 GHz	23.0 GHz	28.4 GHz

Table 2.3: Magnitude of the line width of the pseudo-line of the continuum term in MPM93. Assumed is a total pressure of 1000 hPa and a water vapor partial pressure of 10 hPa.

Inserting Eq. (2.31) into Eq. (2.28) gives a quadratic frequency dependence of the MPM93 continuum, similar to the continuum parameterization expressed in Eq. (2.27). By additionally approximating the temperature dependence to the simple form

$$\begin{aligned}
 n_s \cdot \ln(\Theta) &= \ln\left(\Theta^{3.5} \cdot e^{b_2^* \cdot (1-\Theta)}\right) \\
 n_s &= 3.5 + b_2^* \cdot \frac{1-\Theta}{\ln(\Theta)} \\
 n_s &\approx 3.5 - b_2^* = 2.55 \quad \text{with } \ln(\Theta) \approx (\Theta - 1) \quad (2.32)
 \end{aligned}$$

one can rearrange the pseudo-line continuum to fit Eq. (2.27) (denoted by MPM93*). The so deduced continuum parameter set is given in Table 2.1.

The MPM93* continuum parameters $C_{\text{H}_2\text{O}}^{\text{O}}$ and C_{d}^{O} are 20 % and 15 % larger, respectively, than in the case of MPM87/MPM89. Large discrepancies exist for the temperature exponents n_s and n_d between MPM93* and earlier model versions. The exponent n_s is in MPM93* only 60 % of the corresponding value in MPM89 and the temperature dependence of the H₂O-air term is significant larger than for earlier MPM versions. This reduction of n_s is mainly due to additional measurements considered in MPM93 [Becker and Autler, 1946; Godon et al., 1992], while the continuum parameters in MPM87/MPM89 are determined by a single laboratory measurement at 138 GHz.

2.2.2 Oxygen continuum absorption

As pointed out by Van Vleck [1987], the standard theory for non-resonant absorption is that of Debye (see also Townes and Schawlow [1955]). The Debye line shape is obtained from the VVW line shape function by the limiting case $\nu_k \rightarrow 0$. Both, Liebe et al. [1993] and Rosenkranz [1993] adopted the Debye theory for their models. The only difference is the formulation of the line broadening, where the influence of water vapor is treated slightly different:

$$\alpha_c = C \cdot P_d \cdot \Theta^2 \cdot \frac{\nu^2 \cdot \gamma}{\nu^2 + \gamma^2} \quad (2.33)$$

$$\gamma = w \cdot (P_d \cdot \Theta^{0.8} + 1.1 \cdot P_{\text{H}_2\text{O}} \cdot \Theta) \quad : \text{ Rosenkranz} \quad (2.34)$$

$$\gamma = w \cdot P_{\text{tot}} \cdot \Theta^{0.8} \quad : \text{ MPM93} \quad (2.35)$$

where P_d denotes the dry air partial pressure ($P_d = P_{\text{tot}} - P_{\text{H}_2\text{O}}$). The value for the strength is $C = 2.56 \cdot 10^{-20} \text{ 1/(m Pa Hz)}$ in the case of the Rosenkranz model and

$C = 2.57 \cdot 10^{-20}$ 1/(m Pa Hz) in the case of the MPM93 model. The MPM93 value for C is therefore about 0.4 % larger than in the Rosenkranz model. Since the volume mixing ratio of oxygen in dry air is constant in the lower Earth atmosphere (0.20946 [Goody, 1995]), both models incorporate the oxygen VMR (VMR_{O_2}) in the constant C . In the arts model the separation between the oxygen VMR and the constant C is explicitly done. In this case follows:

$$C = 0.20946 \cdot \hat{C} \quad (2.36)$$

$$\hat{C} = 1.22 \cdot 10^{-19} [1/(\text{m Hz Pa})] \quad : \text{Rosenkranz} \quad (2.37)$$

$$\hat{C} = 1.23 \cdot 10^{-19} [1/(\text{m Hz Pa})] \quad : \text{MPM93} \quad (2.38)$$

The width parameter w is in both models the same, $w = 5.6 \cdot 10^3$ Hz/Pa. If we define the width γ in a more general way like

$$\gamma = w \cdot (A \cdot P_d \cdot \Theta^{n_d} + B \cdot P_{H_2O} \cdot \Theta^{n_w}) \quad (2.39)$$

we can fit both models, the Rosenkranz and the MPM93 model, into the same parameterization with ($A = 1$, $B = 1.1$, $n_d = 0.8$, $n_w = 1.0$) for the Rosenkranz model and ($A = 1.0$, $B = 1.0$, $n_d = 0.8$, $n_w = 0.8$) for MPM93.

The oxygen continuum absorption term is proportional to the collision frequency of a single oxygen molecule with other air molecules and thus proportional to the dry air pressure¹.

2.2.3 Nitrogen continuum absorption

Since molecular nitrogen has in its unperturbed state no electric or magnetic dipole moment (but an electric quadrupole moment), it shows no rotational spectral signature in the microwave region. Regardless of this, nitrogen absorbs radiation in this frequency range due to collision induced absorption (CIA). Far-infrared roto-translational band structures from free-free interactions give rise to far wing absorption below 1 THz.

Different parameterizations of this absorption term for the frequency range below 1 THz are available Rosenkranz [1993]; Liebe *et al.* [1993]; Borysow and Frommhold [1986]. Common to all these models is the quadratic dependency on N_2 partial pressure which is a direct consequence of the underlying CIA processes involved. The simplest model is given by Rosenkranz [1993], which uses the same parameterization as for the water vapor continuum, described in Equation 2.27:

$$\alpha_c = C \cdot \nu^{n_\nu} \cdot \Theta^{n_T} \cdot P_{N_2}^{n_p} \quad (2.40)$$

with $C = 4.56 \cdot 10^{-13}$ dB/(km hPa² GHz²), $n_\nu = 2$, $n_T = 3.55$, and $n_p = 2$, respectively. The laboratory data set for the determination of C is mainly from Dagg *et al.* [1975, 1978] around 70 and 140 GHz, respectively.

The MPM models has compared with Equation 2.40 an additional frequency dependent term which leads to the following expression

$$\alpha_c = \hat{C} \cdot (1.0 - 1.2 \cdot 10^{-5} \cdot \nu^{1.5}) \cdot \nu^2 \cdot \Theta^{3.5} \cdot P_d^2 \quad : \text{MPM89} \quad (2.41)$$

¹The absorption due to weakly bound complexes of O_2 - X with $X = H_2O$, N_2 is treated separately and therefore not included in this Debye formula.

$$\alpha_c = \hat{C} \cdot \frac{\nu^2}{(1.0 + a \cdot \nu^{n_\nu})} \cdot \Theta^{3.5} \cdot P_d^2 \quad : \text{MPM93} \quad (2.42)$$

$$a =$$

where the parameter is $\hat{C} = 2.55 \cdot 10^{-13}$ dB/(km hPa² GHz²), $a = 1.9 \cdot 10^{-5}$ GHz^{- n_ν} , and $n_\nu = 1.5$. based on data from *Stankevich* [1974] and *Stone et al.* [1984]. With respect to the 22 GHz water vapor line, the additional frequency terms in brackets in Equations 2.41 and 2.42 are nearly unity and therefore not essential. Therefore all three parameterizations have the same frequency and temperature relationship, but the absolute magnitude is in the case of Rosenkranz 80 % higher compared with the MPM models.

The model of Borysow and Frommhold² is somewhat different since their focus is mainly on the radiative transfer in the Titan's atmosphere with the infrared interferometer spectrometer, IRIS, on board the Voyager Spacecraft. This detailed model is primarily designed to parameterize each of the roto-translational spectral lines around 200 cm⁻¹ (\approx 6 THz) accurately. The analyzed data set incorporate the data source used by the Rosenkranz but is largely extended with measurements in the far-infrared.

2.2.4 Carbon dioxide continuum absorption

Rosenkranz [1993] gives a similar parameterization for the CO₂-continuum absorption term as for the nitrogen continuum, with

$$\alpha_c = \nu^2 \cdot \left[C_s \cdot P_{\text{CO}_2}^2 \cdot \Theta^{n_s} + C_f \cdot P_{\text{CO}_2} \cdot P_{\text{N}_2} \cdot \Theta^{n_f} \right] \quad (2.43)$$

where the parameter values $C_s = 3.23 \cdot 10^{-11}$ dB/(km hPa² GHz²), $C_f = 1.18 \cdot 10^{-11}$ dB/(km hPa² GHz²), $n_s = 5.08$, and $n_f = 4.7$, respectively, are determined from laboratory measurements of *Ho et al.* [1966]; *Dagg et al.* [1975]. Since the foreign term includes only nitrogen as perturber, one can get an estimate for dry air by replacing P_{N_2} by the dry air partial pressure in Equation 2.43. Because nitrogen is usually a more efficient perturber than oxygen, this estimation can be regarded as an upper limit. Concerning the Earth's atmosphere, the foreign broadening term is more interesting since the carbon dioxide partial pressure is only approximately 0.04 % of the nitrogen partial pressure up to 90 km.

2.3 Complete absorption models

The MPM absorption model of Liebe and coworkers consists of modules for water vapor and oxygen absorption. The Rosenkranz (PWR98) absorption model include also H₂O and O₂ while the Cruz-Pol et al. (CP98) absorption models include absorption due to water vapor. Additionally the CP98 model has a strongly reduced parameter set for the H₂O-line absorption since it is especially intended for the range around the 22 GHz water line. The MPM and R98 are valid from the microwave up to the submillimeter frequency range (1-1000 GHz).

Implemented in ARTS are the following modules of the above mentioned models:

²the source code of this model can be downloaded from the home page of A. Borysow:
<http://www.astro.ku.dk/~aborysow/>

species	model
H ₂ O	MPM87, MPM89, MPM93, PWR98, CP98
O ₂	MPM93, PWR98

2.3.1 Complete water vapor models

In ARTS several complete water vapor absorption models are implemented and can easily be used. Implemented models are the versions MPM87 [*Liebe and Layton, 1987*], MPM89 [*Liebe, 1989*], and MPM93 [*Liebe et al., 1993*] of the Liebe Millimeter-wave Propagation Model and additionally the models of Cruz-Pol et al. (CP98) [*Cruz Pol et al., 1998*] and P. W. Rosenkranz (PWR98) [*Rosenkranz, 1998*]. MPM and PWR98 are especially designed for fast absorption calculations in the frequency range of 1-1000 GHz while the CP98 model is a reduced model for a narrow frequency band around the 22 GHz H₂O-line (especially used by ground-based radiometers).

The total water vapor absorption (α_{tot}) is in all the stated models described by a line absorption (α_{ℓ}) term and a continuum absorption (α_{c}) term:

$$\alpha_{\text{tot}} = \alpha_{\ell} + \alpha_{\text{c}} \quad (2.44)$$

The main differences between the different models is the line shape used for α_{ℓ} and the formulation of α_{c} .

It has to be emphasized that, α_{ℓ} and α_{c} of different models are not necessarily compatible and should therefore not be interchanged between different models.

MPM87 water vapor absorption model

This version, which is described in *Liebe and Layton [1987]* and follows the general line of the MPM model to divide the total water vapor absorption, $\alpha_{\text{tot}}^{\text{MPM87}}$, into a spectral line term, $\alpha_{\ell}^{\text{MPM87}}$, and a continuum term not attributed to spectral lines, $\alpha_{\text{c}}^{\text{MPM87}}$:

$$\alpha_{\text{tot}}^{\text{MPM87}} = \alpha_{\ell}^{\text{MPM87}} + \alpha_{\text{c}}^{\text{MPM87}} \quad \text{dB/km} \quad (2.45)$$

Water vapor line absorption: The MPM87 [*Liebe and Layton, 1987*] water vapor line catalog consists of 30 lines from 22 GHz up to 988 GHz. The center frequencies and parameter values are listed in Table 2.4. To describe the line absorption, a set of three parameters ($b_{1,k}$ and $b_{3,k}$) per line are used: two for the line strength and one for the line width. The total line absorption coefficient (in units of dB/km) is the sum over all individual line absorption coefficients³:

$$\alpha_{\ell}^{\text{MPM87}} = 0.1820 \cdot \nu_k \cdot P_{\text{H}_2\text{O}} \cdot \sum_k S_k(T) \cdot F(\nu, \nu_k) \quad \text{dB/km} \quad (2.46)$$

where $S_k(T)$ is the line intensity described by the parameterization

$$S_k(T) = b_{1,k} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{3.5} \cdot \exp(b_{2,k} \cdot [1 - \Theta]) \quad \text{kHz} \quad (2.47)$$

³The factor $0.1820 \cdot 10^6$ is equal to $(4\pi/c) \cdot 10 \log(e)$ (the term $(4\pi/c)$ comes from the definition of the absorption coefficient in terms of the dielectric constant and the term $10 \log(e)$ is due to the definition of the Decibel.) The velocity of light is defined as $c = 2.9979 \cdot 10^{-4}$ km GHz. The factor 10^6 is incorporated into the line strength and does therefore not appear in the pre-factor.

with ν_k as the line center frequency, $P_{\text{H}_2\text{O}}$ the water vapor partial pressure and $\Theta = 300 \text{ K}/T$.

The line shape function, $F(\nu, \nu_k)$, in Eq. (2.46) is the standard Van Vleck-Weisskopf (VW) function, given by:

$$F(\nu, \nu_k) = \left(\frac{\nu}{\nu_k} \right) \cdot \left[\frac{\gamma_k}{(\nu - \nu_k)^2 + \gamma_k^2} + \frac{\gamma_k}{(\nu + \nu_k)^2 + \gamma_k^2} \right] \quad (2.48)$$

$$(2.49)$$

The pressure broadened line width, γ_k , is calculated with the single parameter $b_{3,k}$ in the following way:

$$\gamma_k = b_{3,k} \cdot (4.80 \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{1.1} + P_d \cdot \Theta^{0.6}) \quad \text{GHz} \quad (2.50)$$

where P_d is the partial pressure of dry air ($P_d = P_{\text{tot}} - P_{\text{H}_2\text{O}}$). The parameterizations of $S_k(T)$ and γ_k are already in use for the early version of MPM81 [Liebe, 1981].

k	ν_k [GHz]	$b_{1,k}$ [$\frac{\text{kHz}}{\text{kPa}}$]	$b_{2,k}$ [1]	$b_{3,k}$ [$\frac{\text{GHz}}{\text{kPa}}$]
1	22.235080	0.1090	2.143	$27.84 \cdot 10^{-3}$
2	67.813960	0.0011	8.730	$27.60 \cdot 10^{-3}$
3	119.995940	0.0007	8.347	$27.00 \cdot 10^{-3}$
4	183.310117	2.3000	0.653	$31.64 \cdot 10^{-3}$
5	321.225644	0.0464	6.156	$21.40 \cdot 10^{-3}$
6	325.152919	1.5400	1.515	$29.70 \cdot 10^{-3}$
7	336.187000	0.0010	9.802	$26.50 \cdot 10^{-3}$
8	380.197372	11.9000	1.018	$30.36 \cdot 10^{-3}$
9	390.134508	0.0044	7.318	$19.00 \cdot 10^{-3}$
10	437.346667	0.0637	5.015	$13.70 \cdot 10^{-3}$
11	439.150812	0.9210	3.561	$16.40 \cdot 10^{-3}$
12	443.018295	0.1940	5.015	$14.40 \cdot 10^{-3}$
13	448.001075	10.6000	1.370	$23.80 \cdot 10^{-3}$
14	470.888947	0.3300	3.561	$18.20 \cdot 10^{-3}$
15	474.689127	1.2800	2.342	$19.80 \cdot 10^{-3}$
16	488.491133	0.2530	2.814	$24.90 \cdot 10^{-3}$
17	503.568532	0.0374	6.693	$11.50 \cdot 10^{-3}$
18	504.482692	0.0125	6.693	$11.90 \cdot 10^{-3}$
19	556.936002	510.0000	0.114	$30.00 \cdot 10^{-3}$
20	620.700807	5.0900	2.150	$22.30 \cdot 10^{-3}$
21	658.006500	0.2740	7.767	$30.00 \cdot 10^{-3}$
22	752.033227	250.0000	0.336	$28.60 \cdot 10^{-3}$
23	841.073593	0.0130	8.113	$14.10 \cdot 10^{-3}$
24	859.865000	0.1330	7.989	$28.60 \cdot 10^{-3}$
25	899.407000	0.0550	7.845	$28.60 \cdot 10^{-3}$
26	902.555000	0.0380	8.360	$26.40 \cdot 10^{-3}$
27	906.205524	0.1830	5.039	$23.40 \cdot 10^{-3}$
28	916.171582	8.5600	1.369	$25.30 \cdot 10^{-3}$

Table 2.4: (continued on next page)

k	ν_k	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$
29	970.315022	9.1600	1.842	$24.00 \cdot 10^{-3}$
30	987.926764	138.0000	0.178	$28.60 \cdot 10^{-3}$

Table 2.4: List of H₂O spectral lines and their spectroscopic parameters (H₂O-air mixture) for the MPM87 model [*Liebe and Layton, 1987*].

Water vapor continuum absorption: The water vapor continuum absorption coefficient in MPM87, α_c^{MPM87} , is determined from laboratory measurements at 137.8 GHz by Liebe and Layton covering the following parameter range:

temperature 282-316 K
relative humidity 0-95 %
dry air pressure 0 - 160 kPa

The mathematical expression of α_c^{MPM87} is derived from the far wing approximation of the line absorption and is expressed as follows

$$\alpha_c^{\text{MPM87}} = \nu^2 \cdot P_{\text{H}_2\text{O}} \cdot (C_{\text{H}_2\text{O}}^{\text{O}} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{n_s} + C_{\text{d}}^{\text{O}} \cdot P_{\text{d}} \cdot \Theta^{n_f}), \quad (2.51)$$

with the continuum parameter set $C_{\text{H}_2\text{O}}^{\text{O}}$, C_{d}^{O} , n_s , and n_f . The determined values of the continuum parameters are:

$$C_{\text{H}_2\text{O}}^{\text{O}} = 6.496 \cdot 10^{-6} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_s = 10.5$$

$$C_{\text{d}}^{\text{O}} = 0.206 \cdot 10^{-6} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_d = 3.0$$

MPM89 water vapor absorption model

MPM89 is described in *Liebe [1989]* and follows the general line of the MPM model to divide the total water vapor absorption, $\alpha_{\text{tot}}^{\text{MPM89}}$, into a spectral line term, $\alpha_{\ell}^{\text{MPM89}}$, and a continuum term not attributed to spectral lines, α_c^{MPM89} :

$$\alpha_{\text{tot}}^{\text{MPM89}} = \alpha_{\ell}^{\text{MPM89}} + \alpha_c^{\text{MPM89}} \quad \text{dB/km} \quad (2.52)$$

All the absorption coefficients are calculated in units of dB/km.

Water vapor line absorption: The MPM89 water vapor line catalog consists of the same 30 lines like MPM87 from 22 GHz up to 988 GHz. The center frequencies and parameter values are listed in Table 2.5. To describe the line absorption, a set of six parameters ($b_{1,k}$ and $b_{6,k}$) per line are used: two for the line strength and four for the line width. The total line absorption coefficient (in units of dB/km) is the sum over all individual line absorption coefficients⁴:

$$\alpha_{\ell}^{\text{MPM89}} = 0.1820 \cdot \nu_k \cdot P_{\text{H}_2\text{O}} \cdot \sum_k S_k(T) \cdot F(\nu, \nu_k) \quad \text{dB/km} \quad (2.53)$$

⁴see footnote for MPM97 line absorption

where $S_k(T)$ is the line intensity described by the parameterization

$$S_k(T) = b_{1,k} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{3.5} \cdot \exp(b_{2,k} \cdot [1 - \Theta]) \quad \text{kHz} \quad (2.54)$$

with ν_k as the line center frequency, $P_{\text{H}_2\text{O}}$ the water vapor partial pressure and $\Theta = 300 \text{ K}/T$.

The line shape function, $F(\nu, \nu_k)$, in Eq. (2.53) is the standard Van Vleck-Weisskopf (VW) function, given by

$$F(\nu, \nu_k) = \left(\frac{\nu}{\nu_k} \right) \cdot \left[\frac{\gamma_k}{(\nu - \nu_k)^2 + \gamma_k^2} + \frac{\gamma_k}{(\nu + \nu_k)^2 + \gamma_k^2} \right] \quad (2.55)$$

where the pressure broadened line width, γ_k , is calculated as

$$\gamma_k = b_{3,k} \cdot (b_{5,k} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{b_{6,k}} + P_d \cdot \Theta^{b_{4,k}}) \cdot 10^{-3} \quad \text{GHz} \quad (2.56)$$

with $P_d = P_{\text{tot}} - P_{\text{H}_2\text{O}}$ as the dry air partial pressure. The only difference between MPM87 and MPM89 with respect to the line absorption is the parameterization of the pressure broadened line width, γ_k , which is calculated with the four parameters $b_{3,k}$ to $b_{6,k}$ in the case of MPM89 whereas in MPM87 a single parameter ($b_{3,k}$) is used (see Eq. (2.50)).

k	ν_k [GHz]	$b_{1,k}$ [$\frac{\text{kHz}}{\text{kPa}}$]	$b_{2,k}$ [1]	$b_{3,k}$ [$\frac{\text{MHz}}{\text{kPa}}$]	$b_{4,k}$ [1]	$b_{5,k}$ [1]	$b_{6,k}$ [1]
1	22.235080	0.1090	2.143	28.11	0.69	4.80	1.00
2	67.813960	0.0011	8.735	28.58	0.69	4.93	0.82
3	119.995940	0.0007	8.356	29.48	0.70	4.78	0.79
4	183.310074	2.3000	0.668	28.13	0.64	5.30	0.85
5	321.225644	0.0464	6.181	23.03	0.67	4.69	0.54
6	325.152919	1.5400	1.540	27.83	0.68	4.85	0.74
7	336.187000	0.0010	9.829	26.93	0.69	4.74	0.61
8	380.197372	11.9000	1.048	28.73	0.69	5.38	0.84
9	390.134508	0.0044	7.350	21.52	0.63	4.81	0.55
10	437.346667	0.0637	5.050	18.45	0.60	4.23	0.48
11	439.150812	0.9210	3.596	21.00	0.63	4.29	0.52
12	443.018295	0.1940	5.050	18.60	0.60	4.23	0.50
13	448.001075	10.6000	1.405	26.32	0.66	4.84	0.67
14	470.888947	0.3300	3.599	21.52	0.66	4.57	0.65
15	474.689127	1.2800	2.381	23.55	0.65	4.65	0.64
16	488.491133	0.2530	2.853	26.02	0.69	5.04	0.72
17	503.568532	0.0374	6.733	16.12	0.61	3.98	0.43
18	504.482692	0.0125	6.733	16.12	0.61	4.01	0.45
19	556.936002	510.0000	0.159	32.10	0.69	4.11	1.00
20	620.700807	5.0900	2.200	24.38	0.71	4.68	0.68
21	658.006500	0.2740	7.820	32.10	0.69	4.14	1.00
22	752.033227	250.0000	0.396	30.60	0.68	4.09	0.84
23	841.073593	0.0130	8.180	15.90	0.33	5.76	0.45
24	859.865000	0.1330	7.989	30.60	0.68	4.09	0.84
25	899.407000	0.0550	7.917	29.85	0.68	4.53	0.90

Table 2.5: (continued on next page)

k	ν_k	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$	$b_{4,k}$	$b_{5,k}$	$b_{6,k}$
26	902.555000	0.0380	8.432	28.65	0.70	5.10	0.95
27	906.205524	0.1830	5.111	24.08	0.70	4.70	0.53
28	916.171582	8.5600	1.442	26.70	0.70	4.78	0.78
29	970.315022	9.1600	1.920	25.50	0.64	4.94	0.67
30	987.926764	138.0000	0.258	29.85	0.68	4.55	0.90

Table 2.5: List of H₂O spectral lines and their spectroscopic parameters (H₂O-air mixture) for the MPM89 model [*Liebe, 1989*].

Water vapor continuum absorption: The MPM89 continuum absorption coefficients in, α_c^{MPM89} , are identical as those in MPM87 (see Sec. 2.3.1 for details):

$$\alpha_c^{\text{MPM89}} = \nu^2 \cdot P_{\text{H}_2\text{O}} \cdot (C_{\text{H}_2\text{O}}^0 \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{\text{ns}} + C_d^0 \cdot P_d \cdot \Theta^{\text{nf}}), \quad (2.57)$$

with

$$C_{\text{H}_2\text{O}}^0 = 6.496 \cdot 10^{-6} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_s = 10.5$$

$$C_d^0 = 0.206 \cdot 10^{-6} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_d = 3.0$$

MPM93 water vapor absorption model

This version, which is described in *Liebe et al. [1993]* and follows the general line of the MPM model to divide the total water vapor absorption, $\alpha_{\text{tot}}^{\text{MPM93}}$, into a spectral line term, $\alpha_\ell^{\text{MPM93}}$, and a continuum term not attributed to spectral lines, α_c^{MPM93} :

$$\alpha_{\text{tot}}^{\text{MPM93}} = \alpha_\ell^{\text{MPM93}} + \alpha_c^{\text{MPM93}} \quad \text{dB/km} \quad (2.58)$$

The continuum absorption is parameterized like a resonant spectral line of H₂O, a so-called pseudo-line. This is a fundamental change in the parameterization of the water vapor continuum in respect to all older versions of MPM, which makes it quite complicate to compare the different versions, especially to distinguish a self- and foreign broadening term in the continuum.

Water vapor line absorption: The water vapor line spectrum of MPM93 [*Liebe et al., 1993*] consists of 34 lines below 1 THz (four more than in MPM89 and MPM87). To describe the MPM93 water vapor line absorption, a set of six parameters ($b_{1,k}$ and $b_{3,k}$) per line are used: two for the line strength and four for the line width. The total line absorption coefficient (in units of dB/km) is the sum over all individual line absorption coefficients⁵:

$$\alpha_\ell^{\text{MPM93}} = 0.1820 \cdot \nu_k \cdot P_{\text{H}_2\text{O}} \cdot \sum_k S_k(T) \cdot F(\nu, \nu_k) \quad \text{dB/km} \quad (2.59)$$

⁵see footnote for MPM97 line absorption

where $S_k(T)$ is the line intensity described by the parameterization

$$S_k(T) = b_{1,k} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{3.5} \cdot \exp(b_{2,k} \cdot [1 - \Theta]) \quad \text{kHz} \quad (2.60)$$

with ν_k as the line center frequency, $P_{\text{H}_2\text{O}}$ the water vapor partial pressure and $\Theta = 300 \text{ K}/T$.

The line shape function, $F(\nu, \nu_k)$, in Eq. (2.46) is the standard Van Vleck-Weisskopf (VW) function, given by:

$$F(\nu, \nu_k) = \left(\frac{\nu}{\nu_k} \right) \cdot \left[\frac{\gamma_k}{(\nu - \nu_k)^2 + \gamma_k^2} + \frac{\gamma_k}{(\nu + \nu_k)^2 + \gamma_k^2} \right] \quad (2.61)$$

$$(2.62)$$

The pressure broadened line width, γ_k , is calculated with the single parameter $b_{3,k}$ in the following way:

$$\gamma_k = b_{3,k} \cdot (4.80 \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{1.1} + P_d \cdot \Theta^{0.6}) \quad \text{GHz} \quad (2.63)$$

where P_d is the partial pressure of dry air ($P_d = P_{\text{tot}} - P_{\text{H}_2\text{O}}$).

The parameterizations of $S_k(T)$ was already in use for the early version of MPM81 [Liebe, 1981]. The expression for γ_k is the same as in MPM89. The main difference between MPM93 and MPM89 concerning the water vapor line absorption is the updated line catalog.

k	ν_k [GHz]	$b_{1,k}$ [$\frac{\text{kHz}}{\text{hPa}}$]	$b_{2,k}$ [1]	$b_{3,k}$ [$\frac{\text{MHz}}{\text{hPa}}$]	$b_{4,k}$ [1]	$b_{5,k}$ [1]	$b_{6,k}$ [1]
1	22.235080	0.01130	2.143	2.811	4.80	0.69	1.00
2	67.803960	0.00012	8.735	2.858	4.93	0.69	0.82
3	119.995940	0.00008	8.356	2.948	4.78	0.70	0.79
4	183.310091	0.24200	0.668	3.050	5.30	0.64	0.85
5	321.225644	0.00483	6.181	2.303	4.69	0.67	0.54
6	325.152919	0.14990	1.540	2.783	4.85	0.68	0.74
7	336.222601	0.00011	9.829	2.693	4.74	0.69	0.61
8	380.197372	1.15200	1.048	2.873	5.38	0.54	0.89
9	390.134508	0.00046	7.350	2.152	4.81	0.63	0.55
10	437.346667	0.00650	5.050	1.845	4.23	0.60	0.48
11	439.150812	0.09218	3.596	2.100	4.29	0.63	0.52
12	443.018295	0.01976	5.050	1.860	4.23	0.60	0.50
13	448.001075	1.03200	1.405	2.632	4.84	0.66	0.67
14	470.888947	0.03297	3.599	2.152	4.57	0.66	0.65
15	474.689127	0.12620	2.381	2.355	4.65	0.65	0.64
16	488.491133	0.02520	2.853	2.602	5.04	0.69	0.72
17	503.568532	0.00390	6.733	1.612	3.98	0.61	0.43
18	504.482692	0.00130	6.733	1.612	4.01	0.61	0.45
19+	547.676440	0.97010	0.114	2.600	4.50	0.70	1.00
20+	552.020960	1.47700	0.114	2.600	4.50	0.70	1.00
21	556.936002	48.74000	0.159	3.210	4.11	0.69	1.00

Table 2.6: (continued on next page)

	ν_k	$b_{1,k}$	$b_{2,k}$	$b_{3,k}$	$b_{4,k}$	$b_{5,k}$	$b_{6,k}$
22	620.700807	0.50120	2.200	2.438	4.68	0.71	0.68
23 ⁺	645.866155	0.00713	8.580	1.800	4.00	0.60	0.50
24	658.005280	0.03022	7.820	3.210	4.14	0.69	1.00
25	752.033227	23.96000	0.396	3.060	4.09	0.68	0.84
26	841.053973	0.00140	8.180	1.590	5.76	0.33	0.45
27	859.962313	0.01472	7.989	3.060	4.09	0.68	0.84
28	899.306675	0.00605	7.917	2.985	4.53	0.68	0.90
29	902.616173	0.00426	8.432	2.865	5.10	0.70	0.95
30	906.207325	0.01876	5.111	2.408	4.70	0.70	0.53
31	916.171582	0.83400	1.442	2.670	4.78	0.70	0.78
32 ⁺	923.118427	0.00869	10.220	2.900	5.00	0.70	0.80
33	970.315022	0.89720	1.920	2.550	4.94	0.64	0.67
34	987.926764	13.21000	0.258	2.985	4.55	0.68	0.90
	ν^*	b_1^*	b_2^*	b_3^*	b_4^*	b_5^*	b_6^*
	[GHz]	[$\frac{\text{kHz}}{\text{hPa}}$]	[1]	[$\frac{\text{MHz}}{\text{hPa}}$]	[1]	[1]	[1]
	1780.000000	2230.00000	0.952	17.620	30.50	2.00	5.00

Table 2.6: List of used H₂O spectral lines and their spectroscopic coefficients of H₂O in air for the MPM93 model [Liebe *et al.*, 1993]. The last separated line is the unphysical pseudo-line used in MPM93. The lines which are marked with a ”+” were not in the MPM87/MPM89 line catalog.

The MPM93 continuum parameterization: In the MPM93 version the water vapor continuum is parameterized as an ordinary spectral line (Eqs. (2.60, 2.61)). The parameters of this continuum ”pseudo-line” (ν^* , b_1^* , b_2^* , b_3^* , b_4^* , b_5^* , b_6^*) are given in Table 2.6. More details about this continuum parameterization and its microwave approximation can be found in Section 2.2.1 of this guide.

CP98 water vapor absorption model

Line absorption component [Cruz Pol *et al.*, 1998] for the water vapor line absorption is based on MPM87 with the main difference that the line catalog consists of only a single line at $\nu_0 = 22$ GHz. The contributions from the other lines is put into the water vapor continuum module. The line absorption is therefore very quickly calculated (in units of Np/km) according to the formula

$$\alpha_\ell^{\text{CP98}} = 0.0419 \cdot S_0(T) \cdot F(\nu, \nu_k) \quad (2.64)$$

with

$$\begin{aligned} S_0(T) &= 0.0109 \cdot C_L \cdot P_{\text{H}_2\text{O}} \cdot \nu_0 \cdot \Theta^{3.5} \cdot \exp(2.143 \cdot [1 - \Theta]) \\ \gamma &= 0.002784 \cdot C_W \cdot (P_d \cdot \Theta^{0.6} + 4.8 \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{1.1}) \end{aligned} \quad (2.65)$$

where $P_{\text{H}_2\text{O}}$ and P_d are the partial pressure of water vapor and dry air in units of hPa, respectively and the Van Vleck-Weisskopf line shape, $F(\nu, \nu_k)$. The numbers correspond to the line parameters from MPM87 for this special line and the factors C_L and C_W are

adjustable scaling factors to match the model with the measurements. Setting the scaling factors to $C_L=1.00$ and $C_W=1.00$ leads to the same results as for MPM87. According to the parameter estimation of Cruz–Pol et al. best agreement between data and model is obtained with $C_L = 1.0639 \pm 0.016$ and $C_W = 1.0658 \pm 0.0096$. The correlation between these two scaling factors was found to be negligible, as can be seen from Table 2.7.

	C_L	C_W	C_C	C_X
value	1.0639	1.0658	1.2369	1.0739
std. dev.	0.016	0.0096	0.155	0.252
correlation				
C_L	1	-0.085	0.045	-0.048
C_W	-0.085	1	-0.513	0.485
C_C	0.045	-0.513	1	-0.989
C_X	-0.048	0.485	-0.989	1

Table 2.7: Scaling parameter values with standard deviation and correlation coefficients according to [Cruz Pol et al., 1998]. The scaling parameters are C_L :22 GHz line strength, C_W :22 GHz line width, C_C :H₂O-continuum, and C_X :O₂-absorption. C_X scales the entire oxygen absorption, the continuum as well as the line absorption. The Cruz-Pol et al. model uses the Rosenkranz [1993] oxygen absorption model.

The main reason why the Cruz-Pol model (CP98) considers only one line lies in the fact that CP98 is especially designed for the data analysis in the 20-31.4 GHz region. The determination of the scaling factors was performed with ground based radiometer data in the frequency range of from different locations⁶ in the USA.

Water vapor continuum absorption: The CP98 model uses the same water vapor continuum parameterization as MPM87, just scaled with an empirical factor, C_C , determined from the above mentioned data:

$$\alpha_c^{\text{CP98}} = C_C \cdot \alpha_c^{\text{MPM87}} \quad (2.66)$$

The scaling factor C_C , as given in Table 2.7, gives a 23.69 % increased continuum absorption compared with MPM87 (see Table 2.1 for a comparison of the parameter values). But one has to keep in mind that C_C has a high correlation with the scaling factor of the oxygen absorption, C_X , since these two components could not be completely distinguished in the data. Therefore the value of 23.69 % has a standard deviation of 15.5 % and is not so reliable than C_L and C_W .

PWR98 water vapor absorption model

The water vapor continuum formulation of Rosenkranz [1998] is a re-investigation of the existing models MPM87/MPM89, MPM93, and CKD_2.1 especially for the frequency region below 1-1000 GHz. in the context of the available laboratory and atmospheric data [Bauer

⁶The data were recorded at San Diego, California (11. December 1991) and West Palm Beach, Florida (8.-21. March 1992)

et al., 1989, 1993, 1995; *Becker and Autler*, 1946; *English et al.*, 1994; *Godon et al.*, 1992; *Liebe*, 1984; *Liebe and Layton*, 1987; *Westwater et al.*, 1980].

Rosenkranz adopted the structure of MPM89 for his improved model (R98). However, some important differences exist compared with MPM89:

- the water vapor line catalogs are different
- the R98 uses the Van Vleck–Weisskopf line shape function with cutoff and MPM89 without cutoff

Water vapor line absorption: The local line absorption is defined as

$$\begin{aligned}\alpha_{\ell}^{\text{R98}} &= N_{\text{H}_2\text{O}} \cdot \sum_k S_k(T) \cdot F_c(\nu, \nu_k) \\ &= N_{\text{H}_2\text{O}} \cdot \sum_k S_k(T) \cdot \left(\frac{\nu}{\nu_k}\right)^2 \cdot [f_c(\nu, +\nu_k) + f_c(\nu, -\nu_k)] \text{ Np/km} \quad (2.67)\end{aligned}$$

where $N_{\text{H}_2\text{O}}$ is the number density of water molecules, ν the frequency and S the line intensity, calculated from the HITRAN92 data base *Rothman et al.* [1992]. Considered for this re-investigation are 15 lines with a frequency lower than 1 THz as listed in Table 2.8.

The line shape function $F_c(\nu, \nu_k)$ has a cutoff frequency, ν_{cutoff} , and a baseline subtraction similar to the CKD model [*Clough et al.*, 1989]. The introduction of a cutoff frequency has two advantages: (1) the cutoff avoids applying the line shape to distant frequencies where the line form is theoretically not well understood and (2) the cutoff also establishes a limit to the summation in Eq. (2.67) where lines far away from the cutoff limit do not contribute to the sum. The Rosenkranz formulation uses the same value for the cutoff frequency as the CKD model:

$$\nu_{\text{cutoff}} = 750 \text{ GHz} \quad (2.68)$$

The explicit mathematical form of the line shape function is defined in such a way that in the limit $\nu_{\text{cutoff}} \rightarrow \infty$ the combination of Eq. (2.67) with the line shape function would be equivalent to a Van Vleck–Weisskopf [*Van Vleck and Weisskopf*, 1945] line shape:

$$f_c(\nu, \pm\nu_k) = \begin{cases} \frac{\gamma_k}{\pi} \left\{ \frac{1}{(\nu \mp \nu_k)^2 + \gamma_k^2} - \frac{1}{\nu_{\text{cutoff}}^2 + \gamma_k^2} \right\} & : |\nu \pm \nu_k| < \nu_{\text{cutoff}} \\ 0 & : |\nu \pm \nu_k| \geq \nu_{\text{cutoff}} \end{cases} \quad (2.69)$$

ν_k is the line center frequency and γ_k the line half width, which is calculated according to

$$\gamma_k = w_{s,k} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{\text{ns}} + w_{f,k} \cdot P_{\text{d}} \cdot \Theta^{\text{nf}} \quad \text{GHz} \quad (2.70)$$

with $P_{\text{H}_2\text{O}}$ and P_{d} as the partial pressure of water vapor and of dry air, respectively. The line depending parameters $w_{s,k}$, n_s , $w_{f,k}$, and n_f are listed in Table 2.8 and the dimensionless parameter Θ is defined as $\Theta = 300 \text{ K}/T$.

Because of the structural similarity to MPM89, the line broadening parameters differ only in minor respects from the values used therein (only the parameters $x_{s,1}$, $w_{f,2}$ and $w_{s,2}$ are significantly different).

index	ν_k	$w_{f,k}$	n_f	$w_{s,k}$	n_s
k	[GHz]	[GHz/kPa]	[1]	[GHz/kPa]	[1]
1	22.2351	0.00281	0.69	0.01349	0.61
2	183.3101	0.00281	0.64	0.01491	0.85
3	321.2256	0.00230	0.67	0.01080	0.54
4	325.1529	0.00278	0.68	0.01350	0.74
5	380.1974	0.00287	0.54	0.01541	0.89
6	439.1508	0.00210	0.63	0.00900	0.52
7	443.0183	0.00186	0.60	0.00788	0.50
8	448.0011	0.00263	0.66	0.01275	0.67
9	470.8890	0.00215	0.66	0.00983	0.65
10	474.6891	0.00236	0.65	0.01095	0.64
11	488.4911	0.00260	0.69	0.01313	0.72
12	556.9360	0.00321	0.69	0.01320	1.00
13	620.7008	0.00244	0.71	0.01140	0.68
14	752.0332	0.00306	0.68	0.01253	0.84
15	916.1712	0.00267	0.70	0.01275	0.78

Table 2.8: Line parameters of the Rosenkranz absorption model (PWR98) (values taken from *Rosenkranz [1998]*).

Water vapor continuum absorption: The continuum absorption in R98 has the same functional dependence on frequency, pressure, and temperature like in MPM87/MPM89 (see Sec. 2.3.1 for details):

$$\alpha_c^{\text{R98}} = \nu^2 \cdot P_{\text{H}_2\text{O}} \cdot (C_{\text{H}_2\text{O}}^{\text{O}} \cdot P_{\text{H}_2\text{O}} \cdot \Theta^{n_s} + C_{\text{d}}^{\text{O}} \cdot P_{\text{d}} \cdot \Theta^{n_f}) \quad (2.71)$$

with

$$C_{\text{H}_2\text{O}}^{\text{O}} = 7.80 \cdot 10^{-8} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_s = 7.5$$

$$C_{\text{d}}^{\text{O}} = 0.236 \cdot 10^{-8} \text{ (dB/km) / (hPa} \cdot \text{GHz)}^2$$

$$n_d = 3.0$$

The main difference to the MPM versions are the values of these parameters, since Rosenkranz used additional data to fit his set of parameters. A second point is the cutoff in the line shape of the line absorption calculation. Since this cutoff decreases the line absorption in the window regions, the continuum absorption tends to compensate this decrease to get the same total absorption as without cutoff. This effects mainly the parameters $C_{\text{H}_2\text{O}}^{\text{O}}$ and C_{d}^{O} but has also an influence in the temperature dependence and therefore on n_s and n_d .

2.3.2 Complete oxygen models

Since the Maxwell equations are symmetric in the electric and magnetic fields, electric as well as magnetic dipole transitions are both possible although magnetic dipoles are in general some orders of magnitudes weaker and therefore not relevant in atmospheric radiative

transfer models. An exception to this is the complex around 60 GHz of the paramagnetic oxygen magnetic dipole transitions. This bulk of lines arise due to the fact that for rotational quantum numbers $K > 1$ the allowed transitions $\Delta J = \pm 1$ have an energy gap of approximately 60 GHz.

The most frequently used absorption model for this absorption effect is that of Liebe, Rosenkranz, and Hufford [*Liebe et al.*, 1992] (also reported in *Rosenkranz* [1993] with a slightly different parameterization).

For oxygen – like for water vapor – the total absorption (α_{tot}) is modelled as the line absorption (α_{ℓ}) plus a continuum absorption (α_{c}):

$$\alpha_{\text{tot}} = \alpha_{\ell} + \alpha_{\text{c}} \quad (2.72)$$

It has to be emphasized that, α_{ℓ} and α_{c} of different models are not necessarily compatible and should therefore not be interchanged.

PWR93 oxygen absorption model

Resonant oxygen absorption The oxygen absorption model of Rosenkranz is described in *Rosenkranz* [1993]. It is based on the investigations made by Liebe, Rosenkranz, and Hufford [*Liebe et al.*, 1992]. The FORTRAN77 computer program of Rosenkranz for the O₂ absorption calculation can be downloaded via anonymous ftp from mesa.mit.edu/phil/ibl_rt.

The oxygen line catalog has 40 lines from which 33 lines build the complex around 60 GHz. The parameterization of the line absorption, $\alpha_{\ell}^{\text{R98}}$, is:

$$\alpha_{\ell}^{\text{R98}} = \frac{n_{\text{O}_2}}{\pi} \cdot \sum_{k=1}^{40} S_k(T) \cdot F(\nu, \nu_k) \quad (2.73)$$

line intensity:

$$S_k(T) = S_k(300 \text{ K}) / \exp(b_k \cdot \Theta) \quad (2.74)$$

line shape function:

$$F(\nu, \nu_k) = \left(\frac{\nu}{\nu_k} \right)^2 \cdot \left[\frac{\Gamma_k + (\nu - \nu_k) \cdot Y_k}{(\nu - \nu_k)^2 + \Gamma_k^2} + \frac{\Gamma_k - (\nu + \nu_k) \cdot Y_k}{(\nu + \nu_k)^2 + \Gamma_k^2} \right]$$

line width:

$$\Gamma_k = w_k \cdot (P_{\text{d}} \cdot \Theta^{0.8} + 1.1 \cdot P_{\text{H}_2\text{O}} \cdot \Theta) \quad (2.75)$$

line coupling:

$$Y_k = P_{\text{air}} \cdot \Theta^{0.8} \cdot [y_k + (\Theta - 1) \cdot v_k]$$

number density of O₂:

$$n_{\text{O}_2} = (0.20946 \cdot P_{\text{air}}) / (k_B \cdot T)$$

where $S_k(300 \text{ K})$ denotes the reference line intensity at T=300 K and the exponential term approximates the exact partition function. All model parameters (see Refs. *Rosenkranz* [1993] and *Liebe et al.* [1992] for the laboratory measurements and the fitting parameters) are tabulated in Table 2.9.

index	ν_k	$S_k(300\text{ K})$	b_k	w_k	y_k	v_k
k	[GHz]	[$\text{cm}^2\text{ Hz}$]	[1]	[$\frac{\text{MHz}}{\text{hPa}}$]	[$\frac{10^{-3}}{\text{hPa}}$]	[$\frac{10^{-3}}{\text{hPa}}$]
1	118.7503	$.2936 \cdot 10^{-14}$.009	1.63	-0.0233	0.0079
2	56.2648	$.8079 \cdot 10^{-15}$.015	1.646	0.2408	-0.0978
3	62.4863	$.2480 \cdot 10^{-14}$.083	1.468	-0.3486	0.0844
4	58.4466	$.2228 \cdot 10^{-14}$.084	1.449	0.5227	-0.1273
5	60.3061	$.3351 \cdot 10^{-14}$.212	1.382	-0.5430	0.0699
6	59.5910	$.3292 \cdot 10^{-14}$.212	1.360	0.5877	-0.0776
7	59.1642	$.3721 \cdot 10^{-14}$.391	1.319	-0.3970	0.2309
8	60.4348	$.3891 \cdot 10^{-14}$.391	1.297	0.3237	-0.2825
9	58.3239	$.3640 \cdot 10^{-14}$.626	1.266	-0.1348	0.0436
10	61.1506	$.4005 \cdot 10^{-14}$.626	1.248	0.0311	-0.0584
11	57.6125	$.3227 \cdot 10^{-14}$.915	1.221	0.0725	0.6056
12	61.8002	$.3715 \cdot 10^{-14}$.915	1.207	-0.1663	-0.6619
13	56.9682	$.2627 \cdot 10^{-14}$	1.260	1.181	0.2832	0.6451
14	62.4112	$.3156 \cdot 10^{-14}$	1.260	1.171	-0.3629	-0.6759
15	56.3634	$.1982 \cdot 10^{-14}$	1.660	1.144	0.3970	0.6547
16	62.9980	$.2477 \cdot 10^{-14}$	1.665	1.139	-0.4599	-0.6675
17	55.7838	$.1391 \cdot 10^{-14}$	2.119	1.110	0.4695	0.6135
18	63.5685	$.1808 \cdot 10^{-14}$	2.115	1.108	-0.5199	-0.6139
19	55.2214	$.9124 \cdot 10^{-15}$	2.624	1.079	0.5187	0.2952
20	64.1278	$.1230 \cdot 10^{-14}$	2.625	1.078	-0.5597	-0.2895
21	54.6712	$.5603 \cdot 10^{-15}$	3.194	1.05	0.5903	0.2654
22	64.6789	$.7842 \cdot 10^{-15}$	3.194	1.05	-0.6246	-0.2590
23	54.1300	$.3228 \cdot 10^{-15}$	3.814	1.02	0.6656	0.3750
24	65.2241	$.4689 \cdot 10^{-15}$	3.814	1.02	-0.6942	-0.3680
25	53.5957	$.1748 \cdot 10^{-15}$	4.484	1.00	0.7086	0.5085
26	65.7648	$.2632 \cdot 10^{-15}$	4.484	1.00	-0.7325	-0.5002
27	53.0669	$.8898 \cdot 10^{-16}$	5.224	.97	0.7348	0.6206
28	66.3021	$.1389 \cdot 10^{-15}$	5.224	.97	-0.7546	-0.6091
29	52.5424	$.4264 \cdot 10^{-16}$	6.004	.94	0.7702	0.6526
30	66.8368	$.6899 \cdot 10^{-16}$	6.004	.94	-0.7864	-0.6393
31	52.0214	$.1924 \cdot 10^{-16}$	6.844	.92	0.8083	0.6640
32	67.3696	$.3229 \cdot 10^{-16}$	6.844	.92	-0.8210	-0.6475
33	51.5034	$.8191 \cdot 10^{-17}$	7.744	.89	0.8439	0.6729
34	67.9009	$.1423 \cdot 10^{-16}$	7.744	.89	-0.8529	-0.6545
35	368.4984	$.6460 \cdot 10^{-15}$.048	1.92	0.0000	0.0000
36	424.7631	$.7047 \cdot 10^{-14}$.044	1.92	0.0000	0.0000
37	487.2494	$.3011 \cdot 10^{-14}$.049	1.92	0.0000	0.0000
38	715.3932	$.1826 \cdot 10^{-14}$.145	1.81	0.0000	0.0000
39	773.8397	$.1152 \cdot 10^{-13}$.141	1.81	0.0000	0.0000
40	834.1453	$.3971 \cdot 10^{-14}$.145	1.81	0.0000	0.0000

Table 2.9: List of O_2 spectral lines of the Rosenkranz absorption model [Rosenkranz, 1993].

Oxygen continuum absorption: As pointed out by Van Vleck [*Van Vleck, 1987*], the standard theory for non-resonant absorption is that of Debye (see also Ref. *Townes and Schawlow [1955]*). The Debye line shape is obtained from the VVW line shape function by the limiting case $\nu_k \rightarrow 0$. Rosenkranz [*Rosenkranz [1993]*] adopt the Debye theory for his models:

$$\alpha_c = C \cdot P_d \cdot \Theta^2 \cdot \frac{\nu^2 \cdot \gamma}{\nu^2 + \gamma^2} \quad (2.76)$$

$$\gamma = w \cdot (P_d \cdot \Theta^{0.8} + 1.1 \cdot P_{\text{H}_2\text{O}} \cdot \Theta) \quad (2.77)$$

The values for the parameters are $C = 1.11 \cdot 10^{-5}$ dB/km/(hPa GHz) and $w = 5.6 \cdot 10^{-4}$ GHz/hPa, respectively. This absorption term is proportional to the collision frequency of a single oxygen molecule and thus proportional to the dry air pressure⁷.

MPM93 oxygen absorption model

Oxygen line absorption: The oxygen line catalog has 44 lines from which 37 lines build the complex around 60 GHz [*Liebe et al., 1993*]. The parameterization of the line absorption, α_ℓ^{MPM} , is (in units of dB/km):

$$\alpha_\ell^{\text{MPM}} = 0.1820 \cdot \nu^2 \cdot \sum_{k=1}^{44} S_k(T) \cdot F(\nu, \nu_k) \quad \text{dB/km} \quad (2.78)$$

with

line intensity:

$$S_k(T) = \frac{a_{1,k}}{\nu_k} \cdot P_d \cdot \Theta^3 \cdot \exp[a_{2,k} \cdot (1 - \Theta)] \quad (2.79)$$

line shape function:

$$F(\nu, \nu_k) = \left[\frac{\gamma_k + (\nu - \nu_k) \cdot \delta_k}{(\nu - \nu_k)^2 + \gamma_k^2} + \frac{\gamma_k - (\nu + \nu_k) \cdot \delta_k}{(\nu + \nu_k)^2 + \gamma_k^2} \right]$$

line width:

$$\gamma_k = a_{3,k} \cdot 10^{-3} \cdot (P_d \cdot \Theta^{a_{4,k}} + 1.10 \cdot P_{\text{H}_2\text{O}} \cdot \Theta) \quad (2.80)$$

line coupling:

$$\delta_k = P_{\text{air}} \cdot \Theta^{0.8} \cdot [a_{5,k} + \Theta \cdot a_{6,k}]$$

where $a_{1-5,k}$ are the fitted parameters due to laboratory measurements [*Liebe et al., 1992*]. All model parameters are tabulated in Table 2.10. One has to note that in the MPM93 code is a threshold value for α_ℓ^{MPM} implemented:

$$\alpha_\ell^{\text{MPM}} = \begin{cases} \alpha_\ell^{\text{MPM}} & : \alpha_\ell^{\text{MPM}} > 0 \\ 0 & : \alpha_\ell^{\text{MPM}} < 0 \end{cases} \quad (2.81)$$

Therefore the oxygen absorption in the wings of the strong O₂-lines is remarkably higher than in the R93 model.

⁷The absorption due to weakly bound complexes of O₂-X with X = H₂O, N₂ is treated separately and therefore not included in this Debye formula.

index	ν_k	$a_{1,k}$	$a_{2,k}$	$a_{3,k}$	$a_{4,k}$	$a_{5,k}$	$a_{6,k}$
k	[GHz]	$[\frac{\text{kHz}}{\text{hPa}}]$	[1]	$[\frac{\text{MHz}}{\text{hPa}}]$	[1]	$[\frac{10^3}{\text{hPa}}]$	$[\frac{10^3}{\text{hPa}}]$
1	50.474238	0.094	9.694	0.890	0.0	0.240	0.790
2	50.987749	0.246	8.694	0.910	0.0	0.220	0.780
3	51.503350	0.608	7.744	0.940	0.0	0.197	0.774
4	52.021410	1.414	6.844	0.970	0.0	0.166	0.764
5	52.542394	3.102	6.004	0.990	0.0	0.136	0.751
6	53.066907	6.410	5.224	1.020	0.0	0.131	0.714
7	53.595749	12.470	4.484	1.050	0.0	0.230	0.584
8	54.130000	22.800	3.814	1.070	0.0	0.335	0.431
9	54.671159	39.180	3.194	1.100	0.0	0.374	0.305
10	55.221367	63.160	2.624	1.130	0.0	0.258	0.339
11	55.783802	95.350	2.119	1.170	0.0	-0.166	0.705
12	56.264775	54.890	0.015	1.730	0.0	0.390	-0.113
13	56.363389	134.400	1.660	1.200	0.0	-0.297	0.753
14	56.968206	176.300	1.260	1.240	0.0	-0.416	0.742
15	57.612484	214.100	0.915	1.280	0.0	-0.613	0.697
16	58.323877	238.600	0.626	1.330	0.0	-0.205	0.051
17	58.446590	145.700	0.084	1.520	0.0	0.748	-0.146
18	59.164207	240.400	0.391	1.390	0.0	-0.722	0.266
19	59.590983	211.200	0.212	1.430	0.0	0.765	-0.090
20	60.306061	212.400	0.212	1.450	0.0	-0.705	0.081
21	60.434776	246.100	0.391	1.360	0.0	0.697	-0.324
22	61.150560	250.400	0.626	1.310	0.0	0.104	-0.067
23	61.800154	229.800	0.915	1.270	0.0	0.570	-0.761
24	62.411215	193.300	1.260	1.230	0.0	0.360	-0.777
25	62.486260	151.700	0.083	1.540	0.0	-0.498	0.097
26	62.997977	150.300	1.665	1.200	0.0	0.239	-0.768
27	63.568518	108.700	2.115	1.170	0.0	0.108	-0.706
28	64.127767	73.350	2.620	1.130	0.0	-0.311	-0.332
29	64.678903	46.350	3.195	1.100	0.0	-0.421	-0.298
30	65.224071	27.480	3.815	1.070	0.0	-0.375	-0.423
31	65.764772	15.300	4.485	1.050	0.0	-0.267	-0.575
32	66.302091	8.009	5.225	1.020	0.0	-0.168	-0.700
33	66.836830	3.946	6.005	0.990	0.0	-0.169	-0.735
34	67.369598	1.832	6.845	0.970	0.0	-0.200	-0.744
35	67.900867	0.801	7.745	0.940	0.0	-0.228	-0.753
36	68.431005	0.330	8.695	0.920	0.0	-0.240	-0.760
37	68.960311	0.128	9.695	0.900	0.0	-0.250	-0.765
38	118.750343	94.500	0.009	1.630	0.0	-0.036	0.009
39	368.498350	6.790	0.049	1.920	0.6	0.000	0.000
40	424.763124	63.800	0.044	1.930	0.6	0.000	0.000
41	487.249370	23.500	0.049	1.920	0.6	0.000	0.000
42	715.393150	9.960	0.145	1.810	0.6	0.000	0.000
43	773.839675	67.100	0.130	1.820	0.6	0.000	0.000

Table 2.10: (continued on next page)

index	ν_k	$a_{1,k}$	$a_{2,k}$	$a_{3,k}$	$a_{4,k}$	$a_{5,k}$	$a_{6,k}$
44	834.145330	18.000	0.147	1.810	0.6	0.000	0.000

Table 2.10: List of O₂ spectral lines of the MPM93 absorption model [*Liebe et al.*, 1993].

Oxygen continuum absorption: As pointed out by Van Vleck [*Van Vleck*, 1987], the standard theory for non-resonant absorption is that of Debye (see also Ref. *Townes and Schawlow* [1955]). The Debye line shape is obtained from the VVW line shape function by the limiting case $\nu_k \rightarrow 0$. *Liebe et al.* [1993] adopt the Debye theory for his model:

$$\begin{aligned}\alpha_c &= C \cdot P_d \cdot \Theta^2 \cdot \frac{\nu^2 \cdot \gamma}{\nu^2 + \gamma^2} \\ \gamma &= w \cdot P_{\text{tot}} \cdot \Theta^{0.8}\end{aligned}\tag{2.82}$$

The values for the parameters are $C = 1.11 \cdot 10^{-5}$ dB/km/(hPa GHz) and $w = 5.6 \cdot 10^{-4}$ GHz/hPa, respectively. This absorption term is proportional to the collision frequency of a single oxygen molecule and thus proportional to the dry air pressure⁸.

⁸The absorption due to weakly bound complexes of O₂-X with X = H₂O, N₂ is treated separately and therefore not included in this Debye formula.

Chapter 3

Cloud absorption

3.1 Liquid water and ice particle absorption

So far only absorption due to air was described. However hydrometeors¹ can have a noticeable effect on the radiative transfer through the atmosphere. To treat hydrometeors you should normally set up a calculation with scattering, which needs input optical properties such as the phase matrix. Several chapters, both in *ARTS User Guide* and here in *ARTS Theory*, deal with such scattering simulations.

This very short chapter is not related to the scattering parts in ARTS. Instead, it describes some functions that handle only the absorption of hydrometeors, not the scattering. They may be useful in some special cases. Practically, they work exactly as the continuum and complete gas absorption models, just the ‘VMR’ is interpreted as a condensate amount.

The MPM93 model provides beside the absorption model of air also an absorption model for suspended liquid water droplets and ice particles [*Liebe et al., 1989, 1991; Hufford, 1991; Liebe et al., 1993*]. The model is applicable for the Rayleigh regime, for which the relation $r < 0.05 \cdot \lambda$ holds where r is the particle radius and λ is the wavelength², e. g. for a frequency of around 22 GHz this means $r < 500 \mu\text{m}$. Considering *Salby [1996]*, this criterium is – except for cirrus – nearly for every aerosol and cloud class satisfied. But one has to bear in mind that these values have a wide range of variability, for example, *Salby [1996]* states that the mean particle radius for stratus, cumulus, and nimbus clouds can be in the range of 10-1000 μm and that the particle radius distribution is highly unsymmetric.

With respect to the imaginary part of the complex refractivity, a unified parameterization of liquid and ice particle absorption is formulated in MPM93:

$$\begin{aligned}\alpha &= 0.1820 \cdot \nu \cdot N'' && \text{dB/km} && (3.1) \\ N'' &= \frac{3}{2} \cdot \frac{w}{m} \cdot \text{Im}[(\epsilon_r - 1)/(\epsilon_r + 2)] \\ N'' &= \frac{3}{2} \cdot \frac{w}{m} \cdot \left[\frac{3 \cdot \epsilon_r''}{(\epsilon_r' + 2)^2 + (\epsilon_r'')^2} \right]\end{aligned}$$

where w is the liquid water ($0.0 < LWC < 5.0 \text{ g/m}^3$) or ice mass ($0.0 IWC < 1.0 \text{ g/m}^3$) content and m is the water or ice bulk density ($\rho_{l,i}=1.0 \text{ g/cm}^3$ and 0.916 g/cm^3 , respectively).

¹We denote liquid water and ice particles, either suspended or precipitating, in the air as hydrometeors.

²See *Brussaard and Watson [1995]*, page 81, for details.

The difference between liquid water and ice absorption is put in the expressions for the complex permittivities (i. e. the relative dielectric constant), $\epsilon_r = \epsilon_r' + i \cdot \epsilon_r''$, which depend on frequency and temperature.

- Complex permittivity for suspended liquid water droplets:

$$\begin{aligned}\epsilon_r' &= \epsilon_o - \nu^2 \cdot \left[\frac{\epsilon_o - \epsilon_1}{\nu^2 + \gamma_1^2} + \frac{\epsilon_1 - \epsilon_2}{\nu^2 + \gamma_2^2} \right] \\ \epsilon_r'' &= \nu \cdot \left[\gamma_1 \cdot \frac{\epsilon_o - \epsilon_1}{\nu^2 + \gamma_1^2} + \gamma_2 \cdot \frac{\epsilon_1 - \epsilon_2}{\nu^2 + \gamma_2^2} \right] \\ \epsilon_o &= 77.66 + 103.3 \cdot (\Theta - 1)\end{aligned}\tag{3.2}$$

$$\epsilon_1 = 0.0671 \cdot \epsilon_o$$

$$\epsilon_2 = 3.52$$

$$\gamma_1 = 20.20 - 146 \cdot (\Theta - 1) + 316 \cdot (\Theta - 1)^2 \text{ GHz}\tag{3.3}$$

$$\gamma_2 = 39.8 \cdot \gamma_1 \text{ GHz}$$

$$\Theta = 300 \text{ K} / T$$

- Complex permittivity for ice crystals:

$$\begin{aligned}\epsilon_r' &= 3.15 \\ \epsilon_r'' &= \frac{a}{\nu} + b \cdot \nu \\ a &= (\Theta - 0.1871) \cdot \exp(17.0 - 22.1 \cdot \Theta)\end{aligned}\tag{3.4}$$

$$b = \left[\left(\frac{0.233}{1 - 0.993/\Theta} \right)^2 + \frac{6.33}{\Theta} - 1.31 \right] \cdot 10^{-5}\tag{3.5}$$

$$\Theta = 300 \text{ K} / T$$

The absorption is directly proportional to the liquid or ice water content LWC/IWC and inversely proportional to the density of a single liquid ice particle $\rho_{1,i}$. Like the mean particle radius, the liquid and ice water content have a high variability. Table 3.1 reflects this variability by summarizing different literature values for several cloud types. Additional uncertainty of this absorption term comes from two sides: (1) the difference to the Rayleigh approximation of the order of 1-6% as reported in *Li et al.* [1997] and (2) from the fit of the complex permittivity. Since $\epsilon(\nu, T)$ was fitted to measurements which were mostly performed above 0°C, the extrapolated values for $T < 0^\circ\text{C}$ for super-cooled clouds are not well established. For example in *Liebe et al.* [1991] itself two different parameterizations for the so called primary relaxation frequency (γ_1 in Equation 3.2) are given, one polynomial in Θ as presented in Equation 3.2) and an exponential function derived from theory. Although the polynomial describes the selected data better than the exponential function, this might not be true for temperatures well below 0°C. The difference in γ_1 according to these two approaches can be more than 2 GHz for very low temperatures [*Lipton et al.*, 1999]. The resulting consequences from this discrepancy for the absorption calculation at three microwave frequencies are shown in Figure 3.1. A more detailed discussion about this source of uncertainty is given in Section 3.2.

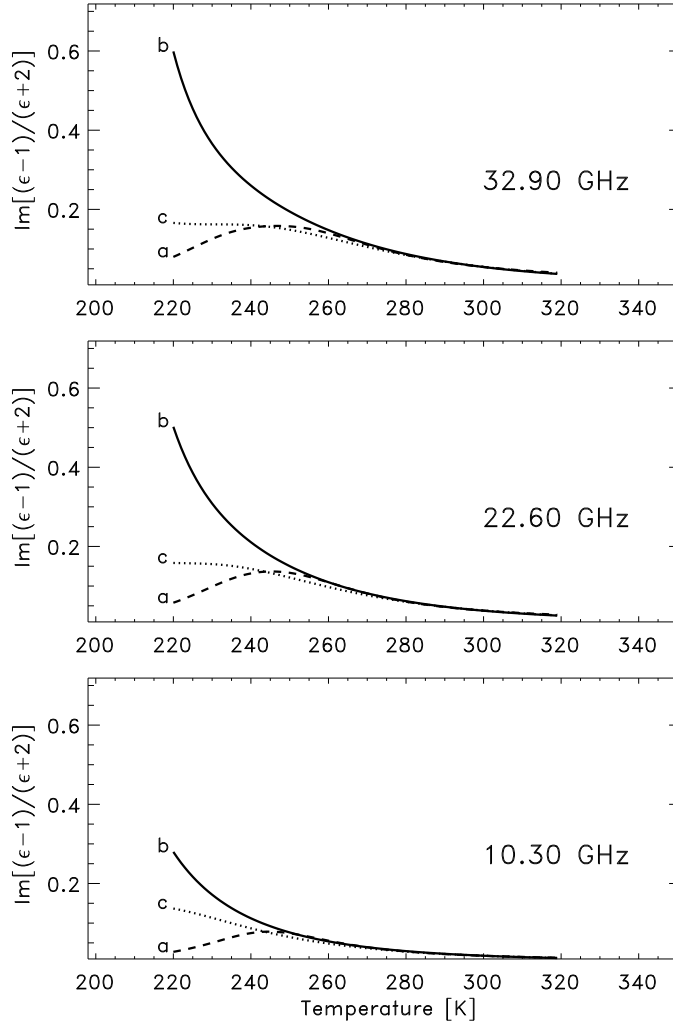


Figure 3.1: Comparison of the imaginary part of the expression $(\epsilon_r - 1)/(\epsilon_r + 2)$ for liquid water at the three frequencies of 32.9, 22.6, and 10,3 GHz. Plotted are the two common models of *Liebe et al.* [1991] (a) and *Ray* [1972] (b). The Ray parameterization is calculated with the F77 program of W. Wiscombe, NASA, GSFC, take from ftp://climate.gsfc.nasa.gov/pub/wiscombe/Refrac_Index/WATER/. Additionally the *Liebe et al.* [1991] parameterization (c) with the alternative expression for the first relaxation frequency, $\gamma_1 = 20.1 \cdot \exp [7.88 \cdot (1 - \Theta)]$, is plotted.

liquid water content (<i>LWC</i>)			
cloud	class	(g/m ³)	reference
stratus	St	0.15	<i>Salby [1996]</i>
		0.09-0.9	<i>Seinfeld and Pandis [1998]</i>
		0.28-0.3	<i>Hess et al. [1998]</i>
		0.29	<i>Kneizys et al. [1996]</i>
nimbostratus	Ns	0.4	<i>Salby [1996]</i>
		0.65	<i>Kneizys et al. [1996]</i>
		0.05-0.3	<i>Berton [2000]</i>
altostratus	As	<0.01-0.2	<i>Seinfeld and Pandis [1998]</i>
		0.41	<i>Kneizys et al. [1996]</i>
		0.1-1	<i>Berton [2000]</i>
stratocumulus	Sc	0.3	<i>Salby [1996]</i>
		<0.1-0.7	<i>Seinfeld and Pandis [1998]</i>
		0.15	<i>Kneizys et al. [1996]</i>
		<0.5	<i>Pawlowska et al. [2000]</i>
cumulus	Cu	0.05-1	<i>Berton [2000]</i>
		0.5	<i>Salby [1996]</i>
		0.26-0.44	<i>Hess et al. [1998]</i>
cumulonimbus	Cb	1.00	<i>Kneizys et al. [1996]</i>
		2.5	<i>Salby [1996]</i>
		0.1-2	<i>Berton [2000]</i>
cumulus congestus	Cg	0.1-3.2	<i>Berton [2000]</i>
FIRE-ACE	-	<0.7	<i>Shupe et al. [2000]</i>

ice water content (<i>IWC</i>)			
cloud	class	(g/m ³)	reference
cirrus	Ci	0.025	<i>Salby [1996]</i>
		0.00193-0.0260	<i>Hess et al. [1998]</i>
		$3.128 \cdot 10^{-4}$ -0.06405	<i>Kneizys et al. [1996]</i>
		0.15-0.3	<i>Larsen et al. [1998]</i>
		<0.1	<i>Berton [2000]</i>
cirrostratus	Cs	0.2	<i>Salby [1996]</i>
		0.05-2	<i>Berton [2000]</i>

Table 3.1: Stated values for the liquid and ice water content of several cloud classes from different sources.

3.2 Variability and uncertainty in cloud absorption

In the case of clouds three sources of uncertainties can be considered at first sight: (1) validity of the Rayleigh approximation (2) the parameterization of the relative dielectric constants (ϵ_r) of water and ice in the microwave region, and (3) the statistical and climatological variability of the cloud liquid water and ice content.

As it was stated above (Section 3.1) the Rayleigh approximation is valid for particle

sizes $< 500 \mu\text{m}$. Figure 3.2 shows a particle size distribution for water clouds and ice clouds (cirrus) from the OPAC model [Hess *et al.*, 1998]. According to this model only cirrus clouds will have particles of size larger than $500 \mu\text{m}$. Nevertheless one has to keep in mind that the variability of the particle size can be very high so that at certain conditions some cloud types (most probable is the cumulonimbus) a non-negligible large particle concentration can occur.

The uncertainty in the relative dielectric constant of water (see e. g. Lipton *et al.* [1999]) is largest below the freezing temperature, since only a few measurements at -4°C contributed to the parameterization of ϵ_r in Liebe *et al.* [1991], which in turn is used in the cloud liquid water absorption model of MPM93. Figure 3.1 shows a comparison of Liebe *et al.* [1991] and Ray [1972]³ parameterizations for the temperature dependence of the expression $\text{Im}[(\epsilon_r - 1)/(\epsilon_r + 2)]$, which is in the Rayleigh approximation one of the relevant terms in the absorption calculation (see Equation 3.1). Additionally the same calculations with the alternative expression of the first relaxation frequency, γ_1 , as stated in Equation 2b of Liebe *et al.* [1991] is shown. The three versions give comparable results for temperatures warmer than 260 K but show significant differences for temperatures below 240 K. However, an uncertainty estimation of $\text{Im}[(\epsilon_r - 1)/(\epsilon_r + 2)]$ is due to the lack of measurements not easy, but it will certainly increase with decreasing temperature.

The largest variability of the involved quantities of cloud absorption is the liquid and ice water content (LWC and IWC) of the clouds (see Table 3.1). Even within a single cloud the LWC (IWC) changes with altitude and the distance from the cloud center as can be seen for example in Figure 10 of Ludlam and Mason [1957] and in the model study of Costa *et al.* [2000].

³The calculations for this parameterization are performed with the computer code of W. Wiscombe, NASA, GSFC (ftp://climate.gsfc.nasa.gov/pub/wiscombe/Refrac_Index/WATER/) For the microwave frequency range this program uses the Ray [1972] temperature parameterization.

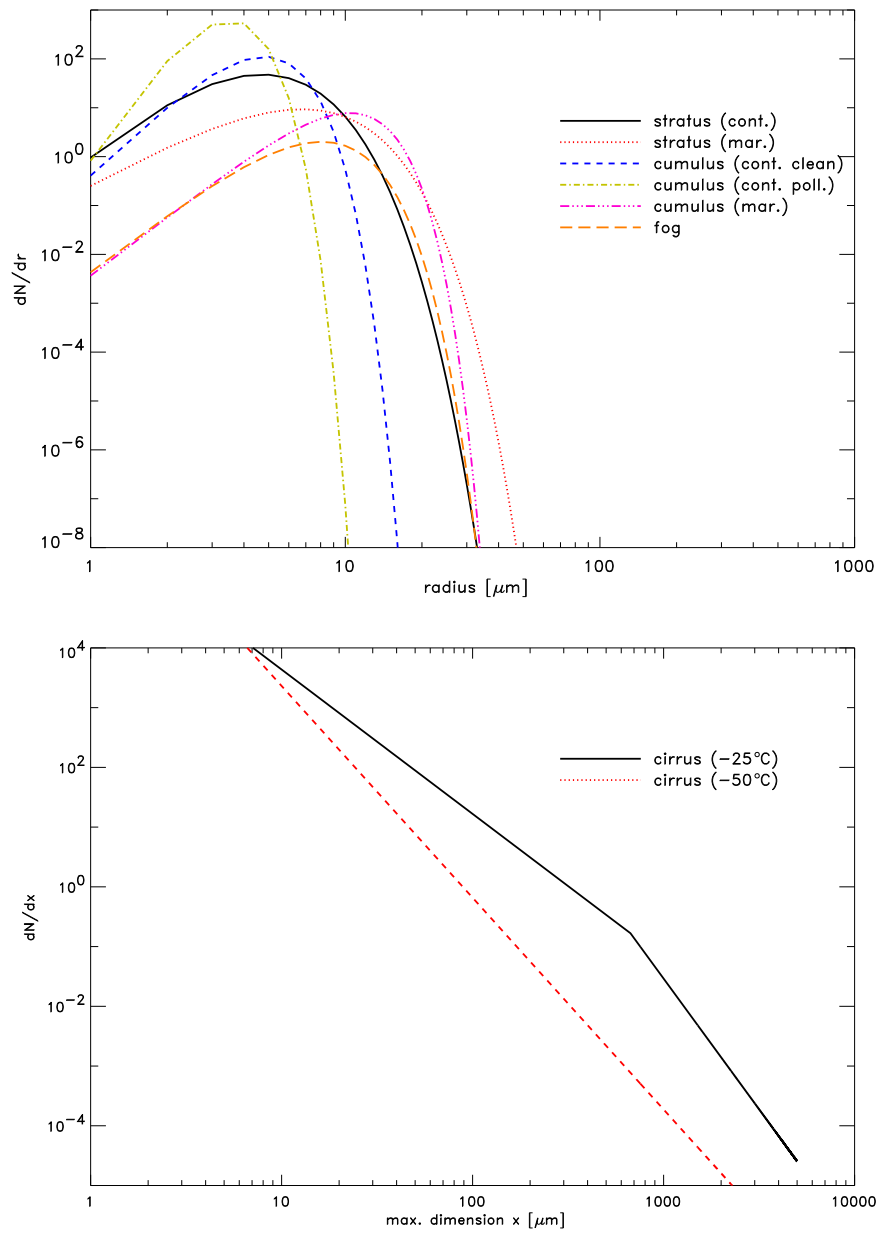


Figure 3.2: Cloud particle size distributions according to Equations 3a and 3c and the microphysical properties are from the Tables 1a and 1b of the OPAC model [Hess *et al.*, 1998]. For the liquid water clouds (upper plot) a modified gamma distribution is assumed whereas for the ice clouds (lower plot) exponential functions are taken.

Chapter 4

Polarisation and Stokes parameters

The present version of ARTS implements the radiative transfer equation in tensor form, i.e., for the 4 components of the Stokes vector, not just for its first component, the intensity or radiance. This means that the model can include polarisation dependence in absorption or scattering processes. It is therefore necessary to give some details on the polarisation of radiation, the definition of the Stokes parameters, and the definition of antenna polarisation.

4.1 Polarisation directions

Electromagnetic waves in homogeneous, isotropic media are transverse waves, i.e., their oscillating electric and magnetic fields are in a plane perpendicular to the propagation direction. The choice of two basis vectors – we shall call them polarisation directions here – that span that transverse plane is arbitrary; often they are called “horizontal” and “vertical” and correspond to some horizontal and vertical direction of the particular setting. Nevertheless, what is meant by horizontal/vertical, or parallel/perpendicular, is purely a matter of definition.

Here, we stick to the system called laboratory frame or fixed frame, used by *Mishchenko et al.* [2002]: We use a coordinate system where the z -axis points toward local zenith. We denote the propagation direction of radiation by a unit vector $\mathbf{n} = \mathbf{k}/k$, where k is the wave number. \mathbf{n} is given by two angles, the zenith angle θ , i.e., the angle between \mathbf{n} and the z -axis, and the azimuth angle ϕ , i.e., the angle between the projection of \mathbf{n} into the xy -plane and the x -axis:

$$\mathbf{n} = \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix} \quad (4.1)$$

Then we define the polarisation directions by the partial derivatives of \mathbf{n} with respect to θ and ϕ . We shall call them θ -direction (also: vertical) and ϕ -direction (also: horizontal), respectively, see Figure 4.1. Their unit basis vectors are

History

040524 Section on scattering matrices added by Patrick Eriksson.

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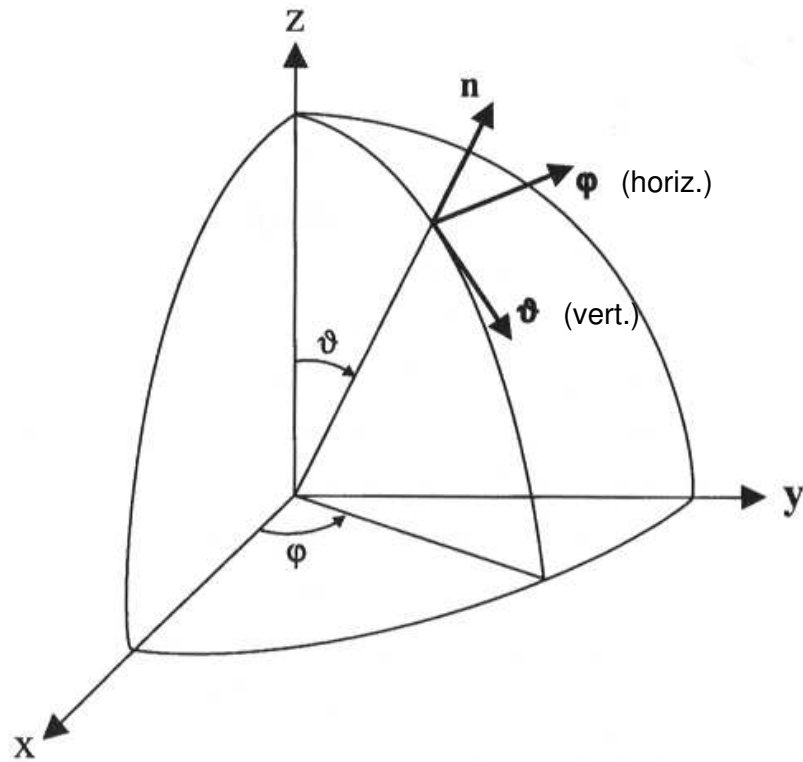


Figure 1 Laboratory coordinate system.

Figure 4.1: The definition of the polarisation directions, adapted from *Mishchenko et al.* [2002]

$$\mathbf{e}_\theta = \mathbf{e}_v = \frac{\partial \mathbf{n}}{\partial \theta} / \left\| \frac{\partial \mathbf{n}}{\partial \theta} \right\| = \begin{pmatrix} \cos \phi \cos \theta \\ \sin \phi \cos \theta \\ \sin \theta \end{pmatrix} \quad (4.2)$$

$$\mathbf{e}_\phi = \mathbf{e}_h = \frac{\partial \mathbf{n}}{\partial \phi} / \left\| \frac{\partial \mathbf{n}}{\partial \phi} \right\| = \begin{pmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{pmatrix} \quad (4.3)$$

The vectors \mathbf{n} , \mathbf{e}_θ ($=\mathbf{e}_v$), \mathbf{e}_ϕ ($=\mathbf{e}_h$) are mutually orthogonal and define (in the mentioned order) a right-handed system, i.e., $(\mathbf{n} \times \mathbf{e}_\theta) \cdot \mathbf{e}_\phi = 1$ and the same for all cyclic permutations.

4.2 Plane monochromatic waves

Plane monochromatic electromagnetic waves are commonly written in the form

$$\mathbf{E}(\mathbf{x}, t) = \begin{bmatrix} E_v \\ E_h \end{bmatrix} e^{i(\mathbf{kx} - \omega t)} = (E_v \mathbf{e}_v + E_h \mathbf{e}_h) e^{i(\mathbf{kx} - \omega t)} \quad (4.4)$$

where \mathbf{E} is the electric field vector, the subscripts v and h denote the components with vertical and horizontal polarisation, respectively. E_v and E_h , the amplitudes, are complex numbers, \mathbf{k} and ω are the wavenumber vector and the angular frequency, respectively, of the plane wave, and the unit vectors $\mathbf{e}_v = (1, 0)^T$, $\mathbf{e}_h = (0, 1)^T$. It is always implicitly understood that the actual, physical, electric field is the real part of the above expression. Rewriting the complex amplitudes E_v and E_h using real, non-negative amplitudes a_v and a_h , and phases δ_v and δ_h ,

$$E_v = a_v e^{i\delta_v}, E_h = a_h e^{i\delta_h} \quad (4.5)$$

the actual electric field vector $\tilde{\mathbf{E}}$ is

$$\tilde{\mathbf{E}}(\mathbf{x}, t) = \text{Re}[\mathbf{E}(\mathbf{x}, t)] = \begin{bmatrix} a_v \cdot \cos(\mathbf{kx} - \omega t + \delta_v) \\ a_h \cdot \cos(\mathbf{kx} - \omega t + \delta_h) \end{bmatrix} \quad (4.6)$$

In general, instruments do not measure the electric or magnetic field vectors of an electromagnetic wave, but rather the time-averaged intensity, i.e., the energy flux, F . This is the time-averaged Poynting vector (which, in turn, is proportional to the square of the electric field), thus:

$$\begin{aligned} F &= \sqrt{\frac{\epsilon}{\mu}} \overline{(\tilde{\mathbf{E}}(\mathbf{x}, t))^2} \\ &= \sqrt{\frac{\epsilon}{\mu}} \left(\overline{a_v^2 \cos^2(\mathbf{kx} - \omega t + \delta_v)} + \overline{a_h^2 \cos^2(\mathbf{kx} - \omega t + \delta_h)} \right) \end{aligned} \quad (4.7)$$

The overline denotes the time average which for cosine squares is $1/2$, thus:

$$F = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (a_v^2 + a_h^2) \quad (4.8)$$

Taking into account that for plane, monochromatic waves the time average always results in a factor $\frac{1}{2}$, we can also directly write the intensity using the electric field vector in complex notation (Equation 4.4).

$$\begin{aligned} F &= \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \mathbf{E}(\mathbf{x}, t) \cdot \mathbf{E}^*(\mathbf{x}, t) \\ &= \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_v^* + E_h E_h^*) \end{aligned} \quad (4.9)$$

where the asterisk denotes complex conjugation.

In addition to the flux, three more intensity quantities are defined as in the following equations. They are called *Stokes parameters*:

$$I = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_v^* + E_h E_h^*) \quad (4.10)$$

$$Q = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_v^* - E_h E_h^*) \quad (4.11)$$

$$U = -\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_h^* + E_h E_v^*) \quad (4.12)$$

$$V = i \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_h E_v^* - E_v E_h^*) \quad (4.13)$$

Written as a row or column vector, (I, Q, U, V) is called *Stokes vector*. Note that sometimes, S_0, S_1, S_2, S_3 is used instead of I, Q, U, V . Using the amplitude/phase notation from Equation 4.5, we can rewrite the Stokes parameters as

$$I = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (a_v^2 + a_h^2) \quad (4.14)$$

$$Q = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (a_v^2 - a_h^2) \quad (4.15)$$

$$U = -\sqrt{\frac{\epsilon}{\mu}} a_v a_h \cos(\delta_v - \delta_h) \quad (4.16)$$

$$V = -\sqrt{\frac{\epsilon}{\mu}} a_v a_h \sin(\delta_v - \delta_h) \quad (4.17)$$

The Stokes parameters fully characterise the electromagnetic wave and therefore contain the same information as the electric field vector (except for one absolute phase). Since instruments generally measure intensities (fluxes), describing electromagnetic radiation by the Stokes parameters is more practical than describing it by the electric (or magnetic) field vector. Furthermore, the Stokes parameters are always real numbers. Note that the Stokes parameters are sometimes defined with different signs of Q, U, V (the definitions and signs used here are based on *Mishchenko et al.* [2000]). Moreover, their normalisation may vary. In particular, the Stokes parameters can be normalised to represent radiance or irradiance (instead of intensity), which is usually done in radiative transfer contexts.

In order to understand what the Stokes parameters mean, we have to go back to the electric field vector and see what polarisation state it describes. To do so, we look at the curve that the tip of the physical electric field vector $\tilde{\mathbf{E}}$ describes with time at a fixed position \mathbf{x}_0 :

$$\tilde{E}_v(t) = a_v \cos(\Delta_v - \omega t) \quad (4.18)$$

$$\tilde{E}_h(t) = a_h \cos(\Delta_h - \omega t) \quad (4.19)$$

where $\Delta_{v,h} = \mathbf{kx}_0 + \delta_{v,h}$. To see that this is an ellipse, we first split the cosines using the addition theorem:

$$\tilde{E}_v(t) = a_v \cos \Delta_v \cos(\omega t) + a_v \sin \Delta_v \sin(\omega t) \quad (4.20)$$

$$\tilde{E}_h(t) = a_h \cos \Delta_h \cos(\omega t) + a_h \sin \Delta_h \sin(\omega t) \quad (4.21)$$

In order to have the tip of $\tilde{\mathbf{E}}$ describe an ellipse with semi-major axis $a_0 \cos \beta$ and semi-minor axis $a_0 \sin \beta$, where $a_0^2 = a_v^2 + a_h^2$, it should have the following form

$$\tilde{E}_v(t) = a_0 \sin \beta \cos(\omega t) \quad (4.22)$$

$$\tilde{E}_h(t) = a_0 \cos \beta \sin(\omega t) \quad (4.23)$$

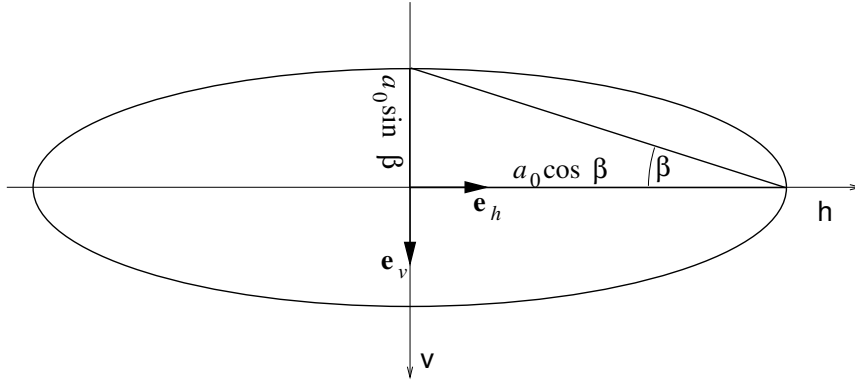


Figure 4.2: The ellipse that the electric field vector describes with time, with the major axis oriented along the h -axis.

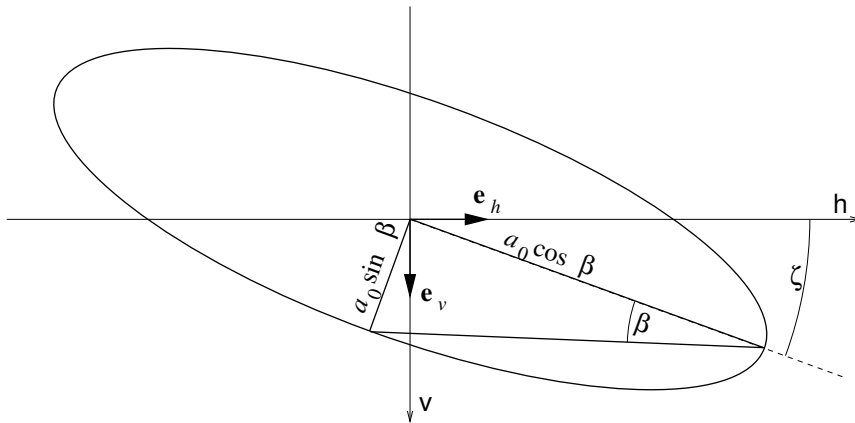


Figure 4.3: The ellipse that the electric field vector describes with time, with the major axis oriented arbitrarily.

Here β must be between -45° and 45° : the tip of the vector $\tilde{\mathbf{E}}$ describes a circle for $\beta = \pm 45^\circ$ (circular polarisation), oscillates along the h -axis for $\beta = 0$ (linear polarisation) and else describes an ellipse (cf. Figure 4.2). The sense of rotation is counterclockwise for positive β (corresponding to left-circular or left-elliptic polarisation) and clockwise for negative β (corresponding to right-circular or right-elliptic polarisation). Since $|\tan \beta|$ is the ratio of the semi-minor and semi-major axes of the ellipse (the ellipticity), β is called the ellipticity angle. Note that the semi-major axis is oriented along the positive h -axis. To have the major axis of the ellipse enclose an arbitrary angle ζ ($0 \leq \zeta < 180^\circ$) with the h -axis, we apply a rotation matrix and get the equation for an ellipse with arbitrary shape (ellipticity) and orientation (cf. Figure 4.3):

$$\tilde{E}_v(t) = a_0(\sin \beta \cos(\omega t) \cos \zeta + \cos \beta \sin(\omega t) \sin \zeta) \quad (4.24)$$

$$\tilde{E}_h(t) = a_0(-\sin \beta \cos(\omega t) \sin \zeta + \cos \beta \sin(\omega t) \cos \zeta) \quad (4.25)$$

With these definitions, horizontal polarisation corresponds to $\beta = 0^\circ$ and $\zeta = 0^\circ$; vertical

polarisation to $\beta = 0^\circ$ and $\zeta = 90^\circ$; left-circular to $\beta = 45^\circ$ and any value of ζ ; right-circular to $\beta = -45^\circ$ and any value of ζ .

Now we want to establish a direct connection between the parameters β and ζ describing the shape (ellipticity) and orientation of the polarisation ellipse on the one hand, and the amplitudes a_v and a_h and phases δ_v and δ_h of the components of the electric field vector on the other hand. Comparing the $\sin(\omega t)$ and $\cos(\omega t)$ terms in Equations 4.24 to 4.25 with the corresponding terms in Equations 4.20 to 4.21, we get:

$$a_v \cos \Delta_v = a_0 \sin \beta \cos \zeta \quad (4.26)$$

$$a_v \sin \Delta_v = a_0 \cos \beta \sin \zeta \quad (4.27)$$

and

$$a_h \cos \Delta_h = -a_0 \sin \beta \sin \zeta \quad (4.28)$$

$$a_h \sin \Delta_h = a_0 \cos \beta \cos \zeta \quad (4.29)$$

Multiplying Equation 4.26 with Equation 4.28, and Equation 4.27 with Equation 4.29 and adding up the results, we get

$$a_v a_h (\cos \Delta_v \cos \Delta_h + \sin \Delta_v \sin \Delta_h) = a_0^2 \sin \zeta \cos \zeta (\cos^2 \beta - \sin^2 \beta) \quad (4.30)$$

Using the addition theorems for sinusoidals and taking into account that $\Delta_v - \Delta_h = \delta_v - \delta_h$:

$$\frac{a_v a_h}{a_0^2} \cos(\delta_v - \delta_h) = \frac{1}{2} \sin(2\zeta) \cos(2\beta) \quad (4.31)$$

In a similar way, subtracting the product of Equation 4.27 with Equation 4.28 from the product of Equation 4.26 with Equation 4.29 and adding up the results, we get

$$-\frac{a_v a_h}{a_0^2} \sin(\delta_v - \delta_h) = \frac{1}{2} \sin(2\beta) \quad (4.32)$$

The above two equations tell us how to translate the amplitudes (a_v, a_h) and phases (δ_v, δ_h) of the vertical and horizontal component of the electric field into the orientation and shape of the ellipse that the tip of the electric field vector describes with time. We can obtain one further relation by subtracting the sum of the squares of Equation 4.28 and Equation 4.29 from the sum of the squares of Equation 4.26 and Equation 4.27:

$$a_v^2 - a_h^2 = -a_0^2 \cos(2\zeta) \cos(2\beta) \quad (4.33)$$

Finally, we use the above 3 equations (4.31, 4.32 and 4.33) to rewrite the Stokes parameters (Equations 4.14 to 4.17) as

$$I = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} a_0^2 \quad (4.34)$$

$$Q = -\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} a_0^2 \cos(2\zeta) \cos(2\beta) \quad (4.35)$$

$$U = -\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} a_0^2 \sin(2\zeta) \cos(2\beta) \quad (4.36)$$

$$V = -\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} a_0^2 \sin(2\beta) \quad (4.37)$$

FIXME: $\beta < 0$ is right-handed pol. (see above, consistent with Jackson and others); thus $V > 0$. This conflicts with Mishchenko's book (p.26).

Thus, we can get the orientation angle ζ of the ellipse from

$$\tan(2\zeta) = \frac{U}{Q} \quad (4.38)$$

Since $0 \leq 2\zeta < 360^\circ$, there are 2 solutions for ζ for a given pair U, Q . This ambiguity is resolved by looking at Equation 4.35, taking into account that $|\beta| \leq 45^\circ$ and thus $\cos(2\beta) \geq 0$: The sign of $\cos(2\zeta)$ must be the same as the sign of $-Q$.

We get the ellipticity angle β from

$$\tan(2\beta) = -\frac{V}{(Q^2 + U^2)^{1/2}} \quad (4.39)$$

I is the total intensity of the radiation, Q is the difference in the intensity of the vertically and horizontally polarised components (cf. Section 4.3). I is always non-negative, and Q, U , and V are between $+I$ and $-I$, since they can be expressed as a product of I with sines and/or cosines (Equations 4.35 to 4.37). Note also that the 4 Stokes parameters are not independent (for completely polarised radiation, see further Section 4.4), since the following equality applies:

$$I^2 = Q^2 + U^2 + V^2 \quad (4.40)$$

Some examples of Stokes parameters for specific polarisations are given at the end of the next section (page 48).

4.3 Measuring Stokes parameters

The three different ways given so far to write the Stokes parameters (Equations 4.10ff., Equations 4.14ff., Equations 4.34ff.) are not very helpful if we actually want to measure the Stokes parameters. So here we are going to rewrite them while keeping in mind that most instruments can just measure intensities of radiation.

We have seen above that the Stokes parameter Q is the difference in the intensity of the vertically and horizontally polarised components (Equations 4.11, or 4.15)

$$Q = I_v - I_h \quad (4.41)$$

where

$$I_v = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_v E_v^* \quad (4.42)$$

$$I_h = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_h E_h^* \quad (4.43)$$

Thus if we measure I_v and I_h using – for optical wavelengths – a polariser aligned with the v - and the h -axis, respectively, or using – for microwaves – two appropriately aligned dipole antennas, we can directly obtain I by taking their sum and Q by taking their difference.

U and V can likewise be expressed as differences of intensities, but not with respect to the linear base \mathbf{e}_v and \mathbf{e}_h . We recall Equation 4.4, omitting the oscillatory term:

$$\mathbf{E} = (E_v \mathbf{e}_v + E_h \mathbf{e}_h) \quad (4.44)$$

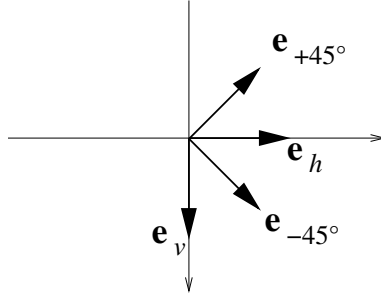


Figure 4.4: Two sets of basis vectors for the linear basis.

Now we want to write \mathbf{E} by two components along polarisation axes at $\pm 45^\circ$ with respect to the h -axis. The basis vectors are thus (cf. Figure 4.4)

$$\mathbf{e}_{+45^\circ} = \sqrt{\frac{1}{2}}(\mathbf{e}_h - \mathbf{e}_v) \quad (4.45)$$

$$\mathbf{e}_{-45^\circ} = \sqrt{\frac{1}{2}}(\mathbf{e}_h + \mathbf{e}_v) \quad (4.46)$$

and we get the field vector in this modified linear basis:

$$\mathbf{E} = \underbrace{\sqrt{\frac{1}{2}}(E_v + E_h)}_{E_{-45^\circ}} \mathbf{e}_{-45^\circ} + \underbrace{\sqrt{\frac{1}{2}}(-E_v + E_h)}_{E_{+45^\circ}} \mathbf{e}_{+45^\circ} \quad (4.47)$$

With the definitions of intensities of the components,

$$I_{-45^\circ} = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_{-45^\circ} E_{-45^\circ}^* \quad (4.48)$$

$$I_{+45^\circ} = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_{+45^\circ} E_{+45^\circ}^* \quad (4.49)$$

we get for their difference:

$$\begin{aligned} I_{-45^\circ} - I_{+45^\circ} &= \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \left[\frac{1}{2} (E_v + E_h)(E_v^* + E_h^*) - \frac{1}{2} (-E_v + E_h)(-E_v^* + E_h^*) \right] \\ &= \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_h^* + E_h E_v^*) \end{aligned}$$

Therefore (cf. Equation 4.12)

$$U = I_{+45^\circ} - I_{-45^\circ} \quad (4.51)$$

Thus if we measure I_{+45° and I_{-45° using – for optical wavelengths – a polariser aligned at $+45^\circ$ and -45° with respect to the h -axis, respectively, or using – for microwaves – two appropriately aligned dipole antennas, we can directly obtain U by taking their difference.

In order to see how to measure the fourth Stokes parameter, V , we have to transform to the circular basis, i.e., express \mathbf{E} by a left-hand (LH) and a right-hand (RH) circularly polarised component. The relevant equations:

Basis vectors

$$\mathbf{e}_{LH} = \sqrt{\frac{1}{2}}(\mathbf{e}_v + i\mathbf{e}_h) \quad (4.52)$$

$$\mathbf{e}_{RH} = \sqrt{\frac{1}{2}}(\mathbf{e}_v - i\mathbf{e}_h) \quad (4.53)$$

Field vector in circular base

$$\mathbf{E} = \underbrace{\sqrt{\frac{1}{2}}(E_v - iE_h)}_{E_{LH}} \mathbf{e}_{LH} + \underbrace{\sqrt{\frac{1}{2}}(E_v + iE_h)}_{E_{RH}} \mathbf{e}_{RH} \quad (4.54)$$

Intensity of the components

$$I_{LH} = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_{LH} E_{LH}^* \quad (4.55)$$

$$I_{RH} = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_{RH} E_{RH}^* \quad (4.56)$$

Their difference

$$\begin{aligned} I_{LH} - I_{RH} &= \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \left[\frac{1}{2} (E_v - iE_h)(E_v^* + iE_h^*) - \frac{1}{2} (E_v + iE_h)(E_v^* - iE_h^*) \right] \\ &= i \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} (E_v E_h^* - E_h E_v^*) \end{aligned} \quad (4.57)$$

Therefore (cf. Equation 4.13):

$$V = I_{RH} - I_{LH} \quad (4.58)$$

Thus if we measure I_{RH} and I_{LH} using – for microwaves – appropriate helical beam antennas, we can directly obtain V by taking their difference. Unfortunately, for optical wavelengths, we cannot measure I_{RH} and I_{LH} directly with the help of filters like polarisers and retarders¹. However, a combination of a retarder and a polarizer can be used to measure the sum of I and V :

The light first passes through a retarder that delays the phase of the horizontally polarised component by 90° with respect to the phase of the vertically polarised component (a quarter-wave plate). A phase delay by 90° can be expressed as a multiplication of the horizontal component by i , so the resulting electric field vector \mathbf{E}' is

$$\mathbf{E}' = (E_v \mathbf{e}_v + iE_h \mathbf{e}_h) \quad (4.59)$$

The light then passes through a polarizer that is aligned at -45° with respect to the h -axis. This means we have to project \mathbf{E}' onto \mathbf{e}_{-45° , resulting in

$$\mathbf{E}'' = (\mathbf{E}' \cdot \mathbf{e}_{-45^\circ}) \mathbf{e}_{-45^\circ} = \sqrt{\frac{1}{2}} (E_v + iE_h) \mathbf{e}_{-45^\circ} \quad (4.60)$$

Measuring the intensity now, we get

$$\begin{aligned} I'' &= |\mathbf{E}''|^2 \\ &= \frac{1}{2} (E_v + iE_h) (E_v^* - iE_h^*) \\ &= \frac{1}{2} (|E_v|^2 + |E_h|^2 - i(E_v E_h^* - E_h E_v^*)) \\ &= \frac{1}{2} (I + V) \end{aligned} \quad (4.61)$$

Here is a summary of the Stokes parameters in terms of intensities of orthogonal components:

$$I = I_v + I_h = I_{-45^\circ} + I_{+45^\circ} = I_{RH} + I_{LH} \quad (4.62)$$

$$Q = I_v - I_h \quad (4.63)$$

$$U = I_{+45^\circ} - I_{-45^\circ} \quad (4.64)$$

$$V = I_{RH} - I_{LH} \quad (4.65)$$

¹A retarder allows the phase of two orthogonal components of light to be varied with respect to each other.

We see that Q and U are both related to linear polarisation, while V is related to circular polarisation.

Here are the Stokes parameters for some standard polarisations:

polarisation	(I, Q, U, V)
horizontal	$(I, -I, 0, 0)$
vertical	$(I, +I, 0, 0)$
linear $\pm 45^\circ$	$(I, 0, \mp I, 0)$
right-circular	$(I, 0, 0, I)$
left-circular	$(I, 0, 0, -I)$

4.4 Partial polarisation

The equality $I^2 = Q^2 + U^2 + V^2$ (Equation 4.40) is valid for the ideal case of a monochromatic plane wave that is completely polarised, i.e., where the amplitudes a_v and a_h and the phases δ_v and δ_h are fixed and do not vary with time. This means that the plane wave is emitted by one coherent source.

In reality, i.e., in the case of natural radiation, the amplitudes and phases fluctuate, since the radiation originates from several sources that do not emit radiation coherently, and since the emission from one source usually has very short coherence times. This means that we usually have a superposition of radiation from several incoherent sources, and that the polarisation state of the radiation from each source fluctuates as well². Typically, such fluctuations have time scales that are longer than the period ($2\pi/\omega$) of the oscillation, but that are still shorter than the integration time of the instrument that measures the radiation. Thus, the instrument measures an incoherent superposition of time averages over of the fluctuating polarisation. If the fluctuations are random for all the sources and if the different sources emit incoherently and are not in any way oriented, then there is no preferred orientation, ellipticity or handedness of the emitted radiation, which is then called unpolarised. This is the case for radiation from the sun. If the fluctuations are not completely random, the radiation is called partially polarised.

To quantify this rather heuristic argumentation, we express the above-mentioned ideas in the language of the Stokes parameters: The Stokes parameters I, Q, U, V derived from measurements result from the superposition of radiation from many sources and/or the average over emission events with individual Stokes parameters I_i, Q_i, U_i, V_i . Since the different sources and/or emission events are incoherent, the Stokes parameters – which are intensity, not amplitude quantities – can simply be added up:

$$I = \sum_i I_i, \quad Q = \sum_i Q_i, \quad U = \sum_i U_i, \quad V = \sum_i V_i \quad (4.66)$$

In the case of unpolarised radiation, i.e., when the amplitudes and phases, or equivalently, the orientation angle ζ and the ellipticity angle β are random (uniformly distributed), $Q, U,$ and V each cancel out.

The equality $I_i^2 = Q_i^2 + U_i^2 + V_i^2$ (cf. Equation 4.40) still holds for each contribution i , but for the resulting I, Q, U, V , we have in general the inequality

$$I^2 \geq Q^2 + U^2 + V^2 \quad (4.67)$$

²This does, of course, not apply to coherent sources like lasers or coherent radars.

To prove it, we must once again go back to the amplitude/phase notation (Equations 4.14ff.), also cf. *Chandrasekhar* [1960, chap. I.15], but we shall omit the factor $\frac{1}{2}\sqrt{\frac{\epsilon}{\mu}}$ on the right-hand sides, for the sake of better readability:

$$I = \sum_i I_i = \sum_i \left(a_v^{(i)}\right)^2 + \sum_i \left(a_h^{(i)}\right)^2 \quad (4.68)$$

$$Q = \sum_i Q_i = \sum_i \left(a_v^{(i)}\right)^2 - \sum_i \left(a_h^{(i)}\right)^2 \quad (4.69)$$

$$U = \sum_i U_i = -2 \sum_i a_v^{(i)} a_h^{(i)} \cos \delta^{(i)} \quad (4.70)$$

$$V = \sum_i V_i = 2 \sum_i a_v^{(i)} a_h^{(i)} \sin \delta^{(i)} \quad (4.71)$$

$$(4.72)$$

where $\delta^{(i)} = \delta_v^{(i)} - \delta_h^{(i)}$. We get

$$\begin{aligned} I^2 - Q^2 - U^2 - V^2 &= 4 \sum_i \left(a_v^{(i)}\right)^2 \sum_i \left(a_h^{(i)}\right)^2 \\ &\quad - 4 \left(\sum_i a_v^{(i)} a_h^{(i)} \cos \delta^{(i)} \right)^2 \\ &\quad - 4 \left(\sum_i a_v^{(i)} a_h^{(i)} \sin \delta^{(i)} \right)^2 \end{aligned} \quad (4.73)$$

The first term on the right-hand side can be rearranged as

$$\sum_i \left(a_v^{(i)} a_h^{(i)}\right)^2 + \sum_{\substack{i,j \\ i \neq j}} \left(a_v^{(i)} a_h^{(j)}\right)^2 \quad (4.74)$$

The other two terms can be rearranged similarly to yield:

$$\begin{aligned} & - \sum_i \left(a_v^{(i)} a_h^{(i)}\right)^2 \left[\cos^2 \delta^{(i)} + \sin^2 \delta^{(i)} \right] \\ & - \sum_{\substack{i,j \\ i \neq j}} a_v^{(i)} a_h^{(i)} a_v^{(j)} a_h^{(j)} \left[\cos \delta^{(i)} \cos \delta^{(j)} + \sin \delta^{(i)} \sin \delta^{(j)} \right] \end{aligned} \quad (4.75)$$

Putting this into Equation 4.73 (and dividing by 4), the sums over just i cancel and we get:

$$\begin{aligned} (I^2 - Q^2 - U^2 - V^2)/4 &= \sum_{\substack{i,j \\ i \neq j}} \left(a_v^{(i)} a_h^{(j)}\right)^2 \\ &\quad - \sum_{\substack{i,j \\ i \neq j}} a_v^{(i)} a_h^{(i)} a_v^{(j)} a_h^{(j)} \cos(\delta^{(i)} - \delta^{(j)}) \end{aligned} \quad (4.76)$$

where the cosine addition theorem was used. In the summation, we now change from $i \neq j$ to $i < j$, so we have to symmetrise the first term (the second term is already symmetric with

respect to i and j and therefore just gets a factor 2):

$$(I^2 - Q^2 - U^2 - V^2)/4 = \sum_{\substack{i,j \\ i < j}} \left[\left(a_v^{(i)} a_h^{(j)} \right)^2 + \left(a_v^{(j)} a_h^{(i)} \right)^2 - 2 \left(a_v^{(i)} a_h^{(j)} \right) \left(a_v^{(j)} a_h^{(i)} \right) \cos(\delta^{(i)} - \delta^{(j)}) \right] \quad (4.77)$$

Each summand of the sum on the right-hand side is positive, since it is greater than or equal to $(a_v^{(i)} a_h^{(j)} - a_v^{(j)} a_h^{(i)})^2$, which completes the proof. The right-hand side vanishes only if $\delta^{(i)} = \delta^{(j)}$ and $a_v^{(i)}/a_h^{(i)} = a_v^{(j)}/a_h^{(j)}$ for all i, j , i.e., if the phase difference and amplitude ratio between the horizontal and vertical component of the electric field is the same for all contributions, in other words: if all contributions have the same polarisation.

For completeness, we shall now restate the definition of the Stokes component, extended to include natural radiation (i.e., including the case of partially polarised and unpolarised radiation). Instead of summing over the individual emission events, we use ensemble averages, denoted by angular brackets:

$$I = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \langle E_v E_v^* + E_h E_h^* \rangle \quad (4.78)$$

$$Q = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \langle E_v E_v^* - E_h E_h^* \rangle \quad (4.79)$$

$$U = -\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \langle E_v E_h^* - E_h E_v^* \rangle \quad (4.80)$$

$$V = i \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} \langle E_h E_v^* - E_v E_h^* \rangle \quad (4.81)$$

Except for the ensemble average $\langle \dots \rangle$, the definition is identical to the one for monochromatic, plane waves (Equations 4.10 to 4.13). The same applies to the second and third definitions of the Stokes parameters (Equations 4.14 to 4.17 and Equations 4.34 to 4.37, respectively). Note that the fourth definition (Equations 4.62 to 4.65) which uses sums and differences of intensities, is equally valid for fully polarised, partially polarised and unpolarised radiation. The definition of intensities, however, has to include the ensemble average: $I_h = \langle E_h E_h^* \rangle$ etc.

Now we can define a measure for the degree of polarisation, p , as:

$$p = \frac{\sqrt{Q^2 + U^2 + V^2}}{I} \quad (4.82)$$

For completely polarised radiation, $Q^2 + U^2 + V^2 = I^2$, so $p = 1$, and for unpolarised radiation, $Q = U = V = 0$, so $p = 0$.

Furthermore, it can be convenient to define the polarised component of radiation by

$$I_p^2 = Q^2 + U^2 + V^2 \quad (4.83)$$

and the unpolarised component as

$$I_u = I - I_p \quad (4.84)$$

Thus, partially polarised radiation, described by a Stokes vector (I, Q, U, V) , can be regarded as a superposition of completely polarised radiation described by the Stokes vector (I_p, Q, U, V) and unpolarised radiation described by the Stokes vector $(I_u, 0, 0, 0)$. We

see that the Stokes parameter formalism can conveniently deal with partially polarised and with unpolarised radiation, much in contrast to the formalism using the electric field (amplitude and phase).

In addition to the degree of polarisation, p , we can define measures for the circularity and the linearity of the polarisation. Recalling Equations 4.64 and 4.65, we can define the degree of linear polarisation, p_{lin} , as

$$p_{lin} = \frac{\sqrt{Q^2 + U^2}}{I} \quad (4.85)$$

and the the degree of circular polarisation, p_{circ} , as

$$p_{circ} = \frac{V}{I} \quad (4.86)$$

4.4.1 Polarisation of Radiation in the Atmosphere

The radiation encountered in atmospheric sounding (for which ARTS is intended) is natural radiation, coming from the sun, space (cosmic background), and/or the atmosphere and the Earth surface (thermal radiation, scattered radiation)³. Radiation from the sun is unpolarised, as already mentioned; the same applies for the cosmic background. In contrast, radiation emitted by the ground can be polarised, dependent on material, texture and direction. Radiation emitted by the atmosphere (thermal radiation) is almost unpolarised because of the random orientation of the air molecules. An exception is caused by the Zeeman effect induced in oxygen molecules by the – anisotropic – Earth’s magnetic field. Scattering of radiation by oriented particles, e.g. cirrus clouds, is sensitive to polarisation, and generally increases the degree of polarisation. Typically $I > |Q| > |U|, |V|$.

4.4.2 Antenna polarisation

Finally we want to know what an antenna of arbitrary polarisation response (antenna polarisation) measures if radiation of some other arbitrary polarisation is incident on it.

In order to clarify the concept, we first consider some trivial examples: We assume an antenna that receives only vertically polarised radiation.

- If the incident radiation is fully horizontally polarised, the antenna will measure nothing.
- If the incident radiation is fully vertically polarised, the antenna will measure the full intensity of the radiation.
- If the radiation is fully left- or right-circularly polarised, the antenna will measure half of the full intensity, for circularly polarised radiation is made up of equal portions of vertically and horizontally polarised radiation, superimposed with a phase lag of 90° .

In order to be able to describe the general case, we first have to formalise the description of the antenna polarisation. Polarised radiation is described by

1. the Jones vector, or

³This is not so for active sounding techniques that use a coherent source, such as lidar.

2. the Stokes vector, or
3. intensity, I , orientation angle, ζ (i.e., the angle between the major axis of the polarisation ellipse and the horizontal polarisation direction), and ellipticity angle, β (see page 43).

Since the intensity of the radiation is the absolute square (the squared “length”) of the complex Jones vector, or, in other words, the first Stokes component, I , the polarisation alone is defined by

1. a normalised Jones vector, or
2. three normalised Stokes components Q , U , and V (where $Q^2 + U^2 + V^2 = 1$), or
3. the orientation angle ζ and the ellipticity angle β (see Equation 4.38 to 4.39).

In the same way, the polarisation of the antenna can be described in one of three ways:

1. a normalised Jones vector

$$\mathbf{e} = \begin{bmatrix} e_v \\ e_h \end{bmatrix} \quad \text{where} \quad \mathbf{e} \cdot \mathbf{e}^* = 1 \quad (4.87)$$

(note that in the scalar product of two complex vectors, the second one has to be complex-conjugated.)

2. a normalised Stokes vector

$$\mathbf{i} = (1, q, u, v) \quad \text{where} \quad q^2 + u^2 + v^2 = 1 \quad (4.88)$$

3. the two angles ζ and β . According to Equation 4.34 to 4.37, we have:

$$q = -\cos(2\zeta) \cos(2\beta) \quad (4.89)$$

$$u = -\sin(2\zeta) \cos(2\beta) \quad (4.90)$$

$$v = -\sin(2\beta) \quad (4.91)$$

Now we can calculate the intensity I' the antenna measures. In terms of the electrical fields, i.e., Jones vectors, we just have to project the Jones vector \mathbf{E} of the incident radiation onto the normalised Jones vector \mathbf{e} of the antenna,

$$\mathbf{E}' = (\mathbf{E} \cdot \mathbf{e}^*)\mathbf{e} \quad (4.92)$$

(this is in effect like passing through a polarizer) and then take its absolute square

$$I' = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} |\mathbf{E}'|^2 = \frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} |(\mathbf{E} \cdot \mathbf{e}^*)|^2 \quad (4.93)$$

With some elementary algebra (mainly using that $\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_v E_v^* = (I + Q)/2$, $\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_h E_h^* = (I - Q)/2$, $\frac{1}{2} \sqrt{\frac{\epsilon}{\mu}} E_v E_h^* = -(U - iV)/2$ which follow immediately from Equation 4.10 to 4.13) this can be rewritten in terms of the of the Stokes vector \mathbf{I} of the incident radiation and the Stokes vector \mathbf{i} of the antenna. It turns out to be just a scalar product:

$$I' = \frac{1}{2} \mathbf{i} \cdot \mathbf{I} \quad (4.94)$$

4.5 The scattering amplitude matrix

The electric field, $[E_v, E_h]^T$, originating from a single scattering event of an incident electric field $[E_v^0, E_h^0]^T$ may in the far field be written as (see further Equation 5.7)

$$\begin{bmatrix} E_v \\ E_h \end{bmatrix} = f(r) \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} \begin{bmatrix} E_v^0 \\ E_h^0 \end{bmatrix}, \quad (4.95)$$

where S_j are the scattering amplitude functions and all distance effects are put into the function $f(r)$. Using Stokes based nomenclature, the equation above becomes

$$\begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix} = g(r) \mathbf{F} \begin{bmatrix} I^0 \\ Q^0 \\ U^0 \\ V^0 \end{bmatrix}, \quad (4.96)$$

where all distance effects are put into the function $g(r)$ and the transformation matrix \mathbf{F} can be expressed as [Liou, 2002, Sec. 5.4.3].

$$\mathbf{F} = \begin{bmatrix} \frac{1}{2}(M_2+M_3+M_4+M_1) & \frac{1}{2}(M_2-M_3+M_4-M_1) & S_{23}+S_{41} & -D_{23}-D_{41} \\ \frac{1}{2}(M_2+M_3-M_4-M_1) & \frac{1}{2}(M_2-M_3-M_4+M_1) & S_{23}-S_{41} & -D_{23}+D_{41} \\ S_{24}+S_{31} & S_{24}-S_{31} & S_{21}+S_{34} & -D_{21}+D_{34} \\ D_{24}+D_{31} & D_{24}-D_{31} & D_{21}+D_{34} & S_{21}-S_{34} \end{bmatrix}. \quad (4.97)$$

The elements of \mathbf{F} are finally given by the following expressions:

$$M_k = |S_k|^2, \quad (4.98)$$

$$S_{kj} = S_{jk} = (S_j S_k^* + S_k S_j^*)/2, \quad (4.99)$$

$$-D_{kj} = D_{jk} = i(S_j S_k^* - S_k S_j^*)/2, \quad j, k = 1, 2, 3, 4. \quad (4.100)$$

Depending on the properties of the scattering event, the structure of the matrix \mathbf{F} differs. Two special cases are:

$$S_1 = S_2, \quad S_3 = S_4 = 0 \quad \rightarrow \quad \mathbf{F} = \begin{bmatrix} x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \\ 0 & 0 & 0 & x \end{bmatrix}, \quad (4.101)$$

$$S_3 = S_4 = 0 \quad \rightarrow \quad \mathbf{F} = \begin{bmatrix} x & x & 0 & 0 \\ x & x & 0 & 0 \\ 0 & 0 & x & x \\ 0 & 0 & x & x \end{bmatrix}, \quad (4.102)$$

where x indicates elements deviating from 0. Many (most?) natural materials have the property that S_4 is the complex conjugate of S_3 ($S_3 = S_4^*$) and this results in that \mathbf{F} is a symmetric matrix (in general with all element positions filled).

Chapter 5

Basic radiative transfer theory

When dealing with atmospheric radiation a division can be made between two different wavelength ranges where the limit is found around $5 \mu\text{m}$, i.e. one range consists of the near IR, visible and UV regions while the second range covers thermal and far IR and microwaves. The first reason to this division is the principal sources to the radiation in the two ranges, for wavelengths shorter than $5 \mu\text{m}$ the solar radiation is dominating while at longer wavelengths the thermal emission from the surface and the atmosphere is more important. A second reason is the importance of scattering but here it is impossible to give a fixed limit. Clouds are important scattering objects for most frequencies but at cloud free conditions scattering can in many cases be neglected for wavelengths $> 5 \mu\text{m}$. If the atmosphere can be assumed to be in local thermodynamic equilibrium the radiative transfer can be simplified considerably, and this is a valid assumption for the IR region and microwaves but not for e.g. UV frequencies.

The radiative transfer in the atmosphere must be adequately described in many situations, as when estimating rates of photochemical reactions, calculating radiative forcing in the atmosphere or evaluating a remote sensing observation. It is not totally straightforward to quantify the radiative transfer with good accuracy because the calculations can be very computationally demanding and many of the parameters needed are hard to determine. For example, situations when a great number of transitions or multiple scattering must be considered will cause long calculations while as a rule scattering is problematic to model because the shape and size distribution of the scattering particles are highly variable quantities.

This chapter introduces the theoretical background which is essential to develop a radiative transfer model including scattering. The theory is based on concepts of electrodynamics, starting from the Maxwell equations. An elementary book for electrodynamics is written by *Jackson* [1998]. For optics and scattering of radiation by small particles the reader may refer for instance to *van de Hulst* [1957] and *Bohren and Huffman* [1998]. The notation used in this chapter is mostly adapted from the book “Scattering, Absorption, and

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- 030305 Copied from a compendium written by Patrick Eriksson.

Emission of Light by Small Particles” by *Mishchenko et al.* [2002]. Several lengthy derivations of formulas, which are not shown in detail here, can also be found in this book. The purpose of this chapter is to provide definitions and give ideas, how these definitions can be derived using principles of electromagnetic theory. For the derivation of the radiative transfer equation an outline of the traditional phenomenological approach is given.

5.1 Basic definitions

From the Maxwell equations one can derive the formula for the electromagnetic field vector \mathbf{E} of a plane electromagnetic wave propagating in a homogeneous medium without sources:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \exp\left(-\frac{\omega}{c} m_{\text{I}} \hat{\mathbf{n}} \cdot \mathbf{r}\right) \exp\left(i\frac{\omega}{c} m_{\text{R}} \hat{\mathbf{n}} \cdot \mathbf{r} - i\omega t\right), \quad (5.1)$$

where \mathbf{E}_0 is the amplitude of the electromagnetic wave in vacuum, c is the speed of light in vacuum, ω is the angular frequency, \mathbf{r} is the position vector and $\hat{\mathbf{n}}$ is a real unit vector in the direction of propagation. The complex refractive index m is

$$m = m_{\text{R}} + im_{\text{I}} = c\sqrt{\epsilon\mu}, \quad (5.2)$$

where m_{R} is the non-negative real part and m_{I} is the non-negative imaginary part. Furthermore μ is the permeability of the medium and ϵ the permittivity. For a vacuum, $m = m_{\text{R}} = 1$. The imaginary part of the refractive index, if it is non-zero, determines the decay of the amplitude of the wave as it propagates through the medium, which is thus absorbing. The real part determines the phase velocity $v = c/m_{\text{R}}$. The time-averaged Poynting vector $\mathbf{P}(\mathbf{r})$, which describes the flow of electromagnetic energy, is defined as

$$\mathbf{P}(\mathbf{r}) = \frac{1}{2} \text{Re}(\langle \mathbf{E}(\mathbf{r}) \rangle \times \langle \mathbf{H}^*(\mathbf{r}) \rangle), \quad (5.3)$$

where \mathbf{H} is the magnetic field vector and the $*$ denotes the complex conjugate. The Poynting vector for a homogeneous wave is given by

$$\langle \mathbf{P}(\mathbf{r}) \rangle = \frac{1}{2} \text{Re} \left(\sqrt{\frac{\epsilon}{\mu}} |\mathbf{E}_0|^2 \exp\left(-2\frac{\omega}{c} m_{\text{I}} \hat{\mathbf{n}} \cdot \mathbf{r}\right) \hat{\mathbf{n}} \right). \quad (5.4)$$

Equation 5.4 shows that the energy flows in the direction of propagation and its absolute value $I(\mathbf{r}) = |\langle \mathbf{P}(\mathbf{r}) \rangle|$, which is usually called intensity (or irradiance), is exponentially attenuated. Rewriting Equation 5.4 gives

$$I(\mathbf{r}) = I_0 \exp(-\alpha^p \hat{\mathbf{n}} \cdot \mathbf{r}), \quad (5.5)$$

where I_0 is the intensity for $\mathbf{r} = \mathbf{0}$. The absorption coefficient α^p is

$$\alpha^p = 2\frac{\omega}{c} m_{\text{I}} = \frac{4\pi m_{\text{I}}}{\lambda} = \frac{4\pi m_{\text{I}} \nu}{c}, \quad (5.6)$$

where λ is the free-space wavelength and ν the frequency. Intensity has the dimension of monochromatic flux [energy/(area \times time)].

5.2 Scattering, absorption and thermal emission by a single particle

A parallel monochromatic beam of electromagnetic radiation propagates in vacuum without any change in its intensity or polarization state. A small particle, which is interposed into the beam, can cause several effects:

Absorption: The particle converts some of the energy contained in the beam into other forms of energy.

Elastic scattering: Part of the incident energy is extracted from the beam and scattered into all spatial directions at the frequency of the incident beam. Scattering can change the polarization state of the radiation.

Inelastic scattering: As above, but the frequency is changed by the scattering. This process is neglected below.

Extinction: The energy of the incident beam is reduced by an amount equal to the sum of absorption and scattering.

Dichroism: The change of the polarization state of the beam as it passes a particle.

Thermal emission: If the temperature of the particle is non-zero, the particle emits radiation in all directions over a large frequency range.

The beam is an oscillating plane magnetic wave, whereas the particle can be described as an aggregation of a large number of discrete elementary electric charges. The incident wave excites the charges to oscillate with the same frequency and thereby radiate secondary electromagnetic waves. The superposition of these waves gives the total elastically scattered field.

One can also describe the particle as an object with a refractive index different from that of the surrounding medium. The presence of such an object changes the electromagnetic field that would otherwise exist in an unbounded homogeneous space. The difference of the total field in the presence of the object can be thought of as the field *scattered* by the object. The angular distribution and the polarization of the scattered field depend on the characteristics of the incident field as well as on the properties of the object as its size relative to the wavelength and its shape, composition and orientation.

5.2.1 Definition of the amplitude matrix

For the derivation of a relation between the incident and the scattered electric field we consider a finite scattering object in the form of a single body or a fixed aggregate embedded in an infinite homogeneous, isotropic and non-absorbing medium. We assume that the individual bodies forming the scattering object are sufficiently large that they can be characterized by optical constants appropriate to bulk matter, not to optical constants appropriate for single atoms or molecules. Solving the Maxwell equations for the internal volume, which is the interior of the scattering object, and the external volume one can derive a formula, which expresses the total electric field everywhere in space in terms of the incident field and the

field inside the scattering object. Applying the far field approximation gives a relation between incident and scattered field, which is that of a spherical wave. The amplitude matrix $\mathbf{S}(\hat{\mathbf{n}}^{\text{sca}}, \hat{\mathbf{n}}^{\text{inc}})$ includes this relation:

$$\begin{bmatrix} E_{\psi}^{\text{sca}}(r\hat{\mathbf{n}}^{\text{sca}}) \\ E_{\omega}^{\text{sca}}(r\hat{\mathbf{n}}^{\text{sca}}) \end{bmatrix} = \frac{e^{ikr}}{r} \mathbf{S}(\hat{\mathbf{n}}^{\text{sca}}, \hat{\mathbf{n}}^{\text{inc}}) \begin{bmatrix} E_{0\psi}^{\text{inc}} \\ E_{0\omega}^{\text{inc}} \end{bmatrix}. \quad (5.7)$$

The amplitude matrix depends on the directions of incident $\hat{\mathbf{n}}^{\text{inc}}$ and scattering $\hat{\mathbf{n}}^{\text{sca}}$ as well as on size, morphology, composition, and orientation of the scattering object with respect to the coordinate system. The distance between the origin and the observation point is denoted by r and the wave number of the external volume is denoted by k .

The amplitude matrix provides a complete description of the scattering pattern in the far field zone. The amplitude matrix explicitly depends on ω^{inc} and ω^{sca} even when ψ^{inc} and/or ψ^{sca} equal 0 or π .

5.2.2 Phase matrix

The phase matrix \mathbf{Z} describes the transformation of the Stokes vector of the incident wave into that of the scattered wave for scattering directions away from the incidence direction ($\hat{\mathbf{n}}^{\text{sca}} \neq \hat{\mathbf{n}}^{\text{inc}}$),

$$\mathbf{I}^{\text{sca}}(r\hat{\mathbf{n}}^{\text{sca}}) = \frac{1}{r^2} \mathbf{Z}(\hat{\mathbf{n}}^{\text{sca}}, \hat{\mathbf{n}}^{\text{inc}}) \mathbf{I}^{\text{inc}}. \quad (5.8)$$

The 4×4 phase matrix can be written in terms of the amplitude matrix elements for single particles [Mishchenko *et al.*, 2002]. All elements of the phase matrix have the dimension of area and are real. As the amplitude matrix, the phase matrix depends on ω^{inc} and ω^{sca} even when ψ^{inc} and/or ψ^{sca} equal 0 or π . In general, all 16 elements of the phase matrix are non-zero, but they can be expressed in terms of only seven independent real numbers. Four elements result from the moduli $|S_{ij}|$ ($i, j = 1, 2$) and three from the phase-differences between S_{ij} . If the incident beam is unpolarized, i.e., $\mathbf{I}^{\text{inc}} = (I^{\text{inc}}, 0, 0, 0)^T$, the scattered light generally has at least one non-zero Stokes parameter other than intensity:

$$I^{\text{sca}} = Z_{11} I^{\text{inc}}, \quad (5.9)$$

$$Q^{\text{sca}} = Z_{21} I^{\text{inc}}, \quad (5.10)$$

$$U^{\text{sca}} = Z_{31} I^{\text{inc}}, \quad (5.11)$$

$$V^{\text{sca}} = Z_{41} I^{\text{inc}}. \quad (5.12)$$

This is the phenomena is traditionally called ‘‘polarization’’. The non-zero degree of polarization Equation 4.82 can be written in terms of the phase matrix elements

$$p = \frac{\sqrt{Z_{21}^2 + Z_{31}^2 + Z_{41}^2}}{Z_{11}}. \quad (5.13)$$

5.2.3 Extinction matrix

In the special case of the exact forward direction ($\hat{\mathbf{n}}^{\text{sca}} = \hat{\mathbf{n}}^{\text{inc}}$) the attenuation of the incoming radiation is described by the extinction matrix \mathbf{K} . In terms of the Stokes vector we get

$$\mathbf{I}(r\hat{\mathbf{n}}^{\text{inc}})\Delta S = \mathbf{I}^{\text{inc}}\Delta S - \mathbf{K}(\hat{\mathbf{n}}^{\text{inc}})\mathbf{I}^{\text{inc}} + O(r^{-2}). \quad (5.14)$$

Here ΔS is a surface element normal to $\hat{\mathbf{n}}^{\text{inc}}$. The extinction matrix can also be expressed explicitly in terms of the amplitude matrix. It has only seven independent elements. Again the elements depend on ω^{inc} and ω^{sca} even when the incident wave propagates along the z -axis.

5.2.4 Absorption vector

The particle also emits radiation if its temperature T is above zero Kelvin. According to Kirchhoff's law of radiation the emissivity equals the absorptivity of a medium under thermodynamic equilibrium. The energetic and polarization characteristics of the emitted radiation are described by a four-component Stokes emission column vector $\mathbf{a}(\hat{\mathbf{r}}, T, \omega)$. The emission vector is defined in such a way that the net rate, at which the emitted energy crosses a surface element ΔS normal to $\hat{\mathbf{r}}$ at distance r from the particle at frequencies from ω to $\omega + \Delta\omega$, is

$$W^e = \frac{1}{r^2} \mathbf{a}(\hat{\mathbf{r}}, T, \omega) B(T, \omega) \Delta S \Delta\omega, \quad (5.15)$$

where W^e is the power of the emitted radiation and B is the Planck function. In order to calculate \mathbf{a} we assume that the particle is placed inside an opaque cavity of dimensions large compared to the particle and any wavelengths under consideration. We have thermodynamic equilibrium if the cavity and the particle is maintained at the constant temperature T . The emitted radiation inside the cavity is isotropic, homogeneous, and unpolarized. We can represent this radiation as a collection of quasi-monochromatic, unpolarized, incoherent beams propagating in all directions characterized by the Planck blackbody radiation

$$B(T, \omega) \Delta S \Delta\Omega = \frac{\hbar\omega^3}{2\pi^2 c^2 \left[\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1 \right]} \Delta S \Delta\Omega, \quad (5.16)$$

where $\Delta\Omega$ is a small solid angle about any direction, \hbar is the Planck constant divided by 2π , and k_B is the Boltzmann constant. The blackbody Stokes vector is

$$\mathbf{I}_b(T, \omega) = \begin{bmatrix} B(T, \omega) \\ 0 \\ 0 \\ 0 \end{bmatrix}. \quad (5.17)$$

For the Stokes emission vector, which we also call particle absorption vector, we can derive

$$a_i^p(\hat{\mathbf{r}}, T, \omega) = K_{i1}(\hat{\mathbf{r}}, \omega) - \int_{4\pi} d\hat{\mathbf{r}}' Z_{i1}(\hat{\mathbf{r}}, \hat{\mathbf{r}}', \omega), \quad i = 1, \dots, 4. \quad (5.18)$$

This relation is a property of the particle only, and it is valid for any particle, in thermodynamic equilibrium or non-equilibrium.

5.2.5 Optical cross sections

The optical cross-sections are defined as follows: The product of the scattering cross section C_{sca} and the incident monochromatic energy flux gives the total monochromatic power removed from the incident wave as a result of scattering into all directions. The product of the absorption cross section C_{abs} and the incident monochromatic energy flux gives the power which is removed from the incident wave by absorption. The extinction cross section C_{ext} is the sum of scattering and absorption cross section. One can express the extinction cross sections in terms of extinction matrix elements

$$C_{\text{ext}} = \frac{1}{I^{\text{inc}}} (K_{11}(\hat{\mathbf{n}}^{\text{inc}})I^{\text{inc}} + K_{12}(\hat{\mathbf{n}}^{\text{inc}})Q^{\text{inc}} + \quad (5.19)$$

$$K_{13}(\hat{\mathbf{n}}^{\text{inc}})U^{\text{inc}} + K_{14}(\hat{\mathbf{n}}^{\text{inc}})V^{\text{inc}}), \quad (5.20)$$

and the scattering cross section in terms of phase matrix elements

$$C_{\text{sca}} = \frac{1}{I^{\text{inc}}} \int_{4\pi} d\hat{\mathbf{r}} (Z_{11}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})I^{\text{inc}} + Z_{12}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})Q^{\text{inc}} + \quad (5.21)$$

$$Z_{13}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})U^{\text{inc}} + Z_{14}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})V^{\text{inc}}). \quad (5.22)$$

The absorption cross section is the difference between extinction and scattering cross section:

$$C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}. \quad (5.23)$$

The single scattering albedo ω_0 , which is a commonly used quantity in radiative transfer theory, is defined as the ratio of the scattering and the extinction cross section:

$$\omega_0 = \frac{C_{\text{sca}}}{C_{\text{ext}}} \leq 1. \quad (5.24)$$

All cross sections are real-valued positive quantities and have the dimension of area.

The phase function is generally defined as

$$p(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}}) = \frac{4\pi}{C_{\text{sca}}I^{\text{inc}}} (Z_{11}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})I^{\text{inc}} + Z_{12}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})Q^{\text{inc}} + \quad (5.25)$$

$$Z_{13}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})U^{\text{inc}} + Z_{14}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})V^{\text{inc}}). \quad (5.26)$$

The phase function is dimensionless and normalized:

$$\frac{1}{4\pi} \int_{4\pi} p(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}}) d\hat{\mathbf{r}} = 1. \quad (5.27)$$

5.3 Scattering, absorption and emission by ensembles of independent particles

The formalism described in the previous chapter applies only for radiation scattered by a single body or a fixed cluster consisting of a limited number of components. In reality, one normally finds situations, where radiation is scattered by a very large group of particles forming a constantly varying spatial configuration. Clouds of ice crystals or water droplets are a good example for such a situation. A particle collection can be treated at each given

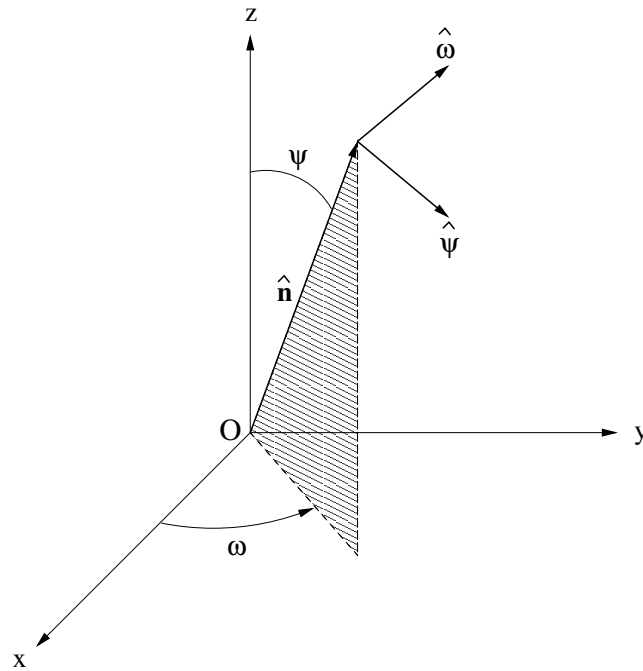


Figure 5.1: Coordinate system to describe the direction of propagation and the polarization state of a plane electromagnetic wave (adapted from Mishchenko).

moment as a fixed cluster, but as a measurement takes a finite amount of time, one measures a statistical average over a large number of different cluster realizations.

Solving the Maxwell equations for a whole cluster, like a collection of particles in a cloud, is computationally too expensive. Fortunately, particles forming a random group can often be considered as independent scatterers. This approximation is valid under the following assumptions:

1. Each particle is in the far-field zone of all other particles.
2. Scattering by the individual particles is incoherent.

As a consequence of assumption 2, the Stokes parameters of the partial waves can be added without regard to the phase. If the particle number density is sufficiently small, the single scattering approximation can be applied. The scattered field in this approach is obtained by summing up the fields generated by the individual particles in response to the external field in isolation from all other particles. If the particle positions are random, one can show, that the phase matrix, the extinction matrix and the absorption vector are obtained by summing up the respective characteristics of all constituent particles.

5.3.1 Single scattering approximation

We consider a volume element containing N particles. We assume that N is sufficiently small, so that the mean distance between the particles is much larger than the incident wavelength and the average particle size. Furthermore we assume that the contribution of

the total scattered signal of radiation scattered more than once is negligibly small. This is equivalent to the requirement

$$\frac{N \langle C_{\text{sca}} \rangle}{l^2} \ll 1, \quad (5.28)$$

where $\langle C_{\text{sca}} \rangle$ is the average scattering cross section per particle and l is the linear dimension of the volume element. The electric field scattered by the volume element can be written as the vector sum of the partial scattered fields scattered by the individual particles:

$$\mathbf{E}^{\text{sca}}(\mathbf{r}) = \sum_{n=1}^N \mathbf{E}_n^{\text{sca}}(\mathbf{r}). \quad (5.29)$$

As we assume single scattering the partial scattered fields are given according to Equation 5.7:

$$\begin{bmatrix} [E_n^{\text{sca}}(\mathbf{r})]_{\psi} \\ [E_n^{\text{sca}}(\mathbf{r})]_{\omega} \end{bmatrix} = \frac{e^{ikr}}{r} \mathbf{S}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}}) \begin{bmatrix} E_{0\psi}^{\text{inc}} \\ E_{0\omega}^{\text{inc}} \end{bmatrix}, \quad (5.30)$$

where \mathbf{S} is the total amplitude scattering matrix given by:

$$\mathbf{S}(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}}) = \sum_{n=1}^N e^{i\Delta_n} \mathbf{S}_n(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}}). \quad (5.31)$$

$\mathbf{S}_n(\hat{\mathbf{r}}, \hat{\mathbf{n}}^{\text{inc}})$ are the individual amplitude matrices and the phase Δ_n is given by

$$\Delta_n = kr_{\text{On}} \cdot (\hat{\mathbf{n}}^{\text{inc}} - \hat{\mathbf{r}}), \quad (5.32)$$

where the vector \mathbf{r}_{On} connects the origin of the volume element O with the n th particle origin (see Figure 5.2). Since Δ_n vanishes in forward direction and the individual extinction matrices can be written in terms of the individual amplitude matrix elements, the total extinction matrix is given by

$$\mathbf{K} = \sum_{n=1}^N \mathbf{K}_n = N \langle \mathbf{K} \rangle, \quad (5.33)$$

where $\langle \mathbf{K} \rangle$ is the average extinction matrix per particle. One can derive the analog equation for the phase matrix

$$\mathbf{Z} = \sum_{n=1}^N \mathbf{Z}_n = N \langle \mathbf{Z} \rangle, \quad (5.34)$$

where $\langle \mathbf{Z} \rangle$ is the average phase matrix per particle. In almost all practical situations, radiation scattered by a collection of independent particles is incoherent, as a minimal displacement of a particle or a slight change in the scattering geometry changes the phase differences entirely. It is important to note, that the ensemble averaged phase matrix and the ensemble averaged extinction matrix have in general 16 independent elements. The relations between the matrix elements, which can be derived for single particles, do not hold for particle ensembles.

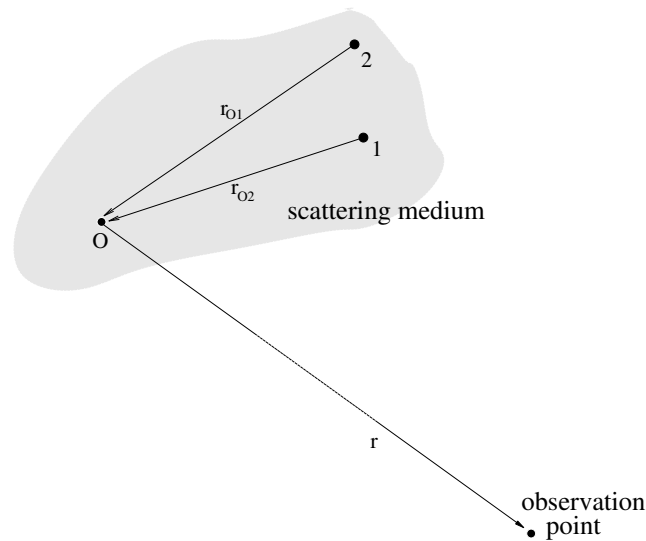


Figure 5.2: A volume element of a scattering medium consisting of a particle ensemble. O is the origin of the volume element, r_{O1} connects the origin with particle 1 and r_{O2} with particle 2. The observation point is assumed to be in the far-field zone of the volume element.

5.4 Phenomenological derivation of the radiative transfer equation

When the scattering medium contains a very large number of particles the single scattering approximation is no longer valid. In this case we have to take into account that each particle scatters radiation that has already been scattered by another particle. This means that the radiation leaving the medium has a significant multiple scattered component. The observation point is assumed to be in the far-field zone of each particle, but it is not necessarily in the far-field zone of the scattering medium as a whole. A traditional method in this case is to solve the radiative transfer equation. This approach still assumes, that the particles forming the scattering medium are randomly positioned and widely separated and that the extinction and the phase matrices of each volume element can be obtained by incoherently adding the respective characteristics of the constituent particles. In other words the scattering media is assumed to consist of a large number of discrete, sparsely and randomly distributed particles and is treated as continuous and locally homogeneous. Radiative transfer theory is originally a phenomenological approach based on considering the transport of energy through a medium filled with a large number of particles and ensuring energy conservation. *Mishchenko* [2002] has demonstrated that it can be derived from electromagnetic theory of multiple wave scattering in discrete random media under certain simplifying assumptions.

In the phenomenological radiative transfer theory, the concept of single scattering by individual particles is replaced by the assumption of scattering by a small homogeneous volume element. It is furthermore assumed that the result of scattering is not the transformation of a plane incident wave into a spherical scattered wave, but the transformation of the specific intensity vector, which includes the Stokes vectors from all waves contributing

to the electromagnetic radiation field.

The vector radiative transfer equation (VRTE) is

$$\frac{d\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}})}{ds} = -\mathbf{K}(\nu, \mathbf{r}, \hat{\mathbf{n}})\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}}) + \mathbf{a}(\nu, \mathbf{r}, \hat{\mathbf{n}})B(\nu, \mathbf{r}) + \int_{4\pi} d\hat{\mathbf{n}}'\mathbf{Z}(\nu, \mathbf{r}, \hat{\mathbf{n}}, \hat{\mathbf{n}}')\mathbf{I}(\nu, \mathbf{r}, \hat{\mathbf{n}}'), \quad (5.35)$$

where \mathbf{I} is the specific intensity vector, \mathbf{K} is the total extinction matrix, \mathbf{a} is the total absorption vector, B is the Planck function and \mathbf{Z} is the total phase matrix. Furthermore ν is the frequency of the radiation, ds is a path-length-element of the propagation path, \mathbf{r} represents the atmospheric position and $\hat{\mathbf{n}}$ the propagation direction. Equation 5.35 is valid for monochromatic or quasi-monochromatic radiative transfer. We can use this equation for simulating microwave radiative transfer through the atmosphere, as the scattering events do not change the frequency of the radiation.

The four-component specific intensity vector $\mathbf{I} = (I, Q, U, V)^T$ fully describes the radiation and it can directly be associated with the measurements carried out by a radiometer used for remote sensing. For the definition of the components of the specific intensity vector refer to Section 4, where the Stokes components are described.

The three terms on the right hand side of Equation 5.35 describe physical processes in an atmosphere containing different particle types and different trace gases. The first term represents the extinction of radiation traveling through the scattering medium, \mathbf{K} . For microwave radiation in cloudy atmospheres, extinction is caused by gaseous absorption, particle absorption and particle scattering. Therefore \mathbf{K} can be written as a sum of two matrices, the particle extinction matrix \mathbf{K}^p and the gaseous extinction matrix \mathbf{K}^g :

$$\mathbf{K}(\nu, \mathbf{r}, \hat{\mathbf{n}}) = \mathbf{K}^p(\nu, \mathbf{r}, \hat{\mathbf{n}}) + \mathbf{K}^g(\nu, \mathbf{r}, \hat{\mathbf{n}}). \quad (5.36)$$

The particle extinction matrix is the sum over the individual specific extinction matrices \mathbf{K}_i^p of the N different particles types contained in the scattering medium weighted by their particle number densities n_i^p :

$$\mathbf{K}^p(\nu, \mathbf{r}, \hat{\mathbf{n}}) = \sum_{i=1}^N n_i^p \mathbf{K}_i^p(\nu, \mathbf{r}, \hat{\mathbf{n}}). \quad (5.37)$$

The gaseous extinction matrix can normally be derived from the scalar gas absorption. This is because there is no polarization due to gas absorption at cloud altitudes, and the off-diagonal elements of the gaseous extinction matrix are zero. On the other hand, at very high altitudes above approximately 40 km there is polarization due to the Zeeman effect, mainly due to oxygen molecules. In addition, in the toposphere and stratosphere molecular scattering can be neglected in the microwave frequency range. Hence the coefficients on the diagonal correspond to the gas absorption coefficient:

$$\mathbf{K}_{l,m}^g(\nu, \mathbf{r}) = \alpha^g(\nu, \mathbf{r}) \quad \text{if } l = m \\ 0 \quad \text{if } l \neq m. \quad (5.38)$$

where α^g is the total scalar gas absorption coefficient, which is calculated from the individual absorption coefficients of all M trace gases α_i^g and their volume mixing ratios n_i^g as:

$$\alpha^g(\nu, \mathbf{r}) = \sum_{i=1}^M n_i^g \alpha_i^g(\nu, \mathbf{r}). \quad (5.39)$$

The second term in Equation 5.35 is the thermal source term. It describes thermal emission by gases and particles in the atmosphere. The absorption vector \mathbf{a} is

$$\mathbf{a}(\nu, \mathbf{r}, \hat{\mathbf{n}}) = \mathbf{a}^p(\nu, \mathbf{r}, \hat{\mathbf{n}}) + \mathbf{a}^g(\nu, \mathbf{r}, \hat{\mathbf{n}}), \quad (5.40)$$

where \mathbf{a}^p and \mathbf{a}^g are the particle absorption vector and the gas absorption vector, respectively. The particle absorption vector is a sum over the individual absorption vectors \mathbf{a}_i^p , again weighted with n_i^p :

$$\mathbf{a}^p(\nu, \mathbf{r}, \hat{\mathbf{n}}) = \sum_{i=1}^N n_i^p \mathbf{a}_i^p(\nu, \mathbf{r}, \hat{\mathbf{n}}). \quad (5.41)$$

The gas absorption vector is simply (if no Zeeman splitting)

$$\mathbf{a}^g = [\alpha^p, 0, 0, 0]^T. \quad (5.42)$$

The last term in Equation 5.35 is the scattering source term. It adds the amount of radiation which is scattered from all directions $\hat{\mathbf{n}}'$ into the propagation direction $\hat{\mathbf{n}}$. The phase matrix \mathbf{Z} is the sum of the individual phase matrices \mathbf{Z}_i weighted with n_i^p :

$$\mathbf{Z}(\nu, \mathbf{r}, \hat{\mathbf{n}}) = \sum_{i=1}^N n_i^p \mathbf{Z}_i(\nu, \mathbf{r}, \hat{\mathbf{n}}). \quad (5.43)$$

The scalar radiative transfer equation (SRTE)

$$\begin{aligned} \frac{dI(\nu, \mathbf{r}, \hat{\mathbf{n}})}{ds} = & -K_{11}(\nu, \mathbf{r}, \hat{\mathbf{n}})I(\nu, \mathbf{r}, \hat{\mathbf{n}}) + a_1(\nu, \mathbf{r}, \hat{\mathbf{n}})B(\nu, \mathbf{r}) \\ & + \int_{4\pi} d\hat{\mathbf{n}}' Z_{11}(\nu, \mathbf{r}, \hat{\mathbf{n}}, \hat{\mathbf{n}}')I(\nu, \mathbf{r}, \hat{\mathbf{n}}') \end{aligned} \quad (5.44)$$

can be used presuming that the radiation field is unpolarized. This approximation is reasonable if the scattering medium consists of spherical or completely randomly oriented particles, where \mathbf{K}^p is diagonal and only the first element of \mathbf{a}^p is non-zero.

5.5 Simple solution without scattering and polarization

If scattering can be neglected and the atmosphere is assumed to be in local thermodynamic equilibrium, the radiative transfer equation gets unusually simple. These assumptions will be made below and they are normally valid for the infrared region and longer wavelengths as in the microwave region. For these conditions the atmospheric absorption and emission are linked and the basic problem to determine the radiative transfer is to calculate the absorption. At the wavelengths considered rotational and vibrational transitions are the dominating absorbing processes.

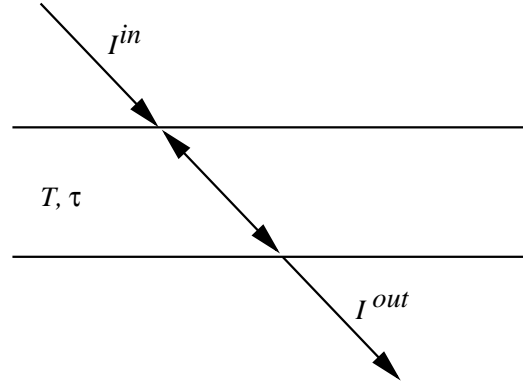
The basic equation describing radiative transfer along a specific direction is

$$\frac{dI(\nu)}{dl} = -k(l, \nu)(I(\nu) + B(l, \nu)) \quad (5.45)$$

where I is the intensity per unit area, ν the frequency, l the distance along the propagation path, k the total absorption coefficient (summed over all species and transitions) and B the Planck function. This differential equation can be solved:

$$I(\nu) = I_0(\nu)e^{-\int_0^l k(l', \nu)dl'} + \int_0^l k(l, \nu)B(T(l), \nu)e^{-\int_0^l k(l', \nu)dl'} dl \quad (5.46)$$

Figure 5.3: Schematic picture of the radiative transfer through a medium with constant temperature.



where the receiver is assumed to be placed at $l = 0$ and h is the distance along the path to the limit of the media. I_0 is the intensity at the point h which can represent thermal emission from the surface, solar radiation at top of the atmosphere or cosmic background radiation depending on the observation geometry. When discussing radiative transfer the quantity optical depth, τ , is commonly used and it is defined as

$$\tau(l, \nu) = \int_0^l k(l', \nu) dl' \quad (5.47)$$

and Equation 5.46 can be written as

$$I(\nu) = I_0(\nu)e^{-\tau(h, \nu)} + \int_0^h k(l, \nu)B(T(l), \nu)e^{-\tau(l', \nu)} dl \quad (5.48)$$

The terms inside the integral found in this equation have a simple physical meaning, the radiation emitted at one point is $kBdl$ and this quantity is attenuated by the factor $e^{-\tau}$ before it reaches the observation point.

5.6 Special solutions

If the total emission along the propagation path can be neglected compared to the transmitted part of the incoming radiation, the radiative transfer equation is simplified to the well known Beer-Lambert law:

$$I(\nu) = I_0(\nu)e^{-\tau(h, \nu)} \quad (5.49)$$

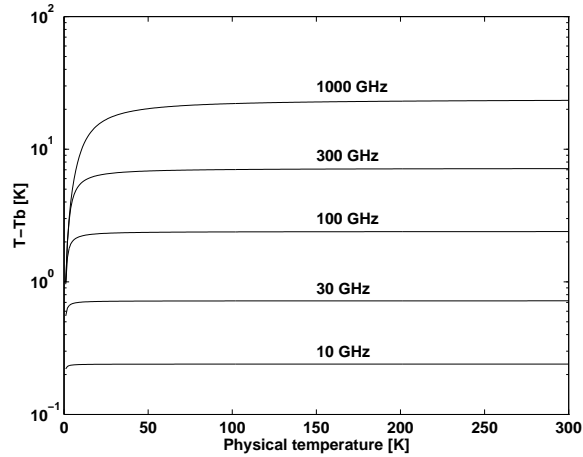
This equation can for example be used when evaluating solar occultation observations.

If the temperature is constant through the medium studied (Fig. 5.3) the integral in Equation 5.46 can be solved analytically:

$$I^{out} = I^{in}e^{-\tau} + B(T, \nu)(1 - e^{-\tau}) \quad (5.50)$$

where τ is the total optical thickness of the medium. Two special cases can be distinguished. If the layer is totally optically thick ($\tau \rightarrow \infty$) then I^{in} is totally absorbed and $I^{out} = B$,

Figure 5.4: The difference between the physical temperature of a blackbody and the equivalent brightness temperature calculated using the Rayleigh-Jeans approximation.



the medium emits as a blackbody. If the layer has no absorption ($\tau = 0$) then Equation 5.50 gives $I^{out} = I^{in}$ as expected.

In microwave radiometry the measured intensity is normally presented by means of the brightness temperature, T_b . This quantity is derived from the Rayleigh-Jeans approximation of the Planck function:

$$B(T, \nu) \approx \frac{2\nu^2 k_b T}{c^2} = \frac{2k_b T}{\lambda^2} \quad (5.51)$$

This equation is valid when $h\nu \ll kT$ which is the case in the microwave region due to the relatively low frequencies. If the temperature is 50 K, $h\nu$ equals kT at 1.04 THz. The important aspect of Equation 5.51 is the linear relationship between the intensity and the physical temperature. The natural definition of brightness temperature, T_b , is then

$$T_b(\nu) = \frac{\lambda^2}{2k_b T} I(\nu) \quad (5.52)$$

The difference between the brightness temperature and the physical temperature (corresponding to the actual intensity) increases with frequency which is exemplified in Figure 5.4. The differences for higher frequencies are certainly not negligible and the brightness temperature shall not be mistaken for the physical temperature. The important fact is that the brightness temperature has a linear relationship to the intensity and gives a more intuitive understanding of the magnitude of the emission. In the Rayleigh-Jeans limit Equation 5.46 can be written as

$$T_b(\nu) = T_{b0}(\nu) e^{-\tau(h, \nu)} + \int_0^h k(l, \nu) T(l) e^{-\tau(l, \nu)} dl \quad (5.53)$$

5.7 Surface emission and reflection

5.7.1 The dielectric constant and the refractive index

The properties of a material can be reported either as the relative dielectric constant, ϵ , or the refractive index, n . Both these quantities can be complex and are related as

$$n = \sqrt{\epsilon}. \quad (5.54)$$

5.7.2 Relating reflectivity and emissivity

Thermodynamic equilibrium can be assumed for natural surfaces, as long as there exist no strong temperature gradients. The Kirchoff law can then be used to relate the reflectivity and emissivity of a surface. For rough surfaces the scattering properties must be integrated to determine the emissivity (Equation 5.72). For specular reflections (defined below) and scalar radiative transfer calculations, the emissivity e is

$$e = 1 - r, \quad (5.55)$$

where r is the reflective (power reflection coefficient) of the surface. Equation 5.55 is valid for each polarisation state individually [Ulaby *et al.*, 1981, Eq. 4.190a].

We have then that

$$I^{\text{up}} = I^{\text{down}}r + (1 - r)B, \quad (5.56)$$

where I^{up} is upwelling radiation, I^{down} is downwelling radiation and B is the magnitude of blackbody radiation. As expected, if $I^{\text{down}} = B$, also I^{up} equals B . Expressing the last observation using vector nomenclature gives

$$\begin{bmatrix} B \\ 0 \\ 0 \\ 0 \end{bmatrix} = \mathbf{R} \begin{bmatrix} B \\ 0 \\ 0 \\ 0 \end{bmatrix} + \mathbf{b}, \quad (5.57)$$

where \mathbf{R} is the matrix (4 x 4) correspondence to the scalar reflectivity, describing the properties of the surface reflection. The vector \mathbf{b} is the surface emission, that can be expressed as

$$\mathbf{b} = (\mathbf{1} - \mathbf{R}) \begin{bmatrix} B \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad (5.58)$$

where $\mathbf{1}$ is the identity matrix.

5.7.3 Specular reflections

If the surface is sufficiently smooth, radiation will be reflected/scattered only in the complementary angle, specular reflection. Required smoothness for assuming specular reflection is normally estimated by the Rayleigh criterion:

$$\Delta h < \frac{\lambda}{8 \cos \theta_1} \quad (5.59)$$

where Δh is the root mean square variation of the surface height, λ the wavelength and θ_1 the angle between the surface normal and the incident direction of the radiation. The criterion can also be defined with the factor 8 replaced with a higher number.

The complex reflection coefficient for the amplitude of the electromagnetic wave for vertical (R_v) and horizontal (R_h) polarisation is for a flat surface (if the relative magnetic permeability (μ_r) of both media is 1) given by the Fresnel equations:

$$R_v = \frac{n_2 \cos \theta_1 - n_1 \cos \theta_2}{n_2 \cos \theta_1 + n_1 \cos \theta_2} \quad (5.60)$$

$$R_h = \frac{n_1 \cos \theta_1 - n_2 \cos \theta_2}{n_1 \cos \theta_1 + n_2 \cos \theta_2} \quad (5.61)$$

where n_1 is refractive index for the medium where the reflected radiation is propagating, θ_1 is the incident angle (measured from the local surface normal) and n_2 is the refractive index of the reflecting medium. The angle θ_2 is the propagation direction for the transmitted part, and is (approximately) given by Snell's law:

$$\text{Re}(n_1) \sin \theta_1 = \text{Re}(n_2) \sin \theta_2, \quad (5.62)$$

where $\text{Re}(\cdot)$ denotes the real part. Equation 5.62 is theoretically correct only if both n_1 and n_2 have no imaginary part. For cases where medium 1 is air, n_1 can (in this context) be set to 1, and an expression allowing n_2 to be complex is found in Section 5.4.1.3 of *Liou [2002]*. We are not aware of any expression for the case when both n_1 and n_2 are complex.

The power reflection coefficients are converted to an intensity reflection coefficient as

$$r = |R|^2, \quad (5.63)$$

where $|\cdot|$ denotes the absolute value. Note that R can be complex, while r is always real.

The surface reflection can be seen as a scattering event and Section 4.5 can be used to derive the reflection matrix values. The scattering amplitude functions of Equation 4.95 are simply

$$S_2 = R_v, \quad (5.64)$$

$$S_1 = R_h, \quad (5.65)$$

$$S_3 = S_4 = 0. \quad (5.66)$$

This leads to that the transformation matrix for a specular surface reflection is (compare to *Liou [2002, Sec. 5.4.3]*)

$$\mathbf{R} = \begin{bmatrix} \frac{r_v + r_h}{2} & \frac{r_v - r_h}{2} & 0 & 0 \\ \frac{r_v - r_h}{2} & \frac{r_v + r_h}{2} & 0 & 0 \\ 0 & 0 & \frac{R_h R_v^* + R_v R_h^*}{2} & i \frac{R_h R_v^* - R_v R_h^*}{2} \\ 0 & 0 & i \frac{R_v R_h^* - R_h R_v^*}{2} & \frac{R_h R_v^* + R_v R_h^*}{2} \end{bmatrix}. \quad (5.67)$$

For the case of $R_v = R_h$ the matrix in Equation 5.67 is strictly diagonal and all the diagonal elements have the same value, $(r_v + r_h)/2$. If the downwelling radiation is unpolarised, the reflected part of the upwelling radiation is

$$\mathbf{R} \begin{bmatrix} I \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} I(r_v + r_h)/2 \\ I(r_v - r_h)/2 \\ 0 \\ 0 \end{bmatrix}. \quad (5.68)$$

as expected.

If \mathbf{R} is given by Equation 5.67, Equation 5.58 gives that the surface emission is

$$\mathbf{b} = \begin{bmatrix} B \left(1 - \frac{r_v + r_h}{2}\right) \\ B \frac{r_h - r_v}{2} \\ 0 \\ 0 \end{bmatrix}. \quad (5.69)$$

5.7.4 Rough surfaces

The scattering of rough surfaces is normally described by the bidirectional reflectance distribution function, BRDF. With the BRDF, $f(\theta_0, \phi_0, \theta_1, \phi_1)$, the scattered radiance in the direction (θ_1, ϕ_1) can be written as (see e.g. *Rees [2001]* or *Petty [2006]*)

$$I'(\theta_1, \phi_1) = \int_0^{\pi/2} \int_0^{2\pi} I(\theta, \phi) \cos(\theta) f(\theta, \phi, \theta_1, \phi_1) \sin(\theta) d\phi d\theta, \quad (5.70)$$

where $I(\theta, \phi)$ is the downwelling radiance for incidence angle θ and azimuth angle ϕ . One important property of the BRDF is

$$f(\theta_0, \phi_0, \theta_1, \phi_1) = f(\theta_1, \phi_1, \theta_0, \phi_0). \quad (5.71)$$

The reflectivity is the half-sphere integral of the BRDF

$$r(\theta_1, \phi_1) = \int_0^{\pi/2} \int_0^{2\pi} f(\theta_1, \phi_1, \theta, \phi) \cos(\theta) \sin(\theta) d\phi d\theta. \quad (5.72)$$

An ideally rough surface is denoted as Lambertian. The BRDF is for this case constant, and normally expressed using the the diffuse reflectivity, r_d [e.g. *Petty, 2006*]:

$$f = \frac{r_d}{\pi}. \quad (5.73)$$

From Eq. 5.72 it follows that $r = r_d$.

Chapter 6

Reversed Monte Carlo Scattering: ARTS-MC

6.1 Introduction

The ARTS Monte Carlo scattering module (ARTS-MC) offers an efficient method for polarized radiative transfer calculations in arbitrarily complex 3D cloudy cases. The algorithm solves the integral form of the Vector Radiative Transfer Equation (VRTE), by applying Monte Carlo integration with importance sampling (MCI) (e.g. [*Press et al., 1997*]). As described in [*Battaglia et al., 2007*], when compared to other techniques for solving the VRTE in 3D domains the ARTS-MC algorithm has the following advantages:

- All computational effort is dedicated to calculating the Stokes vector at the location of interest and in the direction of interest. This is in contrast to forward Monte Carlo and discrete ordinate methods where the whole radiation field is calculated.
- CPU and memory cost scale more slowly than discrete ordinate methods with grid size, so that large or detailed 3D scenarios are not a problem.
- Only parts of the atmosphere that significantly contribute to the observed radiance are considered in the computation. Where the medium is optically thick, only the parts of the atmosphere closest to the sensor are visited by the algorithm. This contrasts with DOM methods, where the whole radiation field is computed, and in particular with forward Monte Carlo methods, where added optical thickness further restricts the number of photons reaching the sensor.

The Monte Carlo integration of the VRTE is over infinite dimensions, where for each scattering order there is a dimension representing: path-lengths, the choice between emission and scattering, and the choice between reflection or emission at the earth's surface. In practice the integrand is always calculated for a finite scattering order, as the dimensionality

History

- 120410 Moved from user guide to theory document.
- 300504 Created and written by Cory Davis.

of the integral is truncated by photon emission or the boundary of the domain. Thus, the algorithm can be pictured as tracing a large number of photons backwards from sensor, in randomly selected multiply scattered propagation paths to either their point of emission, or entry into the scattering domain. This physical picture is identical to the Backward-Forward Monte Carlo algorithm described by [Liu *et al.*, 1996]. However, BFMC did not account for dichroism, which is correctly accounted for in ARTS-MC by importance sampling.

The description of reversed Monte Carlo as tracing photon paths backwards from the sensor gives a useful first-order physical picture for understanding the algorithm, but can lead to difficulty understanding the veracity of the method with regard to polarization. These difficulties are not apparent in the scalar radiative transfer case¹. Specifically, questions I have been asked that highlight the difficulty have included:

- how can you sample a single reversed pathlength when the medium is dichroic? (i.e. different extinction for the different polarized components)
- when reverse tracing, how can you decide on a scattering or emission event when the single scattering albedo depends on the polarization state of the incoming photon?
- How can you sample a single reverse scattered (i.e. incoming) direction when the scattered polarization state depends on the polarization state of the incoming photon?

The answer in each case is to forget the physical picture, focus on the mathematical solution to the VRTE, and realise that MCI permits some freedom in the choice of probability density functions (PDFs), provided the sampled integrand is properly weighted. In the model presented here we choose PDFs that aim to minimise the variance in the 1st element of the Stokes vector. This issue does not arise in the scalar case because it is possible to perfectly sample the phase function to choose new incoming directions, and perfectly sample the transmission function to choose pathlengths, so no weighting terms appear. With the above difficulties in mind, in comparison with [Davis *et al.*, 2005], the algorithm description presented here is more in the context of MCI and with less reference to reversed traced photons. What were referred to as photons in [Davis *et al.*, 2005] we now call Stokes Vector Evaluations (SVE).

The current implementation of the algorithm differs slightly from the description in [Davis *et al.*, 2005]; changes include:

- the initial line of sight is no longer treated differently than the scattered paths
- the algorithm is no longer confined to the ‘cloudbox’,
- MCI is now used for convolving the simulated Stokes vector with a 2D antenna response ([Davis *et al.*, 2005] discusses only pencil beam calculations)
- MCI is now used to treat emission or reflection from the earth’s surface.

These changes make the algorithm simpler and more general.

¹Although this physical picture of reversed Monte Carlo radiative transfer in the scalar case makes intuitive sense, the mathematical demonstration of how this method solves the Schwarzschild equation is often neglected

6.2 Model

The radiative transfer model solves the vector radiative transfer equation (VRTE), here written as (cf. Eq. 5.35)

$$\frac{d\mathbf{I}(\mathbf{n})}{ds} = -\mathbf{K}(\mathbf{n})\mathbf{I}(\mathbf{n}) + \mathbf{K}_a(\mathbf{n})I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}')\mathbf{I}(\mathbf{n}')d\mathbf{n}' \quad (6.1)$$

where \mathbf{I} is the 4 element column vector of radiances $\mathbf{I} = [I, Q, U, V]^T$ with units ($\text{Wm}^{-2}\mu\text{m}^{-1}\text{sr}^{-1}$). This will be referred to as the Stokes vector, although normally the Stokes vector is expressed in units of intensity. s is distance along direction \mathbf{n} and I_b is the Planck radiance. $\mathbf{K}(\mathbf{n})$, $\mathbf{K}_a(\mathbf{n})$, and $\mathbf{Z}(\mathbf{n}, \mathbf{n}')$ are the bulk extinction matrix, absorption coefficient vector and phase matrix of the medium respectively. For brevity these have been expressed as bulk optical properties, where individual single scattering properties have been multiplied by particle number density and averaged over all orientations and particle types. The argument \mathbf{n} has been retained to signify that in general these properties depend on the direction of propagation.

To apply Monte Carlo integration to the problem, the VRTE needs to be expressed in integral form. (e.g. *Hochstadt* [1964])

$$\mathbf{I}(\mathbf{n}, \mathbf{s}_0) = \mathbf{O}(\mathbf{u}_0, \mathbf{s}_0)\mathbf{I}(\mathbf{n}, \mathbf{u}_0) + \int_{\mathbf{u}_0}^{\mathbf{s}_0} \mathbf{O}(\mathbf{s}', \mathbf{s}_0) (\mathbf{K}_a(\mathbf{n})I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}')\mathbf{I}(\mathbf{n}')d\mathbf{n}') ds' \quad (6.2)$$

, where $\mathbf{O}(\mathbf{s}', \mathbf{s})$ is the evolution operator defined by *Degl'Innocenti and Degl'Innocenti* [1985]. \mathbf{u}_0 is the point where the line of sight intersects the far boundary of the scattering domain, and \mathbf{s}_0 is the exit point where the outgoing Stokes vector is calculated.

6.2.1 Integration over the antenna response function

If we consider a scalar antenna response function, $\psi = \psi(\theta, \phi) = \psi(\mathbf{n})$, where $\psi(\mathbf{n})$ is normalised such that $\int_{4\pi} \psi(\mathbf{n})d\mathbf{n} = 1$, then the observed Stokes vector $\mathbf{I}_{\text{ant.}}(\mathbf{n}, \mathbf{s}_0)$ will be

$$\mathbf{I}_{\psi}(\mathbf{n}, \mathbf{s}_0) = \int_{4\pi} \psi(\mathbf{n}')\mathbf{I}(\mathbf{n}', \mathbf{s}_0)d\mathbf{n}' \quad (6.3)$$

If we apply Monte Carlo integration with importance sampling to Eq. 6.3 and sample \mathbf{n}' according to a probability density function (PDF) equal to $\psi(\mathbf{n}')$, an unbiased estimate of Eq. 6.3 is given by (e.g. *Press et al.* [1992])

$$\mathbf{I}_{\psi}(\mathbf{n}, \mathbf{s}_0) = \int_{4\pi} \mathbf{I}(\mathbf{n}', \mathbf{s}_0)\psi(\mathbf{n}')d\mathbf{n}' \quad (6.4)$$

$$\approx \langle \mathbf{I}(\mathbf{n}', \mathbf{s}_0) \rangle_{\psi} \quad (6.5)$$

, where the angled brackets indicate the arithmetic mean, and the ψ subscript indicates the sampled PDF. Eq. 6.5 has an estimated error for each Stokes index, j , of

$$\delta I_j = \sqrt{\frac{\langle I_j^2 \rangle - \langle I_j \rangle^2}{N}}. \quad (6.6)$$

6.2.2 The path integral

We now require a Monte Carlo estimate of the integrand in Eq. 6.5, which is given by Eq. 6.2. First, we re-express 6.2 as a single integral, for simplicity dropping the prime on \mathbf{n}' ,

$$\mathbf{I}(\mathbf{n}, \mathbf{s}_0) = \int_{-\infty}^{s_0} \begin{cases} \mathbf{O}(s', \mathbf{s}_0) (\mathbf{K}_a(\mathbf{n}) I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}') & s' < s'_{boundary} \\ \frac{\mathbf{O}(\mathbf{u}_0, \mathbf{s}_0) \mathbf{I}(\mathbf{n}, \mathbf{u}_0) g}{\int_{u_0}^{\infty} g ds} & s' \geq s'_{boundary} \end{cases} ds' \quad (6.7)$$

, where g is the PDF we will eventually use to sample pathlength, Δs . $s'_{boundary}$ represents the pathlength corresponding to the boundary of the domain opposite the line of sight. The integrand Eq. 6.7 is a piecewise function of the path distance, where path distances corresponding to positions outside the modelled domain give a boundary radiance attenuated by the evolution operator over the length of the path within the model domain, and path distances corresponding to points within the modelled atmosphere give a sum of emission and scattering attenuated by the evolution operator over the distance between the point and the atmosphere exit. The reader could easily verify that evaluating Eq. 6.7 is equivalent Eq. 6.2.

The aim in importance sampling is to choose probability density functions (PDFs) for the independent variables that are as close as possible to being proportional to the integrand *Liu* [2001]. This concentrates computational effort on regions where the integrand is most significant and also reduces the variance in the Stokes Vector evaluations (SVE), thus reducing the number of SVEs and hence CPU time required to give a prescribed accuracy. Eq. 6.2 suggests that the PDF for sampling path length, where path length is the distance traced backwards from the sensor, $\Delta s = |s - s'|$, should be proportional in some way to the evolution operator $\mathbf{O}(s', s)$.

In general there is no closed form expression for $\mathbf{O}(s', s)$. However, in cases where the extinction matrix is constant along a propagation path

$$\mathbf{O}(s', s) = \exp(-\mathbf{K}\Delta s) \quad (6.8)$$

In ARTS a propagation path consists of a set of coordinates indicating where the path intersects with grid surfaces. If the extinction matrix in the path segment between two such points is considered constant, $\mathbf{K} = (\mathbf{K}_j + \mathbf{K}_{j+1})/2$, the evolution operator between two arbitrary points \mathbf{s}_0 and \mathbf{s}_N is

$$\mathbf{O}(\mathbf{s}_0, \mathbf{s}_N) = \mathbf{O}(\mathbf{s}_{N-1}, \mathbf{s}_N) \mathbf{O}(\mathbf{s}_{N-2}, \mathbf{s}_{N-1}) \dots \mathbf{O}(\mathbf{s}_1, \mathbf{s}_2) \mathbf{O}(\mathbf{s}_0, \mathbf{s}_1), \quad (6.9)$$

, where $\mathbf{O}(\mathbf{s}_i, \mathbf{s}_{i+1})$ is given by Eq. 6.8.

Since PDFs are scalar functions, and that we consider the first element of the Stokes vector most important, we choose the pathlength PDF to be proportional to the (1,1) element of $\mathbf{O}(s', s)$,

$$g(\Delta s) = \tilde{k} \tilde{O}_{11}(\Delta s) \quad (6.10)$$

, where $\tilde{O}_{11}(\Delta s)$, is the piecewise exponential function that includes $O_{11}(s', s)$ values at points where the line of sight intersects with grid surfaces. Between two such adjacent intersections, A and B , the function $\tilde{O}_{11}(\Delta s)$ is given by

$$\tilde{O}_{11}(\Delta s) = O_{11}(\Delta s_A) \exp(-\tilde{k}(\Delta s - \Delta s_A)) \quad (6.11)$$

, and

$$\tilde{k} = \frac{1}{(\Delta s_B - \Delta s_A)} \ln \left(\frac{O_{11}^A}{O_{11}^B} \right) \quad (6.12)$$

, which, for cases where the extinction matrix is diagonal, is equal to $K_{11} = (K_{11}^A + K_{11}^B)/2$. Eq. 6.10 is sampled by drawing a random number (from the uniform distribution $[0,1]$), r , and solving

$$\tilde{O}_{11}(\Delta s) = r. \quad (6.13)$$

for Δs . In practise this is done by stepping backwards over grid boundaries until $O_{11} \leq r$, and solving Eqs. 6.11 and 6.13 within the final grid step,

$$\Delta s = \Delta s_A + \frac{1}{\tilde{k}} \ln \left(\frac{O_{11}^A}{r} \right) \quad (6.14)$$

With pathlength sampled according to Eq. 6.13, the Monte Carlo estimate for Eq. 6.7 becomes

$$\begin{aligned} \mathbf{I}(\mathbf{n}, \mathbf{s}_0) &= \int_{\infty}^{s_0} \left\{ \begin{array}{ll} \frac{O(\mathbf{s}', \mathbf{s}_0)}{g(\Delta s)} (\mathbf{K}_a(\mathbf{n}) I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}') & s' < s'_{boundary} \\ \frac{O(\mathbf{u}_0, \mathbf{s}_0) \mathbf{I}(\mathbf{n}, \mathbf{u}_0)}{1 - O_{11}(\Delta s)} & s' \geq s'_{boundary} \end{array} \right\} g(\Delta s) ds' \\ &\approx \left\langle \left\{ \begin{array}{ll} \frac{O(\mathbf{s}', \mathbf{s}_0)}{g(\Delta s)} (\mathbf{K}_a(\mathbf{n}) I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}') & s' < s'_{boundary} \\ \frac{O(\mathbf{u}_0, \mathbf{s}_0) \mathbf{I}(\mathbf{n}, \mathbf{u}_0)}{1 - O_{11}(\Delta s)} & s' \geq s'_{boundary} \end{array} \right\} \right\rangle_{g(\Delta s)} \quad (6.15) \end{aligned}$$

So if the sampled pathlength corresponds to a point outside the atmosphere, or below the earth's surface, the SVE is given by $\frac{O(\mathbf{u}_0, \mathbf{s}_0) \mathbf{I}(\mathbf{n}, \mathbf{u}_0)}{1 - O_{11}(\Delta s)}$. In the top of atmosphere cases, this can be immediately calculated: $O(\mathbf{u}_0, \mathbf{s}_0)$ from Eq. 6.9, and $\mathbf{I}(\mathbf{n}, \mathbf{u}_0)$ from the background radiation from space. As shown in Figure 6.2.8, in this event, we have our SVE and we can begin the calculation for the next one. If however the reversed traced path passes the earth's surface, the calculation of $\mathbf{I}(\mathbf{n}, \mathbf{u}_0)$ requires more steps.

6.2.3 Emission and scattering

If the sampled pathlength corresponds to a point within the atmosphere then the emission and scattering terms in the top term in Eq. 6.15, must be calculated. We also treat this as Monte Carlo integration:

$$\begin{aligned} \mathbf{K}_a(\mathbf{n}) I_b(T) + \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}' &= \int_0^1 \left\{ \begin{array}{ll} \frac{1}{\tilde{\omega}} \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}' & r \leq \tilde{\omega} \\ \frac{\mathbf{K}_a(\mathbf{n}) I_b(T)}{1 - \tilde{\omega}} & r > \tilde{\omega} \end{array} \right\} dr \\ &\approx \left\langle \left\{ \begin{array}{ll} \frac{1}{\tilde{\omega}} \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}' & r \leq \tilde{\omega} \\ \frac{\mathbf{K}_a(\mathbf{n}) I_b(T)}{1 - \tilde{\omega}} & r > \tilde{\omega} \end{array} \right\} \right\rangle_{(6.16)} \end{aligned}$$

. Here we are using a uniform random deviate r , and an albedo-like quantity,

$$\tilde{\omega} = 1 - \frac{K_{a1}(\mathbf{n}_0, \mathbf{s}_1)}{K_{11}(\mathbf{n}_0, \mathbf{s}_1)} \quad (6.17)$$

, to choose between emission and scattering contributions. Note: we can't use the actual single-scattering albedo as this depends on the polarization state of the incident radiation. If $r > \tilde{\omega}$, then the event is considered to be emission. In this case we have all the information required to calculate the SVE,

$$\mathbf{I}^i(\mathbf{n}, \mathbf{s}_0) = \frac{\mathbf{Q}_k \mathbf{O}(\mathbf{s}_{k+1}, \mathbf{s}_k) \mathbf{K}_a(\mathbf{n}_k, \mathbf{s}_{k+1}) I_b(T, \mathbf{s}_{k+1})}{g(\Delta s) (1 - \tilde{\omega})} \quad (6.18)$$

, where $\mathbf{O}(\mathbf{s}_{k+1}, \mathbf{s}_k)$ is the evolution operator pertaining to the preceding pathlength sample, and $g(\Delta s)$, the corresponding importance sampling weight, as indicated in Eq. 6.15. The matrix \mathbf{Q}_k , whose calculation will be described below, holds the multiplicative effect of previous evolution operators, phase matrices, surface reflection matrices, and importance sampling weighting factors, acting on the reversed traced multiply scattered propagation path.

6.2.4 The scattering integral

If, in Eq. 6.16 our sampled $r \leq \tilde{\omega}$, we have sampled a scattering event. In this case we need to evaluate the scattering integral $\int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}'$. Again we apply Monte Carlo integration with importance sampling to this integral.

$$\begin{aligned} \int_{4\pi} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}') d\mathbf{n}' &= \int_0^{2\pi} \int_0^\pi \frac{\mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}')}{g(\theta_{inc}, \phi_{inc})} g(\theta_{inc}, \phi_{inc}) \sin \theta_{inc} d\theta_{inc} d\phi_{inc} \\ &\approx \left\langle \frac{\sin \theta_{inc} \mathbf{Z}(\mathbf{n}, \mathbf{n}') \mathbf{I}(\mathbf{n}')}{g(\theta_{inc}, \phi_{inc})} \right\rangle_{g(\theta_{inc}, \phi_{inc})} \end{aligned} \quad (6.19)$$

Given the desire to use a PDF proportional to the integrand, we choose to sample incoming directions, $\mathbf{n}' = (\theta_{inc}, \phi_{inc})$ from a PDF proportional to $\sin \theta_{inc} \mathbf{Z}(\theta_{scat}, \phi_{scat}, \theta_{inc}, \phi_{inc})$. At the scattering point sample a new incident direction $(\theta_{inc}, \phi_{inc})$ according to

$$g(\theta_{inc}, \phi_{inc}) = \frac{Z_{11}(\theta_{scat}, \phi_{scat}, \theta_{inc}, \phi_{inc}) \sin(\theta_{inc})}{K_{11}(\theta_{scat}, \phi_{scat}) - K_{a1}(\theta_{scat}, \phi_{scat})} \quad (6.21)$$

, which is sampled by the rejection method as described in Liu [2001]. This sampling of the new incoming direction for the evaluation of Eq. 6.20 leads to the calculation of the incoming stokes vector $\mathbf{I}(\mathbf{n}', \mathbf{s})$ at the point of scattering \mathbf{s} in the new incident direction \mathbf{n}' . We thus return to pathlength sampling and evaluation of Eq. 6.15.

6.2.5 Applying the Mueller matrices

The influence of the phase matrix and the preceding evolution operator, along with the importance sampling weights, are stored by calculating the matrix

$$\mathbf{Q}_k = \mathbf{Q}_{k-1} \mathbf{q}_k \quad (6.22)$$

, where

$$\mathbf{q}_k = \frac{\sin(\theta_{inc})_k \mathbf{O}(\mathbf{s}_k, \mathbf{s}_{k-1}) \mathbf{Z}(\mathbf{n}_{k-1}, \mathbf{n}_k)}{g(\Delta s) g(\theta_{inc}, \phi_{inc}) \tilde{\omega}}, \quad (6.23)$$

and $\mathbf{Q}_0 = 1$. The index k represents the scattering order. The \mathbf{Q}_k is updated through precedent scattering events and finally applied to an emission contribution (Eq. 6.18) if an emission event is sampled in Eq. 6.16.

6.2.6 Boundary contributions

If the k^{th} pathlength sampled in Eq. 6.15 is beyond the top of the atmosphere or below the earth surface, \mathbf{Q}_k is applied in

$$\mathbf{I}^i(\mathbf{n}, \mathbf{s}_0) = \frac{\mathbf{Q}_k \mathbf{O}(\mathbf{u}_k, \mathbf{s}_k) \mathbf{I}(\mathbf{n}_k, \mathbf{u}_k)}{O_{11}(\mathbf{u}_k, \mathbf{s}_k)} \quad (6.24)$$

, where $\mathbf{I}(\mathbf{n}_k, \mathbf{u}_k)$ is the incoming radiance at boundary point \mathbf{u}_k . For the top of atmosphere case, $\mathbf{I}(\mathbf{n}_k, \mathbf{u}_k) = I_{space}$. In ARTS it is possible to set I_{space} to any value, but in most cases this is set to the cosmic background radiance associated with a Planck temperature of 2.735K.

For the surface case, if we choose to treat the surface as a blackbody, i.e. there is no reflection, in Eq. 6.24 we set $\mathbf{I}(\mathbf{n}_k, \mathbf{u}_k) = I_{surf}$, where I_{surf} is the Planck radiance associated with the surface temperature, $I_{surf} = I_b(T_{surf})$.

6.2.7 Surface reflection

Currently ARTS-MC can only consider specular reflection. Mostly ARTS-MC has been applied where surface reflections have a small or negligible effect on simulated remote sensing observations. *It would be a straightforward development to handle more complicated reflections. In the same way that the phase matrix is sampled to choose new incoming directions for scattering events, we could sample the Bidirectional reflection distribution (BDRF) for surface reflection events.* In analogy with scattering and emission in Eq. 6.16, \mathbf{I}_{surf} is given by the sum of reflected and emitted radiation:

$$\begin{aligned} \mathbf{I}_{surf}(\mathbf{n}_k, \mathbf{u}_k) &= \mathbf{B}(\mathbf{n}_k, \mathbf{u}_k) + \mathbf{R}(\mathbf{n}_k, \mathbf{n}_{k+1}, \mathbf{u}_k) \mathbf{I}(\mathbf{n}_{k+1}, \mathbf{u}_k) \\ &= \int_0^1 \left\{ \begin{array}{ll} \frac{1}{R_{11}} \mathbf{R}(\mathbf{n}_k, \mathbf{n}_{k+1}, \mathbf{u}_k) \mathbf{I}(\mathbf{n}_{k+1}, \mathbf{u}_k) & r \leq R_{11} \\ \frac{\mathbf{B}(\mathbf{n}_k, \mathbf{u}_k)}{1-R_{11}} & r > R_{11} \end{array} \right. dr \\ &\approx \left\langle \left\{ \begin{array}{ll} \frac{1}{R_{11}} \mathbf{R}(\mathbf{n}_k, \mathbf{n}_{k+1}, \mathbf{u}_k) \mathbf{I}(\mathbf{n}_{k+1}, \mathbf{u}_k) & r \leq R_{11} \\ \frac{\mathbf{B}(\mathbf{n}_k, \mathbf{u}_k)}{1-R_{11}} & r > R_{11} \end{array} \right. \right\rangle_r \end{aligned} \quad (6.25)$$

The reflection matrix $\mathbf{R}(\mathbf{n}_k, \mathbf{n}_{k+1}, \mathbf{u}_k)$ and related surface emission, $\mathbf{B}(\mathbf{n}_k, \mathbf{u}_k)$ are calculated in one of several ways, as described in section **[FIXME: that stuff should be in this document but it isn't yet]**. As in Eq. 6.16, we use a uniform random deviate r ; if $r > R_{11}$, where R_{11} is the (1,1) element of $\mathbf{R}(\mathbf{n}_k, \mathbf{n}_{k+1}, \mathbf{u}_k)$, then the event is considered to be surface emission. In this case we have all the information required to calculate the SVE in Eq.6.24 becomes,

$$\mathbf{I}^i(\mathbf{n}, \mathbf{s}_0) = \frac{\mathbf{Q}_k \mathbf{O}(\mathbf{u}_k, \mathbf{s}_k) \mathbf{B}(\mathbf{n}_k, \mathbf{u}_k)}{O_{11}(\mathbf{u}_k, \mathbf{s}_k)(1 - R_{11})}. \quad (6.26)$$

If our sampled $r \leq R_{11}$ in Eq. 6.25, then we have a surface reflection contribution, and the incoming (downward) stokes vector $\mathbf{I}(\mathbf{n}_{k+1}, \mathbf{u}_k)$ remains unknown. As in the scattering case we record the effect the evolution and reflection operators in the matrix $\mathbf{Q}_k = \mathbf{Q}_{k-1} \mathbf{q}_k$, where

$$\mathbf{q}_k = \frac{\mathbf{O}(\mathbf{s}_k, \mathbf{s}_{k-1}) \mathbf{R}(\mathbf{n}_{k-1}, \mathbf{n}_k)}{O_{11}(\mathbf{u}_k, \mathbf{s}_k) R_{11}} \quad (6.27)$$

, and continue with another path integral (Eq. 6.15) in the direction \mathbf{n}_{k+1} . Since the reflection is specular, \mathbf{n}_{k+1} is described by zenith and azimuthal angles $\theta_{k+1} = \pi - \theta_k$ and $\phi_{k+1} = \phi_k$. With regard to the scattering order k , surface reflection is considered the same as scattering.

6.2.8 Summary

Summarizing sections 6.2.2 to 6.2.7 we see that successively nested Monte Carlo integrals are calculated until atmospheric emission, surface emission, or top of atmosphere contributions are sampled. Mueller matrices encountered in each nested integral (evolution operators, phase matrices, reflection matrices), along with Monte Carlo weights, are recorded in the matrix \mathbf{Q}_k . This matrix applies the Mueller matrices in the correct ‘forward’ order to each emission or top of atmosphere contribution (Eq.s 6.18, 6.26, and 6.24). The algorithm summarized graphically in Figure 6.2.8.

6.3 Practical considerations regarding optical properties

6.3.1 Particle orientation and the evolution operator

The calculation of the evolution operator in Eqs. 6.8 and 6.9 requires evaluation of the matrix exponential. If the scattering particles are spheres (P10), or randomly orientated (p20), as described in Section [FIXME], then Eq. 6.8 is simply

$$O_{jj}(s', s) = \exp(-K_{jj}\Delta s) \quad (6.28)$$

If scattering particles have rotational symmetry, and the axis of symmetry is oriented vertically, or if the particles are have random azimuthal orientation (p30), as described in Section [FIXME], then the extinction matrix has a block diagonal form with 3 independent elements, K_{jj} , K_{12} , and K_{34} (See section [FIXME]).

6.3.2 Particle orientation and the phase matrix

6.4 Variations on the ARTS-MC algorithm

6.4.1 The original ARTS-MC and forcing the original pathlength sample to be within the 3D box

6.4.2 1D clear sky variables and clear sky radiance look up

6.4.3 MCIPA

6.4.4 optical path and ice water path calculations

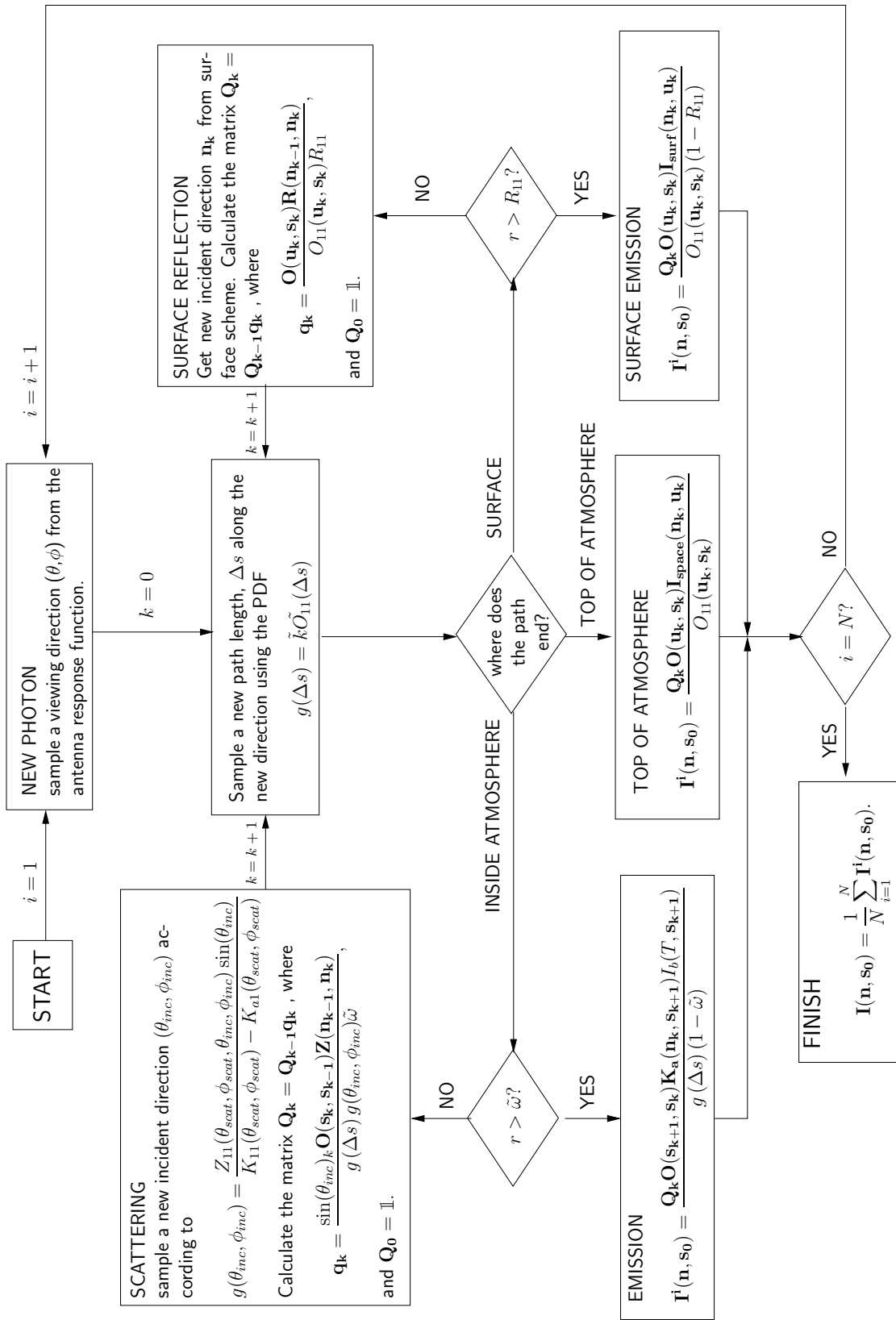


Figure 6.1: Flowchart illustrating MCGeneral algorithm

Part I

Bibliography and Appendices

Bibliography

- Battaglia, A., C. P. Davis, C. Emde, and C. Simmer, Microwave radiative transfer intercomparison study for 3-D dichroic media, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *105*, 55–67, 2007.
- Bauer, A., M. Godon, M. Kheddar, and J. M. Hartmann, Temperature and perturber dependence of water vapor line broadening: Experiments at 183 GHz; calculations below 1000 GHz, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *41*, 49–54, 1989.
- Bauer, A., M. Godon, J. Carlier, Q. Ma, and R. H. Tipping, Absorption by H₂O and H₂O-N₂ mixtures at 153 GHz, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *50*, 463–475, 1993.
- Bauer, A., M. Godon, J. Carlier, and Q. Ma, Water vapor absorption in the atmospheric window at 239 GHz, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *53*, 411–423, 1995.
- Becker, G. E., and S. H. Autler, Water vapor absorption of electromagnetic radiation in the centimeter wavelength range, *Phys. Rev.*, *70*, 300–307, 1946.
- Bernath, P., *Spectra of Atoms and Molecules*, Oxford University Press, 1995, ISBN 0-195-07598-6.
- Berton, R. P. H., Statistical distribution of water content and sizes for clouds above Europe, *Ann. Geophys.*, *18*, 385–397, 2000.
- Bohren, C., and D. R. Huffman, *Absorption and Scattering of Light by Small Particles*, Wiley Science Paperback Series, 1998.
- Borysow, A., and L. Frommhold, Collision induced rototranslational absorption spectra of N₂-N₂ pairs for temperatures from 50 to 300 K, *Astrophysical Journal*, *311*, 1043–1057, 1986.
- Brussaard, G., and P. A. Watson, *Atmospheric Modelling and Millimetre Wave Propagation*, Chapman & Hall, 1995, ISBN 0-412-56230-8.
- Buehler, S. A., P. Eriksson, T. Kuhn, A. von Engeln, and C. Verdes, ARTS, the Atmospheric Radiative Transfer Simulator, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *91*, 65–93, 2005.

- Chandrasekhar, S., *Radiative Transfer*, Dover Publications, New York, 1960.
- Clough, S. A., F. X. Kneizys, and R. W. Davis, Line shape and water vapor continuum, *Atmospheric Research*, 23, 229–241, 1989.
- Costa, A. A., G. P. Almeida, and A. J. C. Sampaio, A bin-microphysics cloud model with high-order, positive-definite advection, *Atmospheric Research*, 55, 225–255, 2000.
- Cruz Pol, S. L., C. S. Ruf, and S. J. Keihm, Improved 20– to 32–GHz atmospheric absorption model, *Radio Science*, 33, 1319–1333, 1998, updated version can be downloaded from <http://ece.uprm.edu/~pol/Atmosphere.html>.
- Dagg, I. R., G. E. Reesor, and J. L. Urbaniak, Collision induced absorption in N₂, CO₂, and H₂ at 2 cm⁻¹, *Canadian Journal of Physics*, 53, 1764–1776, 1975.
- Dagg, I. R., G. E. Reesor, and M. Wong, A microwave cavity measurement of collision-induced absorption in N₂ and CO₂ at 4.6 cm⁻¹, *Can. J. Phys.*, 56, 1037–1045, 1978.
- Davis, C., C. Emde, and R. Harwood, A 3D polarized reversed monte carlo radiative transfer model for mm and sub-mm passive remote sensing in cloudy atmospheres, *IEEE Transactions on Geoscience and Remote Sensing*, 43, 1096–1101, 2005.
- Degl’Innocenti, E. L., and M. L. Degl’Innocenti, On the solution of the radiative-transfer equations for polarized radiation, *Solar Physics*, 97, 239–250, 1985.
- Drayson, S. R., Rapid computation of the Voigt profile, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 16, 611, 1976.
- English, S. J., C. Guillou, C. Prigent, and D. C. Jones, Aircraft measurements of water vapor continuum absorption at millimeter wavelengths, *Quarterly Journal of the Royal Meteorological Society*, 120, 603–625, 1994.
- Eriksson, P., Microwave radiometric observations of the middle atmosphere: Simulations and inversions, Ph.D. thesis, School of Electrical and Computer Engineering, Chalmers University of Technology, Sweden, 1999.
- Eriksson, P., F. Merino, D. Murtagh, P. Baron, P. Ricaud, and J. de La Noë, Studies for the Odin sub-millimetre radiometer: 1. Radiative transfer and instrument simulation, *Canadian Journal of Physics*, 80, 321–340, 2002.
- Eriksson, P., M. Ekström, S. Bühler, and C. Melzheimer, Efficient forward modelling by matrix representation of sensor responses, *International Journal of Remote Sensing*, 27, 1793–1808, 2006.
- Godon, M., J. Carlier, and A. Bauer, Laboratory studies of water vapor absorption in the atmospheric window at 213 GHz, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 47, 275–285, 1992.
- Goody, R. M., *Principles of atmospheric physics and chemistry*, Oxford University Press, 1995.

- Goody, R. M., and Y. L. Yung, *Atmospheric radiation, theoretical basis*, Oxford University Press, 1989, second edition.
- Gordy, W., and R. Cook, *Microwave Molecular Spectra*, Interscience Publishers, 1970, SBN 471 93161 6.
- Herzberg, G., *Infrared and Raman Spectra of Polyatomic Molecules*, Van Nostrand Reinhold Company, 1945, ISBN 0-442-03386-9.
- Hess, M., P. Koepke, and I. Schult, Optical properties of aerosols and clouds: The software package OPAC, *Bulletin of the American Meteorological Society*, 79, 831–844, 1998.
- Ho, W., I. A. Kaufman, and P. Thaddeus, Laboratory measurement of microwave absorption in models of the atmosphere of Venus, *Journal of Geophysical Research*, 71, 5091–5108, 1966.
- Hochstadt, H., *Differential Equations: A Modern Approach*, Holt, Rinehart, and Winston, 1964.
- Hufford, G. A., A model for the complex permittivity of ice at frequencies below 1 thz, *Internatl. J. Infrared & Millimeter Waves*, 12, 677–682, 1991.
- Hui, A. K., B. H. Armstrong, and A. A. Wray, Rapid computation of the voigt and complex error functions, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 19, 509–516, 1978.
- Jackson, J. D., *Classical electrodynamics*, John Wiley & Sons, New York, 1998.
- Kneizys, F. X., et al., The MODTRAN2/3 report and LOWTRAN7 model laboratory studies and propagation modelling, *Tech. Rep. 1/11/96*, Phillips Laboratory, Geophysical Directorate, PL/GPOS, 1996, editors: L. W. Abreu and G. P. Anderson.
- Kuntz, M., and M. Höpfner, Efficient line-by-line calculation of absorption coefficients, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 63, 97–114, 1999.
- Larsen, H., J.-F. Gayet, G. Febvre, H. Chepfer, and G. Brogniez, Measurement errors in cirrus cloud microphysical properties, *Ann. Geophys.*, 16, 266–276, 1998.
- Li, L., J. Vivekanandan, C. H. Chan, and L. Tsang, Microwave radiometric technique to retrieve vapor; liquid and ice; part I – development of a neural network-based inversion method, *IEEE Transactions on Geoscience and Remote Sensing*, 35, 224–235, 1997.
- Liebe, H. J., Modelling attenuation and phase of radio waves in air at frequencies below 1000 ghz, *Radio Science*, 16, 1183–1199, 1981.
- Liebe, H. J., The atmospheric water vapor continuum below 300 GHz, *Internatl. J. Infrared & Millimeter Waves*, 5(2), 207–227, 1984.
- Liebe, H. J., MPM – an atmospheric millimeter-wave propagation model, *Internatl. J. Infrared & Millimeter Waves*, 10, 631–650, 1989.

- Liebe, H. J., and D. H. Layton, Millimeter-wave properties of the atmosphere: Laboratory studies and propagation modelling, *Tech. Rep. 87224*, U.S. Dept. of Commerce, National Telecommunications and Information Administration, Institute for Communication Sciences, 1987, 80p.
- Liebe, H. J., T. Manabe, and G. A. Hufford, Millimeter-wave attenuation and delay rates due to fog/cloud conditions, *IEEE Trans. Antennas Propag.*, *37*, 1617–1623, 1989.
- Liebe, H. J., G. A. Hufford, and T. Manabe, A model for the complex permittivity of water at frequencies below 1 thz, *Internatl. J. Infrared & Millimeter Waves*, *12*, 659–675, 1991.
- Liebe, H. J., P. W. Rosenkranz, and G. A. Hufford, Atmospheric 60-GHz oxygen spectrum: new laboratory measurements and line parameters, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *48*, 629–643, 1992.
- Liebe, H. J., G. A. Hufford, and M. G. Cotton, Propagation modeling of moist air and suspended water/ice particles at frequencies below 1000 GHz., in *AGARD 52nd Specialists Meeting of the Electromagnetic Wave Propagation Panel, Palma de Mallorca, Spain*, 1993, <ftp://ftp.its.blrdoc.gov/pub/mpm93/>.
- Liou, K. N., *An introduction to atmospheric radiation*, 2nd ed., Academic Press, 2002.
- Lipton, A. E., M. K. Griffin, and A. G. Ling, Microwave transfer model differences in remote sensing of cloud liquid water at low temperatures, *IEEE Transactions on Geoscience and Remote Sensing*, *37*, 620–623, 1999.
- Liu, J. S., *Monte Carlo Strategies in Scientific Computing*, Springer-Verlag, 2001.
- Liu, Q., C. Simmer, and E. Ruprecht, Three-dimensional radiative transfer effects of clouds in the microwave spectral range, *Journal of Geophysical Research*, *101*, 4289–4298, 1996.
- Ludlam, F. H., and B. J. Mason, The physics of clouds, in *Encyclopedia of Physics*, edited by S. Flügge, vol. 48, Springer, Berlin, 1957.
- Ma, Q., and R. H. Tipping, Water vapor continuum in the millimeter spectral region, *Journal of Chemical Physics*, *93*, 6127–6139, 1990.
- Mishchenko, M. I., Vector radiative transfer equation for arbitrarily shaped and arbitrarily oriented particles: a microphysical derivation from statistical electromagnetics, *Applied Optics*, *41*, 7114–7134, 2002.
- Mishchenko, M. I., J. W. Hovenier, and L. D. Travis, eds., *Light Scattering by Nonspherical Particles*, Academic Press, 2000, ISBN 0-12-498660-9.
- Mishchenko, M. I., L. D. Travis, and A. A. Lacis, *Scattering, Absorption and Emission of Light by Small Particles*, Cambridge University Press, 2002, ISBN 0-521-78252.
- Oliveiro, J. J., and R. L. Longbothum, Empirical fits to voight line width: A brief review, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *17*, 233–236, 1977.

- Pawlowska, H., J. L. Brenguier, and F. Burnet, Microphysical properties of stratocumulus clouds, *Atmospheric Research*, 55, 15–33, 2000.
- Petty, G. W., *A first course in atmospheric radiation*, Sundog Publishing, 2006.
- Press, W., S. Teukolsky, W. Vetterling, and B. Flannery, *Numerical recipes in FORTRAN*, 2nd ed., Cambridge University Press, 1992.
- Press, W., S. Teukolsky, W. Vetterling, and B. Flannery, *Numerical recipes in C*, 2nd ed., Cambridge University Press, 1997.
- Ray, P., Broadband complex refractive indices of ice and water, *Appl. Opt.*, 11, 1836–1844, 1972.
- Rees, W. G., *Physical principles of remote sensing*, 2nd ed., Cambridge University Press, 2001.
- Rodgers, C., *Inverse methods for atmospheric sounding: Theory and practise*, 1st ed., World Scientific Publishing, 2000.
- Rodgers, C. D., Characterization and error analysis of profiles retrieved from remote sounding measurements, *Journal of Geophysical Research*, 95, 5587–5595, 1990.
- Rosenkranz, P. W., Absorption of microwaves by atmospheric gases, in *Atmospheric remote sensing by microwave radiometry*, edited by M. A. Janssen, pp. 37–90, John Wiley & Sons, Inc., 1993, ftp://mesa.mit.edu/phil/lbl_rt.
- Rosenkranz, P. W., Water vapor microwave continuum absorption: A comparison of measurements and models, *Radio Science*, 33, 919–928, 1998, (correction in 34, 1025, 1999), ftp://mesa.mit.edu/phil/lbl_rt.
- Rothman, L. S., et al., The HITRAN molecular database: editions of 1991 and 1992, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 48, 469–507, 1992.
- Rothman, L. S., et al., The HITRAN molecular spectroscopic database and HAWKS (HITRAN atmospheric workstation): 1996 edition, *Journal of Quantitative Spectroscopy and Radiative Transfer*, 60, 665–710, 1998.
- Salby, M. L., *Fundamentals of Atmospheric Physics*, vol. 61 of *International Geophysics Series*, Academic Press, 1996, ISBN 0-12-615160-1.
- Seinfeld, J. H., and S. N. Pandis, *Atmospheric Chemistry and Physics : from Air Pollution to Climate Change*, Wiley, 1998, ISBN 0-471-17816-0.
- Shupe, M. D., T. Uttal, S. Y. Matrosov, and A. S. Frisch, Cloud water content and hydrometeor sizes during the FIRE-Arctic Clouds Experiment, *Journal of Geophysical Research*, 106, 15015–15028, 2000.
- Stankevich, K. S., Absorption of sub-millimeter-range radio waves in a dry atmosphere, *Radiophys. Quantum Electron. (Engl. Transl.)*, 17, 579–581, 1974.

- Stone, N. W., W. G. Read, A. Anderson, I. R. Dagg, and W. Smith, Temperature-dependent collision-induced absorption in nitrogen, *Can. J. Phys.*, *62*, 338–347, 1984.
- Thorne, A., U. Litzen, and S. Johansson, *Spectrophysics : principles and applications*, Springer, 1999, ISBN 3-540-65117-9.
- Townes, C. H., and A. L. Schawlow, *Microwave Spectroscopy*, Mc Graw-Hill, 1955.
- Ulaby, F., R. Moore, and A. Fung, *Microwave remote sensing: Active and passive, Volume I: Microwave remote sensing fundamentals and radiometry*, Addison-Wesley Publishing Company, 1981, ISBN 0-201-10759-7 (v. 1).
- van de Hulst, H., *Light Scattering by Small particles*, Dover Publications, New York, 1957, corrected republication 1981.
- Van Vleck, J. H., The relation between absorption and dispersion, in *Propagation of Short Radio Waves*, edited by D. E. Kerr, pp. 641–664, Peter Peregrinus Ltd, 1987, first published in 1951 by McGraw-Hill Book Comp. Inc.
- Van Vleck, J. H., and D. L. Huber, Absorption, emission, and linebreadths: a semihistorical perspective, *Reviews of Modern Physics*, *49*, 939–959, 1977.
- Van Vleck, J. H., and V. F. Weisskopf, On the shape of collision-broadening lines, *Reviews of Modern Physics*, *17*, 227–236, 1945.
- Verdes, C., A. von Engeln, and S. A. Buehler, Partition function data and impact on retrieval quality for a mm/sub-mm limb sounder, *Journal of Quantitative Spectroscopy and Radiative Transfer*, *90*, 217–238, 2005.
- Westwater, E. R., J. B. Snider, and M. J. Falls, Ground-based microwave radiometric retrieval of precipitable water vapor in the presence of clouds with high liquid content, *Radio Science*, *15*, 947–957, 1980.

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