Analytical expressions for modeling of radiative transfer and instrumental effects in KOPRA

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Abstract: This paper reports the analytical expressions of radiative transfer and typical instrumental effects the Karlsruhe Optimized and Precise Radiative Transfer Algorithm (KOPRA) is based on. It contains formal expressions of the integrated version of the equation of radiative transfer in the atmosphere, the source function for local thermodynamic equilibrium as well as non-local thermodynamic equilibrium conditions, transmission, slant path column densities of molecules, ray tracing, absorption and extinction coefficients, line intensities as function of temperature, line shape functions, instrument line shape of an interferometer, numerical apodization, aperture effects, and field of view consideration. On this formalism the numeric treatment of spectral modeling in KOPRA is based.

1 Introduction

Computational treatment of radiative transfer processes in the atmosphere requires numeric treatment of many processes. Nevertheless the analytic expression behind the numerics actually coded is important to make a code such as the Karlsruhe Optimized and Precise Radiative Transfer Algorithm (KOPRA) understandable. The intention of this paper is presentation of these analytical expressions, such that interrelations of variables used in this program become traceable. This paper is organized as follows: First radiative transfer physics is discussed in a top to bottom manner, starting with the radiative transfer equation, and consecutively breaking it down to more detail. Second, the degradation functions of a Fourier transform spectrometer with finite field of view as well as numerical apodization are discussed.

2 Radiative Transfer Equation

The following integrated version of Chandrasekhar's [1] radiative transfer equation is used here:

$$S_\Theta(\nu, l_{obs}) \;=\; S_\Theta(\nu, l_o)\,\tau(\nu, l_{obs}, l_o) \;+\; \int\limits_{l_{obs}}^{l_o} J(\nu, l)\,\sigma^{Vol}_{a,total}(\nu, l)\,\tau(\nu, l_{obs}, l)\,dl \qquad (1)$$

where

S_Θ	spectral radiance for the viewing angle Θ
J	source funktion (see Section 2.2)
$\tau(\nu, l_1, l_2)$	transmission between l_1 and l_2 for wavenumber ν (see Section 2.3)
dl	path element (see Section 2.1)
$\sigma^{Vol}_{a,total}$	absorption coefficient including gases and aerosols (per volume) (see Section 2.3.1)
l_{obs}	position of the observer
l_o	position of background radiative source
ν	wavenumber
l	path coordinate

2.1 Ray Tracing

The integration of Eq. 1 is performed along the line of sight of the instrument, which is, through atmospheric refraction, not a straight line. This integration is performed not analytically but numerically for thin atmospheric layers characterized by constant representative state parameters which are derived from the state parameter profiles by mass-weighted integration. In a medium of smoothly varying refractive index $n(z)$, there is refraction as soon as the gradient of $n(z)$ is not parallel to the raypath. After traveling the infinitesimal distance dl, the angular difference between the original and the new direction $d\theta$ is [2]

$$d\theta = dl \times |\vec{e_s}\dot{\bigtriangledown} n_b| / n_b \qquad (2)$$

where $\vec{e_s}$is the component of unity in direction perpendicular to the old direction and the gradient of refractive index. The the length of each path segment l in layer j used for integration of Equation 4 then is

$$l_j = \int dl \qquad (3)$$

The slant path column amount m_g of a species g in the layer j is

$$m_{g,j} \;=\; \int_{l_1}^{l_2} \rho_g(l)\,dl \qquad (4)$$

where the particle density ρ_g of species g is calculated as

$$\rho_g(l) \;=\; C_{V,g} \cdot \frac{N_{avo}}{R} \cdot \frac{p(l)}{T_{kin}(l)} \qquad (5)$$

where N_{avo} is the Avogadro constant, R the universal gas constant, $C_{V,g}$ the volume mixing ration of species g, $T_{kin}(l)$ kinetic temperature at the position l, and p is pressure.

Mass-weighted state parameters are

$$p_{average,g,j} = \frac{1}{m_{g,j}} \int p(l)\rho_g(l)dl \tag{6}$$

and

$$T_{average,g,j} = \frac{1}{m_{g,j}} \int T(l)\rho_g(l)dl \tag{7}$$

This approach supports straight forward consideration of ellipsoidal earth shape, where the local radius R_E is

$$R_E(\Psi) \; = \; \sqrt{\frac{a_E^2 \cdot b_E^2}{b_E^2 \cdot \cos\Psi^2 \; + \; a_E^2 \cdot \sin\Psi^2}} \tag{8}$$

where

$$\tan\Psi \; = \; \left(\frac{b_E}{a_E}\right)^2 \tan\Phi \tag{9}$$

with geocentric latitude Ψ, geographic latitude Φ, major semiaxis a_E, and minor semiaxis b_E.
The refractive index n_b is calculated from the wavenumber-dependent refractive index for dry air n_{b_o}, referring to reference state parameters $T_o = 288.16$ K and $p_o = 1013.25$ hPa, as

$$n_b(l) \; = \; \sqrt{\frac{2\,k\,p(l) \; + \; T_(l)}{T_(l) \; - \; k\,p(l)}} \tag{10}$$

where

$$k \; = \; \frac{T_o\;(n_{b_o}^2 \; - \; 1)}{p_o\;(n_{b_o}^2 \; + \; 2)} \tag{11}$$

The wavenumber dependence of the refractive index is

$$(n_{b_o} \; - \; 1) \cdot 10^6 \; = \; 83.4213 + \frac{24060.3}{130 - 10^8\nu^2} \; + \; \frac{159.97}{38.9 - 10^8\nu^2} \tag{12}$$

where ν must be given in cm^{-1}.

2.2 The Source Function

2.2.1 Local Thermodynamic Equilibrium

In the case of local thermodynamic equilibrium (LTE), the source function J_{LTE} is the Planck function B of the kinetic temperature T_{kin} of the emitting medium:

$$J^{LTE}(\nu, l) \; = \; B(\nu, T_{kin}(l)) \tag{13}$$

The Planck function as a function of frequency f is

$$B(f,T) = \frac{2f^2}{c^2} \cdot \frac{hf}{\exp\left(\frac{hf}{k_B T}\right) \; - \; 1} \tag{14}$$

where h is the Planck constant and c the velocity of light. The Planck function as a function of wavenumber ν can be deduced from Eq. 14 by post-differentiation of the Planck function by $\frac{d\nu}{df}$:

$$B(\nu, T_{kin}(l)) = \frac{2hc^2\nu^3}{\exp\left(\frac{hc\nu}{k_B T_{kin}(l)}\right) \; - \; 1} \tag{15}$$

2.2.2 Non-Local Thermodynamic Equilibrium (NLTE)

Here we follow the formalism of [3] and [4]. For a single line, the source function J in case of non-local thermodynamic equilibrium (NLTE) can be written as:

$$J^{NLTE}(\nu, l) \;=\; \frac{2hc^2\nu^3}{\frac{r_1}{r_2}\exp\left(\frac{hc\nu}{k_B T_{kin}(l)}\right) \;-\; 1} \tag{16}$$

where r_1 and r_2 are the ratios of populations between the general (NLTE) and LTE cases for the lower (1) and upper (2) states of transition n. This ratio of populations between the general (NLTE) and LTE cases for the state m can also be written as

$$r_m \;=\; f_Q(l)\;\exp\left(-\frac{E_{vib,m}}{k_B}\left(\frac{1}{T_{Vib,m}(l)} \;-\; \frac{1}{T_{kin}(l)}\right)\right) \tag{17}$$

where m is the vibrational state under consideration, $E_{vib,m}$ its energy level, T_{Vib} the related vibrational temperature, and $f_Q(l)$ is a correction factor to the vibrational partition sum given by

$$f_Q(l) = \frac{\sum_m g_m \exp\left(-\frac{hcE_{vib,m}}{k_B T_{kin}(l)}\right)}{\sum_m g_m \exp\left(-\frac{hcE_{vib,m}}{k_B T_{vib,m}(l)}\right)}\,. \tag{18}$$

Here, g_m represents the degeneracy factor of state m. For superimposed lines, the NLTE source function is written as

$$J^{NLTE}(\nu, l) \;=\; \beta(\nu, l)\cdot B(\nu, T_{kin}(l)) \tag{19}$$

$$\beta(\nu, l) \;=\; \frac{\sum\limits_{gn} r_{2,gn}(l)\;\sigma^{LTE}_{a,gn}(\nu, l)\;m_g(l)}{\sum\limits_{gn} \alpha_{gn}(\nu, l)\;\sigma^{LTE}_{a,gn}(\nu, l)\;m_g(l)} \tag{20}$$

$$\alpha_{gn} \;=\; \frac{\sigma^{NLTE}_{a,gn}(\nu, l)}{\sigma^{LTE}_{a,gn}(\nu, l)} \tag{21}$$

where

$\sigma^{LTE}_{a,gn}$	absorption coefficient (LTE) (see Eq. 27)
$\sigma^{NLTE}_{a,gn}$	absorption coefficient (NLTE) (see Eq. 28)

2.3 Transmittance

The spectral atmospheric transmission $\tau(\nu, l_1, l_2)$ between two points l_1 and l_2 on the line of sight is calculated as follows:

$$\tau(\nu, l_1, l_2) = \exp\,-\left\{\int\limits_{l_1}^{l_2} \sigma^{Vol}_{a,gas}(\nu, l)\;dl \;+\; \underbrace{\int\limits_{l_1}^{l_2} \sigma^{Vol}_{e,aerosol}(\nu, l)\;dl}_{\text{Aerosol}}\right\} \tag{22}$$

$$= \exp - \left\{ \sum_{g=1}^{G} \int_{l_1}^{l_2} \sigma_{a,g}(\nu,l)\, \frac{\partial m_g(l)}{\partial l}\, dl \;+\; \underbrace{\int_{l_1}^{l_2} \sigma^{Vol}_{e,aerosol}(\nu,l)\, dl}_{\text{Aerosol}} \right\}$$

where

$\sigma^{Vol}_{e,aerosol}$	aerosol extinction coefficient (from external Mie calculation)
$\sigma^{Vol}_{a,gas}$	volume absorption coefficient for gases (see Eq. 24)
$\sigma_{a,g}$	absorption coefficient of the gas g (see Eqs.25)
m_g	slant path column amount of gas g (see Eq. 4)
dl	path element
G	number of gases taken into account

2.3.1 Absorption and -Extinction Coefficients

2.3.1.1 Local Thermodynamic Equilibrium

The aerosol extinction coefficient (per volume) is

$$\sigma^{Vol}_{e,aerosol}(\nu,l) \;=\; \sigma^{Vol}_{a,aerosol}(\nu,l) \;+\; \sigma_s(\nu,l) \tag{23}$$

The gas absorption coefficient is (per volume) is

$$\sigma^{Vol}_{a,gas}(\nu,l) = \sum_{g=1}^{G} \sigma_{a,g}(\nu,l)\cdot \rho_g(l) \tag{24}$$

The absorption coefficient of species g is

$$\sigma_{a,g}(\nu,l) \;=\; \sum_{n=1}^{N_g} \sigma_{a,gn}(\nu,l) + (\text{cross-sections}) + (\text{continua}) \tag{25}$$

where

$\sigma^{Vol}_{e,aerosol}$	aerosol extinction coefficient (per volume)
$\sigma^{Vol}_{a,aerosol}$	aerosol absorption coefficient (per volume)
σ_s	scattering coefficient (from external Mie calculations)
$\sigma_{a,gn}$	absorption coefficient of the transition n of species g (see Eqs. 27 / 28)
ρ_g	particle density of species g (see Eq. 5)
G	number of species under consideration
N_g	number of transitions of species g

Scattering is considered here in terms of extinction only. No additional source term of the type

$$J_s(\nu,l) \;=\; \frac{\Omega_o}{4\pi} \int\!\!\int p(\Omega,\Omega')S(\Omega,\Omega')\, d\Omega' \tag{26}$$

is considered here. The absorption coefficients $\sigma^{LTE}_{a,gn}$ of transition n of species g in LTE is written

$$\sigma^{LTE}_{a,gn}(\nu,l) \;=\; A_{gn}(T_{kin}(l),\nu)\cdot \Phi_{gn}(\nu,p(l),T_{kin}(l)) \tag{27}$$

where

A_{gn}	line intensity of transition n of species g (see Eq.2)
Φ_{gn}	profile function of transition n of species g at position l (see Chapter 2.3.1.4)

2.3.1.2 Non-Local Thermodynamic Equilibrium

In case of NLTE, the absorption coefficient $\sigma_{a,gn}^{NLTE}$ of transition n of species g is derived from the absorption coefficient in LTE by a correction factor α:

$$\sigma_{a,gn}^{NLTE}(\nu,l) \;=\; \alpha_{gn}(\nu,l)\cdot\sigma_{a,gn}^{LTE}(\nu,l) \tag{28}$$

Correction factor α, which is one in case of LTE, is calculated as

$$\alpha_{gn}(\nu,l) \;=\; \frac{\sigma_{a,gn}^{NLTE}(\nu,l)}{\sigma_{a,gn}^{LTE}(\nu,l)} \;=\; \frac{r_1 - r_2\Gamma}{1-\Gamma}. \tag{29}$$

where

$$\Gamma \;=\; \frac{g_1 n_2}{g_2 n_1} \;=\; \exp\left(-hc\nu/k_B T_{kin}\right) \tag{30}$$

$$r_1 \;=\; \frac{n_1^{NLTE}}{n_1^{LTE}} \quad ; \quad r_2 \;=\; \frac{n_2^{NLTE}}{n_2^{LTE}} \tag{31}$$

and where

r_1, r_2	ratios of populations between the general (NLTE) and LTE cases for the lower (1) and upper (2) state (see 17)
n_1^{NLTE}	population of the lower state (NLTE)
n_1^{LTE}	population of the lower state (LTE)
n_2^{NLTE}	population of the upper state (NLTE)
n_2^{LTE}	population of the upper state (LTE)
g_1, g_2	level statistical weights for the lower (1) and upper (2) state

2.3.1.3 Line Intensities

The intensity A_{gn} of line n of species g is

$$A_{gn}(T_{kin},\nu) \;=\; A_{gn}(T_o',\nu)\cdot\frac{Q(T_o')}{Q(T_{kin})}\;\frac{e^{-\frac{E_{gn}''}{k_B T_{kin}}}}{e^{-\frac{E_{gn}''}{k_B T_o'}}}\;\frac{1\;-\;e^{-\frac{hc\nu}{k_B T_{kin}}}}{1\;-\;e^{-\frac{hc\nu}{k_B T_o}}} \tag{32}$$

where

k_B	Boltzmann constant
E_{gn}''	lower state energy of transition n (see Eq. (3))
$Q(T)$	LTE total internal partition function evaluated at T (see Eq.(4))
$Q(T_o')$	LTE total internal partition function at T_o'
$A_{gn}(T_o')$	line intensity at reference temperature T_o'
T_{kin}	kinetic temperature
T_o'	reference temperature (296 K)
ν	wavenumber, usually approximated as $\nu_{o,n}$
$\nu_{o,n}$	central wavenumber of transition n

The lower state energy E'' is calculated from the lower state energy e'' in units of wavenumbers as given in spectroscopic databases by:

$$E''_{gn} \;=\; c\, e''_{gn}\; h \tag{33}$$

The total internal partition function $Q(T)$ describes the temperature dependence of the line intensity of a transition. In LTE it is

$$Q(T) \;=\; \sum_{j=o}^{\infty} g_j \,\exp\left(\frac{E_j}{k_B T}\right) \tag{34}$$

where j is the rotational-vibrational-state, g the factor of degeneration, and E the energy of level j. It is approximated as

$$Q(T) \;=\; a_0 \;+\; a_1 T \;+\; a_2 T^2 \;+\; a_3 T^3 \tag{35}$$

where a_0, a_1, a_2, and a_3 are pretabulated coefficients [5].

2.3.1.4 Profile Function

The Doppler profile function describes the statistical distribution of frequency shifts due to thermal motion:

$$\Phi_{D,n}(\nu, T) \;=\; \frac{1}{\alpha_{D,n}} \sqrt{\frac{\ln 2}{\pi}}\; e^{\,-\,\ln 2 \left(\frac{\nu - \nu_{o,n}}{\alpha_{D,n}}\right)^2} \tag{36}$$

where

$$\alpha_{D,n}(T) \;=\; \frac{\nu_{o,n}}{c} \sqrt{\frac{2 k_B T \ln 2}{M}} \tag{37}$$

and where $\alpha_{D,n}$ is the Doppler halfwidth, M the molecular mass, and $\nu_{o,n}$ central wavenumber of transition n.

The Lorentzian profile function $\Phi_{L,n}$ of transition n, centered at $\nu_{o,n}$, describes pressure broadening, under assumption of infinitesimally short impact between collision partners and elastic collisions:

$$\Phi_{L,n}(\nu, p, T) \;=\; \frac{1}{\pi} \left(\frac{\alpha_{L,n}}{(\nu - \nu_{o,n})^2 \;+\; \alpha_{L,n}^2} \right) \tag{38}$$

The actual Lorentzian halfwidth $\alpha_{L,n}$ is calculated for the actual temperature T and actual pressure p from the related reference Lorentzian halfwidth $\alpha_{L_o,n}$ measured at reference pressure p_o^L and reference temperature T_o^L

$$\alpha_{L,n}(p, T) \;=\; \alpha_{L_o,n}(p_o^L, T_o^L) \frac{p}{p_o^L} \left(\frac{T_o^L}{T}\right)^{\gamma_n} \tag{39}$$

The coefficient of temperature dependence of the halfwidth γ_n, which, following classical collisional theory, should be 0.5, may deviate from this theoretical value; therefore laboratory measurements are used whenever available.

The Lorentzian halfwidth is composed of a self-broadening term and a foreign broadening term:

$$\alpha_{L_o,n} \;=\; (1 \;-\; C_{V,g})\, \alpha_{L_o,n}^{foreign} \;+\; C_{V,g}\, \alpha_{L_o,n}^{self} \tag{40}$$

where

$\alpha_{L_o,n}$	reference Lorentzian halfwidth of transition n
$\alpha_{L_o,n}^{foreign}$	reference foreign-broadening Lorentzian halfwidth of transition n of species g
$\alpha_{L_o,n}^{self}$	reference self-broadening Lorentzian halfwidth of transition n of species g
$C_{V,g}$	volume mixing ratio of species g

The Voigt function $\Phi_{V,n}$ is the convolution of Doppler and Lorentzian broadening:

$$\Phi_{L,n}(\nu,p,T) \otimes \Phi_{D,n}(\nu,T) \tag{41}$$

$$\Phi_{V,n}(\nu,p,T) \;=\; \frac{1}{\alpha_{D,n}} \sqrt{\frac{\ln 2}{\pi}} \, \frac{y}{\pi} \int\limits_{-\infty}^{\infty} \frac{e^{-t^2}}{(x-t)^2 \,+\, y^2}\, dt \tag{42}$$

where

$$y \;=\; \frac{\alpha_{L,n}}{\alpha_{D,n}} \sqrt{\ln 2} \tag{43}$$

and

$$x \;=\; \left(\frac{\nu - \nu_{o,n}}{\alpha_{D,n}}\right) \sqrt{ln2} \tag{44}$$

where $\alpha_{D,n}$ and $\alpha_{L,n}$ are Doppler and Lorentzian halfwidths, respectively, and $\nu_{o,n}$ is the central wavenumber of transition n.

2.3.1.5 Line-mixing

In the case of overlapping lines broadened by collisions, line mixing effects have to be taken into account [6]. The Lorentzian line profile shape is then modified:

$$\Phi_{L,n}^{lm}(\nu,p,T) \;=\; \frac{\tilde{A}(T)}{A(T)} \frac{1}{\pi} \, \frac{\tilde{\alpha}_{L,n} \,+\, (\nu - \tilde{\nu}_{o,n})\tilde{Y}_n(T,p)}{(\nu - \tilde{\nu}_{o,n})^2 \,+\, (\tilde{\alpha}_{L,n})^2} \tag{45}$$

where

$\Phi_{L,n}^{lm}$	pressure broadened profile function of transition n under consideration of line-mixing
$\tilde{A}(T)$	line mixing modified line intensity
$A(T)$	line intensity (see Eq. 2)
$\tilde{\nu}_{o,n}$	line-mixing modified central wavenumber
$\tilde{\alpha}_{L,n}$	line mixing modified Lorentzian halfwidth
$\tilde{Y}_n$	line-mixing coefficient

The determination of the quantities signed by a tilde is discussed in Part VI: 'Line mixing'. Within the Rosenkranz approximation valid for low atmospheric pressures, the quantities $\tilde{A}(T)$, $\tilde{\nu}_{o,n}$, and $\tilde{\alpha}_{L,n}$ are given by their unmodified values.
This modified shape of pressure-broadened lines maps into the Voigt line shape as follows:

$$\Phi_{V,n}^{lm}(\nu,p,T) \;=\; \sqrt{\frac{\ln 2}{\pi}} \, \frac{1}{\alpha_{D,n}} \left[K(\tilde{x}_n,\tilde{y}_n) \,+\, \tilde{Y}_n(p,T)\, L(\tilde{x}_n,\tilde{y}_n)\right] \tag{46}$$

$$K(\tilde{x},\tilde{y}) = \frac{\tilde{y}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{(\tilde{x}-t)^2+\tilde{y}^2}\, dt \tag{47}$$

$$L(\tilde{x},y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{(\tilde{x}-t)e^{-t^2}}{(\tilde{x}-t)^2+\tilde{y}^2}\, dt \tag{48}$$

$$\tilde{x} = \left(\frac{\nu-\tilde{\nu}_{o,n}}{\alpha_{D,n}}\right) \sqrt{ln2} \tag{49}$$

$$\tilde{y} = \frac{\tilde{\alpha}_{L,n}}{\alpha_{D,n}} \sqrt{\ln 2} \tag{50}$$

where

$\Phi_{V,n}^{lm}$	Voigt profile function of transition n under consideration of line-mixing
$\alpha_{D,n}$	Doppler halfwidth (see Eq. 37)
$\tilde{Y}_n$	line-mixing coefficient

2.3.1.6 χ-Faktor

The impact of time-dependence of collisions on the line shape is considered by empirical χ-factors [7]

$$\Phi_\chi(\nu) = \chi \cdot \Phi_V(\nu,p,T) \tag{51}$$

where

Φ_V	Voigt-profile function [cm] (see 42)
χ	χ-factor

For CO_2, asymmetric χ-factors have to be considered. χ-factors for CO_2 self-broadening as published by Refs. [8][9][10] are compiled in Table 1. χ-factors for CO_2 foreign-broadening by N_2 as published by Refs. [11][12][10] and used in KOPRA are compiled in Table 2. The χ-factor for CO_2 foreign broadening by O_2 as published by [11] and [12] is compiled in Table 3.

These χ-factors are added weighted by the partial pressures $p_{\mathrm{CO_2}}$, $p_{\mathrm{N_2}}$ and $p_{\mathrm{O_2}}$ of contributing gases CO_2, N_2 and O_2:

$$\frac{p_{\mathrm{CO_2}}}{p_{total}} \cdot \chi_{\mathrm{CO_2}} + \frac{p_{\mathrm{N_2}}}{p_{total}} \cdot \chi_{\mathrm{CO_2\text{-}N_2}} + \frac{p_{\mathrm{O_2}}}{p_{total}} \cdot \chi_{\mathrm{CO_2\text{-}O_2}} \tag{52}$$

where

$$p_{total} = p_{\mathrm{CO_2}} + p_{\mathrm{N_2}} + p_{\mathrm{O_2}} \tag{53}$$

Table 1: χ-factor for CO_2 self-broadening; $\Delta\nu = \nu - \nu_{o,n}$, $\nu_{o,n}$ is the central wavenumber of transition n, and K_1 is the modified Bessel function of the second kind

Temperature: 296 K	
$0 \leq \lvert\Delta\nu\rvert \leq 3\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 1$
$3 \leq \lvert\Delta\nu\rvert \leq 10\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 1.470\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{7.782}\right)$
$10 \leq \lvert\Delta\nu\rvert \leq 120\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 0.535\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{36.535}\right)$
$\lvert\Delta\nu\rvert \geq 120\ cm^{-1}$	
$\Delta\nu < 0$	$\Delta\nu > 0$
$\chi_{\mathrm{CO_2}} = 0.889\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{31.627}\right)$	$\chi_{\mathrm{CO_2}} = 0.220\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{50.063}\right)$
Temperature: 218 K	
$0 \leq \lvert\Delta\nu\rvert \leq 3\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 1$
$3 \leq \lvert\Delta\nu\rvert \leq 10\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 1.240319\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{13.9296}\right)$
$10 \leq \lvert\Delta\nu\rvert \leq 140\ cm^{-1}$	$\chi_{\mathrm{CO_2}} = 0.68\ \frac{\lvert\Delta\nu\rvert}{28}\ K_1(\frac{\lvert\Delta\nu\rvert}{28})$
$\lvert\Delta\nu\rvert \geq 140\ cm^{-1}$	
$\Delta\nu < 0$	$\Delta\nu > 0$
$\chi_{\mathrm{CO_2}} = 10.04385\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{21.233306}\right)$	$\chi_{\mathrm{CO_2}} = 0.345\ \exp\left(-\frac{\lvert\Delta\nu\rvert}{43.448}\right)$

Table 2: χ-factor for CO_2-broadening by N_2

Temperature: 296 K	
$0 \leq \vert\Delta\nu\vert \leq 0.5\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 1$
$0.5 \leq \vert\Delta\nu\vert \leq 20\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 1.064\ \exp(-0.1235\ \vert\Delta\nu\vert)$
$20 \leq \vert\Delta\nu\vert \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.125\ \exp(-0.0164\ \vert\Delta\nu\vert)$
$50 \leq \vert\Delta\nu\vert \leq 140\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.146\ \exp(-0.0196\ \vert\Delta\nu\vert)$
$\vert\Delta\nu\vert \geq 140\ cm^{-1}$	
$\Delta\nu < 0$	$\Delta\nu > 0$
$\chi_{CO_2\text{-}N_2} = 1.8593\ \exp(-0.03776\ \vert\Delta\nu\vert)$	$\chi_{CO_2\text{-}N_2} = 0.146\ \exp(-0.0196\ \vert\Delta\nu\vert)$
Temperatur: 238 K	
$0 \leq \vert\Delta\nu\vert \leq 5\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 1$
$5 \leq \vert\Delta\nu\vert \leq 22\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 1.968\ \exp(-0.1354\ \vert\Delta\nu\vert)$
$22 \leq \vert\Delta\nu\vert \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.160\ \exp(-0.0214\ \vert\Delta\nu\vert)$
$\vert\Delta\nu\vert \geq 50\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.162\ \exp(-0.0216\ \vert\Delta\nu\vert)$
Temperature: 193 K	
$0 \leq \vert\Delta\nu\vert \leq 9\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 1$
$9 \leq \vert\Delta\nu\vert \leq 23\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 3.908\ \exp\left(-0.1514\vert\Delta\nu\vert\right)$
$23 \leq \vert\Delta\nu\vert \leq 28\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.207\ \exp\left(-3.778\ 10^{-3}\vert\Delta\nu\vert\right)$
$28 \leq \vert\Delta\nu\vert \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}N_2} = 0.219\ \exp\left(-0.0276\vert\Delta\nu\vert\right)$
$\Delta\nu < 0$	$\Delta\nu > 0$
$50 \leq \vert\Delta\nu\vert \leq 130\ cm^{-1}$	$50 \leq \vert\Delta\nu\vert \leq 135\ cm^{-1}$
$\chi_{CO_2\text{-}N_2} = 0.20894\ \exp\left(-0.026694\vert\Delta\nu\vert\right)$	$\chi_{CO_2\text{-}N_2} = 0.146\ \exp\left(-0.0196\vert\Delta\nu\vert\right)$
$130 \leq \vert\Delta\nu\vert \leq 160\ cm^{-1}$	$\vert\Delta\nu\vert > 135\ cm^{-1}$
$\chi_{CO_2\text{-}N_2} = 2.824997\ \exp\left(-0.0467266\vert\Delta\nu\vert\right)$	$\chi_{CO_2\text{-}N_2} = 1.164\ \exp\left(-0.035\vert\Delta\nu\vert\right)$
$\vert\Delta\nu\vert > 160\ cm^{-1}$	
$\chi_{CO_2\text{-}N_2} = 1.192053\ \exp\left(-0.0413334\vert\Delta\nu\vert\right)$	

Table 3: χ-factor for CO_2-broadening by O_2

Temperature: 296 K	
$0 \leq \|\Delta\nu\| \leq 3\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 1$
$3 \leq \|\Delta\nu\| \leq 8\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 3.341\ \exp(-0.4021\ \|\Delta\nu\|)$
$8 \leq \|\Delta\nu\| \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.155\ \exp(-0.0179\ \|\Delta\nu\|)$
$50 \leq \|\Delta\nu\| \leq 70\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.238\ \exp(-0.0266\ \|\Delta\nu\|)$
$70 \leq \|\Delta\nu\| \leq 140\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.146\ \exp(-0.0196\ \|\Delta\nu\|)$
$\|\Delta\nu\| \geq 140\ cm^{-1}$	
$\Delta\nu < 0$	$\Delta\nu > 0$
$\chi_{CO_2\text{-}O_2} = 1.8593\ \exp(-0.03776\ \|\Delta\nu\|)$	$\chi_{CO_2\text{-}O_2} = 0.146\ \exp(-0.0196\ \|\Delta\nu\|)$
Temperature: 238 K	
$0 \leq \|\Delta\nu\| \leq 5\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 1$
$5 \leq \|\Delta\nu\| \leq 22\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 1.968\ \exp(-0.1354\ \|\Delta\nu\|)$
$22 \leq \|\Delta\nu\| \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.160\ \exp(-0.0214\ \|\Delta\nu\|)$
$\|\Delta\nu\| \geq 50\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.162\ \exp(-0.0216\ \|\Delta\nu\|)$
Temperature: 193 K	
$0 \leq \|\Delta\nu\| \leq 11\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 1$
$11 \leq \|\Delta\nu\| \leq 23\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 7.908\ \exp(-0.188\ \|\Delta\nu\|)$
$23 \leq \|\Delta\nu\| \leq 35\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.122\ -(7.539\ 10^{-4}\ \|\Delta\nu\|)$
$35 \leq \|\Delta\nu\| \leq 50\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.349\ \exp(-0.0369\ \|\Delta\nu\|)$
$50 \leq \|\Delta\nu\| \leq 135\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 0.129\ \exp(-0.0170\ \|\Delta\nu\|)$
$\|\Delta\nu\| \geq 135\ cm^{-1}$	$\chi_{CO_2\text{-}O_2} = 1.455\ \exp(-0.0350\ \|\Delta\nu\|)$

3 Field of View and Instrumental Line Shape

While previous sections deal with radiative processes in the atmosphere which are independent of the observing system, in the following the influence of the observing system is discussed.

3.1 Field of View

The observed spectral radiance $S_{\Theta_0}^{FOV}(\nu, l_{obs})$ is the convolution of the radiances related to observation angles Θ with the weighting function W describing the FOV.

$$S_{\Theta_0}^{FOV}(\nu, l_{obs}) = \int_{-\Theta_{max}}^{\Theta_{max}} S_{\Theta}(\nu, l_{obs}) W(\Theta - \Theta_0) d\Theta \tag{54}$$

where

$W(\Theta - \Theta_0)$	weighting function related to field of view (FOV), as integrated for horizontal stripes $d\Theta$
$S_{\Theta_0}^{FOV}$	FOV-convolved spectral radiance for viewing angle Θ_0 $\left[\frac{W}{cm^2 sr \cdot cm^{-1}}\right]$
FOV	field of view
l_{obs}	position of the observer $[cm]$
ν	wavenumber (wavenumber) $[cm^{-1}]$
S_{Θ}	spectral radiance for infinitesimal viewing angle Θ
Θ	viewing angle
Θ_{max}	maximum angle covered by FOV

3.2 Instrumental Line Shape

The instrument line shape (ILS) is a function the atmospheric spectrum has to be convolved with in order to simulate what is seen by the instrument:

$$S_{\Theta}^{AILS}(\nu, l_{obs}) = \frac{\int_{-\infty}^{+\infty} S_{\Theta_0}^{FOV}(\nu', l_{obs}) \cdot AILS(\nu - \nu')\, d\nu'}{\int_{-\infty}^{+\infty} AILS(\nu - \nu')\, d\nu'} \tag{55}$$

where

S_{Θ}	spectral radiance for viewing angle Θ
$AILS$	apparatus function incl. numerical apodization (apodized instrumental line shape) (see Part XII: 'Transformation of irradiated to measured spectral distribution due to finite spectral resolution and field of view extent of a Fourier transform spectrometer')
$\int_{-\infty}^{+\infty} AILS(\nu-\nu')\, d\nu'$	normalization (if necessary; in KOPRA $\int_{-\infty}^{+\infty} AILS(\nu-\nu')\, d\nu' = 1$)

KOPRA determines a single sided ($x \geq 0$) and complex-valued modulation efficiency with symmetric real and antisymmetric imaginary parts. The AILS is the Fourier transform of the modulation efficiency. The modulation efficiency $M(x)$includes the numeric apodization function, the modulation loss due to self apodization, the linear modulation loss and the phase error.

$$AILS(\nu) = \int_{-\infty}^{\infty} M(x) e^{-i\nu x} dx \tag{56}$$

with

$$M(x) = M_{resolution}(x) \times M_{numeric}(x) \times M_{self}(x) \times M_{linear}(x) \times M_{phase}(x) \tag{57}$$

- resolution

  The interferogram is restricted to maximal optical path difference L

  $M_{resolution}(x) = 1$ if $|x| \leq L$
  $M_{resolution}(x) = 0$ else

- apodization function

  1. sinc
     $M_{numeric} = 1$
  2. triangle
     $M_{numeric} = 1 - |x|/L$
  3. Hamming
     $M_{numeric} = 0.53856 + 0.46144 \times \cos(\pi \times x/L)$
  4. Blackmann-Harris 3-term
     $M_{numeric} = 0.42323 + 0.49755 \times \cos(\pi \times x/L) + 0.07922 \times \cos(2 \times \pi \times x/L)$
  5. Blackmann-Harris 4-term
     $$\begin{aligned} M_{numeric} = 0.35875 &+ 0.48829 \times \cos(\pi \times x/L) \\ &+ 0.14128 \times \cos(2 \times \pi \times x/L) \\ &+ 0.01168 \times \cos(3 \times \pi \times x/L) \end{aligned}$$
  6. Norton-Beer weak
     $M_{numeric} = 0.384093 - 0.087577 \times \left(1 - (x/L)^2\right) + 0.703484 \times \left(1 - (x/L)^2\right)^2$
  7. Norton-Beer medium
     $M_{numeric} = 0.152442 - 0.136176 \times \left(1 - (x/L)^2\right) + 0.983734 \times \left(1 - (x/L)^2\right)^2$
  8. Norton-Beer strong
     $M_{numeric} = 0.045335 - 0.554883 \times \left(1 - (x/L)^2\right)^2 + 0.399782 \times \left(1 - (x/L)^2\right)^4$

- self apodization

  The interferometer has finite acceptance angle. It can be shown, that optical path difference depends on the inclination of the wavefront versus the optical axis. In case of homogeneously illuminated circular internal FOV of semidiameter one finds that this leads to an additional loss of modulation:
  $M_{self} = \frac{\sin(\pi \times \Delta\nu \times x)}{\pi \times \Delta\nu \times x}$ with $\Delta\nu = 0.5 \times \nu \times \alpha^2$

  Note that the self apodization (and thereby the resulting AILS) depends on spectral position ν. The additional modulation loss describes the consequences of the finite acceptance angle not completely. In addition, the spectral abscissa is scaled by $0.5 \times (\cos(\alpha) + 1)$.

- linear modulation loss

  This term is used to model the width of the imperfect AILS.

  $M_{linear} = 1 - (1 - a) \times x/L$

  the factor a gives the modulation efficiency at maximal path difference vs ideal instrument.

- phase error

  This term is used to model the asymmetry of the imperfect AILS. The phase error φ is given in radians.

  $M_{phase} = \frac{e^{-i\varphi}}{\cos(\varphi)}$

  The norm of the AILS is fixed by the real part of $M(0)$. The denominator ensures the norm to be unity.

Since the real valued AILS is the Fourier transform of the complex-valued modulation efficiency, the latter is symmetric in the real part and antisymmetric in the imaginary part. Due to this symmetry, the AILS is fully determined by a single sided modulation efficiency interferogram.

Appendix A

Symbols and Acronyms

a_E	major semi-axis
a_0, a_1, a_2, a_3	tabulated coefficients for calculation of total internal partition function (LTE)
b	focal length
b_E	minor semi-axis
c	velocity of light
dl	path element (Eq. 3)
e''	lower state energy (from HITRAN)
f_Q	NLTE correction factor to the partition sum
g	index specifying species
g_1, g_2	level statistical weights
h	Planck constant
j	rotational quantum number
k_B	Boltzmann constant
l	path coordinate
l_{obs}	position of the observer
l_o	position of background emitter
m	vibrational state
m_g	slant path column amount of species g (Eq. 4)
n	index specifying transitions
n_b	refractive index (Eq. 10)
n_{b_o}	wavenumber-dependent refractive index of dry air (Eq. 12)
n_1^{NLTE}	population of the lower state (NLTE)
n_1	population of the lower state (LTE)
n_2^{NLTE}	population of the upper state (NLTE)
n_2	population of the upper state (LTE)
p	pressure
p_{obs}	pressure at observer altitude
p_{CO_2}, p_{N_2}, p_{O_2}	CO_2, N_2 and O_2 partial pressures
p_o	reference pressure for calculation of refractive index n_B ($p_o = 1013.25\,\mathrm{hPa}$)
p_o^L	reference pressure for calculation of Lorentzian halfwidth
r	altitude coordinate + radius of earth
r_A	aperture radius
r_1, r_2	ratio of populations between the general (NLTE) and LTE cases (Eq. 17)
z	altitude coordinate
z_A	upper boundary of atmosphere

z_{obs}	observer altitude
A_{gn}	line intensity of transition n of species g (Eq. 2)
$A_{gn}(T_o')$	line intensity of transition n of species g at reference temperature T_o'
$AILS$	apodized instrumental line shape (apparatus function incl. numerical apodization)(Eq. 56)
B	Planck function (Eq. 15)
$C_0, C_1, .., C_4$	coefficients for calculation of apodization function
$C_{V,g}$	volume mixing ratio of species g
$E_{vib,m}$	energy of vibrational state m
E''_{gn}	lower state energy of transition n of species g
FOV	field of view
$FWHM$	full width at half maximum (nominal spectral resolution)
G	number of relevant species
J	source function
J^{LTE}	source function in case of LTE (Eq. 13)
J^{NLTE}	source function in case of NLTE (Eq. 16)
K_1	modified Bessel function of the second kind
LTE	local thermodynamic equilibrium
M	molecular mass
$M_{resolution}$	modulation efficiency function related to resolution
$M_{numeric}$	modulation efficiency function related to numerical apodization
M_{self}	modulation efficiency function related to self apodization
M_{linear}	modulation efficiency function related to linear modulation efficiency loss
M_{phase}	modulation efficiency function related to phase error
N	apodizing function number
N_{avo}	Avogadro constant
N_g	number of transitions of species g
$NLTE$	non-local thermodynamic equilibrium
OPD_{max}	max. optical path difference
$Q(T)$	LTE total internal partition function evaluated at T (Eq. 4)
$Q(T_o)$	LTE total internal partition function at $T_o = 296$ K
R	universal gas constant
R_E	radius of Earth (Eq. 8)
S_Θ	spectral radiance for viewing angle Θ (Eq. 1)
S^{FOV}	spectral radiance convolved by field of view (Eq. 54)
S^{AILS}	spectral radiance convolved by apodized instrumental line shape (Eq. 55)
T_{kin}	kinetic temperature
T_{obs}	temperature at observer altitude
T_{Vib}	vibrational temperature (in LTE: $T_{Vib} = T_{kin}$)
T_o	reference temperature for calculation of refractive index n_B ($T_o = 288.16$ K)
T_o'	reference temperature ($T_o' = 296$ K)
T_o^{lm}	temperature for calculation of line-mixing coefficients ($T_o^{lm} = 200$ K)
T_o^L	reference temperature for calculation of Lorentzian halfwidth ($T_o^L = 296$ K)
$W(\Theta - \Theta_0)$	weighting function of the FOV
Y_n	line-mixing coefficient (Eq. 45)
$\alpha_{D,n}$	Doppler halfwidth (transition n) (Eq. 37)
$\alpha_{L,n}$	Lorentzian halfwidth (Eq. 39)

$\alpha_{L_o,n}$	reference Lorentzian half width of transition n (Eq. 40)
$\alpha^{foreign}_{L_o,n}$	reference Lorentz half width of transition n
$\alpha^{self}_{L_o,n}$	reference Lorentz half width of transition n
χ	χ-Faktor
$\chi_{\mathrm{CO_2}}$	χ-faktor for self-broadening of $\mathrm{CO_2}$ lines (Eq.18)
$\chi_{\mathrm{CO_2\text{-}N_2}}$	χ-Factor for $\mathrm{N_2}$-broadening of $\mathrm{CO_2}$ lines (Eq.19)
$\chi_{\mathrm{CO_2\text{-}O_2}}$	χ-Faktor for $\mathrm{O_2}$-Verbreiterung von $\mathrm{CO_2}$ (Eq.20)
γ_n	coefficient of temperature dependence of air-broadened halfwidth
ν	wavenumber
$\nu_{o,n}$	central wavenumber of transition n
$\Delta\nu$	wavenumber interval
ρ_g	number density of species g (Eq. 5)
σ^{Vol}_a	volume absorption coefficient (Eq. 24)
$\sigma_{a,g}$	absorption coefficient of species g (Eq. 25)
$\sigma_{a,gn}$	absorption coefficient of transition n of species g
$\sigma^{LTE}_{a,gn}$	$\sigma_{a,gn}$ in LTE (Eq. 27)
$\sigma^{NLTE}_{a,gn}$	$\sigma_{a,gn}$ in NLTE (Eq. 28)
σ^{Vol}_e	volume extinction coefficient (Eq. 23)
$\sigma^{vol}_{e,\mathrm{aerosol}}$	aerosol extinction coefficient (from external Mie calculation
σ_s	scattering coefficient (from external Mie calculation)
$\tau(\nu, l_1, l_2)$	transmission between l_1 and l_2 at wavenumber ν (Eq. 22)
Φ	geographic latitude
Φ_{gn}	profile function of line n of species g
$\Phi_{D,n}$	Doppler profile function of transition n (Eq. 36)
$\Phi_{L,n}$	Lorentzian profile function of transition n (Eq. 38)
$\Phi^{lm}_{L,n}$	Lorentzian profile function of transition n under consideration of line-mixing (Eq. 45)
$\Phi_{V,n}$	Voigt profile function of transition n (Eq. 42)
$\Phi^{lm}_{V,n}$	Voigt profile function of transition n under consideration of line-mixing (Eq. 46)
Ψ	geocentric latitude (Eq. 9)
Θ	viewing angle

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