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Typical atmospheric scenarios in the 0.6 - 5 THz wavelength range (REPORT - DIAST Project)



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### **Typical atmospheric scenarios in the 0.6-5 THz wavelength range** (REPORT - DIAST Project)

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#### **1** Introduction

### 1.1 THz frequency range

This report presents an analysis of the atmospheric characteristics in the terahertz spectral region (frequencies from 300 GHz to 10 THz, wavelengths from 30  $\mu$ m to 1 mm, see Fig. 1.1), with particular attention in the range 1 to 5 THz. This interval is the spectral range of interest in the framework of DIAST project.



Fig. 1.1: Different scales and units.



Fig. 1.2: Absorption spectral windows.

Historically the THz spectral interval has been characterized by a relative lack of convenient radiation sources, detectors and transmission technology (Fig. 1.2).

The simulated atmospheres presented in this document will be considered during the designs of different spectroradiometers and for the simulation of their instrumental responses.

The atmospheres have been chosen to be representative of a realistic working scenario in different acquisition geometries, taking into account the typical gaseous components and pollutants of terrestrial atmosphere.

## 2 Atmospheric scenario in the range 600 GHz - 5 THz 2.1 *Mathematical background*

In a homogeneous medium (i.e. a layer in a constant, stratified atmosphere), the monochromatic radiance *I* (i.e. power for normal area, solid angle units) extincted in an infinitesimal layer *ds* is:

$$dI = I(s + ds) - I(s) = -\beta_e(s)I(s)ds$$

being  $\beta_e$  the extinction (scattering plus absorption) coefficient.

Neglecting the scattering ( $\beta_e = \beta_a$ , being  $\beta_a$  the absorption coefficient) we can express the infinitesimal absorbed radiance  $dI_{abs}$  as:

$$dI_{abs} = -\beta_a I ds$$

On the other hand, the emitted radiance  $dI_{emit}$  is (Kirchhoff's Law):

$$dI_{emit} = \beta_a B(T) ds$$

being B(T) the blackbody radiance (Plank's Law) as a function of temperature T:

- $B(T) = \frac{2hf^3}{c^2} \frac{1}{\frac{hf}{e^{kT}-1}}$ , for the frequency f;  $B(T) = \frac{2hc^2}{\lambda^5} \frac{1}{\frac{hc}{e^{kT}-1}}$ , for the wavelength  $\lambda$ ;  $B(T) = 2hc^2 v^3 \frac{1}{\frac{hcv}{e^{kT}-1}}$ , for the wavenumber  $v = \frac{1}{\lambda}$ ;

with k being the Boltzmann constant and h the Plank constant.

The radiance balance is therefore:

$$dI = dI_{abs} + dI_{emit} = \beta_a(B(T) - I)ds$$

Defining the optical depth as  $\tau = \beta_a s$ , the equation above can be integrated along an optical depth  $\tau$ , bringing to: belling the optical depth as  $t = p_a s$ , the equation above can be integrated as  $I(0) = I(\tau)e^{-\tau} - B(T)(e^{-\tau} - 1)$ where I(0) is the received radiance and  $I(\tau)$  a source term at distance  $s = \frac{\tau}{\beta_a}$ .

The HITRAN interface neglects any source term for simulating the radiance emitted by an homogeneous medium. The simulations shown in next paragraph are obtained by the formula:

$$I = B(T)(1 - T(p,T))$$

being  $T(p,T) = e^{-\tau} = e^{-s\beta_a(p,T)}$  the transmittance depending (through  $\beta_a$ ) by the medium temperature and pressure for taking into account the absorption/emission line shaping effects.

Being the HITRAN a spectral line database, for simulating the emission of a generic custom atmosphere, the HITRAN interface used (HITRAN On The Web applet at hitran.iao.ru/home) calculates the absorption coefficient for a user-selected gas mixture using the following formulas.

Being  $K_{a_{im}}$  the monochromatic absorption line coefficient for a single molecular species for volume unit, for a single spectral line corresponding to a transition between levels j and m at a given pressure p and temperature T, The absorption coefficient  $K_a$  at wavenumber WN (in  $cm^{-1}$ ), for a single molecule per unit volume is obtained by summing over all the transitions  $j \rightarrow m$ :

$$K_{a}(WN,T,p) = \sum_{jm} K_{a_{jm}}(WN,T,p) \left[ \frac{cm^{2}}{molecule} \right]$$

For a gas mixture the partial absorption coefficients are weighted with the mixing ratios of these species.

The absorption coefficient  $\beta_a$  [ $cm^{-1}$ ] is then calculated as:

$$\beta_a(WN,T,p) = N K_a(WN,T,p)$$

being  $N \left[ \frac{molecule}{cm^3} \right]$  the number of absorbing molecules per volume unit considering a perfect gas.

#### Pollutant signal in atmospheric radiance: constant path 2.2

For this analysis, we have chosen the US-Standard 1976 atmosphere as unpolluted representative atmosphere. We have set up three scenarios (using the HITRAN On The Web applet), as shown in the following table:

	Press. (Atm)	Press. (hPa)	Temp.(K)	Altitude a.s.l. (km)	N2 (%) (1)	02 (%)	H2O (ppm)	CO2 (ppm)	03 (ppm)
low stratosphere	0.1	100	216	16	78.26615	21.70000	5.0	333 (2)	0.5
mid stratosphere	0.01	10	227	31	78.26560	21.70000	5.0	333 (2)	6.0
high stratosphere	0.001	1	270	48	78.26595	21.70000	5.0 <sup>(3)</sup>	333 (2)	2.5

(1): N2 concentration is used for normalizing the sum to 100%.

(2): Underestimated with respect to actual values (the reference atmosphere is US 1977) but uninfluential.

(3): for high stratosphere overestimated water value (for worst-case scenario).

For investigating the effects of different pollutants present in the atmosphere and of some interest for remote sensing measurements, we simulated the effects of a pure N2 atmosphere (transparent in the frequency range of interest) with each pollutant in realistic atmospheric concentration. For pollutant present only in traces in atmosphere, we saturated the concentration to the minimum concentration of 1.E-08 (ratio in volume).

The pollutant list is detailed in the following table, together with the concentration used.

Applying the formulas described in par. 2.1, we have simulated the unpolluted atmospheres for each case (Fig. 2.1 - Fig. 2.3), and compared with the ideal corresponding blackbody spectrum.

Using the HITRAN simulation of the polluted atmospheres, the signal due to each single pollutant can be analysed and compared with the background signal, as shown in next paragraphs for each pollutant of the table, compared to the background atmospheric spectrum (Fig. 2.4 - Fig. 2.12).

Pollutant	Atmosphere composition	Concentrations (%)
N20	N2O 0.28ppm + N2	$N_20: 0.000028$ $N_2: 99.999972$
03	O3 2 ppm + N2	O <sub>3</sub> : 0.000200 N <sub>2</sub> : 99.999800
СО	CO 0.47ppm + N2	CO: 0.000047 N <sub>2</sub> : 99.999953
CH4	CH4 1.48 ppm + N2	CH <sub>4</sub> : 0.000148 N <sub>2</sub> : 99.999852
NO	NO 0.01ppm N2	NO: 0.000001 N <sub>2</sub> : 99.999999
SO2	SO2 0.08ppm + N2	SO <sub>2</sub> : 0.000008 N <sub>2</sub> : 99.999992
NO2	NO2 0.01ppm + N2	NO <sub>2</sub> : 0.000001 N <sub>2</sub> : 99.999999
NH3	NH3 0.01ppm + N2	NH <sub>3</sub> : 0.000001 N <sub>2</sub> : 99.999999
ОН	OH 0.01ppm + N2	OH: 0.000001 N <sub>2</sub> : 99.999999
HCl	HCl 0.01ppm + N2	HCl: 0.000001 N <sub>2</sub> : 99.999999
H2CO	H2CO 0.01ppm + N2	$H_2CO: 0.000001$ N <sub>2</sub> : 99.999999
HOCI	HOCl 0.01ppm + N2	HOCl: 0.000001 N <sub>2</sub> : 99.999999
СНЗОН	CH3OH 0.01ppm + N2	N <sub>2</sub> : 99.999999 CH <sub>3</sub> OH: 0.000001
H2S	H2S 0.01ppm + N2	N <sub>2</sub> : 99.999999 H <sub>2</sub> S: 0.000001
<b>SO</b> 3	SO3 0.01ppm + N2	$N_2$ : 99.999999 SO <sub>3</sub> : 0.000001



Fig. 2.1: Simulated unpolluted atmospheric path of 10000 m at 0.1 atm. (16 km altitude) and comparison with the corresponding blackbody spectrum.



Fig. 2.2: Simulated unpolluted atmospheric path of 10000 m at 0.01 atm. (31 km altitude) and comparison with the corresponding blackbody spectrum.



Fig. 2.3: Simulated unpolluted atmospheric path of 10000 m at 0.001 atm. (48 km altitude) and comparison with the corresponding blackbody spectrum.

#### 2.2.1 N20



Fig. 2.4: Radiance spectrum with spectral features of the typical concentration of N2O and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.

#### 2.2.2 СО



Fig. 2.5: Radiance spectrum with spectral features of the typical concentration of CO and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.6: Radiance spectrum with spectral features of the typical concentration of SO2 and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.7: Radiance spectrum with spectral features of the typical concentration of NH3 and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.8: Radiance spectrum with spectral features of the typical concentration of OH and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.9: Radiance spectrum with spectral features of the typical concentration of HCl and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.10: Radiance spectrum with spectral features of the typical concentration of H2CO and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.11: Radiance spectrum with spectral features of the typical concentration of HOCl and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.





Fig. 2.12: Radiance spectrum with spectral features of the typical concentration of H2S and the spectrum for the corresponding unpolluted atmospheres at 16, 31 and 48 km for a 10000 m homogenous path.

## 3 Atmospheric scenario in the range 600 GHz – 5 for different geometry of observation

#### 3.1 Mathematical background

If y(x) is a function tabulated for n points  $x_i$ , i = 0, ..., n so that  $y_i = y(x_i)$ , the integral  $\int y(x) dx$  can be written (linearly interpolating between the values at the points  $x_i$ ):

$$\int_{s_0}^{s_n} y(x) \, dx = \frac{1}{2} \sum_{i=0}^{n-1} (y_i + y_{i+1}) (x_{i+1} - x_i)$$

If n = 2 (3 levels at  $s_0, s_1, s_2$ ) the formula becomes:



#### Fig. 3.1: Geometry of observation for nadir view geometry

Considering the equation introduced in par. 2.1 for a uniform medium, we have (for a linearly interpolated atmosphere between 3 levels, as in Fig. 3.1):

$$\frac{dI}{ds} = \beta_a(s)(B(T(s)) - I(s))$$

whose integral between the levels  $s_0$  and  $s_n$  becomes:

$$I(s_n) - I(s_0) = \int_{s_0}^{s_n} \beta_a(s) (B(T(s)) - I(s)) ds$$

and substituting the integral with the sum we obtain:

$$I(s_n) = I(s_0) + \frac{1}{2} \sum_{i=1}^n (Y_{i-1} + Y_i)(s_i - s_{1-1})$$

being:  $Y_i = \beta_a(s_i)(B(T(s_i)) - I(s_i)), I_i = I(s_i), \beta_{a_i} = \beta_a(s_i)$  and  $B(T(s_i)) = B_i$ . In the following paragraphs we'll consider a simple, 3 level model atmosphere. The equations became then:

$$I_{0} = I(s_{0})$$

$$I_{1} = I_{0} + \frac{1}{2} \{ [\beta_{a_{0}}(B_{0} - I_{0}) + \beta_{a_{1}}(B_{1} - I_{1})](s_{1} - s_{0}) \}$$

$$I_{2} = I_{0} + \frac{1}{2} \{ [\beta_{a_{0}}(B_{0} - I_{0}) + \beta_{a_{1}}(B_{1} - I_{1})](s_{1} - s_{0}) + [\beta_{a_{1}}(B_{1} - I_{1}) + \beta_{a_{2}}(B_{2} - I_{2})](s_{2} - s_{1}) \}$$

$$= I_{1} + \frac{1}{2} \{ [\beta_{a_{1}}(B_{1} - I_{1}) + \beta_{a_{2}}(B_{2} - I_{2})](s_{2} - s_{1}) \}$$

#### 3.2 Nadir view from top of atmosphere: linearly interpolated levels model

The value for  $I_0$  is given by the radiance reaching the level  $s_0$  (for example the radiance emitted by ground and lower atmospheric layers or the power emitted by an active source). The solution for the observed radiance  $I_2$ , as a function of the radiance  $I_0$  is then (with the same signs as in Fig. 3.1):

$$I_{1} = I_{0} + \frac{1}{2} [\beta_{a_{0}}(B_{0} - I_{0}) + \beta_{a_{1}}(B_{1} - I_{1})](s_{1} - s_{0})$$
  

$$I_{2} = I_{1} + \frac{1}{2} [\beta_{a_{1}}(B_{1} - I_{1}) + \beta_{a_{2}}(B_{2} - I_{2})](s_{2} - s_{1})$$

Solving the system and defining:

$$\Delta s_1 = s_1 - s_0$$
  
$$\Delta s_2 = s_2 - s_1$$

we calculate  $I_1$  and  $I_2$  as:

$$\begin{split} I_1 &= \frac{\left(2 - \beta_{a_0} \Delta s_1\right) I_0 + \Delta s_1 \left(\beta_{a_1} B_1 + \beta_{a_0} B_0\right)}{\beta_{a_1} \Delta s_1 + 2} \\ I_2 &= \\ &= \frac{\left[(\beta_{a_0} \Delta s_1 - 2)\beta_{a_1} \Delta s_2 - 2\beta_{a_0} \Delta s_1 + 4\right] I_0 + (\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 B_2 + 2(\Delta s_2 + \Delta s_1)\beta_{a_1} B_1 + (2 - \beta_{a_1} \Delta s_2)\beta_{a_0} \Delta s_1 B_0}{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 + 2\beta_{a_1} \Delta s_1 + 4} \end{split}$$

or, also:

$$I_2 = \alpha_g I_0 + \alpha_2 B_2 + \alpha_1 B_1 + \alpha_0 B_0$$

with:

$$\begin{aligned} \alpha_g &= \frac{(\beta_{a_0} \Delta s_1 - 2)\beta_{a_1} \Delta s_2 - 2\beta_{a_0} \Delta s_1 + 4}{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 + 2\beta_{a_1} \Delta s_1 + 4} \\ \alpha_0 &= \frac{(2 - \beta_{a_1} \Delta s_2)\beta_{a_0} \Delta s_1}{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 + 2\beta_{a_1} \Delta s_1 + 4} \\ \alpha_1 &= \frac{2(\Delta s_2 + \Delta s_1)\beta_{a_1}}{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 + 2\beta_{a_1} \Delta s_1 + 4} \\ \alpha_2 &= \frac{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2}{(\beta_{a_1} \Delta s_1 + 2)\beta_{a_2} \Delta s_2 + 2\beta_{a_1} \Delta s_1 + 4} \end{aligned}$$

The radiance  $I_2$  observed in nadir direction (i.e. observing ground from the top of atmosphere) has been calculated for a stratified *unpolluted* atmosphere. For the layers 0 – 3 the values used are from the atmospheres described in par. 2.2 for the three different altitudes.

The corresponding radiance has been calculated also for different *polluted* atmospheres, in which the absorption coefficient of each pollutant has been added to the absorption coefficient of the unpolluted atmosphere, as in par. 2.2.1 - 2.2.9. In this way, each atmosphere has an observed radiance spectrum as a function of each pollutant.

#### 3.2.1 NO2



Fig. 3.2: Radiance spectrum with spectral features of the typical concentration of N2O for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2.



Fig. 3.3: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of N2O.





Fig. 3.4: Radiance spectrum with spectral features of the typical concentration of CO for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.5: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of CO.

#### 3.2.3 SO2



Fig. 3.6: Radiance spectrum with spectral features of the typical concentration of SO2 for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.7: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of SO2.





Fig. 3.8: Radiance spectrum with spectral features of the typical concentration of NH3 for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.9: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of NH3.





Fig. 3.10: Radiance spectrum with spectral features of the typical concentration of OH for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.11: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of OH.





Fig. 3.12: Radiance spectrum with spectral features of the typical concentration of HCl for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.13: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of HCl.

#### 3.2.7 H2CO



Fig. 3.14: Radiance spectrum with spectral features of the typical concentration of H2CO for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.15: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of H2CO.





Fig. 3.16: Radiance spectrum with spectral features of the typical concentration of HOCl for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.17: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of HOCl.





Fig. 3.18: Radiance spectrum with spectral features of the typical concentration of H2S for a nadir (towards ground) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.19: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of H2S.

#### 3.3 Zenith view from lower atmosphere: linearly interpolated level model

We calculate  $I'_0 = -I_0$  (down-welling radiance received at the lower level) as a function of  $I'_1 = -I_1$  and  $I'_2 = -I_2$  using the same formula:

$${I'}_{1} = \frac{\left(2 - \beta_{a_0} \Delta s_1\right) {I'}_{2} - \Delta s_1 \left(\beta_{a_0} B_0 + \beta_{a_1} B_1\right)}{\beta_{a_1} \Delta s_1 + 2}$$

$$I'_{0} = \frac{\left[(\beta_{a_{0}}\Delta s_{1} - 2)\beta_{a_{1}}\Delta s_{2} - 2\beta_{a_{0}}\Delta s_{1} + 4\right]I'_{2} - (\beta_{a_{1}}\Delta s_{1} + 2)\beta_{a_{2}}\Delta s_{2}B_{2} - 2(\Delta s_{2} + \Delta s_{1})\beta_{a_{1}}B_{1} - (2 - \beta_{a_{1}}\Delta s_{2})\beta_{a_{0}}\Delta s_{1}B_{0}}{(\beta_{a_{1}}\Delta s_{1} + 2)\beta_{a_{2}}\Delta s_{2} + 2\beta_{a_{1}}\Delta s_{1} + 4}$$

and, setting  $I'_2 = 0$  (no source term from space), we obtain:

$$I'_{0} = -\frac{(\beta_{a_{1}}\Delta s_{1}+2)\beta_{a_{2}}\Delta s_{2}B_{2}+2(\Delta s_{2}+\Delta s_{1})\beta_{a_{1}}B_{1}+(2-\beta_{a_{1}}\Delta s_{2})\beta_{a_{0}}\Delta s_{1}B_{0}}{(\beta_{a_{1}}\Delta s_{1}+2)\beta_{a_{2}}\Delta s_{2}+2\beta_{a_{1}}\Delta s_{1}+4}$$

where the minus sign is due to the direction of the system of reference (i.e. the radiance is received oppositely to the vertical axis).



Fig. 3.20: Geometry of observation for nadir view geometry

For the radiance  $I'_0$  and for a zenith view (i.e. observing the top of atmosphere from  $s_0$ ) the same charts as in par.3.2 have been evaluated, comparing the radiance from an unpolluted atmosphere with the radiance of a polluted ones for each pollutant.





Fig. 3.21: Radiance spectrum with spectral features of the typical concentration of N2O for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.22: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of N2O and the corresponding unpolluted atmosphere.





Fig. 3.23: Radiance spectrum with spectral features of the typical concentration of CO for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.24: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of CO and the corresponding unpolluted atmosphere.





Fig. 3.25: Radiance spectrum with spectral features of the typical concentration of SO2 for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.26: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of SO2 and the corresponding unpolluted atmosphere.





Fig. 3.27: Radiance spectrum with spectral features of the typical concentration of NH3 for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.28: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of NH3 and the corresponding unpolluted atmosphere.





Fig. 3.29: Radiance spectrum with spectral features of the typical concentration of OH for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.30: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of OH and the corresponding unpolluted atmosphere.





Fig. 3.31: Radiance spectrum with spectral features of the typical concentration of HCl for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.32: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of HCl and the corresponding unpolluted atmosphere.

#### 3.3.7 H2CO



Fig. 3.33: Radiance spectrum with spectral features of the typical concentration of H2CO for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.34: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of H2CO and the corresponding unpolluted atmosphere.





Fig. 3.35: Radiance spectrum with spectral features of the typical concentration of HOCl for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.36: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of HOCl and the corresponding unpolluted atmosphere.

#### 3.3.9 H2S



Fig. 3.37: Radiance spectrum with spectral features of the typical concentration of H2S for a zenith (towards the top of atmosphere) view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.38: Absolute and relative difference for the radiance spectrum of the atmosphere introduced in par. 2.2 with the typical concentration of H2S and the corresponding unpolluted atmosphere.

#### 3.4 Equivalent constant layer model

The terms  $\alpha_g$ ,  $\alpha_0$ ,  $\alpha_1$ ,  $\alpha_2$  introduced in par. 3.2 can be seen as function of the transmittances  $T_{g0}$ ,  $T_{01}$ ,  $T_{12}$ ,  $T_{2\infty}$  and emissivity  $\varepsilon_0$ ,  $\varepsilon_1$ ,  $\varepsilon_2$  of the layers of an equivalent model with constant (i.e. non-interpolated) absorption coefficients and temperature (Fig. 3.39).





Fig. 3.39: Transmittances of the equivalent constant layers model. Each layer has constant transmittance and temperature. The emissivity of each level can be seen as 1 minus the transmittances of the lower levels.

The inversion of the system brings to the expressions for the equivalent transmittances of the corresponding constant-layer model:

$$T_{g0} = \frac{\alpha_g}{\alpha_g + \alpha_0}$$
$$T_{01} = \frac{\alpha_g + \alpha_0}{\alpha_g + \alpha_1}$$
$$T_{12} = \frac{\alpha_g + \alpha_1}{\alpha_g + \alpha_2}$$
$$T_{2\infty} = \alpha_g + \alpha_2$$

where the terms  $\alpha_g$ ,  $\alpha_0$ ,  $\alpha_1$ ,  $\alpha_2$  have to be calculated considering the absorptions given by all the different species of each level and the right values for  $\Delta s_1$ ,  $\Delta s_2$  (i.e. in case of diagonal crossing of the layer they must be scaled according with the cosine law).

#### 3.5 Limb view

Considering the model described in par. 3.1, we modify the equations for taking into account the limb geometry of Fig. 3.40:

$$I(l_n) - I(l_0) = \int_{l_0}^{l_n} \beta_a(l) (B(T(l)) - I(l)) dl$$



Fig. 3.40: Calculation of *dl* (a) and geometry of observation for two different limb view geometry in black and red (b).

being  $l_0,...,l_n$  the points along the paths l in Fig. 3.40. Following the linear approximation we have:

$$I_{1} = I_{0} + \frac{1}{2} [\beta_{a_{0}}(B_{0} - I_{0}) + \beta_{a_{1}}(B_{1} - I_{1})](l_{1} - l_{0})$$
  
$$I_{2} = I_{1} + \frac{1}{2} [\beta_{a_{1}}(B_{1} - I_{1}) + \beta_{a_{2}}(B_{2} - I_{2})](l_{2} - l_{1})$$

For symmetry, it follows also:

 $I_4 = 2I_2$ 

We solving the system defining (being *R* the Earth radius):

$$\begin{split} \Delta l_{01} &= l_1 - l_0 = \sqrt{(R+s_1)^2 - (R+s_0)^2} \\ \Delta l_{12} &= l_2 - l_1 = \sqrt{(R+s_2)^2 - (R+s_0)^2} \\ l_0 &= 0 \end{split}$$

and we calculate  $I_1$  and  $I_2$  as:

$$I_{1} = \frac{\Delta l_{01} (\beta_{a_{1}} B_{1} + \beta_{a_{0}} B_{0})}{\beta_{a_{1}} \Delta l_{01} + 2}$$

$$I_{2} = \frac{(\beta_{a_{1}} \Delta l_{01} + 2) \beta_{a_{2}} \Delta l_{12} B_{2} + 2(\Delta l_{12} + \Delta l_{01}) \beta_{a_{1}} B_{1} + (2 - \beta_{a_{1}} \Delta l_{12}) \beta_{a_{0}} \Delta l_{01} B_{0}}{(\beta_{a_{1}} \Delta l_{01} + 2) \beta_{a_{2}} \Delta l_{12} + 2\beta_{a_{1}} \Delta l_{01} + 4}}$$

$$I_{4} = 2 \frac{(\beta_{a_{1}} \Delta l_{01} + 2) \beta_{a_{2}} \Delta l_{12} B_{2} + 2(\Delta l_{12} + \Delta l_{01}) \beta_{a_{1}} B_{1} + (2 - \beta_{a_{1}} \Delta l_{12}) \beta_{a_{0}} \Delta l_{01} B_{0}}{(\beta_{a_{1}} \Delta l_{01} + 2) \beta_{a_{2}} \Delta l_{12} + 2\beta_{a_{1}} \Delta l_{01} + 4}}$$

or, as for the nadir view case without ground contribution:

$$I_4 = 2(\alpha_2 B_2 + \alpha_1 B_1 + \alpha_0 B_0)$$

with:

$$\alpha_{0} = \frac{(2 - \beta_{a_{1}}\Delta l_{12})\beta_{a_{0}}\Delta l_{01}}{(\beta_{a_{1}}\Delta l_{01} + 2)\beta_{a_{2}}\Delta l_{12} + 2\beta_{a_{1}}\Delta l_{01} + 4}$$
$$\alpha_{1} = \frac{2(\Delta s_{2} + \Delta s_{1})\beta_{a_{1}}}{(\beta_{a_{1}}\Delta l_{01} + 2)\beta_{a_{2}}\Delta l_{12} + 2\beta_{a_{1}}\Delta l_{01} + 4}$$
$$\alpha_{2} = \frac{(\beta_{a_{1}}\Delta l_{01} + 2)\beta_{a_{2}}\Delta l_{12}}{(\beta_{a_{1}}\Delta l_{01} + 2)\beta_{a_{2}}\Delta l_{12} + 2\beta_{a_{1}}\Delta l_{01} + 4}$$

#### 3.5.1 NO2



Fig. 3.41: Radiance spectrum with spectral features of the typical concentration of N2O for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2.



Fig. 3.42: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of N2O.





Fig. 3.43: Radiance spectrum with spectral features of the typical concentration of CO for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.44: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of CO.





Fig. 3.45: Radiance spectrum with spectral features of the typical concentration of SO2 for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.46: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of SO2.





Fig. 3.47: Radiance spectrum with spectral features of the typical concentration of NH3 for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.48: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of NH3.

#### 3.5.5 OH



Fig. 3.49: Radiance spectrum with spectral features of the typical concentration of OH for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.50: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of OH.

#### 3.5.6 HCl



Fig. 3.51: Radiance spectrum with spectral features of the typical concentration of HCl for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.52: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of HCl.

#### 3.5.7 H2CO



Fig. 3.53: Radiance spectrum with spectral features of the typical concentration of H2CO for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.54: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of H2CO.

#### 3.5.8 HOCl



Fig. 3.55: Radiance spectrum with spectral features of the typical concentration of HOCl for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.56: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of HOCl.

#### 3.5.9 H2S



Fig. 3.57: Radiance spectrum with spectral features of the typical concentration of H2S for limb view in a 3 level linearly interpolated atmosphere introduced in par. 2.2



Fig. 3.58: Absolute and relative difference for the radiance spectrum of the unpolluted atmosphere introduced in par. 2.2 and the same atmosphere with the typical concentration of H2S.

#### 4 Conclusions

This report shows the main characteristics of atmospheric absorbers in the terahertz spectral region, being the interval of interest in the framework of DIAST project. The simulated atmospheres presented in this document have being considered for the designs of different kind of spectroradiometers. The estimate of the instrumental characteristic SNR has been performed for different line of sight in typical working scenarios as a function of the integration time and bandwidth.