CURRENT COMPUTER MODELS OF TRANSMISSION AND RADIATION OF THE ATMOSPHERE IN THE IR SPECTRAL RANGE

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An overview of current software packages for calculating transmission and IR radiation in the absorption bands of atmospheric gases is given in this paper. The algorithms of line–by–line and approximation methods are analyzed. The values of transmission calculated with high or low spectral resolution by different algorithms are compared for individual spectral ranges.

Numerical modeling as a method of investigation is widely used in optics of a gaseous atmosphere. At present various computer models of atmospheric transmission and radiation have been developed to interpret the results of sounding of the atmosphere and underlying surface, to solve the problems of climatology, etc. In 1982 the International Commission on Radiation set up a group with the purpose of comparing the software packages.[1] The algorithms for calculating the molecular absorption were of particular interest there.

The existing software packages can be divided into two groups: 1) algorithms of line–by–line calculation[1–13] and 2) approximation methods.[14–21] The first group of software packages is used to calculate the transmission with high spectral resolution and above all to provide the ground– and space–based systems of sounding of gaseous composition of the atmosphere with information. The second group is used to solve the problems of sounding of the underlying surface temperature, agro–soil resources, etc.

This paper gives an overview of current software packages for calculating the transmission and IR radiation in the atmospheric gas absorption bands. The implemented algorithms for direct calculation and the approximation methods are analyzed. Transmission calculated with high or low spectral resolution by various algorithms is compared for individual spectral regions.

1. ALGORITHMS FOR LINE–BY–LINE CALCULATION

The intercomparison of transmission and radiation algorithms (ITRA) used in the problems of nadir, limb, and microwave sounding of the atmosphere was made by the three international thematic groups[1] which we call here the nadir, limb, and microwave groups for brevity.

The transmission spectra in the nadir and limb groups were analyzed in the 15 μm CO_2 and 6.3 μm H_2O bands. Let us briefly consider the results obtained by the nadir group incorporating six laboratories from four scientific centers of Japan, the USA, France, and DDR.

The participants of the ITRA noted that the line–by–line method is too laborious (for numerical implementation); therefore, simplification is needed to save memory and execution time. This simplification involves the choice of an appropriate frequency grid reflecting the peculiarities of the absorption spectrum and ensuring the required accuracy in calculating an integral over frequency, preliminary selection of absorption lines which make significant contribution to transmission at the frequency ν and removal of weak lines from the calculational scheme, and absorption line profile cutoff at a given frequency separation from the line center that is equivalent to assigning the spectral interval of line selection.

1.1. Salient features of algorithms

The algorithms developed at different institutes are distinguished by the following features:

a) Employed approximation of the absorption line profile. The approximation is classified by the pressure (transition from the Lorentz to Doppler profile), the Voigt profile models, the method of calculating the form factor $\chi(|\nu - \nu_0|)$ which characterizes the deviation of line wings from the Lorentz profile (Table I), the frequency separation of the absorption line cutoff, and the method of consideration of temperature dependence of the Lorentz line halfwidth.

b) Methods of saving the execution time which includes preselection of absorption lines, choice of a frequency grid, change of a frequency grid with altitude increase, choice of the method of integration over frequency, and some other procedures saving the execution time (separation of frequency and altitude dependences of optical thickness for individual line, use of Curtis–Godson approximation, etc).

c) Account of contributions of various physical effects (line interference, induced absorption bands, continuum absorption, etc.).

Conclusions and recommendations given in the ITRA Report are as follows: The spread of transmission calculated with 0.05 cm^{-1} resolution for 15 μm channels of the HIRS instrumentation is mainly 0.02–0.04 for the first three channels used for sounding of the stratosphere (668, 679, and 691 cm^{-1}); maximum deviation from transmission calculated by the NASA software package was 0.08 for the first and 0.07 for the second channels. However, the rms error was 0.01. This value presumably determines the precision threshold of algorithms. On the average, the deviations of calculated spectra increase for higher spectral resolution.

The spread of results may be primarily attributed to different consideration of contributions from line wings. Therefore, the problem of primary importance is to construct a numerical model of line wing profile. Table I lists the approximation of the form factor χ used by different scientists, and Table II gives the models of continuum absorption by H_2O. The models of line wing profiles are parametric. The model parameters are found from experimental data on absorption coefficients. The experimental data of Burch[30] provided a basis for the Roberts[29] and Clough[17] models.

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TABLE I. Method of calculating the form factor $\chi(|\nu - \nu_0|)$ by different algorithms.

Group	Form factor χ
1	2
Meteorological Institute, Japan	Exponential profile $\chi(\lvert\nu-\nu_0\rvert) = \exp[-a(\lvert\nu-\nu_0\rvert - d)^b]$, for $\lvert\nu-\nu_0\rvert > d$, $\chi(\lvert\nu-\nu_0\rvert) = 1$, for $\lvert\nu-\nu_0\rvert < d$, where ν_0 is the line center, d is the frequency separation from the line center, $a = 1.4$ cm, $b = 0.25$, and $d = 3.5$ cm^{-1}
Department of Optical Physics, AFGL, the USA	Algorithm FASCOD[2–4]: for CO_2 $\chi = 1 + (\chi' - 1)\frac{F_4}{L}$, for $\lvert\nu-\nu_0\rvert \le 64\gamma_v$, $\chi = \chi'$, for $64\gamma_v \le \lvert\nu-\nu_0\rvert \le 25$ cm^{-1}, $\chi = 0$, for $\lvert\nu-\nu_0\rvert \ge 25$ cm^{-1}, where $F_4 = \frac{1}{\pi}\left\{\frac{\gamma_L}{(\nu-\nu_0)^2+\gamma_L^2} - \frac{\gamma_L}{25^2+\gamma_L^2}\right\}$, for $64\gamma_v \le \lvert\nu-\nu_0\rvert \le 25$ cm^{-1}, $F_4 = 0$, for $\lvert\nu-\nu_0\rvert \ge 25$ cm^{-1}, $L = \frac{1}{\pi}\left\{\frac{\gamma_L}{(\nu-\nu_0)^2+\gamma_L^2} - \frac{\gamma_L}{25^2+\gamma_L^2}\right\} = F_1 + F_2 + F_3 + F_4$, $\chi' = 1 + C_2\lvert\nu-\nu_0\rvert^2 + C_4\lvert\nu-\nu_0\rvert^4 + C_6\lvert\nu-\nu_0\rvert^6$, for $\lvert\nu-\nu_0\rvert \le 2$ cm^{-1}, $\chi' = \exp(-a\lvert\nu-\nu_0\rvert^b)$, for $\lvert\nu-\nu_0\rvert \ge 2$cm^{-1}, $a = 0.623$, $b = 0.410$, $C_2 = -0.3762$, $C_4 = 0.087\ 18$, $C_6 = 0.007\ 079$. The two portions of the profile are jointed at $\lvert\nu-\nu_0\rvert = 2$ cm^{-1}; at this point the first and second derivatives are continuous. For other molecules $\chi = 1 - \frac{(\nu-\nu_0)^2+\gamma_L^2}{25^2+\gamma_L^2}$, for $\lvert\nu-\nu_0\rvert \le 25$ cm^{-1}, $\chi = 0$, for $\lvert\nu-\nu_0\rvert \ge 25$ cm^{-1}.
Laboratory of Dynamic Meteorology, France	Susskind and Searl approximation [22]: $\chi(\lvert\nu-\nu_0\rvert) = \begin{cases} 1, & \text{for } \lvert\nu-\nu_0\rvert < 0.5 \text{ cm}^{-1}, \\ 1.069\exp[-0.133\lvert\nu-\nu_0\rvert], & \text{for } \lvert\nu-\nu_0\rvert < 23 \text{ cm}^{-1}, \\ 0.05, & \text{for } \lvert\nu-\nu_0\rvert < 50 \text{ cm}^{-1}, \\ 0.133\exp[-0.0196\lvert\nu-\nu_0\rvert], & \text{for } \lvert\nu-\nu_0\rvert < 250 \text{ cm}^{-1}, \\ 0, & \text{for } \lvert\nu-\nu_0\rvert \ge 250 \text{ cm}^{-1}. \end{cases}$ NOAA approximation[69,70]: $\chi(\lvert\nu-\nu_0\rvert) = [1 + A\lvert\nu-\nu_0\rvert]\exp[-A\lvert\nu-\nu_0\rvert]$, for $\lvert\nu-\nu_0\rvert < 4$ cm^{-1}, $\chi(\lvert\nu-\nu_0\rvert) = 0$, for $\lvert\nu-\nu_0\rvert \ge 11$ cm^{-1}, $A = 2/11$ cm^{-1}.
Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences, Tomsk (see Refs. 10 and 11)	Algorithm LARA[10,11]: $\chi = 1$ at all frequencies and for all gases except H_2O in the spectral range 5–6.5 μm. For CO_2 continuum is calculated beforehand for $\Delta\nu = 10$ cm^{-1} in the 1.4, 2.7, and 4.3 μm ranges, for H_2O in the range 5–6.5 μm: for $\lvert\nu-\nu_0\rvert \le 4$ cm^{-1} $\chi = 1$, for the region $10 \ge \lvert\nu-\nu_0\rvert \ge 4$ cm^{-1}, the Tvorogov profile is used[25]: $\chi(\lvert\nu-\nu_0\rvert) = \frac{1}{F_L}\lvert\nu-\nu_0\rvert^{-(1+3/a)}[\kappa_f + \kappa_s]$, $\kappa_{f,s} = d_{f,s}\,\Phi(R_{f,s})$, $\Phi(R_{f,s}) = \frac{1}{R_{f,s}}\int_0^{R_{f,s}} \frac{R\exp(-V(R)/kT)\,dR}{\sqrt{R_{f,s}^2 - R^2}}$, $R_{f,s} = \frac{C_{f,s}}{\lvert\nu-\nu_0\rvert^{1/a}}$, $V(R) = 4\varepsilon\left[\left(\frac{G}{R}\right)^{12} - \left(\frac{G}{R}\right)^{6}\right]$, $\varepsilon/k = 217$ K, $G = 3.24$ Å, $d_{f,s}$, $C_{f,s}$, and a are the adjustable parameters. For H_2O in the spectral region 8–12 μm the Aref'ev continuum model is used.[28]

TABLE I (continued).

<table>
<tr><th>1</th><th>2</th></tr>
<tr><td>Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences, Tomsk (see Refs. 8 and 9)</td><td>
The generalized Fomin profile[26]:
$$\chi(|\nu-\nu_0|)=\frac{\nu}{\nu_0}\frac{[1-\exp(-hc\,\nu/kT)]}{[1-\exp(-hc\,\nu_0/kT)]}\frac{\pi(\nu-\nu_0)^2}{\gamma}[\kappa_f+\kappa_s]\frac{1}{N},$$
$$\kappa_{f,s}=\frac{4\pi R_{f,s}^3 N_{f,s}}{\sum_l l\,C_l^{(f,s)}/R_{f,s}^l}\Phi(R_{f,s}),$$
$$R_{f,s}=\left\{C_3^{f,s}+\sqrt{(C_3^{f,s})^2+4\Delta\nu^{2(m-3)/m}\,(C_m^{(f,s)}(\Delta\nu))^{6/m}}/2\Delta\nu\right\},$$
$$C_m^{f,s}(\Delta\nu)=\left(C_m^{(f,s)}+\sqrt{(C_m^{(f,s)})^2+4\Delta\nu^{2(k-m)/k}\,(C_k^{(f,s)})^{2m/k}\,\Delta\nu}/2\right),$$
$$C_3^{(f,s)}=3\gamma_{f,s}/3\pi^2 N_{f,s},$$
where N_i is the concentration of buffer ($i=f$) and absorbing gas ($i=s$) particles, $C_m^{(f,s)}$ and $C_k^{(f,s)}$ are the adjustable parameters.
</td></tr>
<tr><td></td><td>
The Thomas and Nordstrom profile for H_2O (see Ref. 27):
$$\chi(|\nu-\nu_0|)=[J_1(\Delta\nu)\,\varphi(\Delta\nu)+J_2(\Delta\nu)\,(1-\varphi(\Delta\nu))]\frac{1}{F_L},$$
$$J_1(\Delta\nu)=\frac{1}{\pi}\frac{\gamma}{\Delta\nu^2+\gamma_L^2}\frac{\nu}{\nu_0}\frac{1-\exp(-hc\,\nu/kT)}{1-\exp(-hc\,\nu_0/kT)}\,.$$
$$J_2(\Delta\nu)=\frac{1}{\pi}\frac{1-\exp(-hc\,\nu/kT)}{1-\exp(-hc\,\nu_0/kT)}\left[\frac{0.3198\,\lambda_{a6}\exp\left(-G_{a6}\sqrt{|\Delta\nu|}\right)}{|\Delta\nu|^{1.5}+\lambda_{a6}^3}+\frac{0.4334\,\lambda_{b4}\exp\left(-G_{b4}\sqrt{|\Delta\nu|}\right)}{|\Delta\nu|^{1.75}+\lambda_{b4}^{7/3}}\right],$$
$$\gamma_L=\gamma_{L_0}\left(\frac{296}{T}\right)^{0.83}\left[B\left(\frac{296}{T}\right)^{0.17}P_{H_2O}+P_{N_2}\right],$$
$$\lambda_{a6}=A1(\nu)\left(\frac{296}{T}\right)^{1.5}P_{H_2O},$$
$$\lambda_{b4}=A2(\upsilon)\,(\gamma_{L_0}/0.07)^{1.125}\left(\frac{296}{T}\right)P_{N_2},$$
</td></tr>
<tr><td></td><td>
$$G_{a6}=g_a(\nu)\left(\frac{296}{T}\right)^{\nu_a(\upsilon)},\quad G_{b4}=g_b(\nu)\left(\frac{296}{T}\right)^{\nu_b(\upsilon)},$$
$$\varphi(\Delta\nu)=\begin{cases}\frac{1}{2}+\frac{1}{2}\cos\left(\frac{\pi}{5}\Delta\nu\right), & |\Delta\nu|<5\ \text{cm}^{-1},\\ 0, & |\Delta\nu|\ge 5\ \text{cm}^{-1},\end{cases}$$
$\Delta\nu=\nu-\nu_0$,
$B=5$ for H_2O near the line center.
<table>
<tr><th>Parameters</th><th>Rotational band</th><th>ν_1</th><th>ν_2</th></tr>
<tr><td>$A2$</td><td>2.35</td><td>2.20</td><td>2.65</td></tr>
<tr><td>$A2$</td><td>0.18</td><td>0.18</td><td>0.23</td></tr>
<tr><td>g_a</td><td>0.06</td><td>0.13</td><td>0.10</td></tr>
<tr><td>g_b</td><td>0.115</td><td>0.11</td><td>0.075</td></tr>
<tr><td>γ_a</td><td>−1.2</td><td>0.67</td><td>0.67</td></tr>
<tr><td>γ_b</td><td>0.50</td><td>0.67</td><td>0.67</td></tr>
</table>
</td></tr>
</table>

TABLE II. Models of continuum absorption by H_2O.

The Aref'ev empirical model[28] for the spectral region 8–12 μm: $\alpha(\nu)=f(\nu)[K_1\rho T^n(1+1.95P)+K_2\rho^2\exp(2066/T)]$, km^{-1}, $K_1=0.22\cdot10^{-6}$, ρ is the humidity, in g/m^3, $K_2=0.82\cdot10^{-6}$, P is the air pressure, in atm. $f(\nu)=0.297\exp\{(10^{-4}\nu)^3/[800+0.15(10^{-4}\nu)^3]\}$.
The Roberts, Selby, and Biberman empirical formula[29] a) λ = 8–11 μm: $\alpha(\nu)=0.1\,c(\nu)\,\rho_{H_2O}[P_{H_2O}+0.002(P_T-P_{H_2O})\,\tilde{c}(T)]$, km^{-1}, $c(\nu)=4.18+5578\exp(-7.87\cdot10^{-3}\nu)$, $\tilde{c}(T)=\exp[6.08((296-T)/T)]$, b) λ = 3.5–4.2 μm: $\alpha(\nu)=0.1\,c(\nu)\,\rho_{H_2O}[P_{H_2O}+0.12(P_T-P_{H_2O})]\,\tilde{c}_1(T)$, km^{-1}, $\tilde{c}_1(T)=\exp[4.56((296-T)/T)]$, ρ_{H_2O} is the the humidity, in g/m^3, P_{H_2O} and P_T are the partial (H_2O) and total pressures, in atm.
The Clough et al. model (see Ref. 17) $\alpha(\nu)=c_s(\nu)\left(\frac{n_{H_2O}}{n_0}\right)n_{H_2O}+c_f(\nu)\left(\frac{n_f}{n_0}\right)n_{H_2O}$, in cm^{-1}, $c_s(\nu)=\nu\tanh(hc\nu/2kT)\,\tilde{c}_s$, in cm^2/mol, $c_f(\nu)=\nu\tanh(hc\nu/2kT)\,\tilde{c}_f$, in cm^2/mol, n_{H_2O} is the number density of H_2O molecules, n_0 is the number density of air molecules under normal conditions, and n_f is the number density of molecules of the buffer gas.

1.2. Brief description of functional capabilities of software packages

FASCOD (Fast Atmosphere Signature Code)

The software package FASCOD is most widely used today. The first version of the package was given in Ref. 2. This package was developed at the AFGL (the USA). It can be used to calculate the transmittance and self–radiance for arbitrary atmospheric paths in the 0–120 km layer. The last version FASCOD–3 was reported at the 14th Conference on Atmospheric Transmission Models held in 1991 (see Ref. 4).

Here are the salient features of the software package FASCOD: spectral range extends from the middle UV to microwave region; high resolution (to 1/4 of the absorption line halfwidth); the atlas of spectral data is stored on an external medium; it is possible to calculate transmission and energy brightness under conditions of the local thermodynamic equilibrium (LTE) for six meteorological models included in the package as well as for arbitrary meteorological model; and, the aerosol extinction and molecular scattering are taken into account.

New possibilities of the software package FASCOD–3 are: account of multiple scattering of thermal radiation; account of temperature dependence of interference between the CO_2 and O_2 lines for individual bands; account of diffuse UV absorption by O_3 and O_2; compatibility with the version of the Atlas HITRAN 91 involving a database on the absorption cross sections for some molecules with unresolved structure; and, account of the LTE disturbance in the upper layers of the atmosphere.

SHARC (Strategic High–Altitude Radiance Code)

The software package SHARC has been developed by the three USA firms (Spectral Sciences Inc., Phillips Laboratory, and Yap Analytics). The recent version of this package is given in Ref. 5. The package SHARC is intended for calculation of radiation under conditions of the disturbed LTE and radiation of aurora borealis. The salient features of the package are: the 50–300 m altitude range; spectral region 2–40 μm with 0.5 cm^{-1} resolution; arbitrary path geometry; interactive operational mode with diagnostics of errors; account of mechanisms of chemical kinetics; and, account of the gases H_2O, O_3, CO_2, NO, OH, CO_2, and their isotopes. The model of aurora borealis incorporates the following gases: NO^+, NO, and CO_2; day– and nighttime atmospheres are considered.

The package SHARC uses the formalism of equivalent linewidth in calculating the total transmission for each line and thereby obviates the need for the conventional numerical integration over the line profile.

GENLN 2 (General Line–by–Line)

The first version of the package GENLN 2 was developed at the Robert Hooke Institute (Great Britain, Oxford).[6,7] The package is intended for calculation of transmission and radiation by the line–by–line method. Its salient features are as follows: different line profiles (Voigt, Doppler, Lorentz, and Van–Vleck–Huber) are used; the CO_2 line wings are described by the sub–Lorentz profile; the effect of line shift is taken into account; the continuum absorption by H_2O is calculated for the Clough et al. model[17]; the absorption cross sections are used for heavy molecules with unresolved structure and the pressure–induced O_2 and N_2 absorption bands are taken into account; the Lopez–Puertas model of the LTE disturbance is used; the Curtis–Godson approximation is employed in calculating the mean values of temperature, pressure, and absorbing gas content.

The software package for calculation of the long–wave self–radiation of the atmosphere[8,9] has been developed at the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences and is primarily oriented toward the solution of the problem of determining the temperature of the land and ocean surfaces from satellite measurements of outgoing thermal radiation in the atmospheric transparency windows. The line profile is described by the Voigt formula. The H_2O line wings in the 8–12 μm transparency window are calculated by the generalized Fomin profile[26] (see Table I) with the parameters found by fitting the absorption coefficients to the experimental data of laboratory measurements. The integral over frequency is taken by an adaptive procedure with automatically adjusted step. This software package incorporates the following archives: of absorption line parameters, of meteorological models, of aerosol models, and of the continuum absorption coefficients.

LARA (Light Attenuation in Real Atmosphere)

The software package LARA has been developed at the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences and is oriented toward the calculation of the energy losses of optical (first and foremost laser) radiation in the atmosphere. The recent version of the package is described in Refs. 10 and 11. This software package allows one to calculate the absorptance, optical thickness, and transmission of monochromatic narrow– or wide–band radiation on atmospheric paths in the wavelength range between the near UV and microwave. The salient features of the package are as follows: the atlas of line parameters is stored on an external medium; the aerosol extinction and molecular light scattering are taken into account (the aerosol model has been developed at the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences[31]); the LTE is assumed to be established in the upper layers of the atmosphere; the turbulent broadening of a laser beam in the troposphere is taken into account; five meteorological models of the Institute of Atmospheric Optics[32] and six models of the AFGL[33] are incorporated in the package; moreover, arbitrary meteorological model can be put in.

The software package developed at the Kurchatov Institute of Atomic Energy should also be mentioned here.[12] The first version of this package enables one to calculate the absorption and IR radiation of the atmosphere. The second version is intended for computation of the scattered solar radiation in the atmospheric gas absorption bands.[13] Because of the lack of information about the package structure and its functional capabilities, we do not describe it here.

Analogous software packages have also been developed by the other research groups which are engaged on the problem of IR–radiation transfer in the atmosphere. This is, e.g., the software package for calculation of the absorptance by the line–by–line method, developed at the Institute of Experimental Meteorology at the Scientific–Production Company "Taifun". In 1987 the absorption coefficients at the CO_2 isotope laser transitions calculated by this package were compared with these calculated by the package LARA in the spectral region 8–12 μm. The discrepancy between the calculated results was no more than 1%.

1.3. Comparison of calculated values of transmission

Let us compare the results obtained with the use of the package LARA and those calculated and measured by the other authors.

Comparison in the 15 μm spectral range

Different algorithms were compared in detail by the international group engaged in comparison of the computer codes for calculation of atmospheric transmission and radiation. The results are given in the ITRA Report.[1] Of the six software packages of the nadir group the package NASA was taken as a reference one. We also compare the transmission T_L calculated using the package LARA with T_N obtained using the package NASA.

The following initial data: vertical path extended up to 500 hPa pressure altitude, standard average–annual model of the USA as the meteorological model, and spectral resolution $\Delta\nu = 0.05$ cm^{-1} were used for modeling the transmission. Table III lists the calculated results, T_L, compared to T_N at individual frequencies corresponding to maximum and minimum transmission.

TABLE III. Comparison between the values of transmission T_L (LARA) and T_N (NASA) (see Ref. 61).

ν, cm^{-1}	721.85	721.92	722.10	722.36	722.57	722.90	723.04	723.25
T_N	0.48	0.46	0.63	0.40	0.60	0.81	0.49	0.82
T_L	0.49	0.47	0.64	0.30	0.60	0.81	0.48	0.82
ν, cm^{-1}	723.30	723.35	723.42	723.55	723.60	723.64	723.75	723.80
T_N	0.78	0.80	0.80	0.59	0.70	0.70	0.57	0.35
T_L	0.78	0.81	0.80	0.58	0.70	0.71	0.58	0.37

As seen from this table, the deviation of T_L from T_N does not exceed 0.01. The value 0.01 was taken as a threshold error in the ITRA report. Thus the package LARA ensures the values of transmission within the threshold error accepted by the international group.

Comparison in the 4.2 μm spectral range

Let us consider here the results of comparison with the experimental data. The data of the field experiment reported in Ref. 34 are taken for comparison. The solar spectrum was measured in the frequency range between 2385 and 2430 cm^{-1} using an interferometer with 0.059 cm^{-1} resolution. This spectral range is of interest due to a significant contribution of the continuum absorption by CO_2 within the 4.3 μm band in addition to the selective absorption. The transmission was calculated for a slant path oriented at a 59° angle to the zenith. Table IV gives the calculated and experimental values of transmission. Vertical distribution of pressure and temperature was borrowed from Ref. 32 where synchronous radiosonde measurements of temperature were also presented.

TABLE IV. Comparison between the experimental values of transmission T_{exp} (Ref. 34) and T_L (LARA).

ν, cm^{-1}	2389.0	2389.6	2390.3	2390.8	2391.4	2392.0	2393.0	2394.0
T_{exp}	0.12	0.15	0.20	0.28	0.32	0.36	0.43	0.46
T_L	0.08	0.15	0.23	0.29	0.35	0.39	0.45	0.47
ν, cm^{-1}	2395.0	2397.5	2400.0	2402.5	2405.0	2407.5	2410.0	2412.5
T_{exp}	0.51	0.62	0.70	0.74	0.77	0.83	0.88	0.89
T_L	0.53	0.65	0.77	0.78	0.78	0.84	0.86	0.82

In Table IV the comparison is made for frequencies at which the transmission is determined by both selective and continuum absorption. The discrepancy between the calculated and experimental values is seen to attain 0.02–0.04 at individual frequencies, and at a frequency of 2400 cm^{-1} ΔT is equal to 0.07. This is accounted for by the insufficient accuracy of the initial spectroscopic data.

2. ALGORITHMS OF THE APPROXIMATION METHODS

The three groups of methods: 1) empirical methods, 2) methods using the absorption band models, and

3) method of direct calculation are now widely employed to calculate the transmission functions with intermediate or low spectral resolution. The first two groups were developed at the "pre–laser epoch" and are parametric: their parameters are determined by fitting to laboratory data or to the results obtained by the method of direct calculation. These methods are used for calculation of the extinction of wideband radiation in the atmosphere. The following calculational techniques have been developed for the empirical methods: the SOI technique (State Optical Institute),[35–37] our technique,[38–43] the MGO technique (Main Geophysical Observatory),[44] and the LOWTRAN technique.[14–17] The combined technique for calculation of the transmission functions has been developed which uses the model representation of absorption bands.[45] A common limitation of these techniques is the fixed spectral resolution.

The method of direct calculation (line–by–line method) has no limitations on spectral resolution and allows one to calculate theoretically the absorption functions for any spectral range. In practice, wider spectral range results in greater execution time. This is caused, on the one hand, by the increasing number of lines and, on the other hand, by wider integration interval. Therefore, there is no point in using the line–by–line methods in calculating the wide spectral intervals.

For this reason the fast methods[46–49] of calculation of the transmission function for broadband radiation are beginning to develop recently. They use the model absorption bands obtained by calculation rather then by fitting to the laboratory data.

2.1. Methods for calculation of the transmission functions

2.1.1. Empirical methods for calculation of the transmission functions

Of the empirical methods, the method of calculation of the atmospheric absorption developed at the AFCRL (the USA) has gained wide acceptance.[14–17] This method makes it possible to calculate the transmission function with 20 cm^{-1} resolution in the range 0.25–25 μm. The transmission is given by a function

$$T = f\,(C(\nu)\ W^*)\ ,$$

where W^* is the equivalent absorbing mass

$$W^* = \int \rho(z) \left[\frac{P(z)}{P_0} \left(\frac{T_0}{T(z)} \right)^{0.5} \right]^n \mathrm{d}z\ ,$$

$C(\nu)$ is the empirical coefficient depending on the frequency ν. The values of the parameters n and $C(\nu)$ and the form of the function f were determined by fitting to the laboratory data. Originally this method used nomograms.[14] Its further development is a software package. One of the recent versions of this package is LOWTRAN–7 (see Ref. 18).

The SOI method and the method developed by the authors of Refs. 38–43 are three–parametric and similar. The transmission by the SOI technique[35–37] is calculated by the following formulas:

$$T(\lambda) = \exp\{-\beta_\lambda (W^*)^{m_\lambda}\}\ ,$$

$$W^* = \int \rho(z) \left[\frac{P(z)}{P_0} \right]^{n_\lambda} \mathrm{d}z\ ,$$

where $\rho(z)$ is the concentration of absorbing gas, in cm·km^{-1}; $\rho(z)$ is the air pressure, in atm; β_λ, m_λ, and n_λ are the empirical parameters.

The method reported in Refs. 38–43 gives the following expression for calculation of the transmission:

$$T(\lambda) = \exp\{-\beta_\lambda\ W^{m_\lambda}\ P^{n_\lambda}\}\ .$$

Given in Refs. 41 and 43 are the parameters β_λ, m_λ, and n_λ for the spectral range 1–14 μm, with resolution $\Delta\lambda$ varying in the limits 0.026–0.1 μm.

The MGO method[44] uses the following formulas for calculation of the transmission on the near–ground paths:
– for homogeneously mixed gases (CO_2, N_2O, CO, and CH_4)

$$T(\lambda) = \exp\{-\beta_1(\lambda)\ L^{n_1(\lambda)}\}\ ,$$

$$T_{[N_2]_2}(\lambda) = \exp\{-\beta_2(\lambda)\ L^{n_2(\lambda)}\}\ ,$$

$$T_{O_2}(\lambda) = \exp\{-\beta_3(\lambda)\ L^{n_3(\lambda)}\}\ ,$$

– for water vapor

$$T_{H_2O}(\lambda) = \exp\{-\beta_4(0.1\ \rho_{H_2O}\ L)^{n_4(\lambda)}\}\ .$$

Here $T_{[N_2]_2}(\lambda)$ is the transmission in the induced bands of nitrogen. The continuum absorption by H_2O is described by the expression

$$T_{con}(\lambda) = \exp\{-\beta_5\ k(t)\ \rho^2_{H_2O}\ L\}\ ,$$

where L is the path length, in km, and ρ_{H_2O} is the absolute humidity of air, in g/m^3. The empirical parameters $\beta_i(\lambda)$, $n_j(\lambda)$, $i = 1, \ldots, 5$, $j = 1, \ldots, 4$ were determined from the nomograms.[14] Here $k(t)$ is the temperature factor.

2.1.2. Methods of model representation of absorption spectra

These methods use the idealized model representation of absorption bands which allow their analytical description. They are parametric and have from two to four parameters which are determined from the experimental data or from absorption spectra calculated by the line–by–line method for different thermodynamic parameters of a medium. The model methods are described at length in Refs. 45 and 50.

The following three models have found a wide use in practice: 1) regular model for equally spaced lines with equal intensities and halfwidths (Elsasser model), 2) statistical model of Plass (lines of equal intensity), and 3) statistical model of Goody (exponential distribution of line intensities). A model of individual (isolated) line is also used in theoretical investigation. Formulas for calculation of the transmission functions for these models have the form

$$T_{Sl} = \frac{1}{\pi} \int_0^\pi \exp\left[-\frac{2x\ \beta^2}{t^2 + \beta^2} \right] \mathrm{d}t\ , \qquad (1)$$

$$T_{El} = \frac{1}{\pi} \int_0^\pi \exp\left[-x\beta\ \frac{\sinh(\beta)}{\cosh(\beta) - \cos(t)} \right] \mathrm{d}t\ , \qquad (2)$$

$$T_{Pl} = \exp[-\beta L(x)] , \quad (3)$$

$$T_G = \exp\left[-\frac{\beta x}{(1+2x)^{1/2}}\right] . \quad (4)$$

Here formula (1) is the model of individual line, Eq. (2) is the Elsasser model, Eq. (3) is the Plass model, Eq. (4) is the Goody model, and $L(x)$ is the Landenburg–Raich function

$$L(x) = xe^{-x}[J_0(x) + J_1(x)] ,$$

$J_0(x)$ and $J_1(x)$ are the zeroth and first order Bessel functions of imaginary argument. The parameters x and β are expressed in terms of the parameters of the effective absorption line

$$x = \frac{SW}{2\pi\gamma} , \quad \beta = \frac{2\pi\gamma}{d} ,$$

where S and γ are the average intensity and absorption line halfwidth; d is the mean frequency separation of lines; W is the absorbing mass which for a horizontal path can be represented as $W = \rho L$, ρ is the absorbing gas concentration; and, L is the path length.

For inhomogeneous path, the variability of meteorological parameters along the beam path can be taken into account only in the line–by–line method. A single–parameter method of reduced mass commonly used in empirical techniques,[14–17,35–43,45,50] and a two–parameter method of Curtis–Godson,[45,50] which is more precise and is used for model representation of absorption spectra, are widely used in the approximation methods of calculation.

Using the model absorption spectra, the combined methods of calculation of the transmission functions were developed,[45] which were based on three models: the regular Elsasser model, the Plass model, and the statistical Goody model. In addition to basic formulas (2)–(4), the approximation of the strong Goody line ($x \gg 1$), empirical model (for CO_2 in some spectral ranges), approximation of the strong Elsasser line, etc. were used in the combined methods. The model parameters were determined, as a rule, from laboratory measurements of the transmission functions for different content of absorbing gases and different temperatures. In some individual cases the model parameters were determined by fitting to the calculated data.

All the aforementioned methods of calculation of the atmospheric absorption have limited applicability. They can be used for calculation of the transmission with resolution being not higher than that with which the parameters entering into the formulas were obtained.

In this connection the methods of fast calculation acquire particular importance. In these methods the model representation of absorption spectra is used, and the line parameters are determined from the atlass of spectral lines.

2.1.3. Methods of fast calculation

The methods of the model absorption bands with the parameters found from the data on the fine structure of lines allow one to determine transmission of the atmosphere within wide spectral ranges with arbitrary spectral resolution. The calculational method of determining the band model parameters has been developed owing to, on the one hand, recent advances in high and super–high resolution spectroscopy and, on the other hand, the developed systems for recording, storage, and read–out of the spectroscopic information.

The method for determining the parameters from the spectral line atlas is widely used for the Plass statistical model.[46,52,53] In some cases our model of choice is the model of individual line.[48,49] Figure 1 shows the comparison of the Plass statistical model, the model of individual line, and the regular model. It is seen from this figure that the model of individual line yields intermediate value of the transmission function as compared to the regular and statistical models.

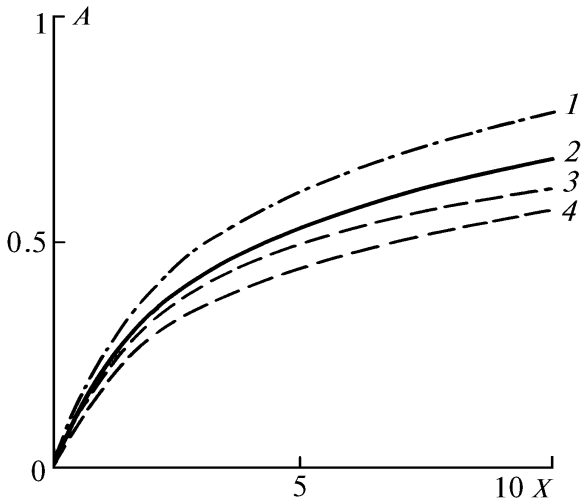

FIG. 1. Comparison of the absorption functions calculated for the band models with $\beta = 0.4$: *1) Elsasser model* A_{El}, *2) model of individual line* A_{Sl}, *3) Plass model* A_{Pl}, *and 4) Goody model* A_G.

The model of individual line and the results of laboratory measurements in the H_2O and CO_2 absorption bands were compared for the 2.7 μm range.[38] Figures 2 and 3 indicate their fairly good agreement.

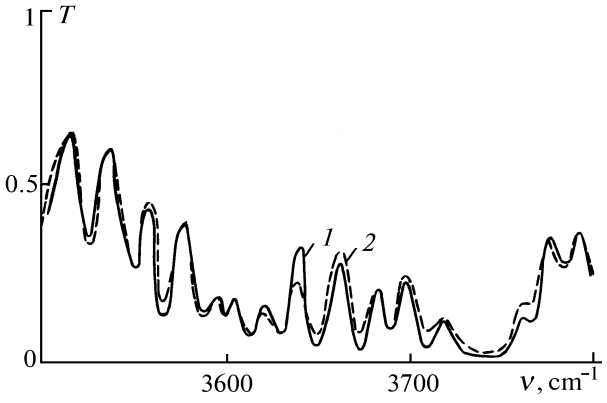

FIG. 2. Comparison of the transmission functions calculated for the model of individual line with the experimental data borrowed from Ref. 38 in the 2.7 μm *band of* H_2O. *Spectral resolution* $\Delta\nu = 10$ cm^{-1}, $W = 0.109$ g/cm^2, $P = 148$ mbar. *1) Experimental data and 2) calculation.*

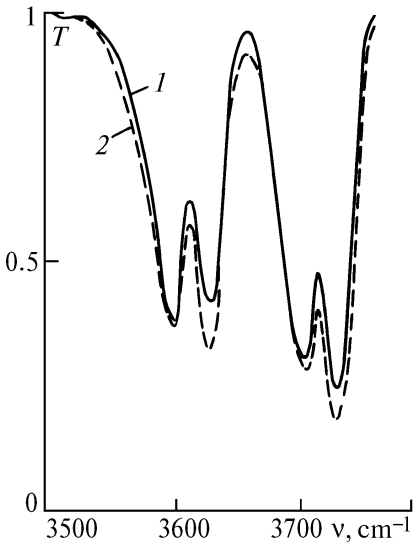

FIG. 3. Comparison of the transmission functions calculated for the model of individual line with the experimental data borrowed from Ref. 38 in the 2.7 μm *band of* CO_2. *Spectral resolution* $\Delta\nu = 8$ cm^{-1}, $W = 6.08$ atm·cm, $P = 676$ mbar. *1) Experimental data and 2) calculation.*

2.2. Software packages for modeling the transmission and radiation of the atmosphere with low spectral resolution

Package LOWTRAN

The package LOWTRAN was developed at the AFCRL based on the technique reported in 1971 (see Ref. 14). Further versions were reported in 1975, 1976, 1978, 1980 (see Refs. 1–16), and 1983 (see Ref. 17). The 7th version of LOWTRAN was reported in Ref. 18.

LOWTRAN–5 enables one to calculate the transmission and self–radiation with 20 cm^{-1} resolution in the spectral range between 350 and 40 000 cm^{-1} (0.25–28.5 μm). In this program a single–parameter molecular absorption model is used, and continuum absorption, molecular scattering, and aerosol extinction are taken into account. The refraction and the Earth's curvature are considered for slant paths. Six models of vertical distribution of meteorological parameters (pressure, temperature, humidity, and ozone concentration) at sub–arctic (winter and summer), moderate (winter and summer), and tropical (average annual) latitudes and the standard model of the USA are incorporated in the package as modules. The volume concentration of gases CO_2, N_2O, CH_4, CO, N_2, and O_2 is taken to be constant and invariable with altitude (homogeneously mixed gases). One model is used for vapor of nitric acid (HNO_3).

Aerosol extinction and molecular scattering are taken into account for the AFGL model. Moreover, it is possible to introduce arbitrary meteorological model and the profile of the aerosol extinction coefficient. The LTE is assumed to be established at all vertical levels.

The version LOWTRAN–6 (1983) has all the options of LOWTRAN–5 and a block for calculation of solar or moon radiation is added. The following sources are taken into account when radiation is calculated: self–radiation along the viewing line, radiation from external sources (the Sun and the Moon), and radiation reflected by the Earth and scattered by aerosol in the direction of the viewing line. The radiation scattered by aerosol is calculated in the single scattering approximation. It is possible to use three types of scattering phase function: the standard one, the Henyey–Greenstein scattering phase function with the asymmetry parameter, and the arbitrary model assigned by the user.

The aerosol LOWTRAN–6 model is complemented by the model describing the coastal regions; the wind is taken into account, the vertical structure of aerosol models is changed, and the models of cirrus clouds and the model of rain are included.

New molecules are additionally taken into account in the calculations of gas constituent transmission: NO, NO_2, NH_3, and SO_2. The scattered solar radiation is computed in the multiscattering approximation. In the 7th version of the package LOWTRAN the altitude range is limited by 50 km.

Package MODTRAN

In Proceedings of the 14th Conference on Atmospheric Transmission Models the MODTRAN package was briefly described.[18] The salient features of the package are as follows: spectral resolution is 2 cm^{-1}; the two–parameter model of the absorption band is used in the package; the altitude range is limited by 60 km; the LTE approximation is used; the initial spectral data are converted to 1 cm^{-1} spectral resolution; it is possible to model the transmission for a triangle instrumental function with arbitrary spectral resolution; the following gases: H_2O, O_3, CO_2, CH_4, N_2O, CO, N_2, O_2, HNO_3, NO, NO_2, NH_3, and SO_2 are taken into account; the model parameters depend on pressure and temperature.

Package AIRA

The applied software package AIRA (Absorption of Infrared Radiation in the Atmosphere) has been developed at the Institute of Atmospheric Optics, Siberian Branch of the Russian Academy of Sciences.[19–21] The following factors of extinction are taken into account in this package: molecular gas absorption, aerosol extinction, and molecular scattering of light.

The main recourse and expense of the package AIRA, similar to the system LARA, are associated with consideration of molecular absorption. However, in contrast to the package LARA, AIRA uses the algorithms of fast calculation with model representation of absorption bands. The parameters of band models are calculated from the atlas of spectral lines. One of the four models [see formulas (1)–(4)] is used for calculation of the transmission.

The package allows for the correction of one parameter using the transmission function obtained experimentally or calculated by the line–by–line method thereby improving the accuracy of the estimate of atmospheric absorption. The absorption function is calculated with arbitrary spectral resolution ($\Delta\nu \geq 1$ cm^{-1}). In the package AIRA it is possible to use either the atlas of spectral data on an external medium or the parameters of absorption band models which were calculated in advance with fixed spectral resolution and then archived.

The aerosol extinction of light is taken into account for the known optical models of atmospheric aerosol which have been developed at the Institute of Atmospheric Optics (IAO).[31]

Used in the package AIRA are both mean–zonal (IAO[32] and AFGL[33]) and regional meteorological models of the atmosphere constructed for individual quasi–homogeneous regions of the globe which were identified based on the objective applied classification and adequately

describe vertical distribution of optically active constituents in each region.

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