Simulation of solar radiation transfer with the allowance for weak water vapor absorption lines under various aerosol conditions

B.A. Voronin, I.M. Nasretdinov, A.B. Serebrennikov, and T.Yu. Chesnokova

Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk

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At present there is a discrepancy between measured and calculated fluxes of solar radiation at the Earth's surface. According to recent investigations, this discrepancy correlates with column density of water vapor. The calculated contribution of numerous weak water vapor absorption lines, which are usually ignored in atmospheric radiation problems, to irradiance of the Earth's surface and sky spectral brightness is considered. Spatial-angular brightness was modeled in several spectral ranges of the near IR and visible regions at different sighting directions and sun positions. Irradiance of the Earth's surface was estimated in the range of 4000–20000 cm^{-1}. The Monte Carlo method was used for calculations.

Introduction

Many investigators noticed the discrepancy (up to 20%) between the calculated and experimentally measured radiative fluxes in the Earth's atmosphere even with no clouds.[1] Possible causes for this discrepancy may be insufficiently correct scattering models,[1] inaccurate determination of continuum absorption by atmospheric gases,[2] and the neglect of numerous weak water vapor absorption lines.[3]

In this paper, which is a continuation of Ref. 4, we estimate the radiative contribution of weak water vapor absorption lines from the Partridge–Schwenke calculation[5,6] that are not included in current versions of spectroscopic databases HITRAN[7] and GEISA.[8] As compared to Ref. 4, this paper considers a wider spectral range and estimates how these lines affect the spectral-angular sky brightness near the horizon. New lines not included in the HITRAN atlas are weak almost everywhere, but since they are numerous, their total contribution to extinction of the solar radiation can be significant for long paths and multiple scattering of radiation.

The contribution of weak lines to the solar radiation transfer was considered when simulating irradiance of the Earth's surface and sky spectral brightness under various aerosol conditions. The spatial-angular brightness was simulated for some spectral ranges in the near IR and visible regions at different sighting directions and sun positions. The irradiance of the Earth's surface was estimated in the region of 4000–20000 cm^{-1}.

Criteria for selection of spectral lines

To apply the results of the variational calculation[5,6] to estimates of the radiation budget of the atmosphere, we have first to analyze the accuracy of *ab initio* calculations of the spectral line intensity for the following molecules: $Í_2{}^{16}Î$, HDO, $Í_2{}^{17}Î$, and $Í_2{}^{18}Î$.

Comparing the spectroscopic databanks (DB) in the number of lines (Table 1) and in the spectral regions covered (Table 2), we can see that the new calculation[5,6] presents more detailed information than other databases. It should be specified here that the number of lines in the Schwenke DB is presented for the room temperature and lines with the intensity lower than 10^{-30} cm / mol are ignored.

Table 1. Number of lines for isotopic modifications of $Í_2Î$ in different DB

DB	Isotopic modifications of H_2O					
	$Í_2{}^{16}Î$	$Í_2{}^{18}Î$	$Í_2{}^{17}Î$	$ÍD^{16}O$	$HD^{17}O$	$HD^{18}O$
HITRAN-96	30117	6357	3744	9226	—	—
GEISA-97	30117	6357	3744	9799	—	200
HITRAN-2000	31646	7423	3755	8493	175	438
Schwenke DB,						
Ref. 5	289806	64734	46003	96102	—	—
Ref. 6				939687		

Table 2. Spectral ranges (cm^{-1}) for isotopic modifications of H_2O in different DB

Isotopic modifications of H_2O	Databank			
	HITRAN-96	HITRAN-2000	Schwenke-97	GEISA-97
$H_2{}^{16}O$	0.4–22656.4	0.4–22656.4	0.1–28279.3	0.4–22656.4
$H_2{}^{17}O$	6.5–11150.8	6.5–11144.0	0.1–17306.5	6.5–11150.8
$H_2{}^{18}O$	6.8–13900.4	6.8–13900.4	0.2–17299.2	6.8–13900.4
$HD^{16}O$:				
Ref. 5,	0.0–5507.5	0.0–5507.5	0.2–15704.4	0.0–5507.5
Ref. 6			0.0–20101.4	
$HD^{18}O$	–	1173.8–1684.2	–	1231–1607
$HD^{17}O$	–	1234.2–1598.8	–	–

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As is seen from Tables 1 and 2, the data from the Schwenke DB are far extended as compared to the other databanks, especially, for HDO, since Ref. 6 presents the new, more accurate Partridge–Schwenke calculation. To estimate the accuracy of the Schwenke calculation, analysis of line positions[9] and intensities[10] was performed. The analysis showed that the mean error is ~ 0.1 cm^{-1} for the line centers and ~ 20–50% for intensities.

The natural abundance of $HD^{18}O$ and $HD^{17}O$ in the atmosphere is very low: 0.0000623 and 0.0000116%, respectively (for comparison: $H_2{}^{16}O$ – 99.7317%; $H_2{}^{18}O$ – 0.199983%, $H_2{}^{17}O$ – 0.0372%; $HD^{16}O$ – 0.031069%), that is, the data on these isotopic modifications can be neglected.

The compared lines from the Schwenke DB and HITRAN-2000 were thought identical, if their following parameters coincide: (1) rotational quantum numbers J', J'' of the lower and upper energy levels of a transition; (2) symmetry of the lower and upper energy levels of a transition as determined from the rotational-vibrational quantum numbers J', $K'_a - K'_c$, V'_3, and J'', $K''_a - K''_c$, V''_3, respectively; (3) transition frequency (the comparison window depended on the transition frequency: the frequency ν (cm^{-1}) divided by 10000 cm^{-1} ($d\nu = \nu / 10000$ cm^{-1}); (4) lower energy level E (the comparison window for the lower energy level was taken as for the transition frequency, but halved ($dE = d\nu / 2$)).

In the HITRAN-2000 DB, about 2000 water vapor lines are unassigned, and the above procedure failed to compare several tens of lines. To compare the rest lines, we applied the following procedure. Those lines from the Schwenke DB and HITRAN DB were thought coinciding, for which value of $(\nu_{\text{Schwenke}} - \nu_{\text{HITRAN}})^2 + \text{Ln}(I_{\text{Schwenke}} / I_{\text{HITRAN}})$ was minimum. Here I is the line intensity. Finally, we have compared 51317 lines and add 448330 from the Schwenke DB to them.

The calculation in Ref. 5 includes no data on self-broadening, air pressure induced broadening and the temperature dependence of line shifts. At the same time, it is inexpedient performing precision calculations of broadening for every line based only on the quantum numbers: on the one hand, it is very laborious and even impossible for a large number of lines (~500000), and, on the other hand, there is no need in this for estimation of absorption in a wide range. Therefore, we calculated the average (over the HITRAN DB) J-dependence for broadening and self-broadening of $H_2{}^{16}O$ and HDO lines. For higher J, we used approximate extrapolation, since now there are no experimental data for $J = 50$ or 55. In particular, the HITRAN BD presents the data for HDO in the case of self-broadening and air pressure induced broadening up to $J = 20$ and for $H_2{}^{16}O$ up to $J = 24$ for air pressure induced broadening and up to $J = 21$ for self-broadening. For $H_2{}^{17}O$ and $H_2{}^{18}O$ the data on broadening and self-broadening were taken as for $H_2{}^{16}O$.

Estimated effect of weak molecular absorption lines on irradiance of the Earth's surface

The results presented in this paper were obtained for the same experimental geometry as in Ref. 4. The only difference is much wider spectral range, in which the irradiance is estimated for models taking into account and ignoring absorption by weak water vapor lines (4000–20000 cm^{-1}).

To calculate the irradiance of the Earth's surface, we took the plane stratified model of the atmosphere / surface system (Fig. 1) and used two models of optical properties of the atmosphere: the model of urban aerosol with the meteorological range (MR) of 5 km in the surface layer of the aerosol atmosphere and the model of advective fog with the meteorological range of 2 km (Ref. 12).

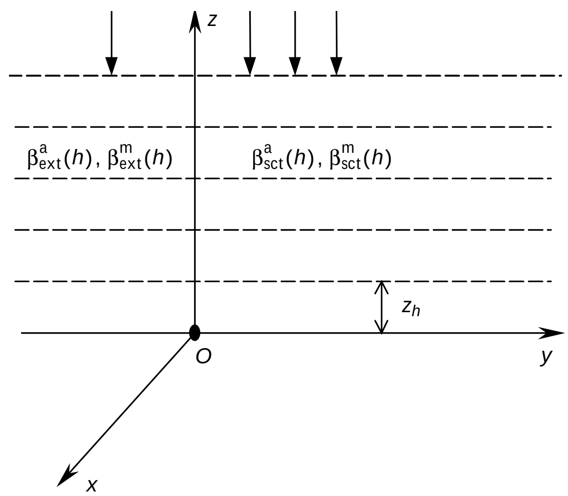

Fig. 1. Geometry of experiment: $\beta^a_{ext}(h)$ and $\beta^m_{ext}(h)$ are the aerosol and molecular extinction coefficients; $\beta^a_{sct}(h)$ and $\beta^m_{sct}(h)$ are the aerosol and molecular scattering coefficients; z_h is the layer thickness.

The process of radiation propagation through the molecular–aerosol atmosphere was imitated through direct simulation by the Monte Carlo method. This method was selected because of its simplicity and low time consumption when calculating irradiance of the Earth's surface at a given wavelength λ (Refs. 11 and 13).

When the molecular absorption was taken into account, the k-distribution method[14] was used, and this significantly shortened the time for calculation as compared to the line-by-line method. Therefore, only ten Monte Carlo estimates of E_j (instead of 10000, as in the line-by-line method with the same resolution) were performed for each of 160 intervals $\Delta\nu$ = 100 cm^{-1} by the equation

$$I = \Delta\nu \sum_{i=1}^{10} C_i I_i S_i,$$

where C_i are the parameterization coefficients; S_i is the solar constant at the spectral interval Δν, $W\cdot cm^{-1} / m^2$.

The calculated results are shown in Fig. 2. The relative contribution δF of weak Í$_2$Î absorption lines to irradiance of the Earth's surface at some 100-cm^{-1} intervals achieves 1.6% in the region of weak absorption bands.

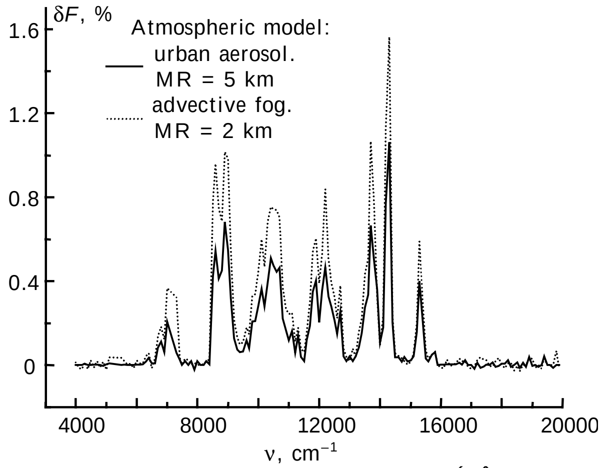

Fig. 2. Relative contribution of weak Í$_2$Î lines to irradiance of the Earth's surface by solar radiation.

The low contribution due to weak lines in the region of 4000–6500 cm^{-1} is caused by the strong molecular absorption, which strongly decreases the fraction of the scattered radiation reaching the Earth's surface. The pattern observed in the interval 16000–20000 cm^{-1} is quite similar. However, this is caused by the sharp decrease in the intensity of water vapor absorption (in particular, in weak lines) against the background of monotonically increasing aerosol extinction.

Simulation of spectral-angular sky brightness taking into account and neglecting absorption by weak water vapor lines

One of the methods frequently used to reconstruct optical characteristics of the atmosphere is the method based on interpretation of measurements of the spectral-angular sky brightness. To estimate the effect of weak water vapor absorption lines, we have performed numerical simulation of the operation of a solar photometer. The following geometry of the experiment was considered. A narrow-beam receiver (field of view ≈1°) is oriented at the horizon (ξ_{det} is the zenith angle of the detector equal to 89.5°). The sun is at some sky point (ξ_0 = 75 and 80°), azimuth scanning is performed at the constant receiver's zenith angle. The atmosphere is assumed spherical and divided into layers, within which the medium characteristics remain constant. The molecular scattering coefficients were calculated at every atmospheric layer with the constant temperature, pressure, and concentration of gases. The major absorbing atmospheric gases, namely, Í$_2$Î, ÑO$_2$, O_3, N_2O, ÑÎ, ÑÍ$_4$, and Î$_3$, were taken into account.

The k-distribution method was used to shorten the time of calculation of the spectral brightness taking into account absorption in the spectral ranges determined by the characteristics of filters. Unlike previous calculations of the irradiance of the Earth's surface, in which the solar radiation was assumed constant within 100 cm^{-1} intervals, in these calculations the spectral intervals are wide (1000 cm^{-1} and wider) and the solar radiation varies widely within the filter pass band, as shown in Fig. 3.

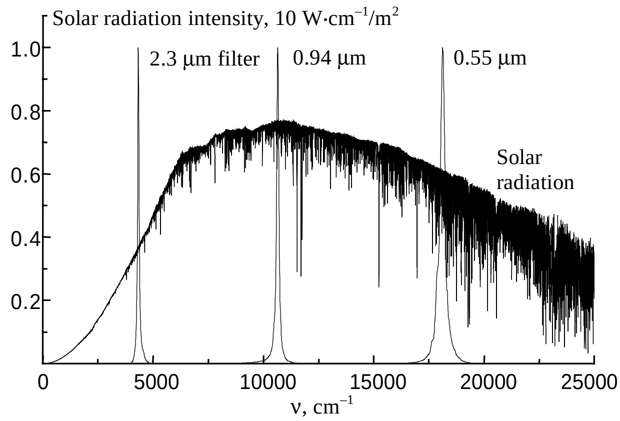

Fig. 3. Solar spectrum and spectral ranges of filter of the solar photometer.

Therefore, the parametric coefficients accounting for molecular absorption were complemented with the spectral characteristics of the filter and the solar constant:

$$\frac{1}{\nu_2-\nu_1}\int_{\nu_1}^{\nu_2} S(\nu)f(\nu)\exp[-k(\nu)]\mathrm{d}\nu =$$

$$= C_0\int_0^1 \exp(-k(g))\mathrm{d}g = \sum_{i=1}^{10} C_i\exp(-k_i),$$

where $S(\nu)$ is the solar constant, in W·cm^{-1}/m^2; $f(\nu)$ is the instrumental function of the filter normalized to unity; k is the molecular absorption coefficient, in km^{-1}.

Tentative estimates by the k-distribution method showed that ten quadratures are also quite sufficient for wide spectral ranges for the parameterization error to be within 0.5%. This accuracy in calculation of molecular absorption allows reliable estimation of the contribution of weak water vapor lines.

Simulation was performed for three filters passing the solar radiation in the spectral intervals: 0.55(±0.02), 0.94(±0.05), and 2.3(±0.1) μm, for each of which we specified the values of the atmospheric parameters: single-scattering albedo ω_0, surface albedo $Â_s$, aerosol scattering phase function $g^a(\theta)$, aerosol extinction, molecular scattering and gas absorption coefficients. Numerical calculations were performed for the single B_S, multiple B_M, and net B components of brightness. The angular dependence of these brightness components of the solar zenith angle ξ_0 and the relative contribution of weak water vapor lines to brightness are depicted in Fig. 4.

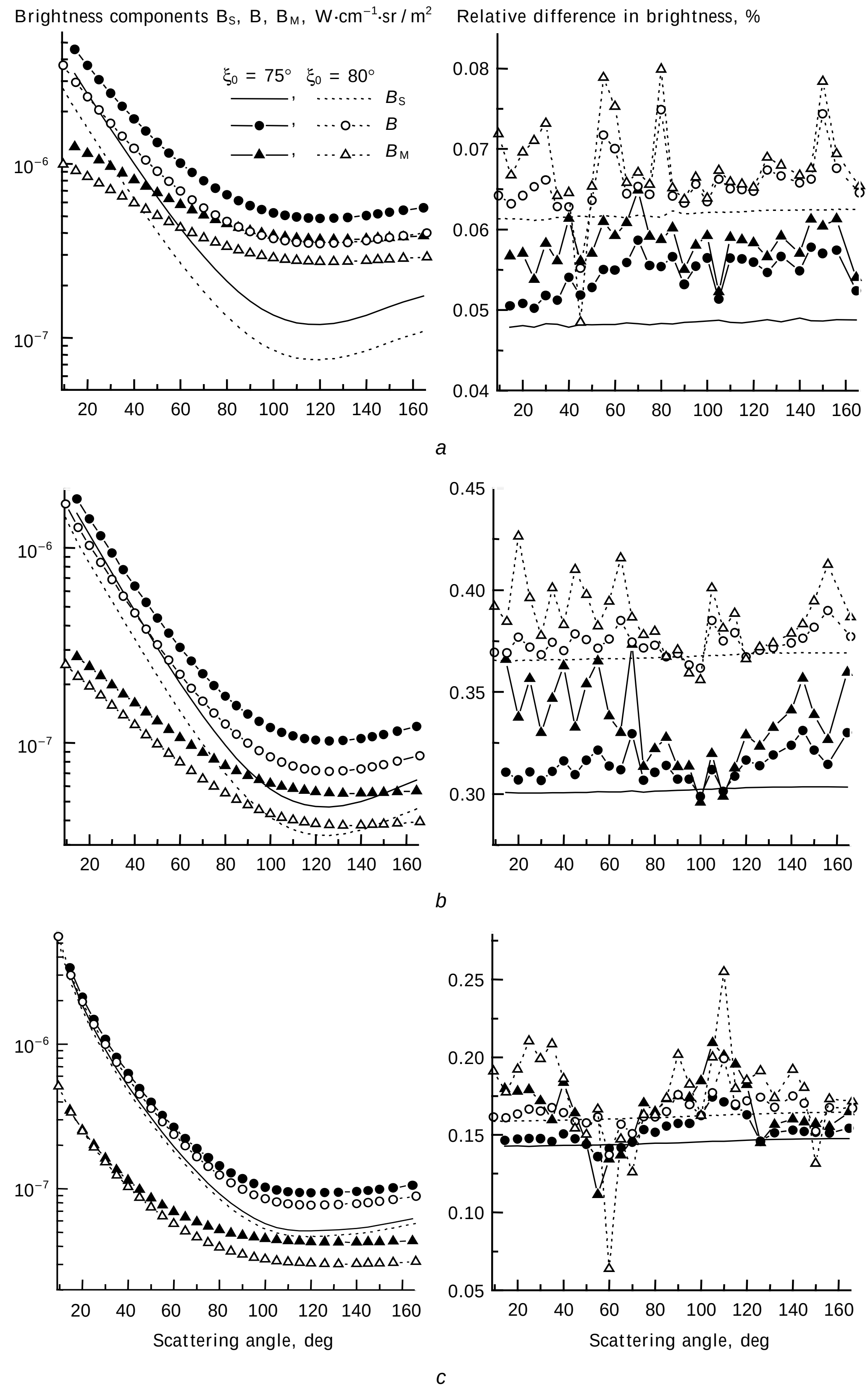

Fig. 4. Angular dependence of the brightness components with the allowance made for the absorption by weak water vapor lines (left) and relative contribution of these lines to brightness (right); A_s = 0.2, ξ_{det} = 89.5°: 0.55 μm filter, ω_0 = 0.891, aerosol optical depth τ_a = 0.17, and molecular scattering optical depth τ_R = 0.1 (*a*); 0.94 μm, ω_0 = 0.827, τ_a = 0.09, τ_R = 0.01 (*b*); 2.3 μm, ω_0 = 0.758, τ_a = 0.027, τ_R = 0.0003 (*c*).

Analysis of the results obtained showed that for the wavelength of 0.55 μm the difference between the intensities calculated with and without the account of absorption by weak water vapor lines is less than 0.1% (Fig. 4*a*), and for other wavelengths (0.94 and 2.3 μm) it is though somewhat larger, but still within 0.5% (Figs. 4*b* and *c*). It should be noted that this difference increases with the increasing solar zenith angle, which can be explained by the increase in the relative contribution of weak lines to the total absorption with the increasing path length.

Conclusion

Consideration of weak water vapor lines that are usually ignored in atmospheric calculations in the region of 4000–20000 cm^{-1} gives an extra contribution up to 1.6% to the irradiance of the Earth's surface by the solar radiation within 100-cm^{-1} -wide spectral ranges in the region of 0.7 μm. Nevertheless, in modeling brightness measured with the solar photometers, weak water vapor lines have the smaller effect (up to 0.5%) onto the radiative transfer because of the wider filter pass bands and the position of its center taken in the ranges of weak water vapor absorption specially for the problems of reconstruction of aerosol optical characteristics.

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