Estimation of the role of weak water vapor absorption lines in solar radiation transfer

B.A. Voronin, A.B. Serebrennikov, and T.Yu. Chesnokova

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

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The contribution of weak water vapor absorption lines to extinction of solar radiation in the gas-aerosol atmosphere is calculated with the use of a new version of HITRAN database and *ab initio* calculation of Partridge and Schwenke. Almost all "new" lines neglected in the previous version of the HITRAN database are weak, but their total contribution to extinction of the solar radiation may reach 1% along vertical atmospheric paths. The contribution of weak lines is essential in atmospheric microwindows, where it can achieve several percent. It is concluded that weak water vapor lines should be taken into account along with the water vapor continuum when estimating the radiative balance.

Introduction

In recent years, many researchers notice that there is a discrepancy between the calculated and experimentally measured radiative budget of the Earth atmosphere even in the absence of clouds. To explain this discrepancy, numerous hypotheses are invoked. Thus, for example, in Ref. 1 the excessive absorption is explained by insufficiently correct account in clouds for scattering effects in the used models. According to Ref. 2, continuum absorption can partially improve the situation, but it does not remove the problem of excessive absorption. In Ref. 3, it is hypothesized that weak water vapor absorption lines that are neglected in current spectroscopic databases such as HITRAN and GEISA can contribute significantly to absorption.

Recently, a new version of the HITRAN database was issued (HITRAN-2000) and new *ab initio* calculations were presented by Partridge and Schwenke.[4] For comparison, in the region of 7600–18000 cm^{-1} the previous version of HITRAN-96 contains 11940 H_2O lines, HITRAN-2000 contains 13575, and *ab initio* calculations give 216670 lines. Almost all "new" lines that were ignored in the previous versions of HITRAN[5] are weak, but numerous, and therefore their total contribution to solar radiation extinction may be marked for long paths and in the case of multiple scattering.

In this paper, we evaluate the contribution of weak water vapor absorption lines to solar radiation transfer. This work continues the study begun in Ref. 3.

1. Spectral line parameters and selection criteria

The HITRAN-96 and HITRAN-2000 databases are most widely used for atmospheric applications. Nevertheless, the information in them on water vapor absorption lines in the near infrared and visible spectral regions is incomplete. The last version of HITRAN-2000 contains the information on HDO lines only up to 5507 cm^{-1}, on $H_2{}^{16}O$ lines up to 22656 cm^{-1}, on $H_2{}^{17}O$ up to 13900 cm^{-1}, and on $H_2{}^{18}O$ up to 11143 cm^{-1}. Besides, in the region of 5850–8200 cm^{-1} the information is absent for all, even rather strong absorption lines of $H_2{}^{17}O$ and $H_2{}^{18}O$ with the intensity ~ 10^{-23} cm/mol.

The data bank used for assessment of the contribution of weak H_2O lines was obtained as follows. Partridge and Schwenke[4] have made *ab initio* calculation of the potential energy surface and dipole moment for isotopic species of water molecule. Then all rovibrational energy levels up to 40000 cm^{-1}, line centers, and intensities were calculated by the variational method. The parameters of the potential energy function were refined through fitting by the least square method to transition frequencies included in HITRAN-92.

The data bank contains much more lines than HITRAN databases. In particular, according to the data of Ref. 4, the number of lines with the intensity lower than 10^{-26} cm/mol. in the region of 12900–14300 cm^{-1} exceeds 19500, whereas the total number of lines with the intensity of 10^{-30} – 10^{-23} cm/mol. is 21800. For example, HITRAN-2000 contains only 2178 lines in this region, and the number of lines with the intensity lower 10^{-26} cm/mol. is less than 50. The database[4] includes lines of hot bands, high overtones of the bending vibration, and absorption lines of isotopic species of water molecule. The accuracy of calculation of line intensities and centers is sufficient to obtain reliable estimates for extinction of broadband radiation at atmospheric paths. The root-mean-square deviation between the calculated line centers and those from HITRAN-96 is only 0.1 cm^{-1}, the root-mean-square deviation of the band integral intensities is about 20%.

Figure 1 presents a comparison of line total intensities in the range 7000–22000 cm^{-1} for HITRAN-96, HITRAN-2000, and *ab initio* calculations. It is seen that HITRAN-96 does not contain lines with the intensity lower than 10^{-27} cm/mol., and lines with the intensity lower than 10^{-28} cm/mol. are absent in HITRAN-2000. Almost all lines given in Ref. 4, but absent in the HITRAN databases, can be treated as weak H_2O absorption lines.

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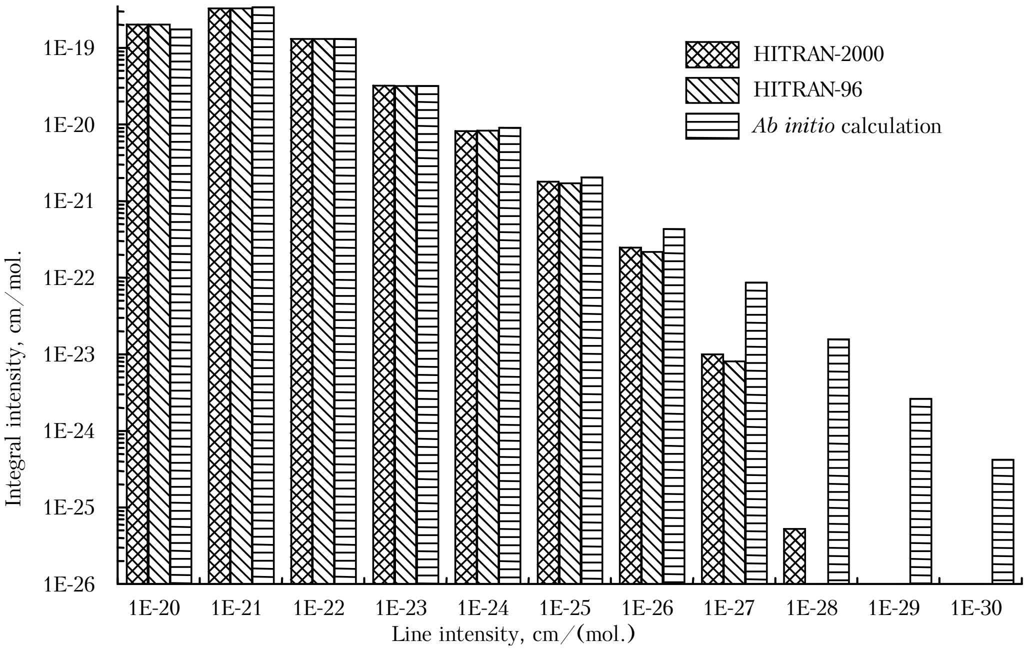

Fig. 1. Integral intensity of lines per one decade of intensity variation as it is given in HITRAN-96, HITRAN-2000, and Partridge–Schwenke databank.

For solar radiation transfer calculation in the region of 7000–22000 cm^{-1}, we excluded the lines presented in HITRAN-2000 (17031 lines) from the Partridge–Schwenke databank.[4] Lines in these two databases were compared by their wavenumbers and lower energy levels. The rest of lines (270145) in the Partridge–Schwenke databank[4] in the same spectral region are mostly weak.

2. Calculation of absorption functions

Absorption functions were calculated by the line-by-line method with the resolution of 20 cm^{-1} for a horizontal path. The path length was chosen so that absorption is close to an inhomogeneous path crossing the entire atmosphere at the angles of 0, 60, 70°. The AFGL meteorological model of midlatitude summer was used.

The contribution of weak H_2O lines to absorption is shown in Fig. 2. The results of calculation show that as the path length increases (the angle changes from 0 to 70°), absorption by weak lines increases more than twice and becomes significant as compared to absorption by all H_2O lines. The relative contribution of weak lines is, as a rule, several percent and increases in the region of weak absorption bands.

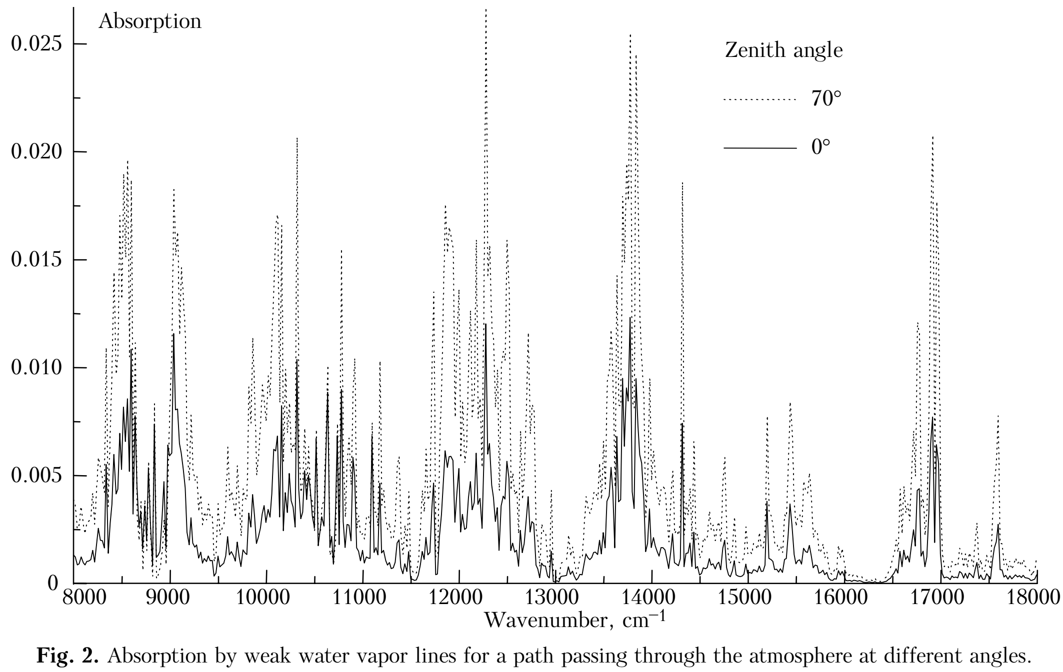

Fig. 2. Absorption by weak water vapor lines for a path passing through the atmosphere at different angles.

Downward fluxes of solar radiation calculated from the line-by-line data, neglecting scattering, for the meteorological model of midlatitude summer, are given in the Table. At the vertical path crossing the entire atmosphere, the contribution of weak water vapor lines to solar radiation absorption was almost 2 W/m^2. The relative contribution of weak lines to the radiation transfer given in the Table and shown in Fig. 3, increases as the path length increases, whereas its absolute value decreases.

Table. Solar radiation flux in the spectral region of 7000–22000 cm^{-1} reaching the surface through the nonscattering atmosphere, in W/m^2

Absorption lines	Zenith angle, deg		
	0	60	70
All Partridge–Schwenke (PS) lines	852.22	410.91	274.44
PS lines similar to HITRAN-2000	853.98	412.40	275.77
Absolute contribution of weak lines to flux	1.76	1.49	1.33
Relative contribution of weak lines to flux, %	0.21	0.36	0.5

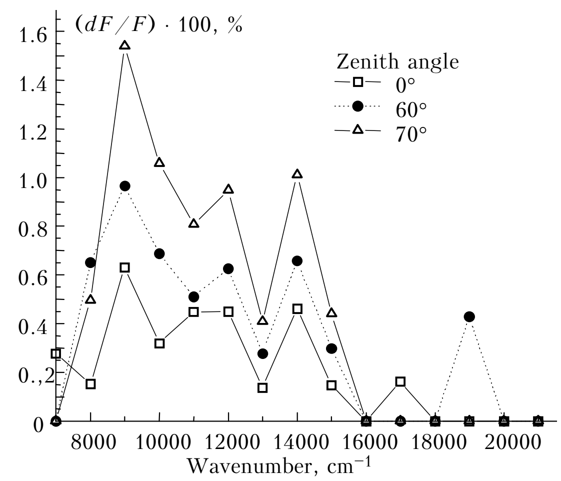

Fig. 3. Relative contribution of weak water vapor lines to solar radiation flux near the surface.

3. Calculation of surface irradiance

For calculation of the surface irradiance, we took the plane-stratified model of the atmosphere–surface system. It was assumed that solar radiation falls normal to the atmospheric top. The integral optical properties of the molecular-aerosol atmosphere were simulated by a set of altitude profiles of the scattering and absorption coefficients. The scattering phase functions were specified in the tabular form as "weighted" aerosol-gas functions determined by the equation[6]:

$$g(\theta) = \frac{\beta^{\rm a}_{\rm sct}}{\beta_{\rm sct}} g^{\rm a}(\theta) + \frac{\beta^{\rm m}_{\rm sct}}{\beta_{\rm sct}} g^{\rm m}(\theta),$$

where $\beta^{\rm a}_{\rm sct}$ and $\beta^{\rm m}_{\rm sct}$ are the coefficients of aerosol and molecular scattering in the jth layer; $\beta_{\rm sct} = \beta^{\rm a}_{\rm sct} + \beta^{\rm m}_{\rm sct}$; $g(\theta)$, $g^{\rm a}(\theta)$ and $g^{\rm m}(\theta)$ are the "weighted," aerosol, and molecular scattering phase functions.

We have selected two models of optical properties of the atmosphere, in which the fraction of the component formed by scattered radiation at total irradiance was 27 and 88%. They are the model of urban aerosol with the visibility of 5 km in the ground layer of the aerosol atmosphere and the model of advective fog with the visibility of 2 km (Ref. 7).

The process of radiation propagation in the molecular-aerosol atmosphere was simulated directly using the Monte Carlo method. This choice was caused by simplicity of the method and its low labor-consuming when calculating surface irradiance at a given wavelength λ (Ref. 8).

To reduce the time-consumption in calculations accounting for molecular absorption, we used the method of "k-distribution,"[9] which allowed us to decrease the number of E_j estimates to 10 (in spite of 10000, as with the use of the line-by-line method with the same resolution). The estimates were made by the Monte Carlo method for each of 55 intervals of 100-cm^{-1} wide by the equation

$$\hat{E} = \Delta\Lambda \sum_{j=1}^{n} C_j\, E_j\, S_{\lambda_j},$$

where C_j are parameterization coefficients; S_λ is the solar constant; $\Delta\Lambda = 100$ cm^{-1}; n is the number of Gauss quadratures ($n = 10$).

The results are shown in Fig. 4.

The relative contribution of weak H_2O absorption lines to the surface irradiance at some 100-cm^{-1} wide intervals can exceed 1% in the region of weak absorption lines, and it can increase significantly at more narrow intervals. In the entire region of 8500–14000 cm^{-1}, the total contribution is less than 0.5%.

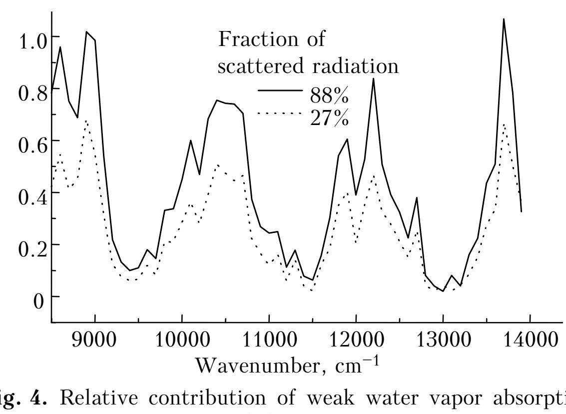

Fig. 4. Relative contribution of weak water vapor absorption lines to surface irradiance (%) by solar radiation in the region of 7000–22000 cm^{-1} for different atmospheric conditions of aerosol and molecular scattering.

Conclusion

The results obtained allow us to conclude the following:

– allowance for weak water vapor lines in the region of 7000–22000 cm^{-1} increases the contribution up to 1% to absorption (up to 2 W/m^2 to flux) along a vertical path crossing the entire atmosphere;

– in atmospheric microwindows this contribution becomes significant and can achieve several percent;

– as the path length increases, the role of weak lines in absorption increases markedly;

– the effect of weak lines can only partially explain the excessive absorption in the atmosphere;

– absorption by weak water vapor lines should be taken into account along with the continuum absorption when estimating the radiative budget.

Acknowledgments

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