Calculation of solar radiative fluxes in the atmosphere: the effect of updates in spectroscopic data

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Line-by-line calculations in the spectral region 2 000–20 000 cm^{-1} (0.5–5 μm) were made to assess the impact of a variety of water vapor spectral databases on the accuracy of solar flux calculation in the atmosphere. The CKD1 and CKD2.4 continuum models were also compared. The maximum disagreement in the calculated solar surface flux due to all the investigated factors can reach 5.9 W/m^2 for midlatitude summer atmosphere and the solar zenith angle 30°. This is ~ 0.8% of the total downward solar flux at the surface and ~ 3.3% of the total atmospheric absorption. The dominant cause of this difference is the extra absorption caused by weak lines, which are not included on the HITRAN databases.

Introduction

The accuracy of the radiative transfer modeling in the atmosphere still remains an important concern for global climate modeling. It was shown more then 10 years ago in Ref. 1 that substantial discrepancies exist among different radiation codes even for the simple case of pure water vapor absorption. The standard deviation ranged from 1% to 3% for the downward fluxes at the surface and from 6% to 11% for the total atmospheric absorption. The situation has hardly improved in recent years. For example, the discrepancy in the amount of the solar energy absorbed in the atmosphere calculated by the two different radiative models reached 12% in the Ref. 2 devoted to the investigation of the excess atmospheric absorption.

In the examples above the same input parameters were used for the models under comparison. A potential source of discrepancies is that different spectroscopic datasets may be used in the different models. This factor has become more important recently as significant changes have taken place in the high-resolution spectroscopic datasets. For example Ref. 3 updates widely used spectral database HITRAN have appeared since 1996. That is HITRAN-96,[3] HITRAN-2000 (or HITRAN-2k)[4] and the latest update for some gases, HITRAN v.11 (see http://www.hitran.com).

Large changes have occurred in the spectroscopic data for H_2O. In addition to the about 51000 H_2O spectral lines in the HITRAN-96, the parameters of a 500 000 (room temperature database) "weak" lines where computed in the *ab-initio* calculations of Partridge and Schwenke.[5] Only a very small proportion of these lines is included in HITRAN v.11.0. In addition, it should be noted that a few updates of the Clough–Kneizys–Davies (CKD) water continuum[6] have been reported during the past 8 years: http://www.aer.com/scienceResearch/rc/rc.html.[7]

The main aim of the present work is to assess what uncertainty in the clear sky flux modeling in the spectral region 0.5–5 μm (2 000–20 000 cm^{-1}) can be caused by using the different HITRAN databases, different versions of CKD continuum, and due to the Partridge–Schwenke weak lines (PSWL). (Here and later the term "weak lines" means those lines in the Partridge–Schwenke (PS) database that are absent from HITRAN-2k).

The absorption of only water vapor was taken into account in the calculations together with the Rayleigh scattering. However, because of the H_2O absorption is dominant in this spectral region the contribution of other gases will not significantly affect our results.

Data and codes used

The line-by-line calculations of the solar irradiance on the surface in the spectral region 2 000–19 900 cm^{-1} were performed and compared to estimate the impact of different spectroscopic datasets. All calculations were performed for the midlatitude summer (MLS) profile used in the Intercomparison of Radiation Codes in Climate Models (ICRCCM),[1] which corresponds to a total atmospheric column of water vapor of 30 kg/m^2. The solar zenith angle (SZA) of 30° was used for the flux calculations.

The fast line-by-line code LBL[8] was used for high (0.002 cm^{-1}) spectral resolution calculation of optical depth for each of 33 atmospheric layers of clear-sky MLS model. The CKD2.4 water continuum[9] was included in the LBL code. The optical depth spectra were then used as input to the Discrete Ordinate (DISORT) code[10] for irradiance calculations with the Rayleigh scattering taken into account. The solar irradiance at the top of the atmosphere compiled by Kurucz[11] is employed, which presents the solar spectrum at the spectral resolution of 1 cm^{-1} (Solar constant = 1368.8 W/m^2). The albedo of the Earth surface was taken to be a spectrally constant value of 0.14, which is close to the global averaged value.

The spectral lines database HITRAN-96, HITRAN-2k, and HITRAN v.11 were used as well as Partridge–Schwenke room temperature water lines database.

Calculations

1. HITRAN database versions

Figures 1*a* and *b* show the spectrum of the calculated solar flux at the surface using HITRAN-96 database and the difference (Δ_{Flux}) between fluxes calculated with HITRAN-96 and HITRAN-2k. The dashed lines in Fig. 1 show cumulative

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differential flux (W/m^2), i.e., ΔFlux integrated over wave number from the beginning of the spectral region to the given wave number. The differential flux in the spectral region 8 000–14 000 cm^{-1} is caused mainly by the Giver et al. correction[12] to HITRAN-96.

The difference between HITRAN-96 and v.11 is shown in Fig. 1*c*. The noticeable disagreement between HITRAN 2k and HITRAN v.11 calculations (Fig. 1*d*) appears only in the spectral interval near 2700 cm^{-1}. The difference is caused by about 1250 lines that were added into HITRAN v.11 in that spectral region, in comparison with HITRAN-2k (there are 2500 lines in the v.11 and 1250 lines in the 2k version in the spectral region 2500–3000 cm^{-1}). The more interesting fact is that all these extra lines were already present in HITRAN-96. That is why there is no marked difference between HITRAN-96 and HITRAN v.11 in the region near 2700 cm^{-1}. It means that HITRAN-96 should be more correct in this spectral region than the later version HITRAN-2k.

As can be seen from Fig. 1 the total difference in the calculated surface flux reaches 0.8 W/m^2 when compared to HITRAN-96 with HITRAN v.11 and 0.2 W/m^2 for the HITRAN-96 versus HITRAN-2k comparison. The lower value of HITRAN-96 – HITRAN-2k disagreement is due to the alternating sign of the differential flux for these versions.

2. CKD1 and CKD2.4 water vapor continuum

Taking into account the fact that at least four new versions of CKD water continuum have appeared since 1994,[7] it is interesting to check what variation of radiative flux can be caused by using some of them. A difference of more than 100% of the radiation absorbed in the atmosphere due to CKD-0 and CKD-2.4[6,9] was found in Ref. 13 by Zhong et al. (19.5 W/m^2 and 7.7 W/m^2, respectively, for SZA = 30°, MLS model, and 1000–22 700 cm^{-1} spectral region).

Figures 2 and 3 demonstrate the comparison of two closer versions of water vapor continuum CKD-1 (1994) and CKD-2.4 (1999). In Fig. 2 the vertical optical depth of the atmosphere due to water vapor continuum is presented. A difference between these two CKD versions of up to an order of magnitude can be seen in the wings of H_2O absorption bands.

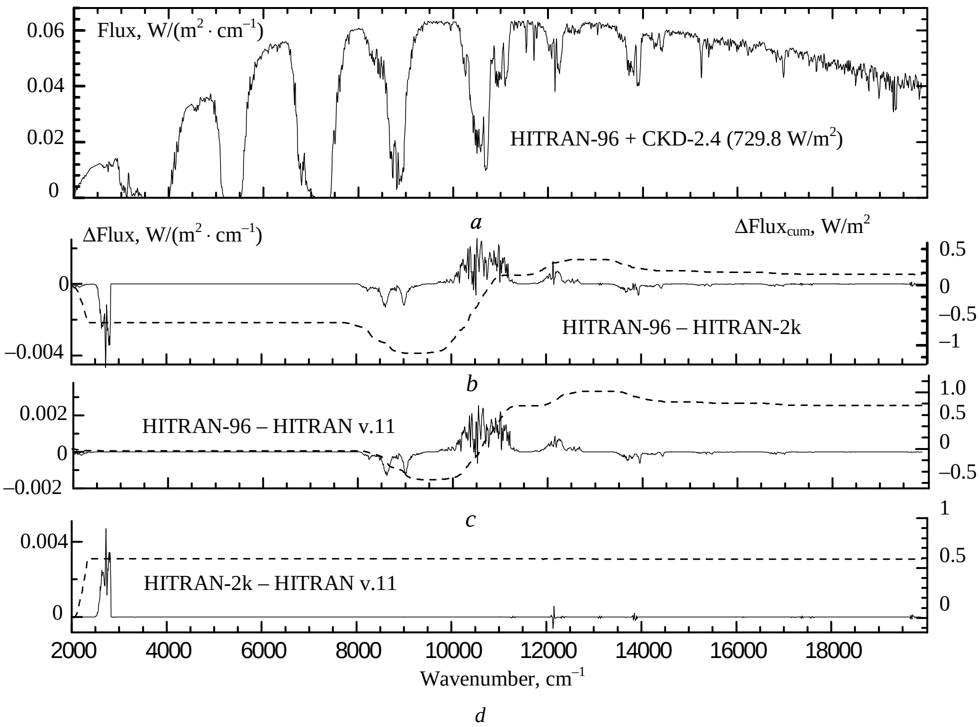

Fig. 1. The spectrum of the solar flux at the surface calculated using HITRAN-96 database and the difference (ΔFlux) (solid line, left-hand axis) between fluxes calculated with different HITRAN databases. The dashed lines (right-hand axis) show the cumulative differential flux (W/m^2) integrated from 2000 cm^{-1}.

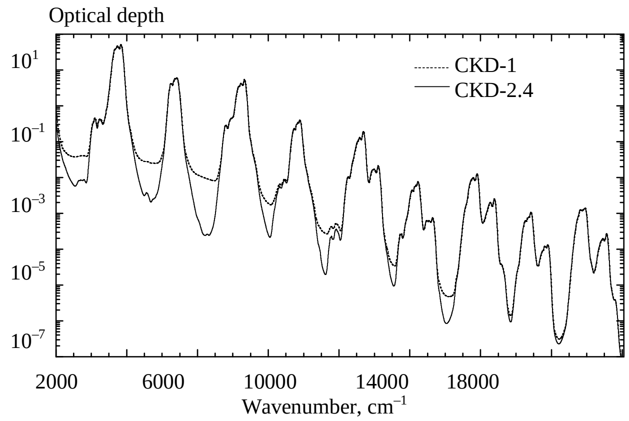

Fig. 2. The vertical optical depth of the atmosphere due to two versions of the CKD water continuum absorption CKD-1 and CKD-2.4.

Figures 3*a* and *b* show this effect with respect to the surface radiative flux. The difference in total absorbed flux is 1.8 W/m^2 for the given conditions. It is about 25% of the total radiation absorbed due to CKD2.4 (7.2 W/m^2) in the spectral region under investigation (Fig. 3*c*). The Voigt profile wings with 25 cm^{-1} cutoff from the line center was used for the calculation without the continuum ('No_CKD' in Fig. 3*c*).

3. Partridge–Schwenke weak lines (PSWL)

There are a few papers where the influence of the PSWL on radiative flux was assessed (see Refs. 13–15). Only in Ref. 13 a wide spectral region (1000–22 700 cm^{-1}) was investigated. The estimation of the weak lines impact was limited by spectral interval 13 200–22200 cm^{-1} and 7 000–22 200 cm^{-1} in Refs. 14 and 15, respectively, although it will be shown below that the spectral range 2 000–7 000 cm^{-1} gives about 30% of the PSWL contribution.

It is not straightforward to use the PS database to estimate PSWL influence, as it includes all lines, including those on HITRAN, although sometimes with different line intensities and positions. We used three different approaches to estimate the PSWL influence.

a) HITRAN-2k – PS

The differential flux between calculations with HITRAN-2k and PS databases is presented in Fig. 4*b*. The total difference in the surface flux is 6.2 W/m^2. This method of PSWL influence estimation is rather crude, as it is known that the PS database has on average more inaccurate values of line intensity and half-width than HITRAN (see Refs. 5 and 16) and so the differences cannot be uniquely attributed to the weak lines. However, such an approach is a useful first assessment.

b) HITRAN-2k – (HITRAN-2k + PSWL)

A separate database of the PSWL was created by removing HITRAN-2k lines from the PS database. The lines were compared by their quantum indices. For about 7 000 lines from the total 52 000 HITRAN-2k lines an equivalent quantum index could not be found among the PS database lines. We believe the errors and disagreements in the quantum indices in these two databases are responsible for that. Most of these lines (about 5 000) were identified with PS lines by simultaneous comparison of their center positions, intensities, and low level energy. About 2 000 of HITRAN-2k lines were left unrecognized and hence not removed from our weak line PS database.

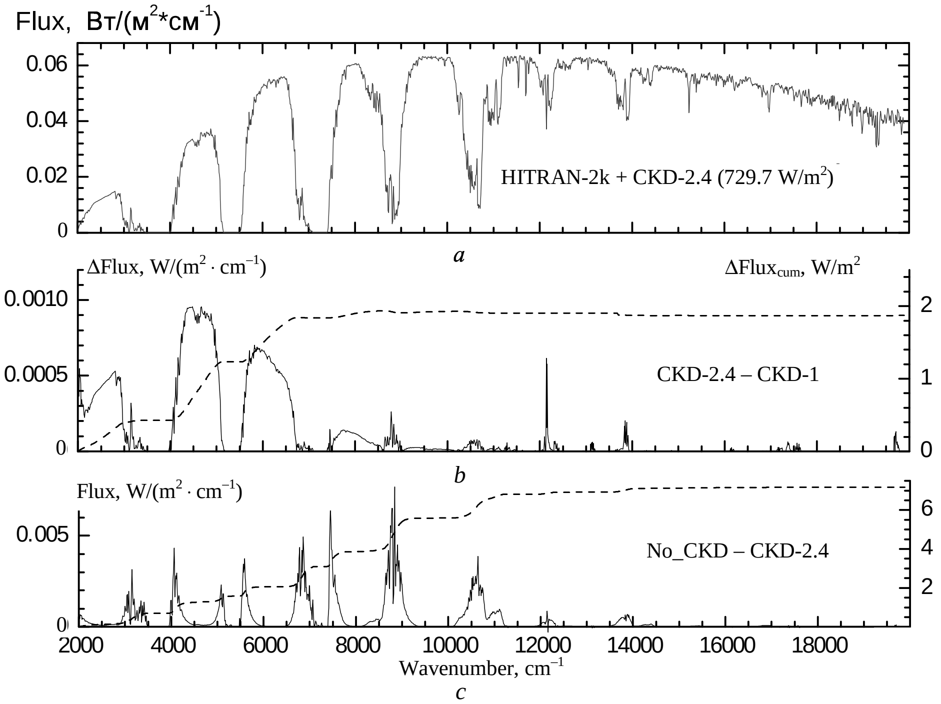

Fig. 3. Solar surface flux (*a*); the differential flux (ΔFlux) (solid line, left-hand axis) between the calculations using CKD2.4 and CKD1 continuum version (*b*) and for the case CKD2.4 versus calculation without continuum (No_CKD) (*c*). The dashed lines (right-hand axis) show the cumulative differential flux (W/m^2) integrated from 2000 cm^{-1}.

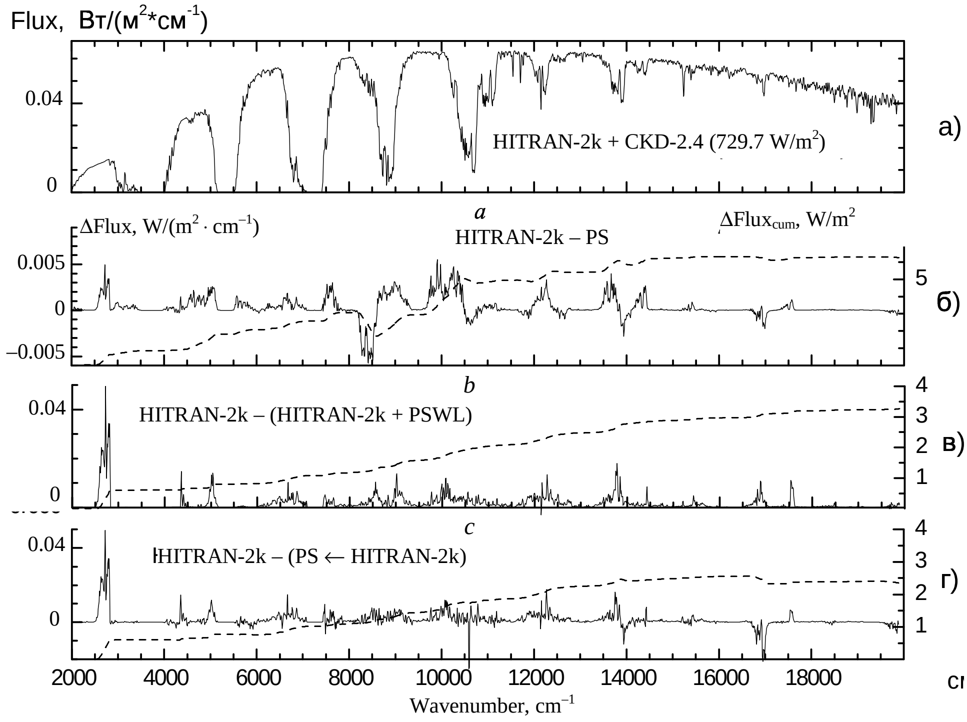

Fig. 4. The solar surface flux (*a*) and the differential flux (solid line, left-hand axis) between calculations using: HITRAN-2k and PS databases (*b*); HITRAN-2k and (HITRAN-2k + PSWL) (*c*); HITRAN-2k and (PS ← HITRAN-2k), where PS ← HITRAN-2k means PS database, in which each line is replaced by its HITRAN's equivalent if it has one (*d*). The dashed lines (right-hand axis) show the cumulative differential flux (W/m^2) integrated from 2000 cm^{-1}.

The influence of PSWL was estimated as a difference in the surface flux between calculation with HITRAN-2k and HITRAN-2k with the PSWL included. The calculated result is presented in Fig. 4*c*. The influence of PSWL reaches 3.3 W/m^2 in this approach. This should be a much more reliable approach for identifying the impact of weak lines than the approach in a).

c) HITRAN-2k – (PS ← HITRAN-2k)

To avoid/assess some possible overestimation of the PSWL influence caused by the HITRAN-2k lines that were left in our PSWL dataset in the previous case, a third approach was tried. The spectral difference in the surface fluxes between HITRAN-2k and (PS ← HITRAN-2k) dataset is presented in Fig. 4*d*. Here (PS ← HITRAN-2k) means the PS database, in which each line is replaced by its HITRAN equivalent if it has one. Hence, if both HITRAN and PS possess the same line but it is in a different position or has a different quantum index, such that the removal process in b) was unsuccessful, this approach will at least ensure that contributions of each of these lines is in both calculations and will at least partially compensate when the difference is taken. Although the spectral dependence of the PSWL influence may be less correct than in approach b), the cumulative extra flux should be more correct. The value of extra absorption 2.5 W/m^2 was found in this case. For a comparison, Zhong et al.[13] found a value of 2.1 W/m^2 for the same conditions as used here, relative to calculations using just HITRAN-96.

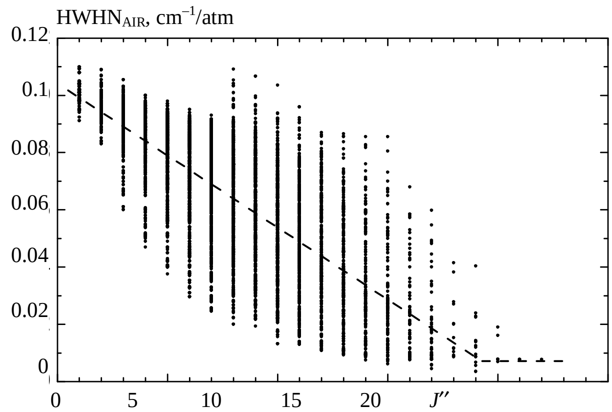

Fig. 5. The dependence of the air-broadened half-width of HITRAN-2k water vapor lines on the low level rotational index J''.

In all the calculations the air-broadened half-width (HWHM) of the PS lines was set according to the following empirical dependence:

$$\mathrm{HWHM} = 0.104 - 0.00457J'' \quad [\mathrm{cm^{-1}/atm}] \quad \text{for } J'' = 0\text{–}21,$$

$$\mathrm{HWHM} = 0.008 \quad [\mathrm{cm^{-1}/atm}] \quad \text{for } J'' > 21,$$

which corresponds on average to the mean dependence of HWHM on the low level rotational index J'' in HITRAN-2k (see the dashed line in Fig. 5). Each point in Fig. 5 corresponds to one HITRAN-2k spectral line. It was found that the impact of PSWL on flux calculations can depend markedly on the

HWHM values chosen for the PS lines. For example, setting the air-broadened half-width equal to 0.068 cm^{-1}/atm for all the PS lines (this value can be determined by averaging all the HITRAN-2k lines' half-widths) leads to up to 100% disagreement with the results of a) and c) assessments, although this does not affect the approach b).

Conclusions

In this work we have discussed the possible impact of the variety of the water vapor spectral databases and some CKD continuum models, existing at present time, on the accuracy of the solar fluxes calculation in the atmosphere. A summary is presented in Table 1.

Table 1. Differences in the solar surface flux (W/m^2) between results using various water vapor datasets in the 2 000–19 900 cm^{-1} region for SZA = 30° and MLS atmospheric profile

HITRAN databases:	
HITRAN-96 – HITRAN-2k	0.2
HITRAN-96 – HITRAN v.11	0.8
HITRAN-2k – HITRAN v.11	0.6
CKD continuum:	
CKD-2.4 – CKD-1	1.8
PSWL:	
HITRAN-2k – (HITRAN-2k + PSWL)	3.3
HITRAN-2k – (PS ← HITRAN-2k)	2.5
Total (maximum available)	~ 5.9

The maximum disagreement in the calculated solar surface flux due to all the investigated factors could reach 5.9 W/m^2 in the spectral region 2 000–19 900 cm^{-1} for the SZA = 30° and MLS atmospheric model (if a model was to use HITRAN-96, CKD-1 and ignore the weak lines, compared to a model using the most recent data, although the value is slightly smaller 5.1 W/m^2) using our best assessment of the impact of the weak lines. It is ~ 0.8% for the total downward solar flux at the surface (~ 729 W/m^2) and 3.3% for the total atmospheric absorption (~ 180 W/m^2) for the case presented here. The dominant cause of the extra absorption is the inclusion of the weak lines.

Acknowledgments

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