Sensitivity of near-infrared transmittance calculations for remote sensing applications to recent changes in spectroscopic information

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Abstract
An accurate determination of atmospheric transmittance relies greatly on the quality of both absorption line parameters and continuum absorption model. A line-by-line radiative transfer model has been used to determine the magnitude of the changes in atmospheric transmittance due to recent updates of HITRAN (High-resolution TRANsmission) line parameters and differences in water vapour continuum formulation. The radiative transfer calculations were carried out at two narrow near-infrared carbon dioxide bands near 4,854 cm$^{-1}$ (2.06 μm) and 6,211 cm$^{-1}$ (1.61 μm), which are currently used by satellite-based instruments for retrieval of atmospheric CO$_2$ concentrations. Transmittance calculations using line parameters from the last three HITRAN editions (2008, 2012 and 2016) show that HITRAN2016 is more similar to HITRAN2012 than HITRAN2008. However, differences of up to about 5% were obtained between transmittances computed using HITRAN2016 and HITRAN2012. Considering the fact that some groups still use HITRAN2012 in forward models for very high (sub percent) accuracy retrievals of CO$_2$ from satellite measurements, these differences are significant and should be accounted for in the uncertainty budget. Transmittances calculated using the semi-empirical MT_CKD 2.5 (Mlawer–Tobin–Clough–Kneizys–Davies) and the laboratory-measured CAVIAR (Continuum Absorption at Visible and Infrared Wavelengths and its Atmospheric Relevance) water vapour continuum models differ by up to about 5–6%. The impact of the continuum formulation adopted for near-infrared transmittance calculations needs to be quantitatively assessed, most especially as the strength of the water vapour continuum in this spectral region is still contested.

KEYWORDS
absorption line parameters, atmospheric transmittance, continuum absorption, near-infrared, remote sensing
1 | INTRODUCTION

Atmospheric transmittance in the near-infrared (near-IR) region is an important physical parameter that must be determined in remote sensing applications such as measurements of vertical columns of atmospheric gases from space using reflected shortwave radiation (e.g., Kuang et al., 2002; Buchwitz et al., 2005; Kuze et al., 2009; Guerlet et al., 2013; Eldering et al., 2017). The importance of atmospheric transmittance is due to the fact that the atmosphere attenuates shortwave radiation passing through it. For clear-sky conditions, and in the near-IR, this attenuation is mainly through absorption by the atmospheric gases such as water vapour, carbon dioxide and methane. Therefore, determining the atmospheric transmittance with a high degree of precision is crucial for accurate and precise retrievals of atmospheric gases from high-spectral resolution clear-sky space soundings, such as, those from the Greenhouse Gases Observatory Satellite (GOSAT) (Kuze et al., 2009) and Orbiting Carbon Observatory-2 (OCO-2) (Eldering et al., 2017) missions.

High accuracy atmospheric transmittance under clear-sky conditions is usually determined through simulation using line-by-line (LBL) radiative transfer models (or codes). However, these modelled transmittances are subjected to a number of uncertainties. Some uncertainties which may lead to errors in these modelled transmittances (and by extension errors in the retrieved atmospheric gases from satellite data) include: uncertainty of the spectroscopic absorption line parameters (such as line strengths, positions and widths) used for LBL calculations (e.g., Dai et al., 2012a), continuum absorption model (e.g., O’Dell et al., 2018), effect of line mixing (e.g., Hartmann et al., 2009) and model of absorption line shape used during the LBL calculations (e.g., Thompson et al., 2012). This work will focus only on the uncertainties of spectroscopic absorption line parameters and continuum absorption. The effects of uncertainties in spectroscopic line parameters and continuum absorption on LBL calculations of transmittances are usually studied by comparing results obtained using different spectroscopic databases and continuum models respectively.

The HITRAN (High-resolution TRANsmission) database, which is the most widely-used source of spectroscopic line parameters for radiative transfer calculations in remote sensing applications, is officially updated at periodic intervals of 4 years (Rothman, 2010; Gordon et al., 2017). Each HITRAN update usually leads to an increase in the number of spectral lines and accuracy of line parameters with respect to its previous version because of improvements in both theoretical and experimental spectroscopy (e.g., Gordon et al., 2017). Despite these regular updates, very little attention has been paid to the effects of these updates on transmittance calculations in the near-IR. Feng and Zhao (2009) studied the effects of upgrades in HITRAN line parameters from the 2000 version to the 2004 version on LBL calculations of atmospheric transmittance in the near-IR from 4,200 to 10,000 cm$^{-1}$ for two standard atmospheres (tropical and sub-arctic winter atmospheres) at different spectral resolutions. Six absorbing species (H$_2$O, CO$_2$, O$_3$, N$_2$O, CO and CH$_4$) were considered in their calculations but the effect of continuum absorption was ignored. Their study showed that an update of the 2000 version of HITRAN led to significant differences in calculated transmittances, especially for the tropical atmosphere. These differences were mainly attributed to changes in line parameters of H$_2$O, CO$_2$ and CH$_4$. Dai et al. (2012a, 2012b) investigated the effect of the modification of the line parameters from the 2004 edition to the 2008 edition of HITRAN on the retrieval of CO$_2$ in some near-IR spectral regions and the calculations of transmittance. Dai et al. (2012a, 2012b) also found out that an improvement in HITRAN line parameters (mainly the CO$_2$ line parameters) from 2004 to 2008 led to significant increases in calculated transmittance (and retrieved CO$_2$). Since 2008, HITRAN has officially been updated twice (in 2012 and 2016), but there is no record in the literature where the effects of these updates on transmittance calculations have been investigated. With each update in HITRAN, it is important to examine how it impacts transmittance modelling as it will assist in the quantification of uncertainties in retrieved atmospheric gases (and other properties) from satellite data (e.g., concentrations of CO$_2$ from GOSAT and OCO-2 satellites).

Both line and continuum absorptions are important for transmittance calculations in remote sensing applications. However, the water vapour continuum (and continua of other gases), is not yet available in these spectroscopic databases (e.g., Shine et al., 2016). Due to this shortcoming, the semi-empirically derived MT_CKD (Clough–Tobin–Clough–Kneizys–Davies) water vapour continuum model (Clough et al., 2005; Clough et al., 2012) is widely employed in radiative transfer models for remote sensing applications in the near-IR (e.g., O’Dell et al., 2018). It should be noted that the MT_CKD also includes the continua model of several gases such as CO$_2$, O$_3$ and O$_2$. There have been unofficial updates of the MT_CKD 2.5 continuum (Lechevallier et al., 2018; O’Dell et al., 2018), but these revisions have not been carried out using adequate experimental constraints. Thus, currently there is no consensus on the strength of the MT_CKD 2.5 continuum in some near-IR windows. A good number of measurements in the near-IR have pointed out that the MT_CKD 2.5 continuum may be underestimating the strength of the water vapour continuum in some spectral windows (e.g., Ptashnik et al., 2011, 2012; Baranov and Lafferty, 2012; Mondelain et al., 2013; Campargue et al., 2016; Reichert and Sussmann, 2016; Lechevallier et al., 2018). Although these measurements do not agree on how
big this underestimation is, the differences are more important for remote sensing techniques that use these windows for retrieval. This is because in atmospheric windows, continuum absorption is usually stronger than absorption due to individual spectral lines, especially under clear-sky conditions (Shine et al., 2012).

Unlike most of the reported near-IR measurements, which were mostly dedicated to validating the MT_CKD continuum model (see, for example, Lechevallier et al., 2018, and references therein), Ptashnik et al. (2011, 2012) used high-resolution laboratory measurements to derive the CAVIAR (Continuum Absorption at Visible and Infrared Wavelengths and its Atmospheric Relevance) water vapour continuum model that can be used at all wavelengths in the near-IR. The CAVIAR continuum is significantly stronger than the MT_CKD 2.5 continuum in most windows of this spectral region. The effect of this strengthened water vapour continuum on the calculation of atmospheric transmittance has not been studied. However, some limited studies have been carried out to examine the consequences of different water vapour continuum models on remote sensing techniques in general. Shine et al. (2012) showed that using the CAVIAR continuum in a narrow-band radiative transfer model leads to a significant modification of the cloud droplets sizes in the 2.1 μm window, compared to the MT_CKD 2.5 continuum. This modification may lead to bias in cloud properties retrieved from spaced-based instruments that use this window. The recent study by O’Dell et al. (2018) briefly examined the effect of different versions of the MT_CKD continuum models on the retrieval of atmospheric CO2. O’Dell et al. (2018) found out that compared to an older version, incorporating a recent version of the MT_CKD continuum into their forward model leads to negligible changes in retrieved column-averaged atmospheric CO2 from the OCO-2 satellite. A limitation of this work is that it does not examine the effect of using continuum models from other sources.

This work is aimed, firstly, at determining the magnitude of the changes in LBL calculated near-IR atmospheric transmittance that result from using the three recent editions of HITRAN (i.e., the 2008, 2012 and 2016 editions). Secondly, the effect of the differences between the strengths of the MT_CKD 2.5 and CAVIAR water vapour continua in the near-IR on the LBL calculations of transmittance will also be examined. Results from this work are expected to assist those using satellite measurements in the near-IR for retrieval of atmospheric gases understand the consequences of their choice of HITRAN version and the continuum model.

The rest of this paper is organized in the following order: Section 2 will present an outline of the radiative transfer calculations. The findings from this work are discussed in Section 3 and Section 4 concludes the paper.

2 | RADIATIVE TRANSFER CALCULATIONS

In this study, the Mitsel et al. (1995) LBL radiative transfer model was used to calculate the atmospheric transmittance in the near-IR region from 4,000 to 10,000 cm$^{-1}$ at a very high-spectral resolution of 0.002 cm$^{-1}$. These modelled transmittances were then averaged over 0.2 cm$^{-1}$ in order for their resolutions to be comparable to the resolutions of space-based spectrometers for measuring atmospheric gases such as that on the GOSAT mission (Kuze et al., 2009). The Voigt line shape with a line cut-off at 25 cm$^{-1}$ from the line centre is used by this model. The Mitsel et al. (1995) model allows the addition of either the MT_CKD or CAVIAR continuum model during the calculations. Both continuum models are derived using the CKD-defined approach (i.e., subtraction of the local lines contribution calculated from the centres out to 25 cm$^{-1}$; Clough et al., 1989). Additionally, the effect of line mixing is not accounted for by this LBL model.

The model tropical (TROP) and sub-arctic winter (SAW) atmospheres, each with 50 vertical levels, were used for these clear-sky calculations (Anderson et al., 1986). The zenith angle of 30° was used for the transmittance calculations. The albedo of the Earth’s surface and Rayleigh scattering were ignored in these calculations. The absorbing gases considered for these calculations are: H$_2$O, CO$_2$, O$_3$, N$_2$O, CO, CH$_4$, and O$_3$. The absorption line parameters for these gases were obtained in turn from HITRAN2008 (Rothman et al., 2009), HITRAN2012 (Rothman et al., 2013) and HITRAN2016 (Gordon et al., 2017). All HITRAN2016 updates available when this study was carried out are included in the model calculations. The effect of continuum absorption was accounted for by using the MT_CKD 2.5 continua for H$_2$O, CO$_2$, O$_3$, and O$_3$. Combining the MT_CKD 2.5 continuum, whose coefficients were calculated using an earlier HITRAN edition, with recent HITRAN editions in the calculations does not affect the results presented here. This is because only relatively strong lines may contribute to the continuum retrieval in microwindows between lines. And the relevant absorption line parameters (e.g., line intensities and half-widths) for LBL calculations of all those lines are known with rather good accuracy and have not changed very much in the last 10 years.

In order to study the effects of the differences in the strength of the water vapour continuum on modelled atmospheric transmittances, some of the calculations were repeated but with the MT_CKD 2.5 H$_2$O continuum replaced by the CAVIAR H$_2$O continuum. In this case, HITRAN2016 was chosen as the only source of the absorption line parameters. All other input into the calculations were the same as described in the preceding paragraph. Note that the MT_CKD 2.5 and CAVIAR continua models
differ only in the water vapour continuum as the MT_CKD 2.5 continua for CO$_2$, O$_3$ and O$_2$ have been incorporated into the CAVIAR continuum model.

### RESULTS AND DISCUSSION

The calculations were carried from 4,000 to 10,000 cm$^{-1}$ (2.5–1.0 μm) but for the sake of brevity, the transmittances are only presented in the two narrow CO$_2$ bands near 4,854 cm$^{-1}$ (2.06 μm) and 6,211 cm$^{-1}$ (1.61 μm) that are currently exploited by the GOSAT and OCO-2 satellites to retrieve the atmospheric concentrations of CO$_2$ (and other gases such as CH$_4$) (Kuze et al., 2009; Eldering et al., 2017; Kataoka et al., 2017). Thus, the results will be presented in the strong CO$_2$ band from 4,800 to 4,895 cm$^{-1}$ (2.0431–2.0834 μm) and weak CO$_2$ band from 6,160 to 6,280 cm$^{-1}$ (1.5906–1.6218 μm).

#### 3.1 Effects of changes in HITRAN database

Figure 1 shows the transmittances over the spectral region 4,800–4,895 cm$^{-1}$ for both the TROP (top left) and SAW (top right) atmospheres computed using line parameters from HITRAN2016. The lower panels of this figure show the relative differences, with respect to HITRAN2016, between the transmittance calculated using the other two editions of HITRAN for TROP (left column) and SAW (right column).

Figure 1 shows that in the CO$_2$ band from 4,800 to 4,895 cm$^{-1}$, the TROP atmosphere is slightly more absorbing than the SAW atmosphere. This is due to the contribution from H$_2$O, whose concentration is higher in the tropics. This figure shows that the relative differences between the transmittances calculated using HITRAN2016 and HITRAN2012 are lower than those between HITRAN2016 and HITRAN2008 for both atmospheres. These results are expected if the HITRAN database is converging towards the truth. The TROP atmosphere is more sensitive to improvements in HITRAN line parameters than the SAW atmosphere (see Figure 1). It can be observed from Figure 1 that the fractional differences are generally higher for the TROP atmosphere than for the SAW atmosphere. For the TROP atmosphere, the relative differences on average are about 0.5% between transmittances calculated using HITRAN2016 and HITRAN2012 and about 1% between HITRAN2016 and HITRAN2008. However, at some wavenumbers, these differences are, respectively, up to about 5% and about 10%.

**FIGURE 1** Simulated atmospheric transmittances from 4,800 to 4,895 cm$^{-1}$ using HITRAN2016 database for the tropical (top left) and subarctic winter (top right) atmospheres. The curves in the lower panels represent the relative differences between the transmittances ($\Delta$transmittance) calculated using HITRAN2016 and HITRAN2012 (middle panels) and HITRAN2016 and HITRAN2008 (bottom panels) for the atmosphere indicated in the top panel of each column. The MT_CKD 2.5 continua and zenith angle of 30° were used for these calculations.
(see Figure 1 middle and bottom left). The average relative difference for the SAW atmosphere is about 0.2% between the modelled transmittances using HITRAN2016 and HITRAN2012 and about 0.4% between HITRAN2016 and HITRAN2008. The maximum relative differences for this atmosphere are, respectively, about 1% and 4% as Figure 1 (middle and bottom right) shows.

Thus, with reference to HITRAN2016, successive increase in the accuracy of HITRAN line parameters (of mostly CO$_2$ and H$_2$O in this band) since 2008 significantly improved the accuracy of modelled transmittances. However, the maximal relative differences between computed transmittances using HITRAN2016 and HITRAN2012 are significant considering the fact that retrievals of CO$_2$ concentrations in this band from satellite measurements are expected at precisions of less than 1% (e.g., Hartmann et al., 2009). HITRAN2016 should therefore be used for remote sensing applications in this band in order to increase the accuracy of the retrievals. However, it is recommended that these discrepancies be accounted for in the uncertainty budget if HITRAN2012 (or HITRAN2008) line parameters are used in forward models in satellite retrievals (see, for example, O’Dell et al., 2018). Other uncertainties such as those in HITRAN2016 line parameters and those due to instrument calibration will also need to be taken in consideration during the retrievals.

The modelled transmittances in the weak CO$_2$ band from about 6,160 to 6,280 cm$^{-1}$ for both the TROP (top, left) and SAW (top, right) atmospheres using line parameters from HITRAN2016 are shown in Figure 2.

As was the case from 4,800 to 4,895 cm$^{-1}$, Figure 2 (top panels) shows that the TROP atmosphere is also slightly more absorbing than the SAW atmosphere in this band. The middle and bottom panels of Figure 2 show that in this spectral region, both the TROP and SAW atmospheres are not very sensitive to improvements in HITRAN line parameters. However, the relative differences between the modelled transmittances using HITRAN2016 and HITRAN2012 are slightly lower than those using HITRAN2016 and HITRAN2008 at some wavenumbers for both atmospheres (e.g., at approximately 6,250.5 cm$^{-1}$ for TROP profile and from 6,160 to 6,200 cm$^{-1}$ for SAW profile). In this spectral region the fractional differences are also generally higher for the TROP atmosphere than the SAW atmosphere. For the TROP atmosphere, the average relative difference in the calculated transmittances using HITRAN2016 and both HITRAN2012 and HITRAN2008 is less than 0.1%. However, for this atmosphere relative differences of up to about 2% were obtained at some wavenumbers.

**FIGURE 2** Simulated atmospheric transmittances from 6,160 to 6,280 cm$^{-1}$ using HITRAN2016 database for the tropical (top left) and sub-arctic winter (top right) atmospheres. The curves in the lower panels represent the relative differences between the transmittances ($\Delta$transmittance) calculated using HITRAN2016 and HITRAN2012 (middle panels) and HITRAN2016 and HITRAN2008 (bottom panels) for the atmosphere indicated in the top panel of each column. The MT_CKD 2.5 continua and zenith angle of 30° were used for these calculations.
(see Figure 2 middle and bottom left). For the SAW atmosphere, the average relative difference is of the order of 0.05% between the modelled transmittances using HITRAN2016 and both the other two editions of HITRAN, with the maximum relative differences of about 0.3% (see Figure 2 middle and bottom right).

The higher accuracy of the line parameters (principally CO2 and H2O lines) for each HITRAN update over the last 10 years in this weak CO2 band (6160–6,280 cm\(^{-1}\)) has also improved the accuracy of modelled transmittances. However, compared to the relatively strong CO2 band (4800–4,895 cm\(^{-1}\)) discussed above, these improvements are moderate. With respect to HITRAN2016, the fractional differences in transmittance calculations due to changes in the HITRAN line parameters in this band generally fall within the expected uncertainties of retrieved CO2 concentrations from GOSAT and OCO-2 satellite measurements (e.g., O’Dell et al., 2018). That notwithstanding, the latest edition of HITRAN should be employed in satellite retrieval algorithms for increased accuracy. If either HITRAN2012 or HITRAN2008 database is used in radiative transfer models in high-precision satellite retrievals in this band, then uncertainties in the choice of the HITRAN database should be accounted for, especially for the TROP atmosphere where these differences are comparatively significant (~1.5%) at some wavenumbers. In these retrievals, it is also important to account for the uncertainties in the HITRAN2016 spectroscopic parameters and other uncertainties (e.g., those from instrument calibration).

### 3.2 Effects of changes in water vapour continuum model

Figure 3 and Figure 4 show the transmittances over the spectral regions 4,800–4,895 cm\(^{-1}\) and 6,160–6,280 cm\(^{-1}\), respectively for both the TROP (top left) and SAW (top right) atmospheres using the MT_CKD 2.5 (red) and CAVIAR (blue) H\(_2\)O continuum. As stated in Section 2 the absorption line parameters were taken from HITRAN2016 in this case. The bottom panels of each figure show the fractional differences between the transmittances calculated using the MT_CKD 2.5 and CAVIAR H\(_2\)O continuum models for TROP (bottom left) and SAW (bottom right).

Figure 3 and Figure 4 (top panels) show that the transmittances calculated using CAVIAR H\(_2\)O continuum is lower than those calculated using the MT_CKD 2.5 H\(_2\)O continuum for both atmospheres. This is obviously due to the fact that the CAVIAR H\(_2\)O continuum is

![FIGURE 3 Modelled atmospheric transmittances from 4,800 to 4,895 cm\(^{-1}\) using MT_CKD 2.5 (red) and CAVIAR (blue) H\(_2\)O continuum for the tropical (top left) and sub-arctic winter (top right) atmospheres. The bottom panels represent the relative differences between transmittances (\(\Delta\)transmittance) computed using the two continuum models for the tropical (bottom left) and sub-arctic winter (bottom right) atmospheres. HITRAN2016 line parameters and zenith angle of 30° were used for these calculations]
stronger than the MT_CKD 2.5 H₂O continuum as discussed in Section 1. However, these differences are relatively bigger for the TROP atmosphere than the SAW atmosphere in both spectral regions. From 4,800 to 4,895 cm⁻¹, the fractional differences in the calculated transmittances using these two H₂O continuum models are about 5–6% for the TROP atmosphere and less than 0.4% for SAW atmosphere (see Figure 3, bottom panels). On the other hand, in the weak CO₂ band from 6,160–6,280 cm⁻¹, these differences are less than 0.5% for TROP atmosphere and less than 0.05% for SAW as Figure 4 (bottom panels) shows.

These results indicate that for a TROP atmosphere, differences in the near-IR water vapour continuum formulation may introduce significant uncertainties in the modelled transmittances. This will in turn have a significant impact on the accuracy of the retrieved CO₂ concentrations over the spectral region from 4,800 to 4,895 cm⁻¹.

4 | CONCLUSIONS

The effects of the recent modifications of HITRAN line parameters and differences in H₂O continuum formulation on near-IR transmittance calculations have been studied for two CO₂ bands of GOSAT and OCO-2 missions (from 4,800 to 4,895 cm⁻¹ and 6,160 to 6,280 cm⁻¹). These radiative transfer calculations were carried out for the tropical and sub-arctic winter atmospheres.

There is a better agreement between the transmittances calculated using HITRAN2016 and HITRAN2012 than between those calculated using HITRAN2016 and HITRAN2008 for both atmospheres. This shows a good convergence in HITRAN database as expected. The maximal relative differences between computed transmittances using HITRAN2016 and HITRAN2012 are about 5% and 1% for the tropical and sub-arctic winter atmospheres, respectively. These differences are in the strong CO₂ band from 4,800 to 4,895 cm⁻¹. Forward models for retrieving CO₂ concentrations from satellite measurements at sub percent accuracy that have been developed using HITRAN2012 (e.g., O’Dell et al., 2018) will need to account for these differences in the uncertainty budgets.

The differences between the calculated transmittances using the CAVIAR H₂O continuum and the widely-used MT_CKD 2.5 H₂O continuum are modest (<0.5%), except for the TROP atmosphere at the strong CO₂ band where the fractional difference is relatively large (5–6%). Although there is still some controversy surrounding the strength of the water vapour continuum in the near-IR, this difference is significant compared to the expected accuracy (<1%) of retrieved CO₂ concentrations from the GOSAT and OCO-2

FIGURE 4  Modelled atmospheric transmittances from 6,160 to 6,280 cm⁻¹ using MT_CKD 2.5 (red) and CAVIAR (blue) H₂O continuum for the tropical (top left) and sub-arctic winter (top right) atmospheres. The bottom panels represent the relative differences between transmittances (Δtransmittance) computed using the two continuum models for the tropical (bottom left) and sub-arctic winter (bottom right) atmospheres. HITRAN2016 line parameters and zenith angle of 30° were used for these calculations.
missions. There is therefore the need to further evaluate the MT_CKD 2.5 water vapour continuum model that is usually adopted for transmittance calculations in high-precision remote sensing applications in the near-IR. In order to validate the water vapour continuum absorption in the near-IR spectral region, it is essential to carry out a radiative closure experiment, such as those performed by, for example, Mlawer et al. (2019) and Liuzzi et al. (2014) at far-infrared wavelengths.

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CONFLICT OF INTEREST
The authors declare no potential conflict of interest.

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