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Evaluation of spectroscopic databases through radiative transfer simulations compared to observations. Application to the validation of GEISA 2015 with IASI and TCCON

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ABSTRACT

The quality of spectroscopic parameters that serve as input to forward radiative transfer models are essential to fully exploit remote sensing of Earth atmosphere. However, the process of updating spectroscopic databases in order to provide the users with a database that insures an optimal characterization of spectral properties of molecular absorption for radiative transfer modeling is challenging. The evaluation of the databases content and the underlying choices made by the managing team is thus a crucial step. Here, we introduce an original and powerful approach for evaluating spectroscopic parameters: the Spectroscopic Parameters And Radiative Transfer Evaluation (SPARTE) chain. The SPARTE chain relies on the comparison between forward radiative transfer simulations made by the 4A radiative transfer model and observations of spectra made from various observations collocated over several thousands of well-characterized atmospheric situations. Averaging the resulting 'calculated-observed spectral' residuals minimizes the random errors coming from both the radiometric noise of the instruments and the imperfect description of the atmospheric state. The SPARTE chain can be used to evaluate any spectroscopic databases, from the visible to the microwave, using any type of remote sensing observations (ground-based, airborne or space-borne). We show that the comparison of the shape of the residuals enables: (i) identifying incorrect line parameters (line position, intensity, width, pressure shift, etc.), even for molecules for which interferences between the lines have to be taken into account; (ii) proposing revised values, in cooperation with contributing teams; and (iii) validating the final updated parameters. In particular, we show that the simultaneous availability of two databases such as GEISA and HITRAN helps identifying remaining issues in each database. The SPARTE chain has been here applied to the validation of the update of GEISA-2015 in 2 spectral regions of particular interest for several currently exploited or planned Earth space missions: the thermal infrared domain and the short-wave infrared domain, for which observations from the space-borne IASI instrument and from the ground-based FTS instruments at the Parkfalls TCCON site are used respectively. Main results include: (i) the validation of the positions and intensities of line parameters, with overall significantly lower residuals for GEISA-2015 than for GEISA-2011 and (iii) the validation of the choice made on the parameters (such as pressure shift and air-broadened width) which has not been given by the provider but completed by ourselves. For example, comparisons between residuals obtained with GEISA-2015 and HITRAN-2012 have highlighted a specific issue with some HWHM values in the latter that can be clearly identified on the 'calculated-observed' residuals.

1. Introduction

Remote sensing of Earth atmosphere from space heavily relies on the quality of spectroscopic parameters involved as input to the forward Radiative Transfer Models (RTMs) used to calculate the top of the atmosphere radiance spectra. The general principle of the inversion process, which aims at interpreting the observed spectra of radiances in terms of geophysical variables (such as vertical distribution of temperature, humidity, gas concentrations, clouds, and surface characteristics), consists in minimizing residuals between radiances spectra actually measured by the instrument at

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any given time and location and simulated spectra generated by RTMs from an initial guess of the atmospheric state vector. Over the years, studies relying on various inverse approaches, such as Bayesian or neural network (e.g. [3,4,8]) have highlighted that errors in the spectroscopic parameters used in the forward RTMs could introduce spatially, temporally, or even altitude-dependent biases in the retrievals. The accuracy of the retrieved geophysical fields thus ultimately depends on the accuracy of the forward model used and on the quality of the under-lying spectroscopy. Reducing the uncertainties in our knowledge of spectroscopic line parameters and continuum absorption is thus important to improve the application of satellite data to weather forecasting, atmospheric composition and climate studies. This also applies to remote sensing from airborne platforms and from the ground.

Spectroscopic parameters used as inputs to RTMs usually come from spectroscopic databases, which provide information on spectral properties of various molecular species: (i) parameters for the molecules having an absorption which can be described in terms of line spectrum (CO_2, H_2O, O_3, CH_4, N_2O, CO, etc.); (ii) far wing absorption and continuum data for H_2O, N_2, O_2, etc.; (iii) far wing absorption and line interference effects data for CO_2 or CH_4; (iv) cross-section parameters for heavy molecules (such as CFCs). The present status of the spectroscopic databases is the result of numerous studies performed during the last 50 years in several dedicated spectroscopic laboratories all over the world. International cooperation contributed to the establishment of widely used spectroscopic databases for atmospheric applications, such as: HITRAN (http://hitran.org; see [19] for its latest version HITRAN-2012) and GEISA (http://www.pole-ether.fr/geisa/; see [12], this issue for its latest version GEISA-2015). The evaluation of existing spectroscopic databases and their update with the latest spectroscopic data requires a continuing effort. In particular, the validation of the spectroscopic parameters in the most extended range of temperature, pressure and absorber amounts appropriate to the specifications of existing or forthcoming instruments is essential to fully exploit their observing capabilities.

The role of molecular spectroscopy in modern atmospheric research has indeed entered a new phase with the advent of highly sophisticated spectroscopic instruments and computers. The launch of high spectral resolution vertical infrared sounders like the Atmospheric Infrared Sounder (AIRS, Aumann et al., 2003; http://airs.jpl.nasa.gov/) on board NASA/Aqua satellite since May 2002, or the Infrared Atmospheric Sounding Interferometer (IASI, Chalon et al., 2001; https://iasi.cnes.fr/) on board the European polar satellites Metop since October 2006, have opened new perspectives for remote sensing applications, for numerical weather prediction, atmospheric composition and climate studies. The launches of the Thermal And Near infrared Sensor for carbon Observation (TANSO) onboard JAXA Greenhouse Gases Observing Satellite (GOSAT, Yokota et al., 2009; http://www.gosat.nies.go.jp/en/) in January 2009 and NASA Orbiting Carbon Observatory (OCO-2, Crisp et al., 2004; http://oco.jpl.nasa.gov/) in February 2014 have called for the need of improved spectroscopic parameters in the short-wave absorption bands of carbon dioxide (CO_2), methane (CH_4) and oxygen (O_2). Moreover, the need to improve and consolidate the spectroscopic parameters and the RTMs that use them will become a priority in order to exploit the increased spectral resolution and radiometric accuracy of new atmospheric instruments like IASI-New Generation (IASI-NG), which has been designed to improve by a factor of 2 the spectral resolution and a factor 2 to 4 the radiometric characteristics as compared to IASI [7]; https://iasi-ng.cnes.fr).

Several studies have focused on the evaluation of the quality of spectroscopic databases by studying the impact of updated spectroscopy on the estimation of various geophysical parameters from remote sensing observation. For instance, Frankenberg et al. [9] identified an error in the methane column retrieved from near-infrared spectra recorded by the SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY (SCIAMACHY) instrument onboard ENVISAT related to inaccuracies in water vapor spectroscopic parameters. This error resulted in a positive correlation of retrieved methane with water vapor abundances and thereby led to a systematic overestimation of tropical methane abundances. Updating the water spectroscopy largely eliminated this dependence. Scheepmaker et al. [21] further evaluated an improved water spectroscopy in the range 4174–4300 cm^{-1}, a region where the spectroscopy of water lines remains a large source of uncertainty, in order to reduce systematic uncertainties observed in the SCIAMACHY retrievals of HDO/H_2O. Similarly, Alvarado et al. [2] evaluated updated spectroscopic parameters for methane (CH_4), water vapor (H_2O) and nitrous oxide (N_2O) by performing thermal infrared retrievals of methane from the NASA Aura Tropospheric Emission Spectrometer (TES) and comparing the bias of the retrieved values when compared to in-situ measurements. Alvarado et al. [1] implemented a validation of spectroscopy by comparing a global dataset of 120 near-nadir, over-ocean, night-time spectra from IASI to calculations from two versions of the RTM (update or previous version of the spectroscopic database) to determine the impact of spectroscopic updates to the model on spectral residuals as well as retrieved temperature and H_2O profiles. Although efficient in detecting potential issues with spectroscopy of the targeted atmospheric variables, these studies were all based on an *a posteriori* evaluation consisting in evaluating the impact of updated spectroscopy on the retrieved geophysical variables. Several issues limit the use of this kind of approach for validating spectroscopic databases: (i) they rely on the existence of a retrieval or assimilation scheme used to interpret the measured radiances in terms of geophysical variables; (ii) they require the availability of a validation dataset for the targeted geophysical variables; and (iii) they are limited to the specific spectral domains used in the retrieval schemes.

This paper aims at introducing an original and powerful approach for evaluating spectroscopy: the Spectroscopic Parameters And Radiative Transfer Evaluation (SPARTE) chain. The SPARTE chain relies on the comparison, throughout the whole spectrum, between forward radiative transfer simulations and observations of spectra made from various instruments, both collocated over several thousands of well-characterized atmospheric situations. Considering that observed spectra come from instruments characterized by high radiometric and spectral stabilities, each individual residual can be affected by two kinds of errors: (i) a random error due to the imperfect description of the atmospheric state or to instrumental noise; (ii) systematic errors more related to the spectral line calculation (spectroscopic parameters, line shape, line mixing, continua, etc.). Averaging the residuals leads to minimizing the random errors to highlight more systematic error due to spectroscopic parameters. This chain is built on the long-term involvement of Laboratoire de Météorologie Dynamique (LMD) in: (i) developing and maintaining the spectroscopic database GEISA; (ii) developing and maintaining forward RTMs and (iii) performing calibration/validation activities of several Earth Observation space missions. Although the SPARTE chain can be used to evaluate spectroscopy from any spectroscopic databases, from the visible to the microwave, taking into account or not the cross-sections or the diffusion by the aerosols, this paper will focus only on the validation of the line parameters sub-databases, for two spectral regions of particular interest for several currently exploited or planned space missions: the thermal infrared domain and the short-wave infrared domain, for which observations from the space-borne IASI instrument and from the ground-based Fourier Transform Spectrometer (FTS) instruments at the Parkfalls Total Carbon Column Observing Network (TCCON) site will be used respectively.