# Sensitivity of microwave downwelling brightness temperatures to spectroscopic parameter uncertainty

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## Abstract

Atmospheric brightness temperatures are simulated through radiative transfer calculations, which rely on spectroscopic parameters for modelling the atmospheric absorption. The uncertainty affecting the spectroscopic parameters contribute to the uncertainty of the simulated brightness temperatures and to the accuracy of atmospheric retrievals obtained with physical approaches (e.g. 1DVAR).

This paper describes the approach to investigate the impact of spectroscopic parameter uncertainties on simulated downwelling microwave brightness temperatures in the 20-60 GHz range. Sensitivities are computed perturbing each parameter individually and considering six different atmospheric climatologies, for the purpose of identifying the parameters with significant impact. Preliminary results are presented, as well as the approach to map the resulting brightness temperatures' uncertainty on the retrieved atmospheric profile space using the full covariance matrices of uncertainties. The analysis can also be extended to higher frequencies and upwelling brightness temperatures in future work.

## Introduction

Atmospheric absorption models are used to simulate the absorption/emission of electromagnetic radiation by atmospheric constituents. Atmospheric absorption models are thus crucial to compute the radiative transfer through the atmosphere, which is needed to simulate and validate passive remote sensing observations, as from microwave radiometer (MWR). Absorption and radiative transfer models, representing the forward operator for atmospheric radiometric applications, are also exploited in physical approaches for the solution of the inverse problem, i.e. the retrieval of atmospheric parameters from remote sensing radiometric observations.

Absorption models are based on quantum-mechanics theory and rely on parametrized equations to compute the atmospheric absorption given the thermodynamic conditions and the abundance of constituents (Rosenkranz, 1993). The spectroscopic parameters entering the parametrized equations are determined through theoretical calculations or laboratory and field measurements, and their values are continuously refined. The uncertainty affecting spectroscopic parameters contributes to the uncertainty of simulated remote sensing observations, and consequently to the uncertainty of remote sensing retrievals of atmospheric thermodynamic and composition profiles (Verdes et al., 2005). In addition, it must be considered that the uncertainty affecting different spectroscopic parameters may be correlated. Therefore, the full uncertainty covariance matrix should be estimated to evaluate the impact on radiative transfer calculations and retrievals (Boukabara et al., 2005; Rosenkranz, 2005).

Here, we present the approach to evaluate the impact of spectroscopic parameters on the simulated brightness temperatures ($T_B$) and the atmospheric profile retrieval from a ground-based MWR. Focusing primarily on clear sky retrievals, the main constituents contributing to atmospheric microwave absorption in the 20-60 GHz range are water vapor and oxygen. Thus, the following approach is used:

(i) review the uncertainty of water vapor and oxygen spectroscopic parameters;

(ii) investigate the dominant uncertainty contributions through a radiative transfer sensitivity study;

(iii) estimate the full uncertainty covariance matrix for the dominant parameters;

(iv) propagate the uncertainty covariance matrix to estimate the impact on MWR simulated observations and atmospheric retrievals.

For this analysis we use a recent update of the Millimeter-wave Propagation Model (MPM), called hereafter R17 (Rosenkranz, 2017). More details on the theory of the microwave absorption by atmospheric gases are given by Rosenkranz (1993).

**Table 1:** List of water-vapor parameters perturbed in the sensitivity analysis.

| Symbol [units] | Parameter | Value | Uncertainty | Reference |
|---|---|---|---|---|
| $\nu_i$ | Resonant line frequency at 22 GHz | 22235079.85 | 0.05 | Kukolich 1969 |
| [kHz] | at 183 GHz | 183310087 | 1 | Golubiatnikov et al. 2006 |
| $S_i$ | Resonant line intensity at 22 GHz | $1.3161 \cdot 10^{-14}$ | 1% | |
| [Hz*cm$^2$] | at 183 GHz | $2.3222 \cdot 10^{-12}$ | 1% | Tretyakov 2016 |
| $E_{low}$<br>[cm$^{-1}$] | Resonant line lower-state energy | HITRAN | 1% | Rothman et al., 2005 + this work |
| $\gamma_a$ | Resonant line air-broadening at 22 GHz | 2.688 | 0.039 | Koshelev et al. 2018 |
| [MHz/mb] | at 183 GHz | 2.945 | 0.015 | Tretyakov, 2016 |
| $\gamma_w$ | Resonant line water-broad. at 22 GHz | 13.281 | 0.034 | Koshelev et al. 2018 |
| [MHz/mb] | at 183 GHz | 14.77 | 0.37 | Tretyakov, 2016 |
| $n_a$ | Resonant line air-broad. temperature dependence exponent at 22 GHz | 0.70 | 0.05 | Payne et al. 2008<br>Tretyakov 2016 |
| [unitless] | at 183 GHz | 0.74 | 0.03 | |
| $n_w$ | Resonant line water-broad. temp. dependence exponent at 22 GHz | 1.20 | 0.5 | Cazzoli et al. 2007<br>Bauer et al. 1989 |
| [unitless] | at 183 GHz | 0.78 | 0.08 | Tretyakov 2016 |
| R | Res. line shift-to-broad. ratio at 22 GHz | -0.0089 | 0.0106 | Koshelev et al. 2018 |
| [unitless] | at 183 GHz | -0.0245 | 0.0026 | Tretyakov, 2016 |
| $C_f$<br>[km$^{-1}$ mb$^{-2}$ GHz$^{-2}$] | Foreign-broadened continuum | $5.96 \cdot 10^{-10}$ | $5.5 \cdot 10^{-11}$ | Rosenkranz 1998<br>Turner et al. 2009 |
| $C_s$<br>[km$^{-1}$ mb$^{-2}$ GHz$^{-2}$] | Self-broadened continuum | $1.42 \cdot 10^{-8}$ | $3.2 \cdot 10^{-9}$ | Rosenkranz 1998<br>Turner et al. 2009 |
| $n_{cf}$<br>[unitless] | Foreign-broadened continuum temperature dependence exponent | 0.0 | 0.8 | Rosenkranz 1998<br>Tretyakov 2016<br>Koshelev et al. 2011 |
| $n_{cs}$<br>[unitless] | Self-broadened continuum temperature dependence exponent | 4.5 | 0.6 | Rosenkranz 1998<br>Tretyakov 2016<br>Koshelev et al. 2011 |

## Sensitivity Analysis

The atmospheric absorption calculated from a model has in general a nonlinear dependence on some spectroscopic parameters. With the assumption of small perturbations, however, one can reasonably linearize that dependence, for a given model:

$$T_B = \mathbf{K}_p \cdot (p - p_0) + T_{B0} \qquad (1)$$

where $p$ is a vector whose elements are the parameters in the model, having nominal value $p_0$; $T_B$ is a vector of calculated brightness temperatures at various frequencies using parameter values $p$, while $T_{B0}$ is calculated for parameter values $p_0$, and $\mathbf{K}_p$ represents the partial derivatives (Jacobian) of model output with respect to model parameters $p$. Thus, for computing the $T_B$ uncertainties due to absorption model parameters, the full covariance matrix of parameter uncertainties is necessary ($^\top$ indicates transpose matrix):

$$\mathbf{Cov}(T_B) = \mathbf{K}_p \mathbf{Cov}(p) \mathbf{K}_p^\top \tag{2}$$

However, the parameter uncertainty covariance matrix is not readily available, as the spectroscopic literature provides at most the uncertainty of individual parameters. To narrow the number of parameters for which the covariance should be evaluated, we investigate the $T_B$ sensitivity to parameter uncertainty, with the purpose of identifying parameters with impact so small that could reasonably be neglected. Spectroscopic parameters used by R17 for water vapor and oxygen absorption are listed in Tables 1 and 2, respectively. The listed uncertainties were either retrieved from the spectroscopic literature or, where not available, were estimated from an independent analysis of measurement methods. Each parameter (or parameter type if known to be highly correlated) is investigated individually by perturbing its value by ±1-σ uncertainty and computing the impact on the modelled $T_B$. Six different climatologic conditions are considered to account for temperature, pressure, and humidity dependences. Examples of the computed sensitivities are shown in Figures 1 and 2 for water vapor and oxygen parameter, respectively. Parameters with 1-σ uncertainty impacting the modelled 20-60 GHz $T_B$ for more than 0.1 K are considered as relevant. The sensitivity analysis indicates that, among all the spectroscopic parameters in Tables 1 and 2, the following dominate the uncertainty of modelled downwelling 20-60 GHz $T_B$:

- 6 for water vapor ($C_s$, $C_f$, $n_{cf}$, and $S_i$, $\gamma_{i,a}$, $R_i$ for $i=1$, i.e. 22 GHz);
- 105 for oxygen ($S_i$, $n_a$, $\gamma_{nr}$, $\gamma_{ai}$, $Y_i$, $v_i$, where the first 3 are scalar, while for the others $i$=1-34). Note that $S_i$ is a scalar because the uncertainty in $O_2$ line intensities is attributed to the calculation of the partition sum, which is a single variable affecting all the lines.

**Table 2:** List of oxygen parameters perturbed in the sensitivity analysis.

| **Symbol [units]** | **Parameter** | **Value** | **Uncertainty** | **Reference** |
|---|---|---|---|---|
| $\nu_i$ [kHz] | Resonant line frequency | Table 1* | Table 1* | Tretyakov et al., 2005 |
| $S_i$ [Hz/cm$^2$] | Resonant line intensity | HITRAN | 1% | Rothman et al., 2005 + this work |
| $E_{low}$ [cm$^{-1}$] | Resonant line lower-state energy | HITRAN | 0.25% | Rothman et al., 2005 + this work |
| $\gamma_i$ [MHz/mb] | Resonant line air-broadening | Table 5* | Table 1* + this work | Tretyakov et al., 2005<br>Koshelev et al. 2016 |
| $n_a$ [unitless] | Resonant line air-broadening temperature dependence exponent | 0.80 | 0.05 | Koshelev et al. 2016 |
| $Y_i$ | Resonant line mixing | Table 5* | This work | Tretyakov et al., 2005 |
| $v_i$ | Resonant line mixing temperature dependence | Table 5* | This work | Tretyakov et al., 2005 |
| $r_{w2a}$ [unitless] | Resonant line water-to-air broadening ratio | 1.20 | 0.05 | Koshelev et al. 2015 |
| $\gamma_{nr}$ [MHz/mb] | Non-resonant pressure broadening | 0.56 | 0.084 | Danese and Partrige, 1989 + This work |

*Table 1 and 5 from Tretyakov et al., 2005.

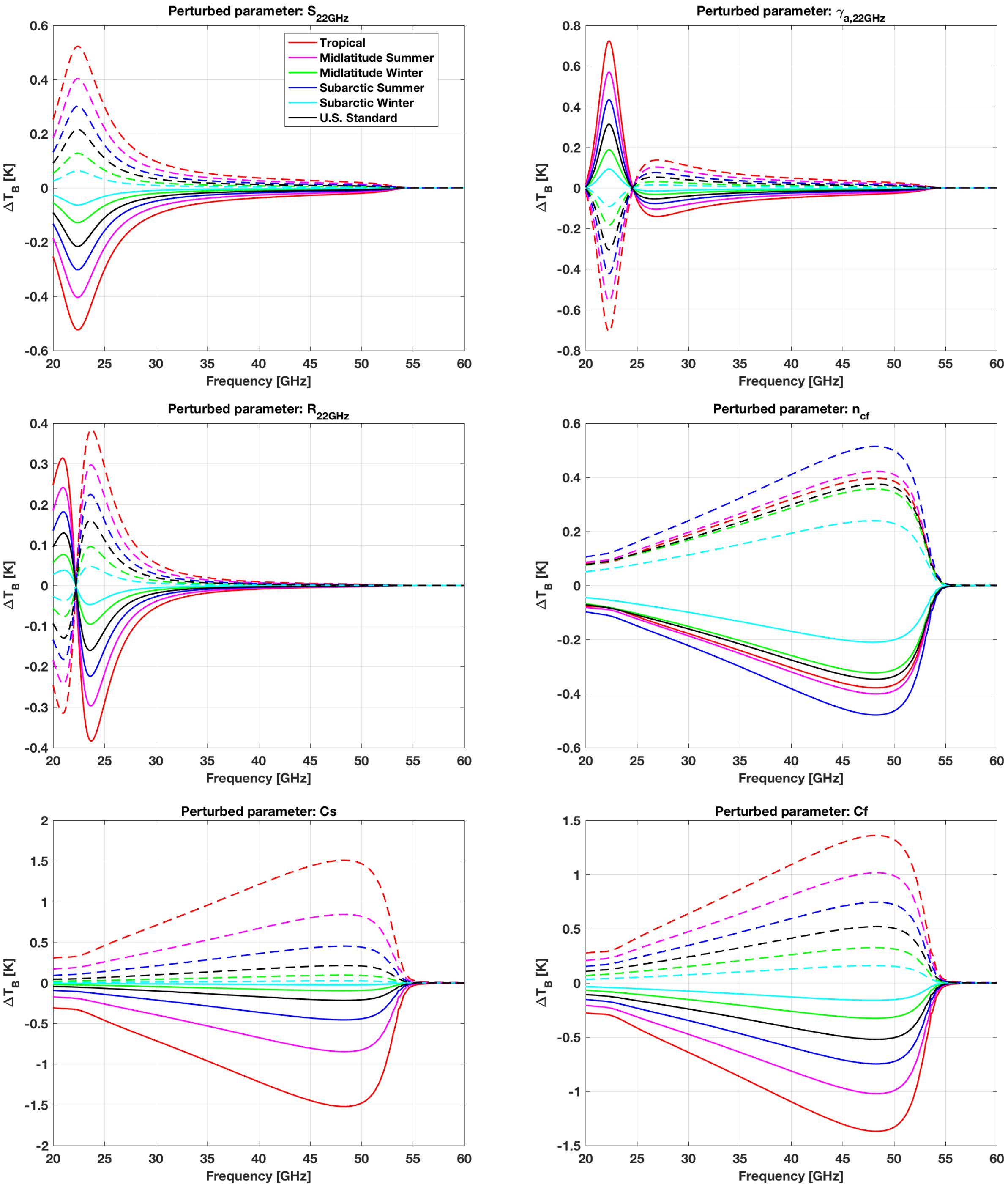

**Figure 1:** Sensitivity of modelled downwelling $\mathrm{T_B}$ to water vapor absorption parameters. Top: line intensity ($S_i$) and air-broadening ($\gamma_{\mathrm{i,a}}$) at 22 GHz. Middle: Shift-to-broadening ratio ($R_i$) at 22 GHz and foreign-broadening temperature-dependence exponents ($\mathrm{n_{cf}}$). Bottom: Self- ($C_s$) and foreign- ($C_f$) induced broadening coefficients.

## Uncertainty propagation

The above sensitivity analysis shows that 111 spectroscopic parameters dominate the uncertainty of modeled downwelling 20-60 GHz $\mathrm{T_B}$. Consequently, the parameter uncertainty covariance $\mathbf{Cov}(p)$ reduces to a (111,111) matrix. $\mathbf{Cov}(p)$ is evaluated in a companion study from the analysis of the measurement methods leading to the parameter values. The results are not shown here but will be included in a manuscript currently being drafted. The propagation of the spectroscopic parameter uncertainty into $\mathrm{T_B}$ uncertainty is described by

Eq. (2). Preliminary results show that the uncertainty contribution to simulated $T_B$ ranges from ~0.3 K (sub-Arctic winter) to 0.9 K (tropical) at 22.2 GHz, and from ~2.6 K (tropical) to 3.2 K (sub-Arctic winter) at 52.28 GHz. The uncertainty on model parameter may be further propagated into the atmospheric retrieval space, giving e.g. the uncertainty of temperature and humidity profiles estimated from a ground-based MWR caused by spectroscopic parameter uncertainty. Following Rodgers (2000), and introducing the Jacobian of $T_B$ with respect to the atmospheric state vector ($\boldsymbol{K_x}$) and the covariance matrices of measurements and a priori uncertainty ($\mathbf{Cov}(\epsilon)$ and $\mathbf{Cov}(a)$, respectively), we can compute the gain matrix $\boldsymbol{G}$ and the covariance matrix of the retrieval $\hat{x}$ as:

$$\boldsymbol{G} = (\boldsymbol{K}_x^{\top}\mathbf{Cov}(\epsilon)^{-1}\boldsymbol{K}_x + \mathbf{Cov}(a)^{-1})^{-1}\mathbf{K}_x^{\top}\mathbf{Cov}(\epsilon)^{-1} \quad (3)$$

$$\mathbf{Cov}(\hat{x}) = (\boldsymbol{G}\boldsymbol{K}_p)\mathbf{Cov}(p)(\boldsymbol{G}\boldsymbol{K}_p)^{\top} \quad (4)$$

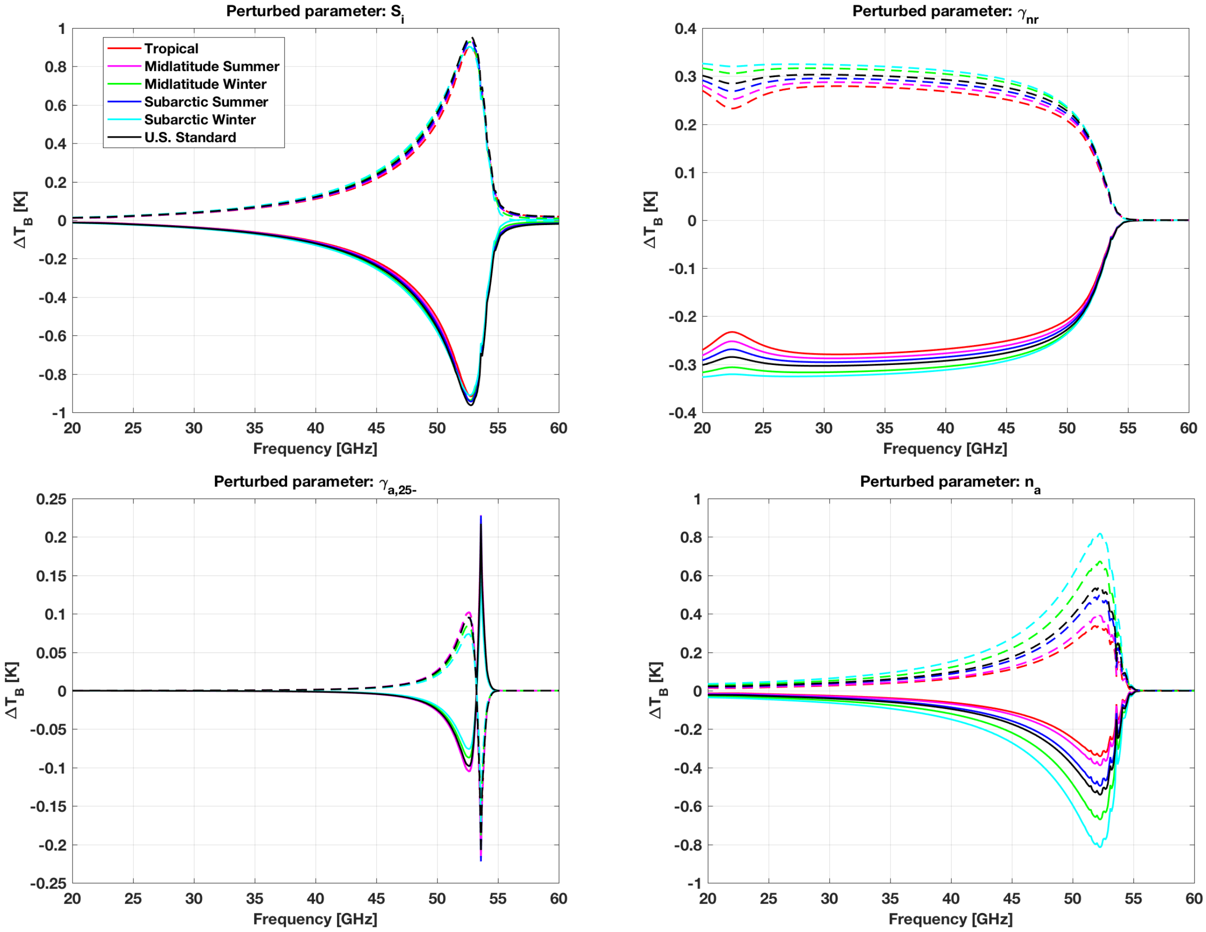

**Figure 2:** Sensitivity of modelled downwelling $T_B$ to oxygen absorption parameters. Top: resonant line intensity ($S_i$) and non-resonant pseudo-line broadening ($\gamma_{nr}$). Bottom: air-broadening ($\gamma_{i,a}$) at 53.59 GHz (N=25-) and air-broadening temperature-dependence exponents ($n_a$).

## Summary and future work

This work describes the approach and preliminary results for estimating the absorption model contribution to the uncertainty of modeled downwelling 20-60 GHz $T_B$ and associated ground-based atmospheric sounding retrievals. The first step towards this goal is to identify a reduced set of spectroscopic parameters that explain most of the modeled $T_B$ uncertainty.

A sensitivity analysis indicates that the uncertainty of modeled downwelling 20-60 GHz $T_B$ is dominated by 6 water vapor parameters (self- and foreign-continuum coefficients, foreign-continuum temperature dependence exponent, and line intensity, air-broadening, and shift-to-broadening at 22 GHz) and 105 oxygen parameters (line intensity, broadening/mixing temperature dependence exponent, non-resonant broadening (scalars) and line air-broadening, mixing, and mixing temperature dependence (34-dimension vectors)). The full covariance matrix for these 111 parameters is performed in a companion study (not shown here) and is used here to give preliminary estimates of the absorption model contribution to the uncertainty of modeled downwelling 20-60 GHz $T_B$ (up to 0.9 K at 22.2 GHz and up to 3.2 K at 52.28 GHz).

The sensitivity analysis, the parameter uncertainty covariance estimation, and the uncertainty propagation into downwelling 20-60 GHz $T_B$ and ground-based sounding retrievals are the subjects of a manuscript currently being drafted. Future work could be dedicated to expanding this analysis to higher frequencies and to upwelling $T_B$ and satellite sounding retrievals.

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