Uncertainties in the Temperature Dependence of the Line-Coupling Parameters of the Microwave Oxygen Band: Impact Study

Sid-Ahmed Boukabara, Shepard A. Clough, Jean-Luc Moncet, Andrei F. Krupnov, Mikhail Yu. Tretyakov, and Vladimir V. Parshin

***Abstract*—A sensitivity study was performed with the commonly used millimeter-wave propagation model (MPM) to assess the impact of prescribed uncertainty in the temperature dependence of the line-coupling factors used to model the oxygen line shape. In some cases, apparent nonphysical behaviors were noticed and their impact on microwave channels was found to be significant and more importantly, nonremovable by simple calibration or bias removal. The Advanced Microwave Sounding Unit configuration in particular was tested because of its prime importance in current data assimilation. This impact, which reached a maximum of a few Kelvin in some channels, is modulated nonlinearly by the amount of water vapor present in the atmosphere, with maximum impact in dry air situations, which makes it dependent on the brightness temperature itself. These errors directly impact the error budget of any physically based geophysical retrieval. The line shape of these O_2 lines has impacts across the microwave spectrum, through the wing effects. This includes channels near 23, 36, and 85 GHz, commonly used in operational radiometry.**

***Index Terms*—Microwave remote sensing, oxygen absorption, spectroscopy, temperature dependence.**

I. Introduction

In MICROWAVE radiometry, absorption by oxygen plays a primary role: temperature sounding is possible only because of the strong oxygen absorption in the 60-GHz band and the 118-GHz line. The modeling of the O_2 absorption, through the nonresonant term and the line wings effects, has also a critical impact on channels in the window regions, which are sensitive to cloud absorption and to the water vapor continuum. In general, spectroscopic uncertainties have long been considered correctable within reasonable margins, by using after-launch calibration. However, new microwave radiometry applications have emerged recently, requiring a significantly higher degree of accuracy from both the measured brightness temperatures and the microwave models used to simulate them. These applications include the sea wind direction and the sea salinity retrievals where a few tenths of a degree are usually the allowed maximum error [1], [2]. Wind direction signal for instance was found to have a peak-to-peak amplitude variation between 0.5 and 3 K depending on frequency in the 10–40-GHz frequency range. This highly demanding requirement induced us to revisit the impact of spectroscopic uncertainties on microwave absorption modeling. This study focuses on the temperature dependence of the line-coupling parameters of O_2. The widely used millimeter-wave propagation model [3]–[5] in microwave remote sensing relies, for the modeling of the oxygen absorption, on data reported in 1991 and 1992 by Liebe *et al.* [6], [7]. These measurements were performed in the temperature range [6 °C to 54 °C]. Behavior of the oxygen absorption is therefore poorly known in an important portion of the earth's atmosphere (both troposphere and stratosphere), where these temperatures cover roughly the range [−90 °C to 55 °C]. The extrapolation to lower temperatures causes uncertainties often not accounted for. Liebe *et al.* felt that the temperature dependence might need to be reevaluated for both the overlapping coefficients and the width. The uncertainty in the coupling coefficients was roughly estimated to be around 12%, but a 15% change was necessary to fit additional data [4]. Another variant of this model is also widely used. The main difference is an update in the formulation of the water vapor continuum [3]. The oxygen modeling is identical. We will use the code associated with this latest version, referred to by the author as MPMf87/s93 and sometimes called Rosenkranz 1998 in the litterature. We will refer to it with the generic name MPM, as the basics of the oxygen absorption modeling are essentially the same.

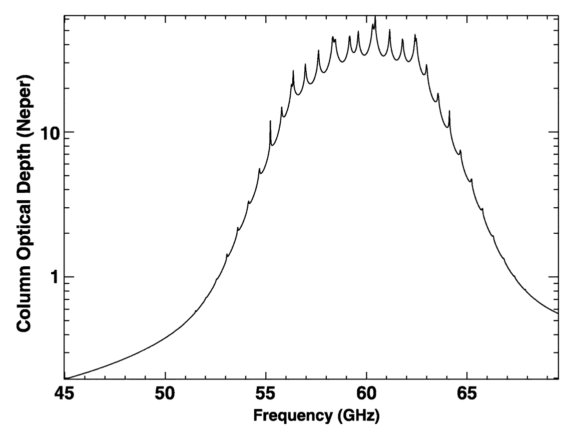

Fig. 1. Total column optical depth, as simulated by MPM, in the 60-GHz oxygen microwave band. A set of 34 spectral lines makes up the band. The U.S. standard atmosphere was used to simulate the optical depth.

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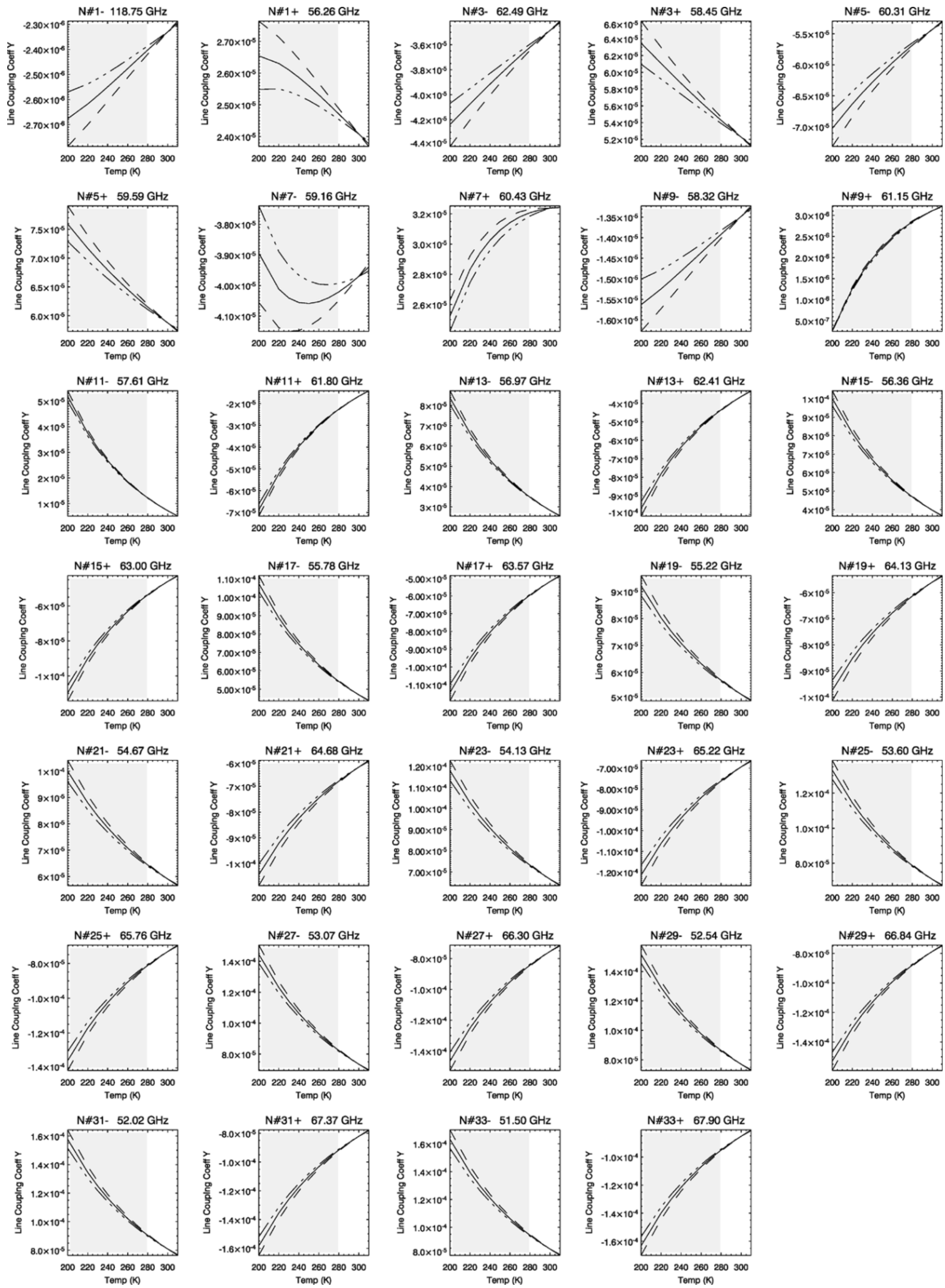

Fig. 2. Variation of the line-coupling factor as a function of temperature, for a pressure of 1000 mbar, for all lines in the 60-GHz microwave band. Lines are ranked by the rotational angular momentum quantum number N. The symbols $\pm$ represent the transition between states of angular momentum, J between $J = N$, and $J = N \pm 1$. The gray area is where no measurement has been made. The solid line corresponds to the current formulation in MPM code. The dashed line corresponds to changing the temperature dependence exponent X to 0.9 (instead of nominal value: 0.8). The dotted–dashed line corresponds to taking $X = 0.7$. The impact of this factor becomes much more important at low temperatures. It has, however, no noticeable effect for the temperatures previously measured at (6 °C to 54 °C). Note also the seemingly nonphysical behavior of the 7-line at 59.16 GHz.

II. Overlapping Coefficients

The oxygen absorption spectrum features a number of absorption spectral lines in the 50–70-GHz band (see Fig. 1). With increasing pressure, their individual widths broaden and their shapes overlap, resulting in their gradual blending. The degree of blending is modeled by line-coupling factors. The line absorption shape of each individual line is therefore affected by these line-coupling factors (also called overlapping factors). In MPM, the line-coupling coefficient at a particular spectral line (index i), is expressed as

$$Y^i = 0.001 \cdot P \cdot \left(\frac{300}{T}\right)^X \left(Y^i_{300} + V^i \cdot \left(\frac{300}{T} - 1\right)\right) \quad (1)$$

where T is the temperature, in Kelvin, and P the pressure of the layer, in millibar. The temperature dependence exponent X is equal to 0.8 for all lines in MPM. Y_{300} and V are prestored values for a number of frequencies (34 lines in the microwave spectral range and six in the submillimeter wavelength range). The previous formulation (1) of the line-coupling parameters is equivalent to [7, eq. 27]. It is based on a modified version of a previous overlapping coefficients retrieval algorithm, developed by Rosenkranz [8], accounting for the effect of the departure of temperature from the 300-K value, previously used in [8]. The second term in (1) reflects that. These line-coupling coefficients were extracted from the absorption at 70.1 kPa, using a temperature-normalized line-coupling coefficient. In their paper, Liebe *et al.* showed that two terms in powers of $300/T$ (represented by θ in their paper) are necessary but not sufficient to represent the temperature dependence of the Y^i, especially in the higher rotational levels, away from the center of the band. They found that the two-term expansion in temperature was adequate enough for the set they used and for the temperature range they had, but warned that it might fail outside the temperature range investigated. They also cited the first-order expansion in pressure as a possible source of error although the systematic residuals found at different pressures were small.

III. Temperature Dependence

The line-coupling coefficients, which have a major impact on the line shape of the oxygen line and therefore on the brightness temperature simulation, are virtually unknown in the range of low to medium atmospheric temperatures. Fig. 2 shows the variations of these coupling factors with temperature, at the prestored spectral lines, extended to the whole atmospheric temperature range. Note that the spectral lines are ranked in ascending order of the quantum number N which defines the structural transition between states of total angular momentum. The gray area corresponds to the temperature range where we have no measurements. The values in this region are pure extrapolation. Three values for the temperature dependence exponent X were tested: the nominal value 0.8 as well as a $\pm 12\%$ error on this value, as estimated by Liebe *et al.*, corresponding to values of X of 0.7 and 0.9. From these plots, a number of observations could be made.

- The effect of any uncertainty on X is impacting the line-coupling factor in the subfreezing temperatures but not much at temperatures where the measurements were made [279–320 K]. So by fitting X using only the upper bound temperature range, one cannot ensure a proper representation for the lower bound temperatures. Relative errors up to 5% can occur in some of the lines between the nominal $X = 0.8$ and either $X = 0.7$ or $X = 0.9$.
- The absolute value of the line-coupling coefficient in the low to medium temperature range cannot be assessed obviously because of the lack of measurements, but certain behaviors could be noticed. A clearly nonphysical variation with respect to temperature is noticed in the line 59.16 GHz ($N = 7-$). There are indeed no physical reasons to expect that the line-coupling factor will decrease with temperature and then to start increase at around 240 K, especially given that this is the only line featuring this kind of variation. If we assume a relatively smooth variation (to mimic the other lines), then differences up to 12% could be reached in this line. In the 60.43-GHz frequency line, the coupling factor seems to vary in a strongly quadratic way. If again, we assume only a weakly nonlinear behavior as in almost all the rest of the lines, then differences up to 20% occur.
- General patterns could also be mentioned from Fig. 2. (a) The temperature dependencies of the Y_i for corresponding lines in the two branches $N = \pm n$ almost always vary in opposed senses. The exceptions are the (7-, 7+) pair where the apparent anomaly occurs, and the (9-, 9+) pair which signals the sign reversal. (b) The Y coefficients in each branch change sign at the (9-, 9+) pair. This is consistent with [7] and [8]. (c) It may or may not be coincidence that the unphysical anomaly mentioned above, for which $N = 7$, is close to the most populated rotational level at 300 K and therefore comes close to the switch between the two temperature regimes mentioned in (b). This could be a hint that the two-term expansion in temperature of (1) is less justified and that a higher order expansion might be necessary for these rotational levels.

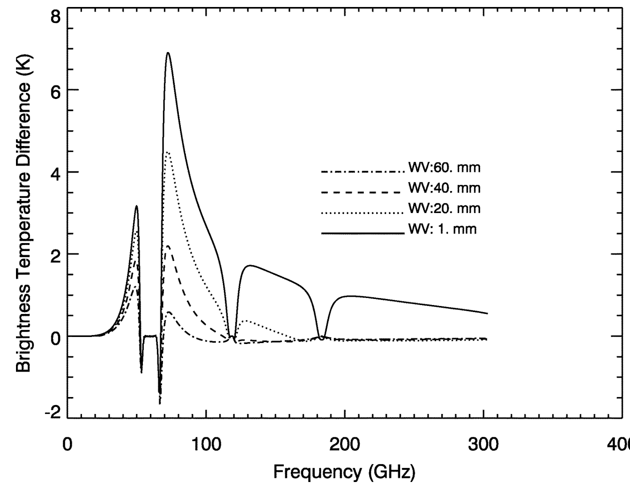

Fig. 3. Impact of modifying by 10% the line-coupling coefficient (only for temperatures below 279 K), on the whole microwave spectrum. The U.S. standard atmosphere served as an input with a flat surface to compute the top of the atmosphere brightness temperature. Horizontal polarization was used. The curves correspond to four values of integrated water vapor. Error is maximal for dry cases, at the edge of the 60-GHz band, where the wing effect is important. An earth incidence angle of 53° was used for these simulations.

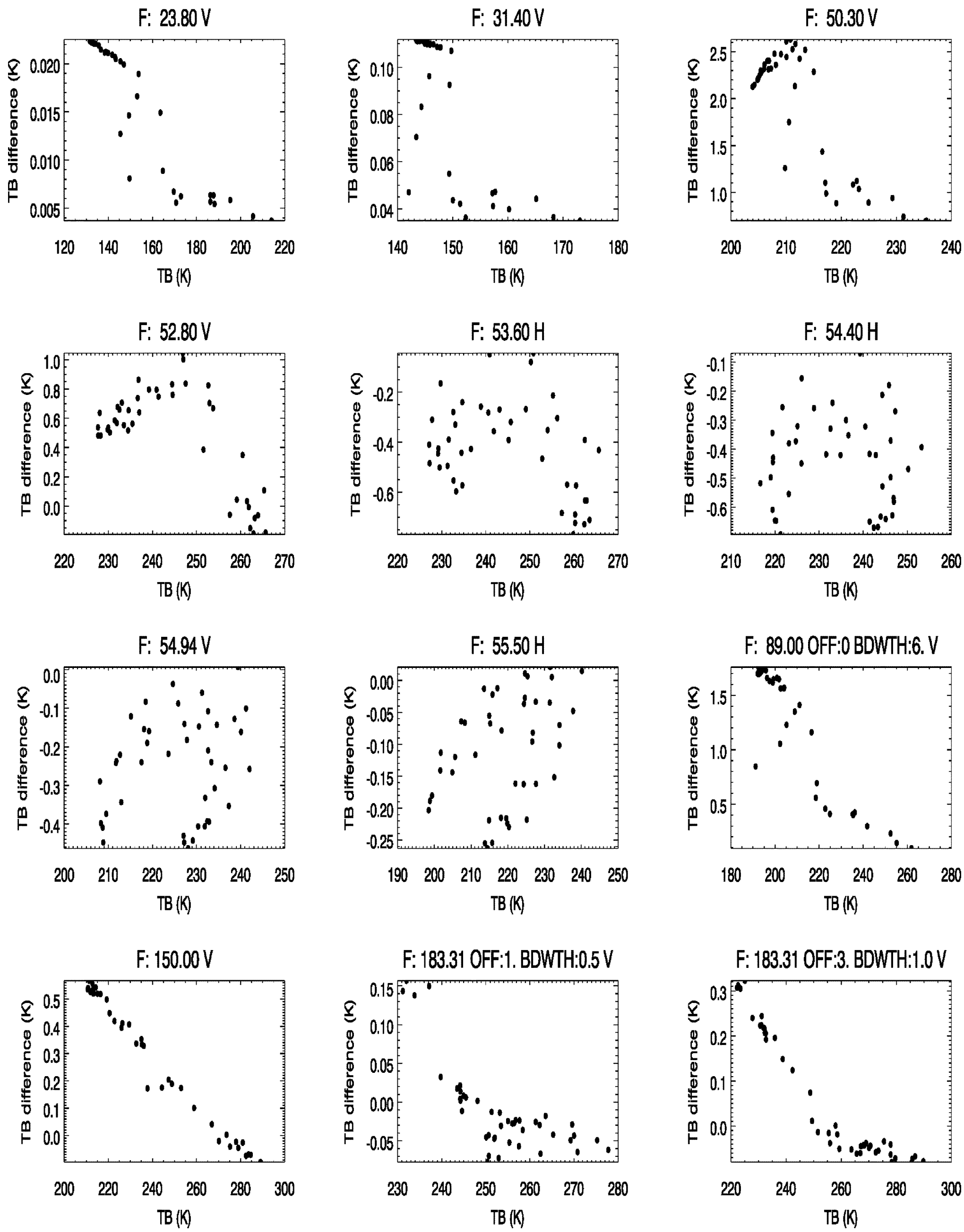

Fig. 4. Impact of a 10% change in the line-coupling coefficient computed for temperatures below 279 K, on some of the AMSU channels. They are plotted versus the TB itself to show the nonlinear aspect, which cannot be canceled by a simple bias removal at the postlaunch calibration stage. Note there are two 183 water vapor sounding channels shown in this plot that differ by the side-band offsets and their respective bandwidths. Frequencies (F), bandwidths (BDWTH), and side-band offsets (OFF) are all in Gigahertz. V or H symbols represent the signal polarization.

IV. Impact on Brightness Temperatures

The impact of an uncertainty of 10% in the line-coupling coefficients Y in the low to medium temperatures range, on the brightness temperatures, has been assessed. Line-coupling factors for upper temperatures were left unchanged. The absolute value of the line-coupling coefficients for lower temperatures was decreased by 10% to make the temperature dependence in this range more consistent with the variation in the higher temperature range. The 10% value tested here is believed to be near the lower end of the uncertainty range. Fig. 3 represents the impact of this 10% uncertainty on the whole microwave spectral range. The U.S. standard atmosphere was used. A tropical atmosphere was also used with essentially the same results (not shown). The water vapor profile was scaled to encompass four different values of total precipitable water (1, 20, 40, and 60 mm). A perfectly flat surface (zero wind speed) was used. Fresnel equations served to compute the emissivity with the dielectric constant of saline water obtained using the Klein and Swift model [9]. Maximum errors, reaching 7 K at the edge of the 60-GHz band, occur where the effect of the oxygen lines wings is important. For water vapor-saturated channels, the impact is minimal. For opaque sounding channels, the impact is also small.

V. Impact on the Advanced Microwave Sounding Unit (AMSU) Configuration

A similar assessment was performed for the 20 AMSU channels. AMSU was chosen for its prime importance in microwave data assimilation. We used 43 profiles that the U.K. Meteorological Office developed [10], to represent a wide range of temperature and water vapor variations. The line-coupling coefficients were perturbed in the same way described in Section IV. Also, the surface modeling follows the same approach adopted in the previous section. The incidence angle used here corresponds to the nadir viewing configuration. Fig. 4 shows a series of plots representing impacts on some of the AMSU channels for all profiles. The impact (brightness temperature difference) is plotted versus brightness temperatures (TB). The main remarks to be drawn from these plots are as follows.

- Errors can reach up to 2.5 K. This is probably a worst case scenario for the 10% error figure. In reality, the wind will increase the surface emissivity and therefore decrease the atmosphere–surface contrast, thus reducing the importance of the atmospheric absorption in the computation of the radiance.
- The differences are not removable by a simple shift since they depend on the brightness temperature itself. Therefore, reducing these errors has the potential for reducing the standard deviation. Errors are especially high for channels at the edge of the 60-GHz band. Other AMSU channels do not show a significant impact.

VI. Conclusion

The temperature dependencies of the oxygen spectral overlapping factors in the widely used MPM model were tested. The current formulation of the temperature dependence is based on a two-term expansion in $300/T$ and relies on a unique exponent that is applied to all oxygen spectral lines in the 60-GHz band. This parameter was determined statistically in the limited temperature range between 6 °C and 54 °C. We have shown that any error in this factor or in the two-term expansion formalism would not be apparent within the measurement range used to determine this factor (between 6 °C and 54 °C). A change in this factor causes, however, a significant departure (from not changing it) in the lower to medium temperatures. We showed that any determination of this parameter in the [6 °C to 54 °C] range, could not satisfy the whole range of atmospheric temperatures which vary roughly between -90 °C and 55 °C. The extrapolation to lower temperatures of the line-coupling coefficients, showed also a seemingly nonphysical behavior of some oxygen band lines. A potential improvement in the modeling of these line-coupling coefficients would be the revision of the two-term expansion formalism. A three-term expansion could be an alternative to better model all the range of temperatures, but additional data, like those recently reported in [11] and [12], would be necessary in the subfreezing temperatures range, in order to be able to detect the potential benefit in better fitting the temperature dependence of the line-coupling coefficients. An assessment was made to gauge the impact that an assumed uncertainty in these dependencies has on the simulated brightness temperatures, first on the whole spectrum between 3 and 300 GHz and then on AMSU channels.

It was found that a 10% error on these factors could lead to nonlinear errors in the range between few tenths of a degree to few degrees, depending on the frequency. Situations with dry air atmosphere are the most impacted. Most errors occur in the channels at the edge of the oxygen band, but they also propagate to the tails of the band shape through the wing effects, reaching frequencies as low as 30 GHz and as high as 160 GHz. Clearly these errors are not correctable by simple bias removals at the calibration stage. The 10% figure is deemed to be in the lower boundary of the possible uncertainty range. Liebe has estimated that it is likely that the temperature dependence is known within a 12% margin, although a 15% change was necessary later on to fit additional data. The uncertainty could in fact be higher than 10% if we consider the temperature dependence of other important spectroscopic parameters such as the pressure-broadening width and the nonresonant absorption, not treated here.

These potential spectroscopic errors in the oxygen absorption modeling could lead to only marginal errors in terms of traditional geophysical performances (temperature and water vapor profiles, skin temperature, etc.), but it is expected that with emerging applications such as microwave remote sensing of wind direction and salinity, increasing accuracy requirements will be put on absorption models and the spectroscopic data they utilize.

This study highlights the need for extending the current spectroscopic measurements of the oxygen absorption in the 60-GHz band to subfreezing atmospheric temperatures, to meet those requirements.

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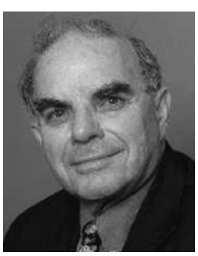

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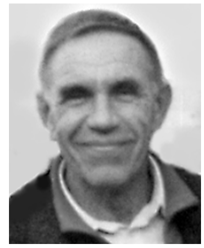

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