Simplified Molecular Absorption Loss Model for $275 - 400$ Gigahertz Frequency Band

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Abstract—**This paper focuses on giving a simplified molecular absorption loss model for a $275 - 400$ GHz frequency band, which has significant potential for variety of future short and medium range communications. The band offers large theoretical data rates with reasonable path loss to theoretically allow even up to kilometer long link distances when sufficiently high gain antennas are used. The molecular absorption loss in the band requires a large number of parameters from spectroscopic databases, and, thus, the exact modeling of its propagation characteristics is demanding. In this paper, we provide a simple, yet accurate absorption model, which can be utilized to predict the absorption loss at the above frequency band. The model is valid at a regular atmospheric pressure, it depends on the distance, the relative humidity, and the frequency. The existing simplified model by ITU does not cover frequencies above 350 GHz and has more complexity than our proposed model. The molecular absorption loss increases exponentially with the distance, decreasing the utilizable bandwidth in the vicinity of the absorption lines. We provide a model to approximate the window widths at the above frequency band. This model depends on the distance, the relative humidity, the frequency, and the maximum tolerable loss. It is shown to be very accurate below one kilometer link distances.**

I. INTRODUCTION

The millimeter wave frequency band (mm-wave, 30–300 GHz) is of interest for future wireless communications systems and applications, such as 5G and beyond [1]. These frequencies can be utilized in both medium and short range communications, with the former requiring large antenna gains. Up to 850 meter link has been shown to be feasible at 240 GHz frequency [2]. The main benefit of higher frequencies are the large available bandwidths that make it possible to provide extremely high data rates, or the possibility to share the spectral resources among vast numbers of devices. The latter case is very interesting because of the ever increasing numbers of internet of things (IoT) devices.

One challenge of utilizing the mm-wave frequencies and above is the proper channel modeling. The free space path loss and the associated antenna gain terms are very well known and easy to implement and adjust based on the antennas in hand. On the other hand, molecular absorption loss plays a role in the accurate channel modeling. At short distances (few meters) around the 300 GHz frequency band, the molecular absorption is not significant in comparison to the large free space path loss. However, its importance becomes more evident at high distances or high frequencies due to exponentially increasing loss as a function of distance [3]. Modeling of the absorption

is very well known, but requires large numbers of parameters from the spectroscopic databases, such as HITRAN database [4]. Our aim herein is to present a simplified molecular absorption loss model that predicts this loss component with high accuracy without a need for large numbers of parameters.

ITU has presented accurate model for calculation of gaseous attenuation up to 1000 GHz in ITU-R P.676-8 [5]. The model in [5] is line-by-line based and the results from it correspond to those obtained by using HITRAN database, confirming its validity (Fig. 1). The full model is not suitable for analytical calculations or for quick use, since it requires using a significant number (553) of tabulated parameters and complicated functions. In [5], a polynomial based approximation has also been presented. It is valid up to 350 GHz. Please note that a newer version ITU-R. 676-11 also exists but that version does not have a specified polynomial model. We use the older version, since the polynomial model therein is related to our work in this paper. However, compared to our models, those models have several weaknesses. First of all, even though [5] includes lines even at 1780 GHz, it is only specified to be valid for frequencies up to 350 GHz. The simple reason is that the model gives erroneous results above 350 GHz (see Fig. 1). The simplified model in the newer version is also limited to 350 GHz. The model also (only for water absorption, oxygen absorption is handled separately) includes 9 terms and if some of the terms are removed, they may also affect frequencies in different bands. For example, the term involving 1780 GHz needs to kept or the level of the attenuation between the peaks at lower frequencies is way off. In general, the ITU model is accurate below 350 GHz, but in this paper we will extend the frequency range and simplify the estimation for it.

Our model is targeted for the frequency range 275–400 GHz, which is not covered by the simplified ITU model. Also, our model, which uses two polynomials is much simpler than the ITU model which involves at least 4 to 9 polynomial functions. The presented model is valid in the standard atmospheric pressure and is accurate at the standard atmospheric temperatures, and it only depends on the distance, the frequency, and the relative humidity. The presented absorption model is aligned towards future standardization in WRC 2019, where the use of frequency band 275 to 450 GHz is on the agenda. Our new simplified model covers 275–400 GHz and can be modified easily to cover also frequencies up to 450 GHz by including a third term. Our simplified model is
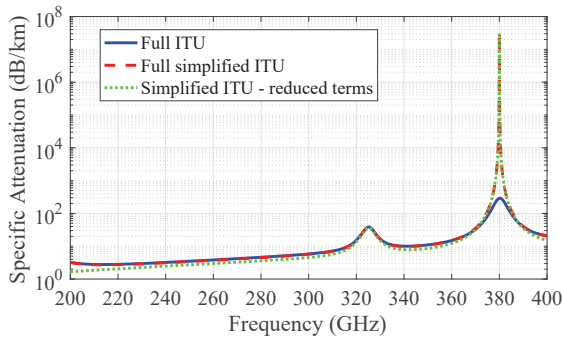
Fig. 1. ITU-R models for the molecular absorption loss.

aimed at analytical studies and simple calculations without the need of calculating the full complicated model. It is hoped to be valuable for wireless communication engineers in their research by enabling easy approximation of the molecular absorption loss.

As the molecular absorption is exponentially increasing with distance, it has been shown that the available bandwidth of the transmission is decreasing with distance (see, e.g., [6], [7]). Utilizing a similar approach as that in the case of molecular absorption loss, we show a simplified model to estimate the transmission window width as a function of the distance, the frequency, the humidity, and the maximum tolerable loss in the vicinity of the center frequency of the transmissions. This model estimates the available bandwidth very accurately up to about one kilometer distances. This helps researchers to easily estimate the bandwidth of the specific systems with known transmission distances.

The rest of this paper is organized as follows. Section II derives the molecular absorption model and shows its validity. Section III gives the available bandwidth model and shows its validity and Section IV concludes the paper.

II. SIMPLIFIED MOLECULAR ABSORPTION LOSS MODEL

A. Path Loss Model

A common path loss model for the higher frequency bands is composed of the free space path loss and molecular absorption loss. The latter is given by the Beer-Lambert law [3], [8]

$$\tau(f,r) = \frac{P_r(f)}{P_t(f)} = e^{-\Sigma_i \kappa_a^i(f) r}, \tag{1}$$

where $\tau(f,r)$ is the transmittance, f is the frequency, r is the distance from transmitter (Tx) to receiver (Rx), $P_t(f)$ and $P_r(f)$ are Tx and Rx power, respectively, and $\kappa_a^i(f)$ is the absorption coefficient of the ith absorbing species at frequency f. Combining this to the free space path loss, we get a total path loss for the LOS paths as

$$\text{PL}(r,f) = \frac{(4\pi r f)^2 \exp(\kappa_a(f) r)}{c^2} G_{\text{Rx}} G_{\text{Tx}}, \tag{2}$$

where c is the speed of light and G_{Rx} and G_{Tx} are the antenna gains of the Rx and Tx, respectively, that further are usually

functions of frequency and antenna orientation. The absorption coefficient can be calculated with the help of databases, such as the HITRAN database [4], as it will be detailed below.

B. Absorption Coefficient

The main point of interest here is to model the absorption loss due to the interest in showing an easy estimate for it. First, we need to define the absorption coefficient as a whole before showing the approximation in the next section. The absorption coefficient depends on pressure, temperature and molecular composition of the channel as

$$\kappa_a^i(f) = \mu_i N \sigma_i(f), \tag{3}$$

where μ_i is the fraction of the molecules of kind i, N is the number density of all molecules, and $\sigma_i(f)$ is the absorption cross section of the ith molecular species. The absorption cross section is a product between spectral line intensity $S^i(T)$ and spectral line shape $F^i(f,p,T)$. The absorption cross section tells the effective area for absorption for a single molecule. The spectral line intensity tells the strength of the absorption per absorption line and the spectral line shape tells the width and shape of the spectral lines. The center frequency of the absorption line i (f_c^i) is dependent on pressure through [3], [9]

$$f_c^i = f_0^i + \delta_i \frac{p}{p_0}, \tag{4}$$

where, p is the atmospheric pressure, p_0 is the standard pressure (101325 Pa), f_0^i is the center frequency of the absorption line at standard pressure, and δ_i is the linear pressure shift.

In the regular atmospheric pressures, the discrete absorption lines experience pressure broadening that we model with the line shapes. This broadening can be modeled with the Lorentz half-width α_L^i at normal pressure conditions and that is composed of foreign and self-broadened half-widths α_0^f and α_0^i, respectively, [8], [9]

$$\alpha_L^i = [(1 - \mu_i)\alpha_0^f + \mu_i \alpha_0^i] \left(\frac{p}{p_0}\right) \left(\frac{T_0}{T}\right)^\delta, \tag{5}$$

where T is the temperature of the atmosphere in Kelvin, T_0 is the standard temperature (296 K reference temperature of HITRAN catalogue [4]), and δ is temperature broadening coefficient. Self-broadening is caused by the collisions between molecules of the same species, while foreign-broadening is due to the inter-molecular collisions.

The most well known line shape is the Lorentz line shape [8], [10]

$$F_L^i(f \pm f_c^i) = \frac{1}{\pi} \frac{\alpha_L^i}{(f \pm f_c^i)^2 + (\alpha_L^i)^2}, \tag{6}$$

where the minus sign is chosen when the Lorentz line shape is utilized alone. This line shape is simple, but it also overestimates the absorption at far wings and it never reaches zero [8]. This line shape was enhanced by Van Vleck and Weisskopf in

1945 [10]. The Van Vleck-Weisskopf line shape is defined as [10]–[12]

$$F_{VVW}^i(f) = \left(\frac{f}{f_c^i}\right)^2 [F_L^i(f - f_c^i) + F_L^i(f + f_c^i)]. \quad (7)$$

The Van Vleck-Weisskopf line shape with far wing adjustments is often called the Van Vleck–Huber line shape

$$F_{VVH}^i(f) = \frac{f}{f_c^i}\frac{\tanh(\frac{hcf}{2k_BT})}{\tanh(\frac{hcf_c^i}{2k_BT})}[F_L^i(f - f_c^i) + F_L^i(f + f_c^i)], \quad (8)$$

where h is the Planck constant, because of the derivation by Van Vleck and Huber [11]. In reality, the difference of this line shape to the Van Vleck–Weisskopf line shape is very small in the mm-wave frequencies.

The line intensity S_0^i can be obtained from HITRAN database for the reference temperature (296 K), but it has to be scaled for the other temperatures by [13]

$$S^i(T) = S_0^i \frac{Q(T_0)}{Q(T)} \frac{e^{(-\frac{hcE_L^i}{k_BT})}}{e^{(-\frac{hcE_L^i}{k_BT_0})}} \left(\frac{1 - e^{(-\frac{hcf_c^i}{k_BT})}}{1 - e^{(-\frac{hcf_c^i}{k_BT_0})}}\right) \quad (9)$$

where k_B is the Boltzmann constant, E_L^i is the lower state energy of the transition of absorbing species i. The partition function $Q(T)$ and its definitions can be found in [13, Appendix A].

Combining the above theories, the total absorption loss becomes

$$\text{PL}_{\text{abs}}(f) = \exp(\mu_i N F^i(f) S^i(T)). \quad (10)$$

Using the different line shapes in the place of $F^i(f)$, we can compare their differences in Fig. 2. We can see that as predicted, the Lorentz line shape overestimates the wing absorption and the Van Vleck–Weisskopf and Van Vleck–Huber line shapes are in practice identical. Fortunately, the error of the Lorentz line shape is nearly linear to the more sophisticated line shapes, which gives us tools to simplify the absorption loss based on the Lorentz line shape.

C. Simplified Absorption Model

The main goal here is to introduce a simplified molecular absorption model that is valid at 275–400 GHz frequency band, although, the model is equally accurate from 200 to 400 GHz. This band has two major absorption lines, one at about 325 GHz and second at 380 GHz. The proposed simplified channel model starts from the assumption of the Lorentz line shape holding for the relative loss. This line shape gives the easiest way to give a simple molecular absorption model that only depends on volume mixing ratio of water (humidity) and frequency. The absorption model is given by

$$y_1(f, \mu_{\text{H}_2\text{O}}) = $$
$$\frac{0.2205\mu_{\text{H}_2\text{O}}(0.1303\mu_{\text{H}_2\text{O}} + 0.0294)}{(0.4093\mu_{\text{H}_2\text{O}} + 0.0925)^2 + \left(\frac{100f}{c} - 10.835\right)^2}, \quad (11)$$
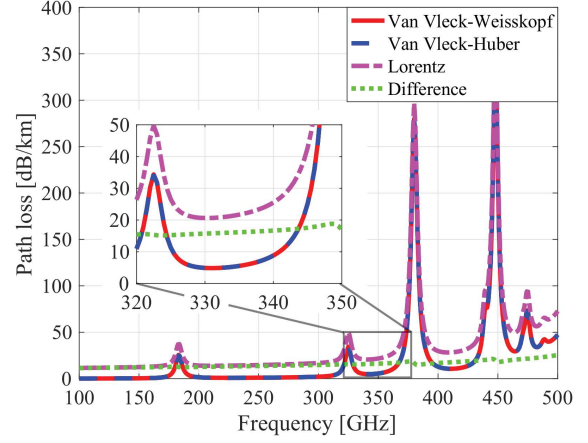

Fig. 2. Comparisons of the common line shapes for modeling the absorption loss. Figure also shows the relative error of the Lorentz line shape to the more sophisticated line shapes.

$$y_2(f, \mu_{\text{H}_2\text{O}}) = $$
$$\frac{2.014\mu_{\text{H}_2\text{O}}(0.1702\mu_{\text{H}_2\text{O}} + 0.0303)}{(0.537\mu_{\text{H}_2\text{O}} + 0.0956)^2 + \left(\frac{100f}{c} - 12.664\right)^2}, \quad (12)$$

$$\boxed{\text{PL}_{\text{abs}}(f, \mu_{\text{H}_2\text{O}}) = e^{d(y_1(f,\mu_{\text{H}_2\text{O}})+y_2(f,\mu_{\text{H}_2\text{O}})+g(f))},} \quad (13)$$

where f is the desired frequency grid, $\mu_{\text{H}_2\text{O}}$ is the volume mixing ratio of water vapor, which is given in terms of relative humidity ϕ by

$$\mu_{\text{H}_2\text{O}} = \frac{\phi}{100}\frac{p_w^*(T, p)}{p}, \quad (14)$$

where $\phi p_w^*(T, p)/100$ is the partial pressure of water vapor, for which the saturated water vapor partial pressure p_w^* under pressure p and temperature T can be estimated, e.g., by the Buck equation [14]

$$p_w^* = 6.1121(1.0007 + 3.46 \times 10^{-6}p)\exp\left(\frac{17.502T}{240.97 + T}\right), \quad (15)$$

where p is given in hectopascals and T is given in degrees Celsius. The factor $g(f)$ is an equalization factor given by a polynomial

$$g(f) = p_1f^3 + p_2f^2 + p_3f + p_4, \quad (16)$$

where coefficients $p_1 = 5.54 \times 10^{-37}$, $p_2 = -3.94 \times 10^{-25}$, $p_3 = 9.06 \times 10^{-14}$, and $p_4 = -6.36 \times 10^{-3}$, to take into account the difference between the Lorentz and Van-Vleck Huber line shapes. This factor is a simplified approximation of the real difference. The model above is obtained by utilizing the line-specific data from HITRAN and by leaving only the humidity (with pressure and temperature dependencies) and frequency grid floating. Therefore, the accuracy of this model is very high as the only sources of error come from the rounding errors and a small error caused by the correction factor $g(f)$.

The difference difference of the above simplified line shape is compared to the fully theoretical one calculated with Van
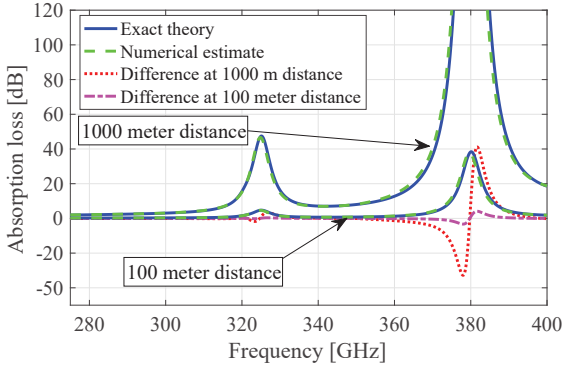
Fig. 3. Comparison of the exact absorption loss to the numerical estimate and the error caused by the numerical estimate.
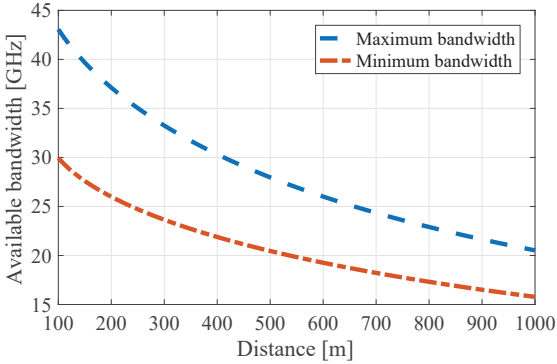

Fig. 4. The estimated available bandwidth based on one sided three dB loss (minimum bandwidth) and the maximum bandwidth allowed by the full transmission window.

Vleck–Huber line shape in Fig. 3. Two distances are utilized, 100 and 1000 meters. We can see that the expected performance of the simplified model is extremely high. As it can be seen, the error is mainly at the absorption peaks, which is not that important as the power loss is high at the absorption peaks at high distances. Thus, they should be avoided in any case. Instead, the performance of the numerical approximation at the wing absorption is more important where the numerical estimate is more or less perfect.

III. TRANSMISSION WINDOW MODEL

We saw in the previous section that the relative loss between the frequencies is roughly the same among different line shapes, although, the absolute loss is different. Assuming that we have a certain linear threshold γ for maximum absorption loss, i.e., to calculate available $10\log_{10}(\gamma)$ dB bandwidth within a transmission window, we can calculate the limiting frequencies by

$$\exp(d\mu N F(f)S(T)) = exp(d\mu N F(f_c)S(T))\gamma, \quad (17)$$

where $F(\cdot)$ is the line shape and f is the frequency at which the left-hand side of the equation is equal to the loss at center frequency of the transmission f_c multiplied with the threshold
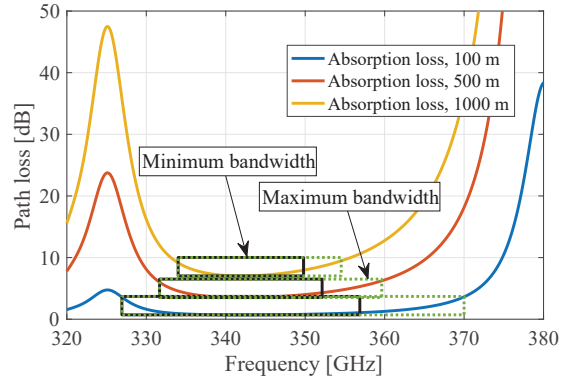

Fig. 5. The estimated transmission window widths in comparison to the absorption loss at different distances.

γ. Then,

$$F(f) = F(f_c) + \frac{\ln(\gamma)}{d\mu N S(T)}. \quad (18)$$

by applying the Lorentz line shape in (6) and assuming that the line shape is roughly symmetric around the line center, we get the frequency deviations from the line centers ($\Delta f = f - f_c^i$, where f_c^i is absorption line center) for the two meaningful absorption lines (325 and 380 GHz) as presented in Eqs. (19) and (20). In these equations, Δf_l is the frequency deviation from the 325 GHz absorption line where the absorption loss has increased by factor γ from the center frequency and Δf_h is the same for the 380 GHz line, and indices l and h refer in general to the lower and higher frequency absorption line parameters, respectively. The simplified versions are given by Eqs. (21) and (22).

Then the available bandwidths become

$$W_{\max} = f_c^h - \Delta f_h - (f_c^l + \Delta f_l), \quad (23)$$

$$W_{\min} = 2\min\{f_c^h - \Delta f_h - f_c, f_c - (f_c^l + \Delta f_l)\}, \quad (24)$$

where $W_{\max}$ indicates the maximum bandwidth limited by the preset threshold to upper and lower frequency band, and $W_{\min}$ tells the minimum bandwidth by single side limitation, i.e., when either side of the transmission center frequency reaches the preset threshold, the bandwidth is considered to be limited by it.

Figure 4 shows the available bandwidths according to (23) and (24) and for three-dB threshold at a transmission center frequency of 342 GHz. This particular frequency experiences the lowest loss between the two major absorption lines between 325 and 380 GHz. As it has been predicted earlier, e.g., in [6], [7], the available bandwidth decreases as a function of frequency because of the exponential molecular absorption loss as a function of distance. Fig. 5 shows the predicted available band as a function of frequency. We can see that the prediction is not exact due to error caused by the usage of the Lorentz line shape, similarly as in the previous section for the numerical prediction of the absorption loss. However, the error is not major and is about 2 GHz at one kilometer

$$\Delta f_l = c\sqrt{\left[\left(\left(\frac{f_c - f_c^l}{c}\right)^2 - (\alpha_L^l)^2\right)^{-1} + \frac{\pi \ln \gamma}{\alpha_L^l d\mu_{\mathrm{H_2O}} N S_l(T)}\right]^{-1} - (\alpha_L^l)^2}, \qquad (19)$$

$$\Delta f_h = c\sqrt{\left[\left(\left(\frac{f_c - f_c^h}{c}\right)^2 - (\alpha_L^h)^2\right)^{-1} + \frac{\pi \ln \gamma}{\alpha_L^h d\mu_{\mathrm{H_2O}} N S_h(T)}\right]^{-1} - (\alpha_L^h)^2}. \qquad (20)$$

$$\Delta f_l = \frac{c}{100}\sqrt{\left(\left[\left(\frac{100 f_c}{c} - 10.842\right)^2 + 0.0098\right]^{-1} + \frac{0.449\pi \ln(\gamma)}{\mu_{\mathrm{H_2O}}}\right)^{-1} - 0.0098}, \qquad (21)$$

$$\Delta f_h = \frac{c}{100}\sqrt{\left(\left[\left(\frac{100 f_c}{c} - 12.679\right)^2 + 0.0107\right]^{-1} + \frac{0.047\pi \ln(\gamma)}{\mu_{\mathrm{H_2O}}}\right)^{-1} - 0.0107}. \qquad (22)$$

distance. If we would increase the distance, also the error would increase. Thus, we see the one kilometer link distance as a maximum distance where this model can be considered relatively accurate.

IV. CONCLUSION

We have shown simple estimates for the molecular absorption loss and the expected bandwidths within the transmission windows in the 200 to 400 GHz frequency band. Despite of the simplicity, they provide an accurate way to estimate the molecular absorption loss without a need to implement complex absorption models and obtaining values from the databases. We showed that these models are very accurate and reliable at the given frequency range. Furthermore, the models can easily be extended to any possible frequency band. However, the complexity of the approximation increases as the number of absorption lines increases. Therefore, the links operating below one terahertz are easier to model numerically. The shown numerical models are very useful for millimeter and low terahertz band communications analysis. Both being among the potential frequency ranges for the future communications. Via accurate information on the absorption loss, one can easily predict the additional loss, and the maximum utilizable and application specific bandwidths.

V. ACKNOWLEDGEMENT

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