Time and Frequency Domain Analysis of Molecular Absorption in Short-range Terahertz Communications

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***Abstract*—Graphene is enabling a plethora of applications in wide range of fields due to its unique electrical, mechanical and optical properties. In this context, graphene antennas are envisioned to enable ultra-high-speed wireless communication in short transmission ranges, due to both their reduced size and their radiation frequency in the terahertz band. Despite its high potential bandwidth, the terahertz band presents several phenomena which may impair the communication and reduce the achievable data rate. In this paper, the phenomenon of molecular absorption is quantitatively analyzed, evaluating the scalability of both time- and frequency-domain performance metrics with the transmission distance. The results of this analysis show that molecular absorption creates a trade-off between the achievable throughput and the maximum transmission distance at which short-range terahertz wireless communications can successfully take place.**

***Index Terms*—Terahertz, Molecular absorption, Graphene antennas, Graphene-enabled Wireless Communications, Time domain.**

I. Introduction

Nanonetworks [1], communication networks of nanosystems, will boost the range of applications of nanotechnology, bringing new opportunities in fields as diverse as Information and Communication Technologies (ICT), biomedical technology or environmental research. Due to the unique characteristics of the electromagnetic physical channel at the nanoscale, classical communication paradigms need to undergo a profound revision before being applied to this new scenario.

A novel paradigm has recently emerged to implement nanonetworks: *Graphene-enabled Wireless Communications* (GWC) [2], whose key component are *graphene antennas* [3]. Graphene [4] exhibits novel plasmonic properties due to its internal structure, which allow a graphene antenna of a size in the order of 1 μm to radiate electromagnetic waves in the terahertz band (0.1–10 THz) [3], [5].

In this paper, we consider a communication channel in the terahertz frequency band, focusing on transmission distances from one centimeter to several meters. Based on a recent channel model for short-range wireless communications in the terahertz band [6], we study the impact of molecular absorption on the performance of GWC. In particular, we derive several performance metrics from the impulse response of molecular absorption in the time and frequency domains, as well as their scalability with respect to the transmission distance. A sample scenario where this study may be useful is that of Graphene Wireless Networks-on-Chip (GWNoC) [7], a novel approach that considers GWC to share information among the cores in a multiprocessor.

The remainder of this paper is structured as follows. Section II reviews a physical channel model for short-range terahertz communications, focusing on its differences with respect to the microwave radio channel. Section III details the environment and assumptions of this channel model. Next, Section IV shows the results of our analysis, which determine the achievable communication throughput in the considered scenario. Finally, Section V concludes the paper.

II. Background: Channel Models for the Terahertz Band

Short-range high-bandwidth terahertz wireless communications have been proposed for indoor scenarios with the objective of their standardization within the IEEE 802.15 Terahertz Interest Group, but they are aimed for transmission distances of several meters. In those cases, the propagation of terahertz waves is usually modeled by means of ray tracing and the atmospheric attenuation shows several peaks in the terahertz band [8].

However, these models are not directly applicable to a scenario of GWC, which usually comprise communication distances of less than 1 meter. Even at this short range, the phenomenon of molecular absorption will influence the propagation of the terahertz signals in the atmosphere [6].

Molecular absorption is the process by which part of the wave energy is converted into internal kinetic energy of the excited molecules in the medium. Indeed, since several molecules present in the standard atmosphere (such as water vapor molecules) have thousands of resonances in the terahertz band, they are excited by the terahertz electromagnetic waves radiated by antennas, converting part of the radiation into internal vibrations [8]. In addition to other factors such as spreading loss or fading, molecular absorption attenuates the propagated signals in wireless communications in the terahertz band. It can be modeled by the following analytical expression [6]:

$$\alpha_M(f,d) = \frac{1}{\tau} = e^{k(f)d} \tag{1}$$

where f is frequency, d is distance, τ is defined as the transmittance of the medium and k is the medium absorption coefficient. This last parameter depends on the medium composition, i.e., the particular mixture of molecules that the propagating wave finds along the channel.

We will analyze next the key impact of the highly frequency-dependent molecular absorption on the communication performance of GWC. In particular, its influence will depend on the transmission distance, which determines the number of molecules that the radiated terahertz waves will find along their path. Whereas narrowband signals may be attenuated by a constant absorption factor, molecular absorption will particularly degrade the propagation of wideband signals.

III. System Model

In this work, we consider a scenario of GWC where the transmission distance ranges from one centimeter up to several meters. The channel is modeled as a standard medium with 10% of water vapor molecules. Moreover, since current propagation models for GWC have not been experimentally validated, we analyze uniquely the effect of molecular absorption without considering other factors affecting the propagation loss. We assume a single point-to-point wireless link where communication is performed by the transmission of subpicosecond pulses, which allows using the whole terahertz band and maximizes the achievable data rate, in the order of Tbits/s.

In this context, we focus on the phenomenon of molecular absorption in the terahertz band and analyze it from both the frequency domain and, most importantly, the time domain, focusing in the channel impulse response due to molecular absorption. This dual analysis allows the evaluation of different performance metrics of a molecular absorption-impaired channel. For instance, from the frequency domain, we can compute the *available bandwidth* for transmission, defined as the frequency band where the attenuation caused by molecular absorption is below a given threshold.

The channel transfer function accounting for the effects of molecular absorption can be obtained from Eq. (1) as $H_M(f,d) = 1/\alpha_M(f,d)$. The impulse response of molecular absorption is the inverse Fourier transform of this channel transfer function: $h_M(t,d) = \mathcal{F}^{-1}\left[1/\alpha_M(f,d)\right]$. Convolving the impulse response of molecular absorption with the impulse response accounting for the remaining propagation effects (such as fading or multipath propagation) would allow obtaining the complete impulse response of the short-range terahertz channel. The impulse response of molecular absorption $h_M(t,d)$ allows the calculation of several relevant performance metrics [9], such as:

- *Response amplitude:* the amplitude A of the molecular absorption impulse response is defined as the maximum value of its instantaneous power: $A = \max_t |h_M(t,d)|^2$. A high amplitude value means that the energy is highly concentrated around the response peak. In most applications, receiving a signal with a high amplitude allows for a precise detection of the transmitted information.
- *Response width:* the width W of the impulse response is defined as the time interval during which the impulse response has a higher value than half the response peak, i.e., $W = t_0 : (h_M(t_0,d) < A/2) \wedge (\forall t : t < t_0 \rightarrow h_M(t,d) \geq A/2)$. A high W means that the molecular absorption distorts the transmitted pulses by increasing their width. Due to this pulse widening effect, molecular absorption might reduce the achievable data rate in GWC.
- *Response energy:* the energy E of the impulse response is defined as the integral of its instantaneous power over its duration: $E = \int_t |h_M(t,d)|^2 \mathrm{d}t$. The value of E indicates how molecular absorption affects the energy of transmitted pulses. A high pulse energy will improve the detection performance of non-coherent receivers in GWC.

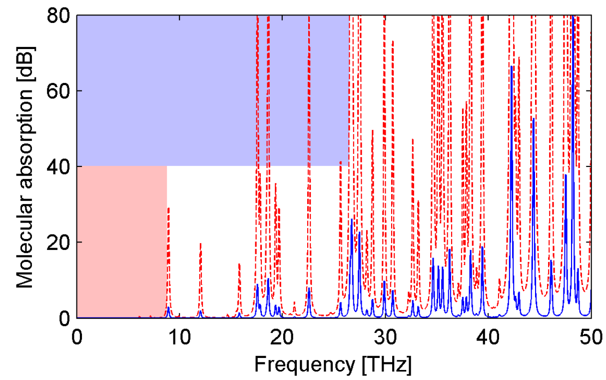

Fig. 1. Molecular absorption in dB for transmission distances of 1 cm (blue solid line) and 10 cm (red dashed line). The top blue (bottom red) background shows the frequency region which determines the available bandwidth for a transmission distance of 1 cm (10 cm).

IV. Results

We obtain next quantitative results which show some properties of the short-range terahertz channel with molecular absorption and the design parameters in a GWC system. Fig. 1 shows the molecular absorption of the terahertz channel as a function of frequency, for transmission distances of 1 cm and 10 cm. We observe that molecular absorption is highly dependent on the transmission distance, derived from its exponential dependence with the distance, as shown in Eq. (1). In this particular case, both the number of absorption peaks and their amplitude notably increase when the transmission distance changes from 1 to 10 cm.

Fig. 1 shows that molecular absorption creates several peaks of very high attenuation, which will create a limitation in the available bandwidth in GWC (defined in Section III). In order to quantify the available bandwidth as a function of the transmission distance, we consider the frequency band at which the value of molecular absorption is below a given threshold. Since this threshold will depend on the final implementation and the tolerable distortion, we choose 10 dB as an example. A different threshold would result in different quantitative values for the effective bandwidth, but with the same dependence on the transmission distance. In line with the pulse-based modulations which have been proposed in short-range terahertz communications [3], the range of frequencies considered ranges from baseband to 50 THz.

Fig. 1 allows measuring the range of frequencies which determine the available bandwidth for transmission distances of 1 cm (27 THz, top blue background) and 10 cm (9 THz, bottom red background). Fig. 2 shows a semi-log plot of the scalability of the available bandwidth with respect to

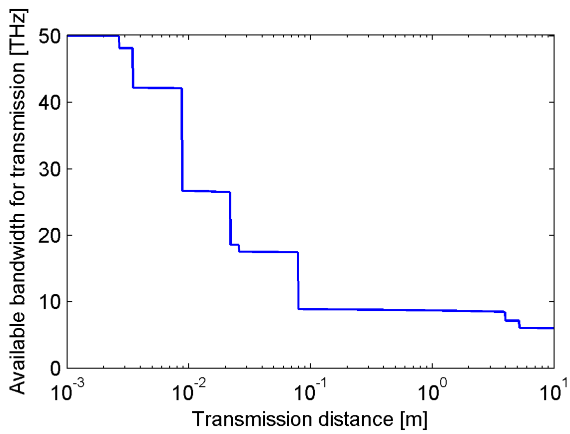

Fig. 2. Available bandwidth in the frequency band up to 50 THz due to molecular absorption.

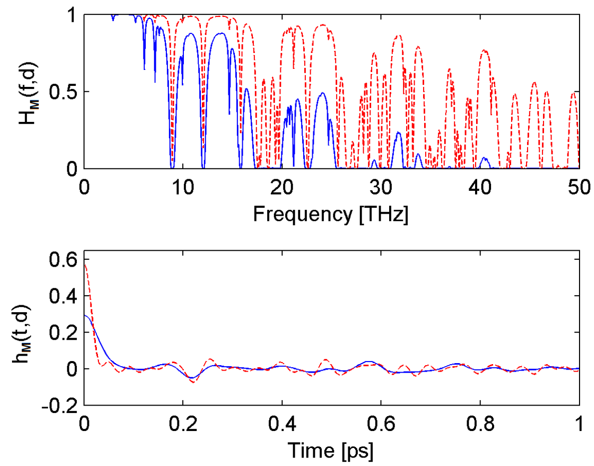

Fig. 3. Absorption-driven channel transfer function $H_M(f,d)$ (top) and channel impulse response $h_M(t,d)$ (bottom) of the molecular absorption for transmission distances of $d = 10$ cm (red dashed line) and $d = 1$ m (blue solid line).

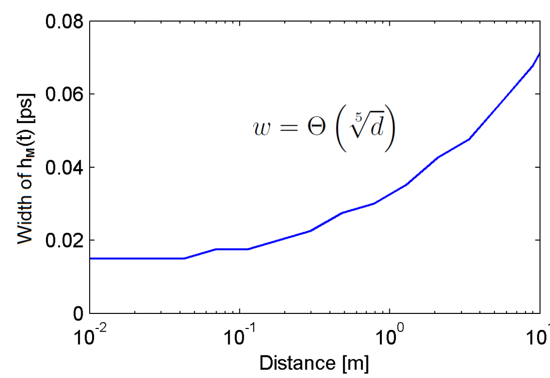

Fig. 4. Semi-log plot of the width of the channel impulse response due to molecular absorption.

the transmission distance. We observe a rapid decrease of the bandwidth as the distance increases, with several steps of different sizes corresponding to the molecular absorption peaks. For instance, molecular absorption has a negligible effect at short transmission distances and the whole 50 THz band is usable for distances up to 2.5 mm. On the other hand, for distances greater than 5 m, less than 6 THz are available for a molecular absorption-free transmission.

As mentioned in the previous section, the expression of the frequency-dependent molecular absorption can be used to obtain the channel impulse response due to molecular absorption. Fig. 3 shows both the channel transfer function and the impulse response of molecular absorption for two transmission distances. We see that, for a transmission distance of 10 cm (red dashed line), the channel transfer function shows a significant spectral content throughout most of the frequency band; whereas, when the distance is increased to 1 m (blue solid line), the molecular absorption blocks almost all the frequency components above 25 THz of the transmitted signal. Furthermore, this attenuation of the high-frequency components of the signal causes the channel impulse response to lower peak amplitude, a larger width and a smoother shape for the higher transmission distance. Assuming that the transmitted signals consist of subpicosecond pulses [3], the main implication of the dispersive behavior of the channel impulse response is that molecular absorption distorts the transmitted pulses, decreasing their amplitude and increasing their width. We will study these effects in more detail next.

Fig. 4 shows a semi-log plot of the width of the molecular absorption impulse response w as a function of the transmission distance d. A clear dependence of the width of the impulse response on the distance between transmitter and receiver is observed, with a scaling trend of $w/w_0 = \Theta\left(\sqrt[5]{d}\right)$ (notice the logarithmic horizontal axis in Figure 4). In particular, in order to achieve a communication throughput in the order of 1 Tbit/s, the received pulses will need to have a width of less than 1 ps. This result shows that, for instance, for a transmission distance of 3 m, the distortion introduced by molecular absorption is limited to 0.05 ps, thereby reducing the maximum achievable throughput by around 5 %. In short, given a target throughput, the width of the impulse response allows deriving the maximum transmission distance, as limited by molecular absorption.

The amplitude of the channel impulse response A is related to the attenuation caused by molecular absorption to a signal propagating in the terahertz channel. In Fig. 5 we can observe that, as expected, the amplitude of the impulse response decreases as the transmission distance increases, with a scaling trend of $A = \Theta\left(1/\sqrt{d}\right)$. For instance, the amplitude decreases by a factor of 10 when the transmission distance changes from 1 cm to 1 m. This substantial decrease indicates that the amplitude of the transmitted pulses will be highly attenuated by molecular absorption, thereby potentially impairing their detection by the receiver.

Another important metric to consider is how molecular absorption affects the energy of the transmitted signals. Since we have found that molecular absorption attenuates the transmitted signal (Fig. 5) but it also increases their width (Fig. 4), it is not clear how the signal energy measured by the receiver will scale with the transmission distance. Fig. 6 shows that the energy of the channel impulse response due to molecular absorption decreases with respect to the distance, with a

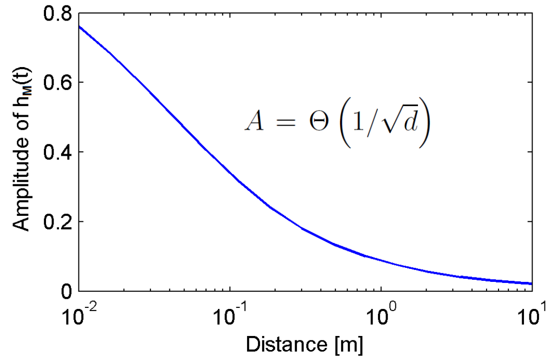

Fig. 5. Semi-log plot of the amplitude of the channel impulse response due to molecular absorption.

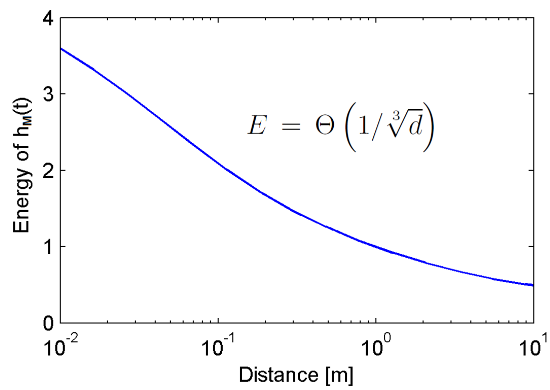

Fig. 6. Semi-log plot of the energy of the channel impulse response due to molecular absorption.

scaling trend of $E = \Theta\left(1/\sqrt[3]{d}\right)$. This result shows that the reduction of the signal energy occurs at a lower pace than that of its amplitude; by comparison, the energy decreases only by a factor of 4 when increasing the transmission distance by two orders of magnitude, from 1 cm to 1 m. As a consequence, an non-coherent detection scheme based on the signal energy may be better suited than a coherent detector in GWC affected by molecular absorption.

For the sake of comparison, in a scenario of an ideal free-space wireless communication channel with no molecular absorption, the channel impulse response would be a delta function independently of the transmission distance (without considering other factors affecting the loss). To summarize the results of this section, the scalability of the analyzed performance metrics in GWC is compared to the case of ideal free-space wireless communications, as a function of the transmission distance d, in the following table:

Metric	**Molecular absorption**	**No molecular absorption**
Width of $h_M(t,d)$	$\Theta(\sqrt[5]{d})$	$\Theta(1)$
Amplitude of $h_M(t,d)$	$\Theta(1/\sqrt{d})$	$\Theta(1)$
Energy of $h_M(t,d)$	$\Theta(1/\sqrt[3]{d})$	$\Theta(1)$

V. Conclusions

Graphene antennas offer great potential to implement wireless communications among nanosystems, due to their small size and high achievable bandwidth at short transmission distances, giving rise to Graphene-enabled Wireless Communications (GWC). The operation range of these antennas lies in the terahertz range, a frequency band which has not been widely explored for short distances of up to a few meters.

At the small scale of GWC, the phenomenon of molecular absorption will have a key impact on the atmospheric propagation of electromagnetic waves and, in consequence, in the communication performance of GWC. In this work, we analyze molecular absorption from both the frequency and the time domain, and in particular how its effects scale with respect to the transmission distance. We find that, on the one hand, for short transmission distances (below one meter), the effects of molecular absorption in the communication performance of GWC are limited to frequencies above 8 THz. On the other hand, for transmission distances greater than a few meters, molecular absorption presents a noticeable impairment in the propagation of terahertz wireless signals and its effects should be considered in order to achieve the target throughput rates of Tbits/s. Moreover, several performance metrics of GWC affected by molecular absorption are evaluated and they are found to show unique scaling trends with respect to traditional wireless communications, with implications in the design of GWC networks. For instance, the results show that in GWC receivers using an energy detection scheme may scale better with respect to the transmission distance than receivers based on amplitude detection.

These results provide guidelines for the design of modulations, protocols and architectures for future GWC systems that take advantage of the unique characteristics in the physical channel while minimizing the impairments of molecular absorption in order to optimize their communication performance. Further work modeling other propagation effects (such as fading) will enable the derivation of a complete channel model and link budget analysis for short-range terahertz communications.

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