The physical theory and propagation model of THz atmospheric propagation

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Abstract. Terahertz (THz) radiation is extensively applied in diverse fields, such as space communication, Earth environment observation, atmosphere science, remote sensing and so on. And the research on propagation features of THz wave in the atmosphere becomes more and more important. This paper firstly illuminates the advantages and outlook of THz in space technology. Then it introduces the theoretical framework of THz atmospheric propagation, including some fundamental physical concepts and processes. The attenuation effect (especially the absorption of water vapor), the scattering of aerosol particles and the effect of turbulent flow mainly influence THz atmosphere propagation. Fundamental physical laws are illuminated as well, such as Lamber-beer law, Mie scattering theory and radiative transfer equation. The last part comprises the demonstration and comparison of THz atmosphere propagation models like Moliere(V5), SARTre and AMATERASU. The essential problems are the deep analysis of physical mechanism of this process, the construction of atmospheric propagation model and databases of every kind of material in the atmosphere, and the standardization of measurement procedures.

1. Introduction
Terahertz radiation is the electromagnetic wave in the frequency interval from 0.1 to 10 THz (1THz=10^{12} Hz). It lies in the so-called “unexplored” range between visible light and radio wave, due to the difficulty of generating and detecting techniques in this region [1]. Recently, basic research and development in terahertz technologies are now underway for an increasing wide variety of applications, including information and communication technology (ICT), biomedical field, safety and security, non-destructive examination, quality control of food and agricultural products, and global
environmental monitoring [1,2]. The rapid development can be attributed to the nature of terahertz radiation, which offers the advantages of both microwave and light wave.

The atmospheric transmittance of terahertz wave now ranks among the most critical issues in the principal application of space communication and atmospheric remote sensing [2].

![Atmospheric transmission in the terahertz region at various locations and altitudes](image)

**Figure 1.** Atmospheric transmission in the terahertz region at various locations and altitudes

(a) 0-500 GHz, (b) 500-2000GHz.

The atmospheric opacity severely limits the communication application at terahertz range, which has been shown in figure 1[3]. Terahertz communication will benefit from the high-bit-rate wireless technology which takes advantage of higher frequency and broader information bandwidth allowed in this range than microwave [4]. Some THz frequency bands can be used for communications between locations separated several kilometers, and knowing accurately the location and width of atmospheric transmission windows will be of great importance. Other terahertz waves propagate less than 1m due to the significant attenuation of rotational transitions of molecules in the air and can be used for certain applications such as short-range secure communication.

As for the atmospheric remote sensing, THz technology is important in the environmental monitoring of atmospheric chemical species (water, oxygen, ozone, chlorine and nitrogen compounds, etc.), cloud and ice as well as taking temperature and other measurement [2]. A special emphasis has been put on the troposphere and lower stratosphere to learn climate evolution and the influence of pollution or biomass burning on the atmospheric composition. The knowledge about atmospheric attenuation will illustrate the optimum bands for sensing systems while the material database will discriminated atmospheric components. The overview of the THz remote sensing from the National Institute of Information and Communications Technology (NICT) in Japan is given in figure 2[5].
With respect to the research on terahertz atmospheric propagation, there are three fundamental problems as follow: [6]

1) To confirm the atmospheric transparency in the THz range and find out the air transmission windows for communicating and sensing system.

2) To collect the spectroscopic fingerprinting of atmospheric molecules for Terahertz atmospheric monitoring.

3) To improve the signal to noise ratio and restore the original signal from the observed signal by the process of deconvolution [7].

Based on these considerations, for many types of practical application, it is essential to understand the actual effects on the amplitude and phase of THz wave propagating through the atmosphere, which depends on the frequency of incident wave, gas components, and ambient temperature or barometric pressure in different atmospheric conditions.

This investigation aims to construct a terahertz radiation propagation model on the basis of the theoretical analysis and material database. It comprises the construction of an atmospheric radiative transfer equation as well as the collection of accurate spectroscopic parameters including standardization of the measurement protocol [8]. Section 1 outlines the significance and application of THz atmospheric propagation, including space communication and atmospheric remote sensing. Section 2 describes the fundamental theory in the THz atmospheric propagation, with the physical process of Lamber-beer law, Mie scattering theory and so on. The atmospheric absorption, emission and scattering are taken into account, and a special focus is put on the detailed derivation and physical significance of radiative transfer equation. Several THz atmospheric propagation model are introduced in Section 4, including Moliere, SARTre and AMATERASU. The last one has a strong heritage from the former two, respectively in the non-scattering case and scattering version. The conclusions are drawn in section 5 by giving the future evolutions and suggestions of further study in this region.
2. The fundamental physical theories

2.1. The framework of atmospheric propagation characteristics of THz-Wave

In the process of terahertz atmospheric propagation, there are several fundamental physical concepts and theories as figure 3:

![Diagram](image)

**Figure 3.** The fundamental physical concepts and theories.

1. Atmospheric extinction

The atmospheric extinction consists of the absorption and scattering effects, described by Lamber-Beer law and mainly causing the energy attenuation of incident wave. The differential and integral forms of the mathematical expression is

\[
\frac{dI}{d\nu} = -\alpha_v(z)I(\nu)dz
\]

\[
I_{r_i}(\nu) = I_{r_0}(\nu)\exp[-\int_{r_0}^{r_i} \alpha_v(z)dz]
\]  

(1)

\(\alpha_v(z)\) is the extinction coefficient and can be expressed as the summation of the absorption and scattering coefficient. But in accordance with most literatures at present, \(\alpha_v(z)\) only represents the absorption coefficient while the scattering effect has been discussed separately, so did we in this paper. 

\(I_{r_0}(\nu)\) denotes the incident radiance entering the optical path \((r_0, r_i)\) at the frequency \(\nu\) and \(I_{r_i}(\nu)\) is the outgoing radiance. The opacity or optical thickness is defined as

\[
\tau_v(r_0, r_i) = \int_{r_0}^{r_i} \alpha_v(z)dz
\]

and the transmission is

\[
\eta_{r_0, r_i} = \frac{I_{r_i}}{I_{r_0}} = \exp[-\tau_v(r_0, r_i)].
\]

The atmospheric absorption involves the linear absorption and continuum absorption, which will be described particularly in the next part.

The scattering effect comprises the molecular Rayleigh scattering and the Mie scattering by aerosols. The former can be neglected with the wavelength of THz radiation being in the order of...
aerosols. Aerosol particles mainly refer to the solid and liquid particles suspending in the atmosphere, for example, dusts, salts, ice particles and water droplets, and the Mie scattering effect mainly depends on their size-distribution, complex refractive index and the wavelength of incident radiation.

(2) Atmospheric turbulence

The essence of turbulence effect is the impact of medium disturbance on the transmission of incoming wave, due to the fluctuation of atmospheric refractive index. Fully coherent light beams are sensitive to the properties of the medium through which they are propagating and the turbulence-induced spatial broadening is the major limiting factor in most applications. Partially coherent beams are less affected by atmospheric turbulence than fully ones [9].

(3) Atmospheric refraction

The atmospheric refraction results from the uneven distribution of air in horizontal and vertical directions. When passing through the atmosphere, the line of sight is refracted and bended towards the surface of the planets. Taking refraction into account will correct and promote the radiative transfer path with some elementary geometrical relationships, as figure 4 shows.

![Figure 4. The radiation path and its modification due to atmospheric refraction.](image-url)
The background radiation of THz wave in atmosphere, depending on the geometries, mainly results from many kinds of electromagnetic radiation in the interstellar space or from the planet surface. For limb-sounding and up-looking, it is the cosmologic radiation at 3K, and for nadir-sounding (or down-looking), it is the earth surface emission.

In conclusion, the general idea to solve these problems above is to study the various effects independently and superpose them. Currently, most researches are mainly focused on the atmospheric extinction and the establishment of radiative transfer model, which will be introduced in the following text.

2.2. The absorption of water vapor

The linear and continuum absorption constitutes the atmospheric absorption of terahertz waves. The former is comprised most of the water vapor absorption lines in the air, which is due to the molecular rotational transitions. Their spectroscopic parameters, including the center frequency, oscillator intensity, and pressure broadening coefficient, should be measured by laboratory experiments precisely, as they will directly influence the accuracy of atmospheric propagation model [10]. There are several databases, such as JPL [11] and HITRAN [12], to stimulate the line by line absorption.

The continuum absorption is arbitrary because it is what remains after subtraction of linear contributions from the total absorption that can be measured directly [13]. Its generating mechanism is not sufficiently understood while several theories have proposed various causes, including anomalous far-wing absorption [14], absorption by dimmers and larger clusters of water vapor, and absorption by collisions between atmospheric molecules [15]. An empirical CKD model [16], proposed by Clough, Kneizys, and Davis, is applicable in a wide frequency range and has been proven successful in some aspects. For the simulation at frequencies below 400GHz, Liebe model [17] should be used for dry air and water vapor continua. Figure 5 [10] illustrates the discrepancy between radio-wave and infrared wave propagation models. The radio-wave model is calculated with JPL line catalog and Liebe model for continuum absorption while the infrared model is on the basis of HITRAN line catalog and CKD continuum model.

![THz wave propagation](image)

**Figure 5.** The linear and continuum absorption of THz wave from NICT.

It is difficult to measure spectroscopic parameters accurately in THz region due to the limitations of
measurement instruments in the past. Currently, Terahertz Time-domain Spectroscopy (THz-TDS) technology and Fourier-transform Infrared Spectroscopy (FT-IR) have attracted a great deal of attention in precise measurement of spectroscopic parameters. The former is advantageous at low frequencies less than 3 THz, while Fourier transform spectroscopy works better at frequencies above 5 THz [18].

2.3. The derivation of radiative transfer equation

The radiative transfer equation is determined by absorption and emission processes occurring along the line-of-sight. It is the foundation of atmospheric propagation model, and the derivation is as follow [19,20]:

\[ I_{v} + dl_{v} = \int I_{v} d\sigma \omega d\nu d\Omega dt \]  
\[ \text{where } I_{v} \text{ is radiant intensity, } d\sigma \text{ solid angle, } d\nu \text{ frequency interval, } d\sigma \text{ basal area, and } dt \text{ denotes the time of radiation. And the emergent radiant energy from surface II is:} \]
\[ dE_{\text{out}} = (I_{v} + dl_{v}) d\sigma \omega d\nu d\Omega dt \]  
\[ \text{According to the Lamber-beer law, with the absorption coefficient } \alpha_{v}, \text{ the radiant energy absorbed by the medium is:} \]
\[ dE_{a} = -\alpha_{v} dE_{\text{in}} dr = -\alpha_{v} I_{v} d\sigma \omega d\nu d\Omega dr \]  
\[ \text{With the emission coefficient } j_{v}, \text{ the radiant energy of medium emission is:} \]
\[ dE_{e} = j_{v} d\sigma \omega d\nu d\Omega dr \]  
\[ \text{In accordance with energy conservation law, we get:} \]
\[ dE_{\text{out}} = dE_{\text{in}} + dE_{e} + dE_{a} \]
Substituting equation (2)–(5) into equation (6):

\[
dl = j_v d\omega d\nu d\sigma d\tau dt + (-\alpha_v I_\nu) d\omega d\nu d\sigma d\tau dr
\]  

(7)

The source function is defined as \( S_v \equiv j_v / \alpha_v \), and assuming the local thermodynamic equilibrium (LTE), it equals the Planck function, according to Kirchhoff’s law:

\[
S_v \equiv j_v / \alpha_v = B_v (T)
\]

(8)

Given the definition of opacity or optical thickness: \( d\tau = \alpha_v d\tau \), we get the differential form of radiative transfer equation from equation (7):

\[
\frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu
\]

(9)

To solve this single-order partial differential equation along integral path \((r_0, r_1)\), with the integral variable \(r\), we get the integral form of radiative transfer equation:

\[
I_\nu (r_1) = I_\nu (r_0) \exp[-\int_{r_0}^{r_1} \alpha_v (r) dr] + \int_{r_0}^{r_1} \exp[-\int_{r_0}^{r_1} \alpha_v (r') dr'] S_v (r) \alpha_v (r) dr
\]

(10)

Under the assumption of local thermodynamic equilibrium, the equation can be written as:

\[
I_\nu (r_1) = I_\nu (r_0) \exp[-\int_{r_0}^{r_1} \alpha_v (r) dr] + \int_{r_0}^{r_1} B_v (T) \alpha_v (r) \exp[-\int_{r_0}^{r_1} \alpha_v (r') dr'] dr
\]

(11)

The physical significance of radiative equation lies in the processes of absorption and emission of atmosphere at the position \(r\) along a given optical path \((r_0, r_1)\), with the first term on the right side describing the background radiation attenuated by atmosphere while the second one standing for atmospheric emission and absorption. \(I_\nu (r_1)\) is the outgoing radiance reaching the sensor at the frequency \(\nu\) and \(I_\nu (r_0)\) corresponds to the background radiance entering the optical path, either the cosmologic radiation at 3K or the Earth surface emission, depending on geometries mentioned above. \(B_v (T)\) denotes the atmospheric source function which is given by Planck’s function describing the radiation of a black-body at temperature \(T\):

\[
B_v (T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp[h\nu/k_B T] - 1}
\]

(12)

where \(h\) is Planck’s constant, \(c\) the speed of light, and \(k_B\) denotes Boltzmann’s constant.

Note that the radiative transfer equation results from energy conservation law, so it is applicable to the whole electromagnetic spectrum, from radio wave to visible light including THz wave.

For the special case when the optical path goes through a medium at a constant temperature \(T\), the
equation above simply becomes:

\[ I_v(s_r) = I_v(s_e) \exp[-\int_{s_e}^{s_r} \alpha_v(s)ds] + \int_{s_e}^{s_r} B_v(T)\alpha_v(s) \exp[-\int_{s_e}^{s'} \alpha_v(s')ds']ds \]

\[ = I_v(s_e) \cdot \eta_{s_e,s_r} + B_v(T) \int_{s_e}^{s_r} \alpha_v \exp[-\alpha_v(s_r - s)]ds \]

\[ = I_v(s_e) \cdot \eta_{s_e,s_r} + B_v(T) \cdot (1 - \eta_{s_e,s_r}) \]  

3. THz atmospheric propagation model

3.1. Moliere

Microwave Observation Line Estimation and Retrieval (Moliere) is the versatile forward and inversion model for millimeter and sub-millimeter wavelength observations on board the Odin satellite, including a non-scattering radiative transfer model, a receiver simulator and an inversion code. The forward models comprise spectroscopic parameters, atmospheric radiative transfer model, and instrument characteristics in order to model and compute the searched atmospheric quantities. In parallel, inversion techniques have been developed to retrieve geophysical parameters such as temperature and trace gas mixing ratios from the remotely measured spectra [21].

Moliere is presently applied to data analysis for ground-based and space-borne heterodyne instruments and definition studies for future limb sensors dedicated to Earth observation and Mars exploration. However, this code can not be used when both up-looking and down-looking geometries should be considered together, and for limb geometry if the receiver is inside the atmosphere, such as balloon and airplane.

3.2. SARTre

The new radiative transfer model [Approximate] Spherical Atmospheric Radiative Transfer model (SARTre) has been developed to provide a consistent model that accounts for the influence of aerosols and clouds, e.g. water droplets or ice particles. It includes emission and absorption as well as scattering as sources/sinks of radiation from both solar and terrestrial sources in the spherical shell atmosphere and is able to analyze data measured over the spectral range from ultraviolet to microwaves [24]. SARTre is designed for monochromatic, high spectral resolution forward modeling of arbitrary observing geometries, especially for the limb observation technique.

The line-by-line calculation of molecular absorption cross sections has been adapted from the radiative transfer package MIRART (Modular Infrared Atmospheric Radiative Transfer). And the DISORT (Discrete Ordinate Radiative Transfer Model) package is used for the calculation of the incident radiation field when taking multiple scattering into account, under the assumption of a locally plane-parallel atmosphere [22].

3.3. AMATERASU

The Advanced Model for Atmospheric Terahertz Radiation Analysis and Simulation (AMATERASU) is developed by the National Institute of Information and Communications Technology (NICT) THz project. This project aims to develop THz technology for various applications concerning the telecommunications, atmospheric remote sensing and the study of the thermal atmospheric emission in
the Earth energy budget.

The first stage of this model concerns a non-scattering and homogeneous atmosphere, based on the original Moliere receiver simulator and retrieval codes. The absorption coefficient module has been extent to THz region and a more general radiative transfer module has been implemented to handle different geometries of optical paths and any location for the receiver [23].

The advanced version has a strong heritage from the SARTre model, considering the scattering effect. Modules related to optical properties of atmospheric particles and to scattering have been adapted from SARTre. The complex refractive index data of aerosols in THz region should be emphasized as a crucial parameter for single scattering properties of monodispersions and bulk optical properties, which are the necessary input of radiative transfer algorithms [24].

4. Conclusion
In this paper, we have discussed the fundamental theory in the process of THz atmospheric propagation, including Lamber-beer law, Mie scattering theory and the radiative transfer equation in detail. The key problems lie in the construction of radiative transfer algorithm, the collection of accurate spectral parameters, such as linear and continuum absorption and complex refractive index in THz region, and the standardization of measurement procedures. However, due to the lack in terahertz source and receiver technology, few experimental measurements have been made within this special region. Several kinds of THz atmospheric propagation model are introduced as well. There is a close inheritance relationship between them and these models should be compared with each other and validated against real laboratory measurements in order to check the correctness of the data accuracy and the algorithm hypothesis. The ultimate aim is to construct the atmospheric propagation model under different kinds of climatic conditions on the basis of the theoretical analysis and the material database.

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