Postprint: Simulation Study of Microwave and Submillimeter Wave Radiation in Planetary Atmospheres

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Date: 2017-01-22T00:00:00+00:00

Abstract

To analyze the radiative transfer characteristics of planetary atmospheres in the microwave-submillimeter wave band, the line-by-line integration method is employed to calculate the absorption coefficients of various atmospheric gas components within this band. Based on parameters such as transition frequencies and line strengths of gas molecules from the HITRAN database, the absorption characteristics of various gas molecules in the 1-3 THz frequency range are effectively simulated and compared with existing Earth atmospheric microwave radiative transfer models. As a special case, the composition and characteristics of Earth and Martian atmospheres are analyzed, and brightness temperature simulations for Earth atmospheric radiative transfer are performed using the radiative transfer equation, providing a model and theoretical basis for subsequent selection of detection bands and profile retrieval of planetary atmospheric composition.

Full Text

Preamble

Simulation of Microwave and Sub-Millimeter Wave Radiation of Planetary Atmospheres

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Abstract

To analyze the radiative transfer characteristics of planetary atmospheres in the microwave and sub-millimeter wave bands, we calculate the absorption coefficients of atmospheric gas components using the line-by-line integration method. Based on molecular transition frequencies, line intensities, and other parameters from the HITRAN database, we effectively simulate the absorption features of various gas molecules in the 1-3 THz frequency range and compare them with existing Earth atmospheric microwave radiative transfer models. As a case study, we analyze the composition and characteristics of Earth’ s and Mars’ atmospheres, and simulate the brightness temperature of Earth’ s atmospheric radiative transfer using the radiative transfer equation. This work provides a model and theoretical foundation for the selection of detection frequency bands and atmospheric profile retrieval for planetary atmospheric composition sensing.

Keywords: line-by-line integration, absorption coefficient, HITRAN database, radiative transfer characteristics of planetary atmospheres

0 Introduction

Several planets in the solar system possess atmospheres, including Earth, Mars, Jupiter, and Venus. These planetary atmospheres contain various gas components, and detecting their composition holds significant scientific importance. Microwave and sub-millimeter wave (hereinafter referred to as microwave) remote sensing represents a crucial tool for studying planetary atmospheres and surfaces because this band can typically penetrate the atmosphere, offers good directionality, and enables all-day, all-weather observations independent of light sources. Additionally, microwave radiation exhibits characteristics such as transient nature, broadband capability, coherence, low energy, and penetrative ability [1].

In the microwave band, planetary atmospheric components exhibit distinct absorption spectral lines that enable remote sensing detection. For Earth remote sensing, the 183.31 GHz water vapor absorption peak is utilized for atmospheric humidity profiling, while the 50-60 GHz and 118.75 GHz oxygen absorption bands enable temperature profiling through atmospheric oxygen detection [2]. Furthermore, limb sounding of atmospheric trace gases can be performed using their characteristic absorption lines in the microwave band [3].

For most microwave remote sensing observations of Earth’ s atmosphere, the lower atmosphere is the primary region of interest because it contains the majority of atmospheric mass and significantly influences surface remote sensing. In Earth microwave remote sensing, the atmospheric components that predominantly affect microwave-submillimeter wave radiation processes include oxygen, water vapor, and nitrogen. Other gases are present in such minute quantities that their effects are negligible. Consequently, atmospheric absorption is commonly simulated using microwave millimeter-wave atmospheric absorption models such as MPM/PWR [4], which typically consider only oxygen lines, nonresonant oxygen absorption, water vapor lines, water vapor continuum absorption, nitrogen, suspended cloud particles, and rain absorption and scattering coefficients.

However, when studying the middle and upper atmosphere of Earth or the surface atmospheres of other planets, these simplified models prove insufficient. The absorption spectral lines of additional gases such as O , SO , and NO in the microwave-submillimeter wave band must also be considered.

Foreign atmospheric radiative transfer models in the microwave band, including ARTS [5], LBLRTM [6], LinePak [7], MODTRAN, and RTTOV [8], have already incorporated gases beyond oxygen, water vapor, and nitrogen. To address these limitations, this paper employs the line-by-line integration method to calculate gas absorption coefficients in the microwave-submillimeter wave band and simulates radiative brightness temperatures. We first introduce planetary atmospheric composition and the radiative transfer process. Then, based on the HITRAN database and using the line-by-line integration method, we calculate the absorption coefficient of each gas under specific temperature, pressure, and density conditions, analyzing their absorption characteristics to inform future gas detection frequency band selection. Finally, we analyze atmospheric profile data for Earth and Mars, simulating Earth' s atmospheric transmittance and detection system brightness temperature to provide a model and theoretical basis for various atmospheric information retrieval algorithms.

1.1 Planetary Atmosphere

In the solar system, planets with atmospheres include Earth, Mars, Jupiter, and Venus. Earth' s atmosphere comprises various gas molecules, including nitrogen, oxygen, hydrogen, carbon dioxide, water vapor, ozone, helium, and neon. Based on concentration levels, Earth' s atmospheric gases are generally classified into major, minor, and trace components. Major components, with concentrations above 300 ppmv, include N (78.08%), O (20.95%), and Ar (0.93%). Minor components have concentrations between 1-20 ppmv, such as CO and H O. Trace components have concentrations below 1 ppmv and include O , SO , NO , nitrogen oxides (NO), sulfides, and anthropogenic pollutants such as chlorofluorocarbons. Atmospheric gas density decreases gradually with altitude.

The atmosphere surrounding Mars is far more tenuous than Earth' s, with a density less than one percent of Earth's atmosphere. Observational data indicate that Mars' atmospheric composition is dominated by CO (95.32%), followed by N (2.7%), with O content being relatively low at only 0.03%. The CO concentration decreases with altitude; at 100 km altitude, CO constitutes 50% of the atmosphere, while at 140 km, oxygen content is six times greater than CO [9]. Mars' surface pressure is 5.6 mbar (560 Pa), equivalent to Earth' s atmospheric pressure at 37 km altitude. The average surface temperature is approximately 210 K, ranging from 140-300 K, with highly asymmetric thermal conditions between the northern and southern hemispheres exhibiting significant seasonal and latitudinal variations [10][11][12].

Mars' atmosphere is divided into three layers: lower, middle, and upper. The lower atmosphere extends below 45 km, where temperature decreases with increasing altitude. In the middle atmosphere (45-110 km), temperature remains essentially constant. Above 110 km lies the upper atmosphere, where temperature increases with altitude; this layer is also known as the thermosphere.

1.2 Principles of Planetary Atmospheric Radiative Transfer

Atmospheric radiative transfer refers to the propagation process of electromagnetic waves through atmospheric media. When illuminated by external electromagnetic radiation, the atmosphere undergoes absorption, reflection, scattering, and transmission, while also emitting energy itself. The interaction between electromagnetic waves and atmospheric constituents is governed by wave properties and atmospheric physical characteristics (pressure, temperature, etc.) as well as atmospheric composition. Atmospheric microwave radiation features can be described by absorption spectra [13]. In the microwave-submillimeter wave band, numerous atmospheric molecules exhibit absorption lines.

Under ideal conditions, we consider only atmospheric microwave radiation emission and absorption processes. The radiation field is typically described by microwave radiation intensity I_f, which propagates along a specific direction. The differential form of the radiative transfer equation is:

$$\frac{dI_f}{ds} = -\alpha I_f + S_f$$

where α represents the atmospheric absorption coefficient, I_f denotes the microwave radiation intensity at frequency f propagating in direction s, and S_f is the source term describing energy loss and gain along a given direction. According to Kirchhoff' s law, thermal radiation and absorption coefficients are proportional to the Planck function [14]. Therefore, the source term S_f can be expressed as:

$$S_f = \alpha B_f(T)$$

where $B_f(T)$ is the Planck function representing blackbody radiation intensity:

$$B_f(T) = \frac{2hf^3}{c^2} \frac{1}{e^{hf/kT} - 1}$$

where T is thermodynamic temperature, c is the speed of light, f is frequency, h is Planck' s constant, and k is Boltzmann' s constant.

For planetary surface microwave-submillimeter wave atmospheric detection systems, substituting the source term yields:

$$I_f(s) = I_f(0)e^{-\tau(s)} + \int_0^s \alpha(s')B_f[T(s')]e^{-[\tau(s)-\tau(s')]}ds'$$

where $I_f(s)$ is the microwave radiation intensity at frequency f at the planetary surface, $I_f(0)$ represents the initial radiation intensity at boundary $s = 0$, $B_f[T(s')]$ is the blackbody radiation intensity at point s', $\alpha(s')$ is the absorption coefficient at point s', and the optical thickness τ from point s' to s is:

$$\tau(s) = \int_0^s \alpha(s')ds'$$

Thus, simulating the forward process of planetary atmospheric transmission requires obtaining the atmospheric absorption coefficient profile. For mixed gases, the total absorption coefficient equals the sum of individual gas absorption coefficients. We calculate each gas' s absorption coefficient using the line-by-line integration method based on the HITRAN database.

2.1 Line-by-Line Integration Principle

The line-by-line integration method is the most accurate approach for addressing atmospheric radiative transfer problems involving non-uniform paths and overlapping absorption bands, enabling calculation of absorption coefficients for various gas molecules in planetary atmospheres [15].

In the microwave-submillimeter wave band, atmospheric gases exhibit rotational transitions. According to molecular spectroscopy theory, energy absorption or emission occurs when molecules transition between energy levels. When a molecule transitions from a higher to a lower energy state with energy reduction ΔE, Einstein' s formula dictates that it radiates energy at frequency $\nu = \Delta E/h$ into the surrounding space. Consequently, all possible transitions constitute the gas' s radiation spectrum, with each transition corresponding to a spectral line. In the microwave-submillimeter wave band, various gases possess numerous characteristic absorption lines. Figure 1 [Figure 1: see original paper] shows the relationship between absorption line intensity and transition frequency for the H O molecule in the HITRAN2012 database under 1 atm and 296 K conditions, containing 224,515 lines across 1–800 THz, with 3,093 lines in the 1–3 THz range.

The line intensity at a specific temperature can be transformed to other temperatures using:

$$S(T) = S(T_0)\frac{Q(T_0)}{Q(T)}\exp\left[-\frac{E''}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]$$

where $S(T_0)$ is the line intensity at reference temperature T_0, E'' is the lower state energy, k is Boltzmann' s constant, and exponent β varies by molecule (generally 1 for linear molecules, 1.5 for non-linear molecules, and 1 for O).

In practice, each absorption line does not exhibit ideal line absorption at a single frequency. Three effects influence line width and shape, causing line broadening.

When molecules are excited and transition between energy levels, a finite time is required. According to quantum mechanics' uncertainty principle, this introduces a frequency uncertainty, creating a natural line width that is extremely small. Molecular collisions and Doppler frequency shifts from thermal motion further broaden the lines through pressure broadening and Doppler broadening.

At low gas densities with minimal intermolecular collisions, Doppler broadening dominates. The Doppler-broadened line shape is:

$$F_D(\nu) = \frac{1}{\gamma_D\sqrt{\pi}}\exp\left[-\frac{(\nu-\nu_0)^2}{\gamma_D^2}\right]$$

where the Doppler width γ_D is:

$$\gamma_D = \frac{\nu_0}{c}\sqrt{\frac{2kT}{M}}$$

At high gas densities with frequent molecular collisions, pressure broadening dominates, which we approximate using the Lorentzian function:

$$F_L(\nu) = \frac{1}{\pi}\frac{\gamma_L}{(\nu-\nu_0)^2 + \gamma_L^2}$$

where the Lorentzian width γ_L is:

$$\gamma_L = \gamma_{air}\left(\frac{P_t}{P_0}\right)\left(\frac{T_0}{T}\right)^n$$

with γ_{air} as the air-broadened half-width, P_t as total pressure, and n as the temperature dependence coefficient (0-1).

In regions where both pressure and Doppler broadening are significant, the Voigt line shape function approximates the convolution of Lorentzian and Doppler functions:

$$F_V(\nu) = \int_{-\infty}^{\infty} F_L(\nu')F_D(\nu - \nu')d\nu'$$

For Earth atmospheric absorption calculations, the Lorentzian shape is used below 30 km, the Doppler shape above 50 km, and the Voigt shape between 30-50 km. Figure 2 [Figure 2: see original paper] shows the Lorentzian line shape for the H O molecule transition at 183.4370 GHz under 1 atm and 296 K conditions.

Given the line intensity and shape for a single line, the absorption cross-section is:

$$\sigma(\nu) = S \cdot f(\nu)$$

where S is line intensity and $f(\nu)$ is the line shape function. The single-line absorption coefficient is:

$$\alpha(\nu) = n \cdot \sigma(\nu)$$

where n is number density (units of m ³).

When the shape and intensity information for each spectral line of a gas molecule are known, the absorption coefficient at any frequency ν equals the sum of contributions from all lines:

$$\alpha(\nu) = \sum_i \alpha_i(\nu)$$

2.2 HITRAN Database

Practical implementation of the line-by-line integration method requires spectroscopic information for target gases, including transition frequencies, line intensities, and line widths, which must be obtained from databases. Available databases include JPL, HITRAN, and GEISA. The JPL database lacks complete information for simulating atmospheric spectral lines, such as line broadening parameters, necessitating data merging. The HITRAN database offers broad spectral coverage and comprehensive line information, making it the most widely used database.

All simulations in this paper are based on the HITRAN2012 database. The High-resolution Transmission Molecular Spectroscopy Database (HITRAN) compiles spectroscopic parameters for multiple gases, primarily for atmospheric research in the 0-20,000 cm ¹ spectral region, using computer codes to predict and simulate atmospheric light transmission and emission. Initiated in the late 1960s by the Air Force Cambridge Research Laboratories (AFCRL) and first released in 1973 (AFCRL-TR0096), the database has undergone numerous updates (1978, 1983, 1992, 1996, 2000, 2004, 2008, 2012), forming a comprehensive database of absorption line parameters for 47 important gas molecules including H O, CO , and O . The choice of HITRAN version affects calculation accuracy [16]. This paper utilizes the HITRAN2012 database [17] and its JavaHAWKS application software to obtain spectral parameters for target gas molecules under specified temperature, pressure, and wavelength conditions. Table 1 lists the molecular species and number of lines in HITRAN2012, while Table 2 details the spectroscopic parameters included for each line.

2.3 Calculation of Absorption Coefficients for Various Gases

Figure 3 [Figure 3: see original paper] presents a flowchart for calculating gas absorption coefficients using the line-by-line integration method. The process begins with input atmospheric parameters and HITRAN spectroscopic data, selects appropriate line shapes, calculates single-line absorption cross-sections and molecular densities, and determines single-line absorption coefficients. The line-by-line integration method then computes single-species absorption coefficients, with the total absorption coefficient for mixed gases being the sum of individual species contributions.

Using H O as an example under 1 atm and 296 K conditions with a mass concentration of 1 g/m^3, Figure 4 [Figure 4: see original paper] shows the relationship between absorption coefficient and frequency for lines at 22.2507 GHz, 67.8508 GHz, 183.4370 GHz, 321.4479 GHz, 390.8782 GHz, 437.6495 GHz, and 557.3216 GHz. Figure 5 [Figure 5: see original paper] displays the H O absorption coefficient across 1-3000 GHz under the same conditions.

Comparing our line-by-line integration results with existing microwave-millimeter wave atmospheric absorption models (MPM89, MPM93, PWR98, PWR04) for H O at 1 atm, 296 K, and 1 g/m^3 concentration over 0-800 GHz reveals close agreement (Figure 6 [Figure 6: see original paper]).

Figures 7 [Figure 7: see original paper] through 13 [Figure 13: see original paper] present absorption coefficients for O , N O, CO, CH , O , N , and CO gases at 1 atm, 296 K, and 1 g/m^3 concentration across 1-3000 GHz. These results demonstrate that each gas exhibits multiple absorption peaks in the microwave-submillimeter wave band, enabling selection of appropriate bands for specific gas detection. When selecting detection frequencies, both the target gas’ s prominent absorption peaks and potential interference from other gases absorbing in the same band must be considered.

3 Simulation of Planetary Atmospheric Radiative Transfer Process

For Earth, atmospheric profile data are provided by the 1976 U.S. Standard Atmosphere, including altitude, pressure, temperature, density, and volume mixing ratios of various gases. For Mars, atmospheric data were obtained from the Mariner 9 and Viking 1 and 2 landers. Figure 14 [Figure 14: see original paper] shows temperature profiles for Earth and Mars, while Figure 15 [Figure 15: see original paper] displays volume mixing ratio profiles for H O, O , N O, CO, CH , O , and N from the U.S. Standard Atmosphere.

Given planetary atmospheric profile parameters, we calculate the total atmospheric absorption coefficient using the line-by-line integration method. Optical thickness and transmittance are then computed layer by layer, and brightness temperature is simulated using the radiative transfer equation (Figure 16 [Figure 16: see original paper]).

For a ground-based Earth observation system considering only H O, O , and N effects, layer-by-layer transmittance calculations yield the simulated brightness temperature shown in Figure 17 [Figure 17: see original paper]. Adding O and comparing the results reveals brightness temperature differences of 0–3.5 K across 1-1000 GHz for ground-based systems (Figure 18 [Figure 18: see original paper]).

4 Conclusion

This paper analyzes the radiative transfer process in planetary atmospheres within the microwave-submillimeter wave band. Based on the HITRAN database and using the line-by-line integration method, we obtain absorption coefficients for individual gases under specific conditions and analyze the atmospheric characteristics of Earth and Mars. Simulations of Earth' s atmospheric microwave radiative transfer forward process provide a model and theoretical foundation for gas detection frequency band selection and various atmospheric information retrieval algorithms.

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