Observation Capability of a Ground-based Terahertz Radiometer for Vertical Profiles of Oxygen and Water abundances in Martian atmosphere

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Abstract—We present expected performance for a ground-based Terahertz (THz) radiometer, plan to be launched on the TEREX-1 (TERahertz EXplore-1) Mars exploration micro spacecraft. The small THz passive radiometer has been developed for the TEREX series of future micro spacecrafts. This spacecraft is an opportunity for organizations with limited resources and technology to conduct frequent missions to Mars well suited for resource exploration in contrast to all of the current and past Mars missions of large/giant class missions with fully government lead. The observation frequencies of TEREX-1 radiometer are 474.64–475.64 and 486.64–487.64 GHz with 100 kHz resolution, and the double-sideband noise temperature less than 3000 K. A theoretical error analysis is performed with the instrument characteristics to assess for the first time up-looking observations of atmospheric Oxygen molecules (O$_2$) and water vapor (H$_2$O). Measurement errors for O$_2$ and H$_2$O are 7–22% and 14–25% with 8–17 km and 5–10 km vertical resolution in the vertical ranges 0 to 55 km and 0 to 25 km, respectively. TEREX-1 is also capable to measure minor species, O$_3$ and H$_2$O$_2$, with a precision better than 30% within two independent layers. We used the integration time of 1 hour for all simulations. Our theoretical simulation showed the instrument characteristics of the TEREX-1 sensor is able to observe vertical profiles of O$_2$ and H$_2$O abundances with the same level of the large class missions.

Index Terms—Mars, terahertz, atmospheric observation, lander, error analysis.

I. INTRODUCTION

The Vertical profiles of molecular oxygen (O$_2$) and water vapor (H$_2$O) have important roles to understand the oxygen and water cycle on Mars [e.g. 1, 2, 3, 4]. Especially, previous studies suggested that the vertical profiles of O$_2$ and H$_2$O at lower altitude is influenced by surface processes on Mars. The global distribution and seasonal variations of water vapor and clouds have been relatively well understood since the first detection in 1963 [5]. A perturbed vertical profile of water vapor below 30 km altitude, which was previously thought to be uniform, was suggested [2]. This is likely to be affected by a more complex Martian water environment near the surface than expected, and future observations at various seasons, locations, and times are needed to understand the heterogeneity up to 30 km especially the variability below 5 km [2]. Molecular oxygen in the Martian atmosphere has been measured by in-situ instruments of a rover [6] and landers [7], by remote sensing on Earth-orbiting satellite [8] and from ground-based telescopes on the Earth [9, 10]. The high signal-to-noise ratio spectral data of Herschel/HIFI (The Heterodyne Instrument for the Far-Infrared) observations indicate a potential increase of O$_2$ concentration near the surface [8], although the O$_2$ has been considered to have a vertically constant profile of about 1400 ppmv. The low-altitude O$_2$ profile is a key for understanding possible emission of O$_2$ from the surface, and to assess oxidation capacity of the Martian atmosphere (oxidizing water-vapor, methane, and various hydrogen radicals). However, the low-altitude O$_2$ and H$_2$O profiles have not been properly measured yet.

Remote sensing the submillimetre-wave range up to frequencies of approximately 5 terahertz (THz) were able to measure with high-frequency resolution, individual rotational transitions of molecules in the thermal emission of atmospheres of the astrophysical targets. Previous observations using the submillimetre-wave range have been conducted by ground-based or earth-orbiting satellite measurements for the study of Mars. Ground-based observations have mainly detected minor species using its high-frequency resolution and signal-to-noise ratio rather than water and oxygen lines because they are absorbed by the Earth’s atmosphere. The ground based measurement have suggested upper limits of volatile gases such as SO$_2$, SO$_3$, H$_2$S, and OCS by using disk-averaged spectra [e.g. 11, 12, 13]. The H$_2$O$_2$ observation with the James Clerk Maxwell Telescope (JCMT) suggested that the observed amount, 18±0.4 ppbv at 0–30 km of altitude, is three times larger than the upper-limit level of the previous study [14]. The Submillimeter Wave Astronomy Satellite (SWAS) demonstrated high sensitivity of CO and H$_2$O observations and found a ~20 K drop in surface brightness temperature.
during a global dust storm [15, 16]. The Odin satellite provided constraints on the surface H$_2$O mixing ratios of 2–3 × 10$^{-4}$ in disk-averaged spectrum [17]. Using Herschel/HIFI observations, Hartogh et al. [8] derived a constant volume mixing ratio (vrm) of 1400±120 ppm for O$_2$ and determined upper limits of 2 ppm for H$_2$O$_2$. For further investigations, measurements from Mars-orbiting satellites are expected to improve the precision and the resolution, and to expand the observation coverage of local-time, vertical and spatial distributions, especially during dust events.

Space-borne THz limb sounders orbiting Mars are under study to measure global vertical profiles of parameters such as water vapor, oxygen molecules, carbon monoxide, trace gases (e.g. O$_3$ and H$_2$O$_2$), their isotopologues, winds, and temperature [18, 19, 20, 21]. However, these projects have not been realized yet. Larsson et al. [21] proposed a limb and nadir submillimeter sensor under construction, named Terahertz Explore (TEREX) and a sensitivity study for the measurement of O$_3$, O$_2$, H$_2$O, and H$_2$O$_2$ volume mixing ratios as well as the wind speed and magnetic field strength. The estimated errors in 1 h nadir observation are approximately 1% from 10–40 km of altitude with about 20 km vertical resolution for O$_2$ and H$_2$O. It was decided that the realization of the TEREX orbiter comes after a lander mission due to the limitation of the amount of the propellant for the satellite thruster required for limb observations [22, 23].

The same TEREX, named TEREX-1, is now considered for Ground-based observations on the Martian surface and will be the main payload of a lander under design [22, 23]. The lander is designed such that it can be constructed and operated by organizations with limited resources and technology such as universities or emerging countries. Such observations will be complementary to those performed by Mars orbiters by providing continuous measurements over the same position. Compared to the satellite measurement [18, 19, 20, 21], the ground-based measurement is less sensitive especially for resolving the vertical profile of the atmospheric parameter. The advantage of ground-based observations is the possibility of increasing the observation time to improve the precision. TEREX-1 would be the first terahertz remote sensing instrument operating from the surface of a planet other than Earth, and this study is the first simulation study for such an instrument. The study aims at specifying the scientific value of this instrument by assessing the measurement errors, the vertical and time resolutions of the targeted molecules of O$_2$, H$_2$O, O$_3$, and H$_2$O$_2$.

The contents of the manuscript are organized as follows. Section II provides an overview of TEREX-1 including the measurement method. In Section III, we describe the measurement simulation setup including radiative transfer calculation, i.e. the forward model, retrieval error analysis, and parameters for these calculations. In Section IV, we present the results of error analysis for the targeted molecules. Finally, in Section V we summarize our main results and future implications.

II. TEREX-1

TEREX is the name of the series of future micro-satellite missions to Mars. It is a microsatellite to realize frequent opportunities to go to Mars for resource exploration, such as O$_2$ and H$_2$O as a piggyback spacecraft of another large Mars orbiter or lander [21, 22, 23]. As explained in the Introduction, the lander will be the first mission and subsequent will be orbiters [21]. The lander was conceptually designed for a novel, small, and simple Mars lander with simulations of Entry, Descent, and Landing processes, and a feasible thermal and power plan while conducting a THz sensor mission on the Martian surface [22, 23].

A. Instrument description

Since the sensor is to be mounted on the micro lander, it is expected to be light (<8 kg), small (384 × 384 × 357 mm$^3$), and with low power budget (30 W). The instrument configuration is mostly inherited from the orbiter design [21], which was under development. The local oscillator changed from 484.15 GHz to 481.14 GHz with a central intermediate frequency of 6 GHz due to the specification of a phase-locked dielectric resonator oscillator. It will operate in double-side-band (DSB) mode so that the measured radiation will be between 474.64–475.64 and 486.64–487.64 GHz which includes absorption lines of O$_2$ at 487.25 GHz, H$_2$O at 474.69 GHz, H$_2$O$_2$ at 475.20 and 487.20 GHz, and O$_3$ at 487.35 GHz. As discussed in Larsson et al. [21], this frequency range is decided by the trade-off between O$_2$ at the upper-sideband and H$_2$O at the lower-sideband frequency. After down-converted to the IF signals, the power level is amplified to turn this analog signal into a digital signal by a digital fast Fourier transform (FFT) spectrometer [24]. The system noise temperature is expected to be approximately 3000 K in DSB mode. The frequency resolution is expected to be less than 100 kHz. The antenna is made of carbon fiber reinforced plastic, and its diameter is about 20 cm. The antenna design is also inherited from the original limb sounder, which is used to avoid sidelobe contamination due to the surface emission. The observation time was supposed to be ∼1 hour during a day according to the power plan [22]. Further information related to TEREX-1 instrument such as an optical system including calibration loads and spectrometer can be found in Nakagawa et al. [24, 25].

B. Measurement method

The sensor was originally developed for the orbiter system, although it was modified minimally to enable the observation by the lander system. Fig. 1 shows the optical paths when observing the atmosphere, the calibration hot load ($T_c$), and the subcalibration load ($T_d$). The backend is a dual polarized receiver, but only one channel is used at a time. The second one will be a back-up system. TEREX-1 will operate with an up-looking geometry with a single FOV. The landing procedure is defined so that the antenna part faces the zenith to measure the atmosphere [22]. The precise antenna direction will depend on the attitude of the lander that will be derived from a three-axis accelerometer. The observation procedure uses a beam switching technique to calibrate the measured power. Unlike for the original orbiter, the cold space cannot be
used as the zero reference temperature. Calibration of the measured power will be performed using the hot and subcalibration loads whose temperatures will be monitored accurately. They are expected to be approximately 300 and 235 K for \( T_h \) and \( T_c \), owing to the internal heat generation of mission instruments and the exposure to the outside atmosphere (Fig. 1).

Typically, the raw power \( P \) measured with the radiometer is

\[
P_i = G(T_{sys} + T_i)
\]

where \( G \) is the radiometric gain, and \( T_{sys} \) is the double-sideband system temperature, and \( T_i \) is the measured intensity expressed in Rayleigh-Jeans temperature [26]. Note that these parameters are frequency dependent. The subscript \( i \) denotes the source of the signal, namely, \( a \), \( h \) or \( c \), for atmosphere, hot and subcalibration loads, respectively. The calibrated spectrum \( T_a \) is estimated by linear interpolation of the signals emitted by a hot and cold load:

\[
T_a = \frac{T_h - T_c}{P_h - P_c} (P_a - P_c) + T_c.
\]

The random noise on the calibrated spectra is

\[
\sigma_{n,T}^2 = \frac{1}{\Delta \nu T^4/4} \left[ \frac{(T_a + T_{sys})^2}{2} + \frac{(T_a - T_a)^2}{(T_h - T_a)^2} (T_h + T_{sys})^2 \right. \\
\left. + \frac{(T_h - T_a)^2}{(T_h - T_c)^2} (T_c + T_{sys})^2 \right],
\]

where \( \sigma_{n,T} \) is the measurement noise, \( \Delta \nu \) the frequency resolution and \( \tau \) the total observation time including the integration of the atmospheric, hot and cold loads spectra. This equation is derived from the radiometric equation:

\[
\frac{\delta T_i}{T_{sys} + T_i} \sqrt{\Delta \nu T_i^4}
\]

\[
t_a = \frac{\tau}{\alpha} \quad \text{for } i = a \\
t_h = \frac{\tau}{\alpha} \quad \text{for } i = h \\
t_c = \frac{\tau}{\alpha} \quad \text{for } i = c,
\]

where \( \tau_a \), \( \tau_h \), and \( \tau_c \) are the integration times for observing atmosphere, hot load, and cold load, respectively.

A measurement bias can be induced by spectrally correlated uncertainties on the emission of the calibration signal intensity such as errors induced by the load physical temperature. The bias \( \sigma_{b,T} \) can be derived as

\[
\sigma_{b,T}^2 = \frac{(T_h - T_a)^2 \delta T_a^2 + (T_h - T_c)^2 \delta T_c^2}{(T_h - T_c)^2},
\]

where \( \delta T_i \) is the uncertainty on the brightness temperature of the cold and hot loads.

Usually, the cold load is cold enough such that its brightness temperature has a value of the same order of magnitude as that of the atmospheric lines \( T_a \). For the orbiter version of the instrument, the cosmic background at 2.7 K will be used. For TEREX-1, the temperature of both calibration loads will be significantly higher than \( T_a \) and a proper strategy to calibrate the measurement needs to be defined based on laboratory studies. In particular, the radiometer non-linearity and the spectral shape of the receiver temperature will be characterized with respect to the signal intensity. The results will be validated and constrained when the instrument operates on Mars using the spectral windows between the lines, typically between 5.5 and 5.9 GHz intermediate frequency (IF). This study is not within the scope of this paper, and, here, we assume that the cold-spectrum represents a black body with a brightness temperature of approximately 7 K, namely, the atmospheric CO2 continuum intensity. The retrieval errors will also be calculated for the case that the subcalibration load emission will be used as the cold spectrum (\( T_c \sim 235 \) K) to define a range that encompasses the actual retrieval performance.

Fig. 2 shows \( \sigma_{n,T} \) and \( \sigma_{b,T} \) with respect to \( T_a \) for both strategies. The method with \( T_a \sim 7 \) K is strongly influenced by the level of CO2 continuum emission intensity that is very uncertain for temperatures below 200 K [27], as well as atmospheric pressure and temperature. For this reason, the systematic error of the sub-calibration brightness temperature is set to 1 K, a value much higher than the error induced by uncertainties on the physical temperature of the load. The latter uncertainty is set 0.1 K. For \( T_a = 10 \) K, the random errors are 1.6 K and 0.27 K for methods 1 and 2, respectively. The differences on the systematic errors of these methods is insignificant (0.28 K and 0.78 K at \( T_a = 10 \) K).

III. MEASUREMENT SIMULATION SETUP

A. Forward model

The signals by the TEREX-1 measurements were simulated by our radiative transfer model named Atmospheric Terahertz Radiative Transfer Simulator (ATRASU) [28]. This model performs line by line radiative transfer calculation [26] and we assume local thermodynamic equilibrium in this study. The macroscopic radiative transfer equation can be expressed as

\[
\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu,
\]

where \( I_\nu \) is the specific intensity [J m\(^{-2}\) sr\(^{-1}\) Hz\(^{-1}\) s\(^{-1}\)], \( j_\nu \) is the emission coefficient [J m\(^{-3}\) sr\(^{-1}\) Hz\(^{-1}\) s\(^{-1}\)], and \( \alpha_\nu \) is the absorption coefficient [m\(^{-1}\)]. The intensity passing from
Fig. 2: Typical random (noise) and systematic (bias) errors on calibrated spectra with respect to $T_a$. Two scenario are shown: 1) $T_c = 235$ K and $\Delta T_c = 0.1$ K (red lines) and 2) $T_c = 7$ K and $\Delta T_c = 1$ K (black lines). Other parameters are $T_{sys} = 3000$ K, $T_h = 300$ K, $\delta T_h = 0.1$ K, $\Delta \nu = 100$ kHz and $\tau = 1$ h.

$s_0$ (boundary condition of the path) to 0 (e.g. position of the sensor) along the path can be described by

$$I_v(0) = I_v(s_0) \exp(-\tau_v(s_0)) + \int_0^{s_0} j_v(s')\exp(-\tau_v(s')) ds'$$  \hspace{1cm} (7)

where $\tau_v$ is the optical depth defined by $d\tau_v = \sum \alpha_v ds$. The sum is performed over all active absorber contributions at the given frequency (nonoverlapping lines). For the targeted low altitudes, LTE is assumed as in previous studies [8, 17, 18, 20]. Therefore, the source function, $S \equiv j_v/\alpha_v$, is simply equal to the Planck black body radiation intensity. In this study, we use a pencil beam path without refraction for the line-of-sight and the Voigt line shape for $\alpha_v$.

The atmospheric profiles for inputs were taken from a three-dimensional general circulation model of the Martian atmosphere [1, 29], as shown in Fig. 3. The solar longitude, landing position, observation local time were assumed to be at 49°, 10.5°N of latitude and 85.5°E longitude, and noon, respectively, to be consistent with a previous study [22]. The measurement conditions follow the TEREX-1 measurement, i.e. the altitude is zero and zenith angle is zero degrees.

Spectroscopic line parameters for the line-by-line calculation are taken from the HITRAN (high-resolution transmission) molecular absorption database (www.hitran.org) [30]. Moreover, broadening parameters for target lines were adapted to Martian conditions by using of measured or calculated values for CO$_2$ broadening or, if measurements were not available, air-broadening parameters scaled by a factor of 1.65 as estimated from the ratio of collisional broadening coefficients in air and CO$_2$ for molecules and lines already studied by Urban et al. [18]. Collisional line width parameters of the H$_2$O broadened by CO$_2$ are taken from theoretical calculations [31].

Fig. 4 shows the simulated spectrum of TEREX-1 with estimated noise levels. The DSB spectrum is the sum of the half powers of the upper sideband spectrum and lower sideband spectrum on the IF range. There are 10,000 channels due to 100 kHz frequency resolution to resolve the line shape. The estimated random noise level is less than 0.4 K. The signal heights at line center frequency for each molecule from the baseline are 14.1, 0.6, 98.1, and 0.6 K for O$_2$, O$_3$, H$_2$O, and H$_2$O$_2$, respectively.

B. Error analysis

We follow the formalism of the “maximum a posteriori (MAP) solution” [32] which deals with the retrieval of unknown state $x$ related to a noisy measurement $y$ by forward model $F(x,b)$

$$y = F(x,b) + \epsilon_y$$  \hspace{1cm} (8)

where $b$ and $\epsilon_y$ describe the forward model parameters and the measurement error, respectively. We use our radiative transfer model as the forward model. The MAP leads to the maximum likelihood solution, $\hat{x}$, which minimizes the generalized $\chi^2$

$$\chi^2 = (y-F(x,b))^T S_y^{-1} (y-F(x,b)) + (x-x_0)^T S_x^{-1} (x-x_0)$$  \hspace{1cm} (9)

where superscripts “-1” and the “T” indicate the inverse and transpose of the matrix, respectively; $x_0$, $S_x$, and $S_y$ are an a priori knowledge of $x$, the covariance matrix representing the natural variability of $x$, and the covariance matrix representing the variability of the measurement error. The solution $\hat{x}$ is calculated by finding the partial derivatives of $\chi^2$ with respect to each element of $x$ when it becomes zero which is described as

$$\frac{\partial \chi^2}{\partial x(j)} = 0$$  \hspace{1cm} (10)

where $x(j)$ is the $j$th element of $x$.

Solving Eq.(10) is not straightforward due to the nonlinearity of radiative transfer equation with respect to $x$ mostly for optically thick conditions. For the error analysis, we use the standard linear formalism which leads to the retrieved state, $\hat{x}$,

$$\hat{x} = x_0 + D(y - Kx_0)$$  \hspace{1cm} (11)

where $K$ and $D$ are the matrices of weighting function and the contribution function described as

$$K = \frac{\partial y}{\partial x}$$  \hspace{1cm} (12)

and

$$D = \frac{\partial \hat{x}}{\partial y} = (K^T S_y^{-1} K + S_x^{-1})^{-1} K^T S_y^{-1}$$  \hspace{1cm} (13)

respectively.

The averaging kernel matrix $A = DK = \partial \hat{x}/\partial x$ represents the sensitivity of the retrieved state with respect to the true state. The measurement response, $m(i) = \Sigma_j A(i,j)$, is useful to indicate the weight of the true state in the retrieved value at the altitude level $i$. We chose the altitude range where $m(i)$ is higher than 0.7 as the good measurement response. The trace of $A$ gives the degrees of freedom for signal (DFS), which indicates the number of distinct pieces of information in the retrieved profile. By using $A$, Eq. (11) can be rewritten as

$$\hat{x} = (I - A)x_0 + Ax + De_y$$  \hspace{1cm} (14)
Fig. 3: Atmospheric conditions obtained from the three-dimensional general circulation model of the Martian atmosphere [1, 29] used in this study. a) Vertical profiles of pressure (solid line) and temperature (dashed line) as true profiles in this study. b) Vertical profiles of volume mixing ratios of CO$_2$ (black), O$_2$ (red), H$_2$O (blue), O$_3$ (yellow), and H$_2$O$_2$ (green).

Fig. 4: Simulated spectrum (solid line) and 1-sigma noise level for 1 h integration (dashed line). Noise is assessed for the total observation time $\tau = 1$ h and system temperature $T_{sys} = 3000$ K. Noise level is estimated using the second calibration approach described in Section II-B.

where $I$ is the identity matrix.

For simultaneous retrieval of several atmospheric profiles such as some molecular species and temperature, the $x$ can be also represented as

$$x = \begin{pmatrix} x^1 \\ \vdots \\ x^k \end{pmatrix}$$

(15)

in which $x^1$ and $x^k$ are the state representing the vertical profiles of the first and $k$th profiles, respectively. Consequently, $A$ is rewritten in the following form:

$$A = \begin{pmatrix} A^{1,1} & \cdots & A^{1,k} \\ \vdots & \ddots & \vdots \\ A^{k,1} & \cdots & A^{k,k} \end{pmatrix}$$

(16)

where $A^{m,n} = \frac{\partial \hat{x}^m}{\partial x^n}$ with $m$th atmospheric profile and $n$th atmospheric profile.

The total error in the estimated profile results from the three components: (1) measurement noise errors $\epsilon_y$, (2) the error on the a priori profile $\epsilon_a$ meaning $\hat{x} - x_a$, and (3) forward model parameter errors $\epsilon_b$. The error in $\hat{x}$ can be expressed by

$$\hat{x} - x = D\epsilon_y + (I - A)\epsilon_a + DK_b\epsilon_b$$

(17)

where $K_b = \frac{\partial y}{\partial b}$ representing the sensitivity of the calculated spectrum to the forward model parameters $b$. Thus the estimated covariance matrix of the retrieval can be separated into (1) the measurement $S_M$, (2) smoothing error $S_A$, and (3) forward model parameter $S_B$, defined as

$$S_M = DS_yD^T$$

(18)

$$S_A = (A - I)S_a(A - I)^T$$

(19)

$$S_B = D K_b S_b K_b^T D^T$$

(20)

where $S_a$ and $S_b$ are the covariance matrices associated with the a realistic a priori error and the forward model parameter error, respectively. In this study, we follow Baron et al. [33] for interpreting the blocks of $S_A$ (e.g. $S_{A,1}^{m,n}$). The diagonal block elements represent the vertical resolutions which include the effects of the smoothing errors. The nondiagonal blocks correspond to the contamination errors caused by uncertainty of other atmospheric profiles. The covariance matrix corresponding to the contamination error of $m$th profile by $n$th profile changes, $S_{A,1}^{m,n}$ is represented as $S_{A,1}^{m,n} = A_{m,n} S_a^{(A_{m,n})^T}$, where $S_a^{(A_{m,n})^T}$ is the a priori error of $n$th profile. Furthermore, as described in [34], we show the averaging kernel and full width of half maximum (FWHM) for
each of its component to evaluate the smoothing error instead of including this in the error budget.

C. Retrieval conditions

The calibration of $S_y$ takes into account of the measurement noise for its diagonal elements. In this study, we take into account of Eq. 3 in which the parameters $T_{sys}$, $T_{b}$, $T_c$, $\delta T_x$, $\delta T_c$, $\Delta \nu$, and $\tau$, are 3000 K, 300 K, 7 K, 0.1 K, 1 K, 100 kHz, and 1 h, respectively. For more realistic estimation of $S_y$, the calibration uncertainty and measurement noise including Off-diagonal components will be published elsewhere.

The calculation of $S_x$ takes into account a priori standard deviation, $\sigma_x$, at each vertical profile of 100 % except for 30 K error for temperature profile with adjacent levels correlation. Then $S_x$ is considered as

$$S_x(i,j) = \sigma_x(i)\sigma_x(j) \exp \left( \frac{|z(i) - z(j)|}{\sigma_{corr}} \right)$$ (21)

where $z$ and $z_{corr}$ represent altitude grid and a distance correlation between $i$th and $j$th altitudes for the a priori parameter, respectively. We set $z_{corr}$ to 10 km to defuse the constraint from a priori value at one altitude to neighboring layers. The value of 10 km matches the typical resolution that is expected for the retrievals.

We set $S_a$ and $S_b$ for estimating the total error budget as followings. We consider an error of 50 % with respect to the atmosphere for diagonal elements except for 15 K error for temperature profile, and correlations of 10 km (Eq.21) for $S_a$. The errors related to the forward model parameters include the uncertainty of antenna elevation and spectroscopic parameters. The uncertainty of the antenna direction depends on the accuracy of the three-axis accelerometer, and arbitrary value of 0.025 degrees is chosen. The retrieved error calculated in this study can be scaled linearly to any pointing uncertainty we might assess in the future. Except for the H$_2$O broadening parameter, the spectroscopic parameters are taken from HITRAN \[27, 30\]. The uncertainties follow the higher values reported in the catalog. The H$_2$O broadening parameters are from Bauer et al. \[31\], and the uncertainty is arbitrary set to 5 %.

We calculate $K$ (Eq.12) by differentiation of the modeled signals with respect to the atmospheric vertical profiles. The state vector grid spacing for the error analysis is set to be 3 km. The absolute values of $K$ scaled by $x$ at each altitude for each profile are shown in Fig. 5. The scaled $K$ values of O$_2$, H$_2$O$_2$, and O$_3$ have symmetric shape about their center frequencies. The increase of the $K$ values of O$_3$ above 30 km of altitude is caused by the strong increase of O$_3$ vmr as shown in Fig. 3.

IV. RESULTS AND DISCUSSION

A. O$_2$

The measurement sensitivity to the O$_2$ profile is shown in Fig. 6 when the temperature is retrieved simultaneously. The scaled averaging kernel matrix, $A(i,j)x_a(j)/x_a(i)$ \[33\], and the measurement response are plotted on the left panel. The altitude range of the good measurement response is 0–55 km. The DFS is 4.9. The peak altitudes and FWHM of the scaled $A$ for each altitude are also shown in the Fig. 6. The FWHM is computed from the Gaussian fitting of $A$ for each altitude. The peak altitudes show the most related altitudes of the retrieved state. The peak altitude of the averaging kernels is consistent with the retrieved altitude where the measurement response is good. The FWHM within the good measurement response is 8–17 km of altitude. The right panel of the Fig. 6 shows the retrieval errors related to the a priori contamination, forward model parameters, and thermal noise error. The largest error component for O$_2$ retrieval is line parameter errors which are dominated by the 20 % uncertainty of O$_2$ line strength parameter. The error due to the uncertainty of the antenna direction is less than 0.0023%. Such an error remains negligible even if a pointing error 10 times larger than that assumed in this study is considered. Most of the error from line parameters is regarded as systematic error. On the other hand, the noise and a priori contamination including temperature profile errors are random errors which can be reduced by the observation integration time. Consequently, the random error for retrieving O$_2$ profile is 7–22 % with the systematic error of 15–27 %.

The retrieval errors increase if we consider the calibration strategy for which the subcalibration load is used as the the cold spectrum ($T_c \sim 235$ K). The spectral noise level increases from approximately 0.4 K to 2.0 K. The altitude range of the good measurement response is narrowed to 0–52 km. The peak altitude of the averaging kernels is consistent with the retrieved altitude below 40 km. The DFS decreases to 3.5. The FWHM increases by 1.2–1.4 times compared to the calibration strategy using the atmospheric CO$_2$ continuum intensity as the cold spectrum ($T_c \sim 7$ K). The random error for retrieving O$_2$ profile increases to 10–28 % with the systematic error of 15–22 %.

B. H$_2$O

The measurement sensitivity to the H$_2$O profile is shown in Fig. 7 when the temperature is retrieved simultaneously. The altitude range of the good measurement response is 0–25 km.
Fig. 6: O$_2$ retrieval by TEREX-1 up-looking with 1 hour integration time observation and with simultaneous temperature retrieval. (left) Scaled averaging kernels of the retrieved O$_2$ profile for each altitude and measurement response (black line). The colorbar shows the related altitude of the state of averaging kernels. DFS value is shown at the top of the panel. Peak altitude and FWHM values for each component of averaging kernels are shown on the right side of the panel. (right) Expected retrieval errors. Dashed, dotted, and solid lines represent contamination error from the other profiles, forward model errors from spectroscopic parameters, and thermal noise error, respectively. The shaded area represents the altitude range where measurement response is less than 0.7.

The DFS is 3.5 and the FWHM within the good measurement response is 5–10 km of altitude. The random error for retrieving H$_2$O profile is 13–25% with the systematic error of 5–17%. The main source of the systematic errors is 20% uncertainty of broadening coefficient parameters for H$_2$O. The error due to the uncertainty of the antenna direction is less than 0.0036%. For H$_2$O K, an optically thick condition that has no sensitivity owing to low transparency between an atmospheric layer and sensor, can be seen around the center frequency of H$_2$O as shown in Fig. 5. This implies the information of the center frequency of H$_2$O only corresponds to the state near the surface, and there is no sensitivity to upper-layer information. This causes a decrease in the observational sensitivity of the water vapor content of the upper atmosphere and an increase in the error due to the temperature profile because the line intensity at optically thick condition linearly depends on the temperature in the considered atmospheric layer.

We demonstrate error analysis without retrieving temperature profile which reduces the retrieved sensitivity to atmospheric species especially H$_2$O profile below an altitude of 30 km. Note that a reliable information of the temperature profile is needed to retrieve the vmr profiles without retrieving temperature. If we average 25 1-hour integrated spectra (25 Martian days), the uncertainty of the temperature profile reduces to about 3 K, which allows us to avoid retrieving temperature. Two scenarios were considered for the error analysis. One is retrieving vertical profiles in vmrs of atmospheric constituents from all the spectral range. The other retrieving vertical profiles in vmrs of atmospheric constituents without optically thick frequency near the H$_2$O line. This condition sets the frequency range at which the information of K is ignored in the retrieval procedure. For the frequency range, we consider optically thick frequency which has a transparency of radiations from surface to the top of the atmosphere of less than 0.2. The level of thermal noise in Eq. (13) is set to the same as that used for the 1-hour integration time case. This allows us to get vmr retrievals with the DFS close to those obtained with temperature retrieval. Also the estimated retrieval error (Eq. 18) due to the thermal noise will be divided by factor $5(\sqrt{25})$.

The left panel on Fig. 8 shows the results of an error analysis without temperature retrieval. The DFS for retrieving H$_2$O increased by 1.3 compared to the retrieval with temperature. The vertical resolution of H$_2$O profile becomes 1 km higher than that of the retrieval with temperature. However, the H$_2$O retrieval error from temperature uncertainty increases up to 130% because of the strong dependency of the H$_2$O line intensity on temperature. The random error, due to the contamination from other retrieved species and the measurement noise, is less than 5%. Consequently, this scenario is suitable if users are interested only in vmrs of H$_2$O and other species and can use a reliable temperature profile.

The Right panel on the Fig. 8 shows the results of the error
analysis with the optically thick conditions. This condition ignores $K$ values at 6431.8–6469.6 MHz, which is an IF range that corresponds to the transparency less than 0.2. The DFS of the H$_2$O decreased to 3.0 with a decrease of the temperature uncertainty to 5–21% due to the loss of the signal information around the H$_2$O centerline. The vertical resolution of H$_2$O profile becomes approximately 1 km lower than that of the retrieval with temperature. This retrieval scenario allows us to not depend on a good knowledge of the temperature profile and reduce the contamination due to other retrieved species. This error assessment is based on an uncertainty of 3 K on the temperature profile which is questionable due to the lack of data. However, the error found in this study can be easily updated because it is linearly proportional to the assumed temperature error.

The altitude range of the good measurement response is 0–15 km. The DFS is 2.8 and the FWHM within the good measurement response is 5–16 km of altitude. The random error for retrieving temperature profile is 2–5 % with the systematic error of 2–3 %. The main source of the systematic errors is the uncertainty of broadening coefficient parameters for H$_2$O.

![Fig. 8: Expected retrieval errors for H$_2$O without temperature retrieval when using the full-frequency range of TEREX-1 observation spectra (left) and ignoring optically thick frequency range (right) in the retrieval process. DFSs are shown at the top of each panel. Dashed, dotted, dash-dotted, and solid lines represent contamination error from the other profiles, forward model errors from spectroscopic parameters, forward model errors of temperature uncertainty, and thermal noise error multiplied by 5, respectively. The shaded area represents the altitude range where measurement response is less than 0.7.](image)

**C. Temperature**

As shown in Fig. 5, the sensitivity of temperatures below 30 km mostly originates from the H$_2$O spectrum. The transition from positive values to minus values occurs from the H$_2$O line frequency to its outer frequency region. The O$_2$ line also contributes to the temperature at upper 30 km. Fig. 9 shows the measurement sensitivity to the temperature profile.

![Fig. 9: Same manner as Fig. 6 but for temperature profile](image)

**D. Minor species and detection limits**

The atmospheric profiles of minor species, O$_3$ and H$_2$O$_2$, are also expected to be retrieved with approximately two-layer vertical resolution. The measurement sensitivity to the O$_3$ profile is shown in Fig. 10. The peak altitudes of O$_3$ averaging kernels are not consistent with retrieved altitude and are 0–4 km for all averaging kernels peaking below 20 km and 40–43 km between for those peaking between 30–45 km, despite the good measurement response. TEREX-1 has the sensitivity to the O$_3$ profile at approximately 42 km altitude with about 13 km vertical resolution because of the strong increase of O$_3$ vmr above 30 km altitude. The random error for O$_3$ profile is 22–30% with 15–22% of systematic errors. In the case of the H$_2$O$_2$, the altitude range of the good measurement response is 0–30 km with 12–30 km of FWHM as shown in Fig. 11. The random error for H$_2$O$_2$ profile is 14–30% with 10–34% of systematic errors, respectively.

We present the trade-off between DFSs and integration time from one second to one day for both calibration scenarios in Fig. 12. The integration time to obtain at least a column layer profile of H$_2$O$_2$ and O$_3$ are 100 and 400 seconds, respectively for the best calibration method. The retrieval scenario without temperature retrieval gives higher values of DFS for atmospheric constituents than the retrieval with the temperature profile, especially for longer integration time. This implies a
better signal-to-noise ratio of spectra has more information of temperature profile for each atmospheric constituent. The decrease of the DFS of H$_2$O with respect to the increase of the integration time for the optically thick condition implies that a higher signal-to-noise ratio of H$_2$O spectra has more information about temperature and vmr profile around the surface altitude. An integration time of one second gives more than one DFS value for H$_2$O, O$_2$, and temperature retrieval, i.e., at least a column layer can be retrieved from the measurement signal. For the calibration strategy for which subcalibration load is used as the cold spectrum, the required integration time is ten times longer to obtain similar results.

**V. CONCLUSIONS**

We studied the observation capability of the ground-based Terahertz radiometer for vertical profiles of O$_2$ and H$_2$O in the Martian atmosphere. Considering the up-looking geometry and 1 h observation time, the expected measurement errors for O$_2$ and H$_2$O are 7–22% and 14–25% with 8–18 km and 5–10 km vertical resolution in the vertical range 0 to 55 km and 0 to 25 km, respectively. The measurement error for temperature retrieval is 2–5% with 5–16 km vertical resolution in the altitude range from 0 to 15 km. Scenarios without the retrieval of the temperature profile show improvements of the measurement error for H$_2$O profile in case of the large amount of H$_2$O vmr or reliable temperature profiles from other sources are available. Further investigations will be conducted on the use of ancillary information on the temperature profile. For instance, the error of 3 K could be obtained from proposed limb sounders [18, 21]. TEREX-1 is also capable to measure O$_3$ and H$_2$O$_2$ signals and retrieve vertical profiles in two independent layers with 30% measurement error. The minimum integration time to obtain at least one DFS values are <1, 400, <1, 100, <1 seconds for O$_2$, O$_3$, H$_2$O, H$_2$O$_2$, and temperature profiles, respectively. These errors correspond to the best scenario for the calibration. If we consider the worst case scenario, namely $T_c \sim 235$ K used as cold load spectrum, we found that the retrieval errors and DFS are degraded by about 20–40% in the case of O$_2$. The laboratory measurements of pressure broadening parameters in CO$_2$ gas are important for reducing systematic spectroscopic errors. Further laboratory study using two calibration loads is needed to assess the errors on the
calibrated spectra and to define a more optimal calibration strategy. The error ranges and vertical resolutions of TEREX-1 will certainly improve past and current observations. We believe this unique dataset will allow us to better understand source and sinks of Oxygen and water vapor on the Martian surface and to go on with further innovations related with human activity on Mars.

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