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A compact breath gas sensor system based on terahertz/millimeter-wave gas spectroscopy

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Abstract: We demonstrate a full-cycle breath gas sensor system based on terahertz/millimeter-wave gas spectroscopy. The sensor consists of a transmitter and receiver working around 250 GHz based on SiGe BiCMOS technology. Typical detection thresholds are in the ppm range depending on the respective molecule. The data analysis provides partial pressures of the investigated molecules by fitting of spectra which are measured by wavelength modulation. Beside the spectroscopic measurement and the data analysis, a full cycle of breath analysis includes the sampling and the conditioning of the sample tubes. The full cycle takes about 35 min per sample in average. As the system is compact and easy to operate, it allows for on-site analysis of breath samples in medical laboratories or hospitals.

Keywords: breath analysis; gas spectroscopy; millimeter-waves; terahertz.

1 Introduction

The analysis of exhaled human breath is a very promising field of research as the breath contains many compounds that can deliver information about a patient's metabolism and health [1, 2]. Despite the large potential it has not yet

found the way into doctors' offices or hospitals for everyday use. Besides costs, one major criterion for this application is the simplicity of the whole process of analysis which includes sampling, measurement, and the analysis. It is highly desirable to realize this whole process on-site in a short time with a compact system. So far, most studies on breath analysis are based on complex methods such as gas chromatography–mass spectrometry which requires mailing the samples to dedicated laboratories. In turn, this results in a high effort and a large time delay. A rather novel measurement approach is the analysis of breath based on terahertz/millimeter-wave gas spectroscopy [3–6]. The method is highly sensitive and specific. Even very similar molecules such as conformers can be identified unambiguously [7]. The advance of silicon-based technologies allows for cost-efficient and compact systems [8, 9]. In this work, we present a breath gas sensor based on terahertz/millimeter-wave gas spectroscopy which can perform a full cycle of breath analysis (including conditioning, sampling, measurement and data analysis) on-site in a short time.

2 System overview

Figure 1 shows our full-cycle on-site breath analysis system on a cart and a scheme of the sensor. It consists of a commercially available RECIVA breath sampling station including the air supply (bottom right) and the sampling device with mouth piece (right). With this device, up to four sampling tubes based on thermal desorption can be loaded simultaneously. We use Tenax tubes, which are commonly used for breath analysis. The tubes have an outer diameter of 6.35 mm and a length of 88.9 mm and are filled with Tenax TA with a mesh size of 60/80. Typically, around 500 mL of exhaled breath is sampled at a flow rate of around 100 mL/min which results in a total sampling time of approximately 5 min. The measurement of the samples is performed with a compact sensor based on terahertz/millimeter-wave gas spectroscopy which is placed on a 45 cm × 60 cm breadboard (left). It includes the transmitter and receiver modules, a compact gas absorption cell as well as the vacuum pumps (in the background). Details of the sensor system will be described below.

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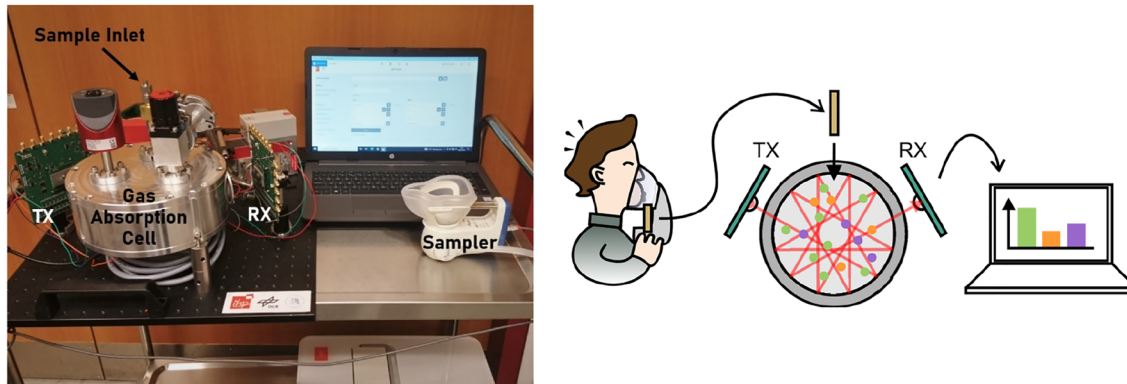


Figure 1: Photograph (left) and schematics (right) of the on-site breath gas sensor based on terahertz/millimeter-wave gas spectroscopy.

3 TX/RX performance

3.1 Circuit design

The transmitter (TX) and a receiver (RX) each with bowtie-antenna and silicon lens are fabricated in IHP's 0.13 μm SiGe BiCMOS technology. The TX and RX use two integrated local oscillators for 222–256 and 250–270 GHz, which are switched for dual-band operation [9]. The frequency of TX and RX can be tuned and modulated by a fractional- n phase-locked loop (PLL) which is controlled by a Serial Peripheral Interface (SPI). Figure 2 (left) shows microscopic images of the TX and RX circuits with the bowtie antennas. The areas are $2.64 \times 1.34 \text{ mm}^2$ and $3.25 \times 1.34 \text{ mm}^2$, respectively. The TX and RX are mounted on a baseband board (12 cm \times 12 cm) which provides the supply voltages, the PLL and functionalities for the evaluation of the circuits. A baseband board with the TX and the silicon lens is shown in Figure 2 (right).

3.2 TX/RX characterization

For the performance of the gas spectroscopy system, the characteristics of the TX and RX chips are of major importance. First, the bandwidth of the system is important, because a larger bandwidth covers more absorption lines. In turn, this means that a larger variety of molecules can be detected and the covered lines are more likely to have large line intensities. Generally, the strongest rotational transitions tend to shift to higher frequencies for smaller molecules. For symmetrical tops, the maximum line intensities are expected at around $\nu_{\text{max}} \sim B + 11(BT)^{1/2}$ with the rotational constant B and the temperature T [10]. By using two local oscillators, our system covers frequencies between 222 and 270 GHz (see Figure 3), which is a spectral range with a lot of strong transitions of relevant breath gases such as acetone, ethanol, or acetaldehyde. We have successfully demonstrated spectroscopy in the full available bandwidth [9]. Second, the emitted power P of the transmitter is a key figure. Due to the relatively high

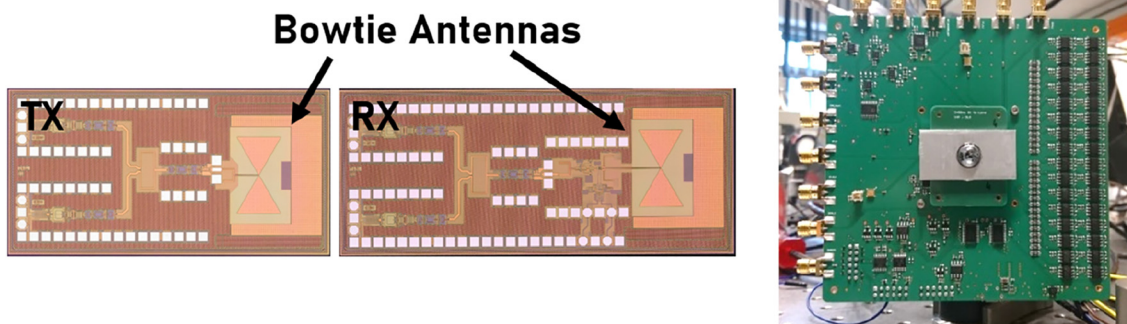


Figure 2: Microscopic images of the TX and RX circuits (left) and photograph of the TX with silicon lens on the 12 \times 12 cm² baseband board (right). The areas of the circuits are $2.64 \times 1.34 \text{ mm}^2$ and $3.25 \times 1.34 \text{ mm}^2$, respectively.

power compared to the small absorption signal (typical absorptions are well below 0.1%), the dominant noise source is Townes noise [10]. In this case, the minimum detectable absorption scales with $1/\sqrt{p}$ [11]. Earlier, we have observed this relationship with our setup [12]. Thus, a high power is required to achieve a high sensitivity. We have measured output powers between 360 and 870 μW (see Figure 3) using a TK power meter [9]. The third important characteristic is the noise performance of the receiver. We were able to determine noise temperatures around 20,000 K, that even allow for passive heterodyne spectroscopy for space applications (see Figure 3) [13]. Furthermore, the RX should have a high dynamic range to allow detection of a wide range of power levels. We have shown an input-related 1 dB compression point of -10 dBm [14]. Finally, Gaussian-like beam profiles with a high directivity are required in order to couple the radiation appropriately into the gas absorption cell [15]. We determined FWHM opening angles between 6.6° (E-plane) and 9.2° (H-plane) by rotation of the TX and detection by a Golay cell, as can be seen in Figure 3 [9]. These beam characteristics are well suited to be coupled into our gas cell.

4 Spectroscopic system

4.1 Spectroscopic setup

The spectroscopic setup is based on the TX/RX described above and a gas absorption cell containing the sample. The characteristics of the gas cell are similarly important for the system performance as the TX/RX. First of all, the absorption path length L should be as long as possible to

allow for a sensitive detection, because the absorption signal scales approximately with L in the limit of weak absorptions. Our gas cell is based on a circular multi-pass design and provides a path length of 1.9 m. The details of the design of the gas cell are described in [15]. On the other hand, the gas volume should be low due to the following reason. Typically, sampling volumes are only about 0.5–1 L and the samples are collected in pre-concentrator tubes based on adsorption and thermal desorption. Therefore, only a limited number of molecules are adsorbed in the tubes. In turn, the molecules can only produce a certain pressure in the gas cell after thermal desorption. However, a pressure of a few Pa is required for a sensitive detection. At lower pressures, the absorption signal will be very weak and at higher pressures, the lines will get too broad. Pressures of a few Pa are the optimum, because in this regime, line widths from Doppler broadening and from pressure broadening are typically similar. Due to the compact design of our gas cell, it has a gas volume of only 1.5 L. This is very well suited since we achieve pressures of around 1–2 Pa after thermal desorption of breath samples. Despite the small volume, there shouldn't be too much overlap between the beams in the gas cell, because it increases the risk of saturation of the gas absorption. In contrast to other designs such as Herriott-cells, our beams overlap only slightly close to the cell center, such that the volume is efficiently used with little overlap. Another important aspect are losses which mainly result from coupling, reflections, and absorptions. These should be low to increase the received power which increases the signal-to-noise-ratio (SNR) as described above. For the coupling, the optics need to be adapted to the beam profiles of the TX/RX and the apertures should be large enough to minimize diffraction. This is a limiting factor with respect to the size of the

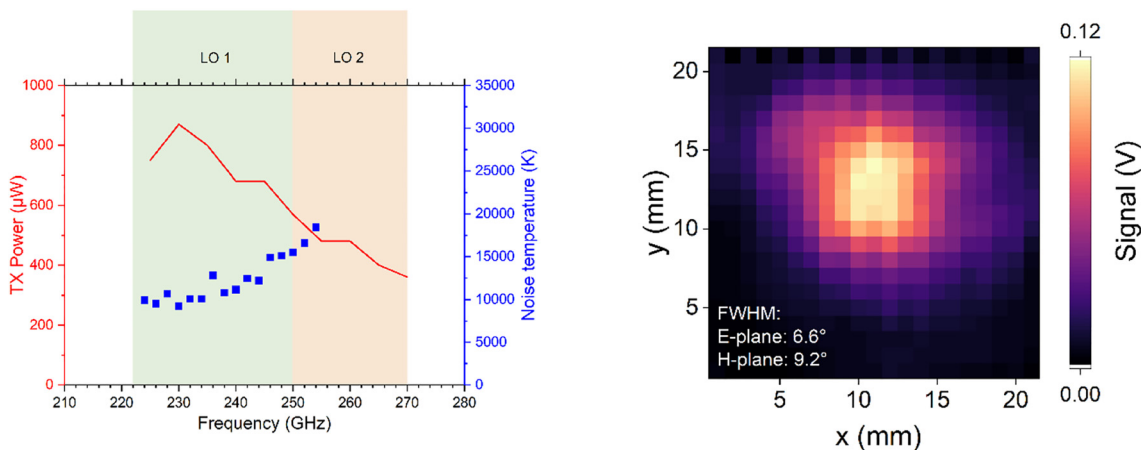


Figure 3: Measured performance parameters (left) and beam profile (right) of the TX and RX.

system. Note, that the wavelengths are larger than 1 mm. We have carefully measured the beam profiles (see descriptions above) and adapted the gas cell optics accordingly. The beam is focused at the input and output of the gas cell and after each internal reflection. Focusing at the internal reflections is realized by a spherical surface. The losses from these reflections are relatively small due to the smooth surface compared to the wavelength. To minimize absorption losses, the lenses serve also as windows of the cell and are made from high-density polyethylene. The total losses of the gas cell amount to only 3 dB. Interferences play another important role in MMWGS. For instance, Fabry–Pérot interferences can occur from partial reflections at coupling optics or the antennas. Typically, the periods of the standing waves (e.g. 75 MHz for a 2 m long resonator) are close to the linewidths of the transitions. Thus, the baseline can affect the measurements significantly which makes it difficult to detect and to quantify the absorptions. If the interferences are strong, the signal at certain frequencies can be almost completely lost. In our design, we have suppressed interference modulations of 100% by a factor of four (to only ~25% modulation) by using an aperture mask. Together with modulation techniques (see description below), this allows for an almost complete suppression of the baseline variations. Finally, the size of the system should be small such that it can be used for medical screenings or similar applications. Obviously, a compromise between the system size and other characteristics such as the absorption path length or losses has to be found. In this regard, our system is very compact with an outer diameter of 21.5 cm and a height of 8 cm. The system including the TX/RX, the gas cell and the pumps fits on a portable 45 × 60 cm breadboard [16].

4.2 Measurement parameters

The measurement parameters have to be chosen carefully to optimize the sensitivity of the system. In most cases, we use wavelength modulation of the TX and phase-sensitive detection by a lock-in amplifier. In wavelength modulation spectroscopy, the wavelength is modulated by a certain deviation (similar to the width of the absorption line) with a certain modulation frequency. If the center frequency is scanned across an absorption line, the frequency modulation is translated into an amplitude modulation of the signal which can be detected by a lock-in amplifier. The first harmonic content will resemble the derivative of the absorption line [17]. Compared to direct absorption spectroscopy, this scheme offers two main advantages. First, the sensitivity is much higher due to noise suppression by the lock-in amplifier and second, the baseline variations are suppressed. Figure 4 shows two exemplary measurements of a water line from the same breath sample, one of them taken by direct absorption spectroscopy and the other one measured by lock-in detection of the wavelength-modulated signal. One can clearly see that baseline variations are suppressed (~100 vs. ~0.1% relative to the signal) and the SNR has increased (30 vs. 7000) in the latter measurement. Note that for other molecules measured in breath samples, the absorption lines are usually completely hidden in the noise in the direct absorption measurements. In this example, the second harmonic ($2f$) of the modulation is detected, which resembles the second derivative of the absorption line. In contrast to $1f$ detection, the signal peak can be found at the center frequency of the absorption and the baseline is even more suppressed. The width of the modulation has to be

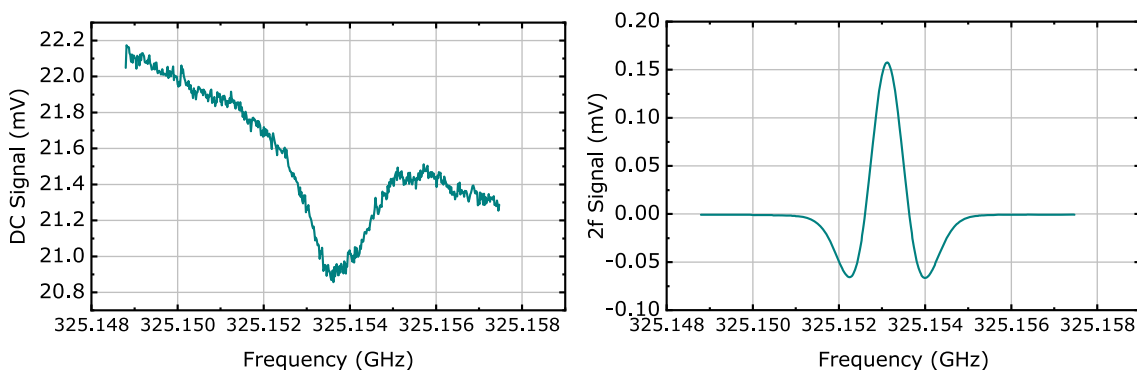


Figure 4: Measurement of water in a breath sample acquired with direct absorption spectroscopy (left) and wavelength modulation (right). Through the modulation technique, the SNR is increased and the baseline variations are reduced.

adapted to the linewidth of the absorption (see also next section) in order to maximize the signal. Since Doppler widths are different for each absorption line (scales with the center frequency and with $1/\sqrt{\text{molecular mass}}$) and the pressure broadening is unknown in an unknown gas mixture, the best modulation has to be estimated. We found a modulation width of 500 kHz best suited as it matches well with most detectable molecules in the almost Doppler-limited regime. Other important parameters are the scan range and the scan time. A very simple approach is to scan the entire available bandwidth to cover all possible absorption lines. However, this measurement would contain a lot of empty spectral range. Typically, the line widths are about 1 MHz wide whereas the bandwidth of our system is in the order of 100 GHz, which is a factor of 100,000 larger. Furthermore, not all detected lines might be assigned to known molecular species. More importantly, the scan would consume a lot of time, specifically about 14 h with our typical parameters. It makes sense, to scan only known absorption lines. To increase the specificity, at least three lines should be scanned. The slower each line is scanned, the longer the integration time τ can be chosen. In turn, a longer integration time increases the sensitivity as the SNR scales with $\sqrt{\tau}$. For the analysis of breath samples, we scan a range of 10 MHz per line, which provides sufficient baseline to recognize weak lines. The scan time is 5 s and the corresponding integration time 50 ms.

4.3 Data analysis

Our system can operate in two different modes that require two different data analysis methods. In the first case, the measurements are performed as direct absorption spectroscopy. Although it is usually noisier than wavelength modulation spectroscopy (WMS), it can be advantageous in certain scenarios, e.g. if the pressure of the gas sample can't be controlled and is rather high (as in direct sampling instead of using pre-concentrators). In this case, the detection of gases is not limited by noise, because the absorption signal is rather high. Instead, the analysis of the data is limited by the difficulty of interpretation due to strong overlap of the absorption lines. Here, direct absorption spectroscopy is much better suited since the data is easier to interpret. For this scenario, we analyze the data based on Independent Component Analysis (ICA) [18]. We have demonstrated unambiguous identification and quantification of a binary mixture at pressures up to 300 Pa with strong overlap [18].

The second case is much more common for the analysis of breath samples. Here, the pressure of the sample is low such that the absorption lines are narrow and well

isolated. WMS is well suited for this case because the sensitivity is much higher as described above. However, the data is more complicated to interpret [17]. In addition to the absorption line shape itself, the signal is also affected significantly by the modulation as illustrated in Figure 5. Figure 5 (left) shows the shape of the measured signal of an exemplary Voigt profile (with equal contributions from Gaussian and Lorentzian profiles) in dependence of the modulation index. The modulation index is defined as the amplitude of the modulation over the half width at half maximum of the absorption line. Two things can be recognized in this illustration. First, the amplitude of the signal changes with the modulation index. The optimum modulation is around two for Gaussian, Lorentzian as well as Voigt profiles (cf. Figure 5, right). Second, the shape changes with the modulation index. It gets broader and the height of the positive amplitude (P) relative to the negative amplitude (N) gets smaller with increasing modulation index. In the optimum case, this ratio is approximately two for all line shapes, cf. Figure 5 (right), which is a good indicator for a properly chosen modulation. Based on the underlying theory, we have developed and verified a routine to quantify the partial pressure of a molecular species from the 2f signals precisely [19]. Input parameters of the model are the modulation width, the center frequency, the molar mass of the molecule, the temperature, the absorption path length, and the line intensity.

4.4 Spectroscopic performance

The spectroscopic performance of the system depends on many variables such as the TX power, the RX noise performance, the detection scheme, the measurement parameters, the absorption path length or the line intensity of the molecular transition. To evaluate the performance of our system we have performed reference measurements to estimate the detection threshold for various molecules. Typical detection thresholds range between 20 ppt/ $\sqrt{\text{Hz}}$ for hydrogen cyanide and 24 ppm/ $\sqrt{\text{Hz}}$ for acetone [9]. These values refer to the mixtures in the gas cell, i.e. the actual detection limit after pre-concentration of the samples can be higher by orders of magnitude. An exemplary measurement of an acetone absorption line from a breath sample is shown in Figure 6. The spectrum is an average of six scans with 8 ms integration time each and the SNR amounts to 40. Using the fitting procedure described above, the derived partial pressure of acetone is $9 \cdot 10^{-3}$ Pa. As demonstrated, the performance of the SiGe-BiCMOS based system clearly allows for the detection of volatile organic compounds in typical exhaled human breath samples.

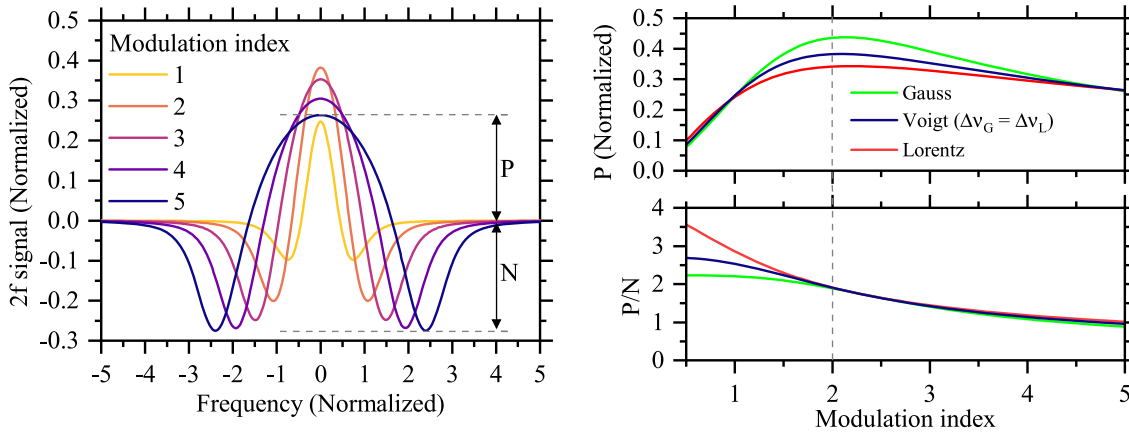


Figure 5: Theoretical waveforms acquired with wavelength modulation spectroscopy for different modulation widths (left) and the resulting signal parameters (right). The maximum signal is achieved with a modulation index of about two.

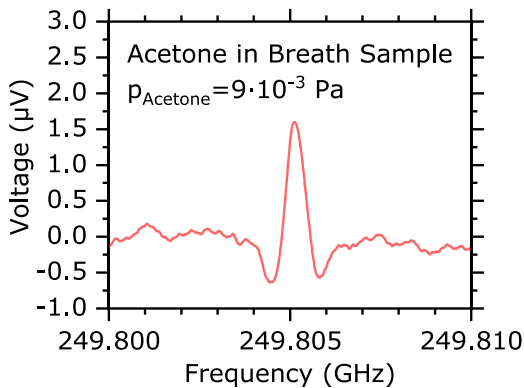


Figure 6: Acetone in a breath sample of a COPD patient acquired with the SiGe-based breath gas sensor.

5 On-site breath analysis

To demonstrate the feasibility of our system for on-site medical screenings, we have performed full-cycle measurements of breath samples in our laboratory. The process includes the conditioning of the tubes, the sampling, the measurements, and the data analysis. The conditioning was performed with a TC-20 from Markes. This process is required prior to any measurement to remove adsorbed molecules from previous measurements from the tubes. After conditioning, the tubes can be stored for several days or even for weeks if the tubes are stored in a refrigerator. As recommended for new tubes, we have conditioned at 320 °C for 2 h with a nitrogen flow of approximately 50 mL/min. Note that regularly, the conditioning will take only 30 min for up to 20 tubes at the same time, i.e. the conditioning takes 1.5 min per sample in average. The sampling was carried out with the RECIVA sampling device from Owlstone [20]. We have collected 500 mL of exhaled breath of a

healthy volunteer at a flow rate of 100 mL/min such that the sampling took about 5 min. To control the reliability of the measurement, we have acquired two duplicate samples at the same time. The spectroscopic measurements of the samples were performed with our laboratory setup as described previously with samples taken externally in a hospital [5, 21]. The measurements took 5 s per line scan plus approximately 15 min per sample which includes mounting, heating and the actual measurements. This time can be reduced by optimizing mechanical interfaces and scanning less molecules of interest. The data was analyzed as described above to determine the partial pressures of the detected molecular species. As this process is in principle fully-automatic and does not require trained technicians, this step doesn't consume any time in the breath analysis cycle. In conclusion, the full cycle consumes only 35–40 min which is suitable for a screening scenario in a doctor's office. Most of this time does not require any action of the physician or medical doctor. Some results of the measurements from an exemplary sample are shown in Figure 7.

To validate the outcome of our method, we have compared results of our laboratory setup to reference measurements taken by gas chromatography–mass spectrometry (GC-MS), which is a well-established method in breath analysis. In that study, we have compared 28 duplicate samples, which were taken in a hospital from patients suffering from the Chronic Obstructive Lung Disease (COPD) [21]. We found that the variation in the duplicate samples is very similar for both methods and the abundances of acetone and ethanol agree very well. Figure 8 shows the very good correlation ($R = 0.93$) between the ethanol abundances as measured with both methods [21].

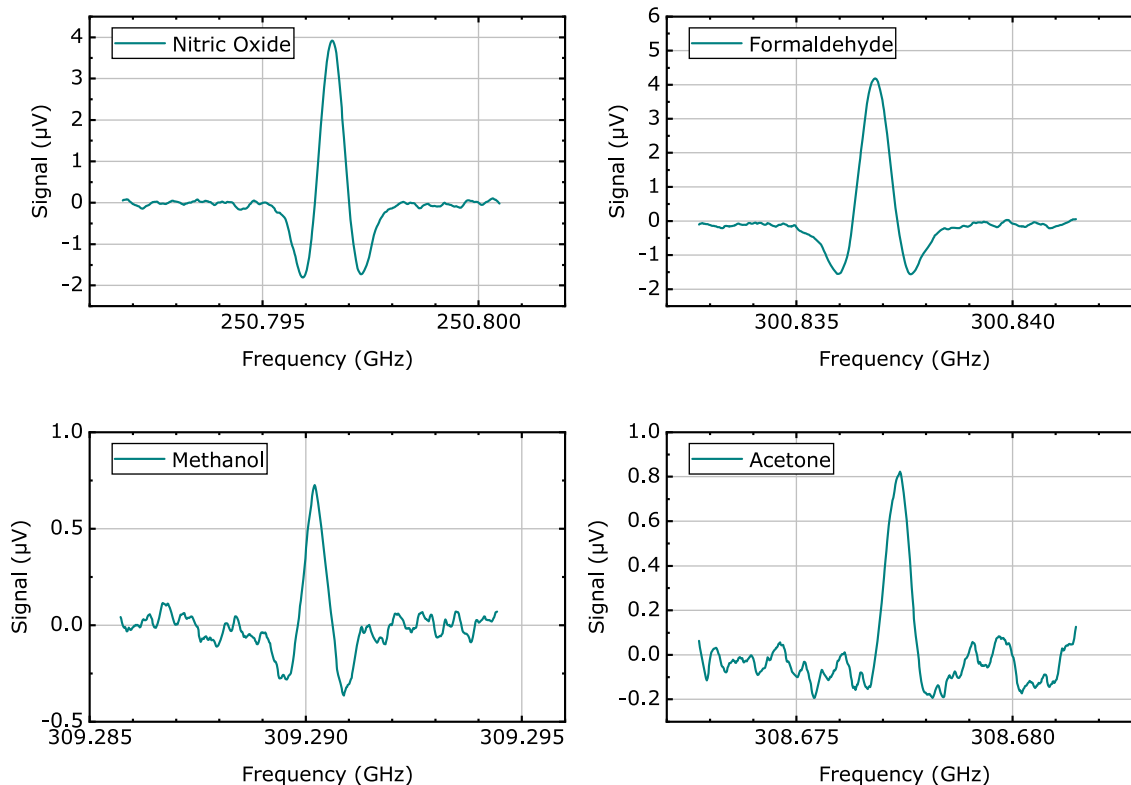


Figure 7: Exemplary results of a complete on-site measurement of a breath sample of a healthy volunteer. The measurement including sampling and measurement was performed in a total of approximately 35 min.

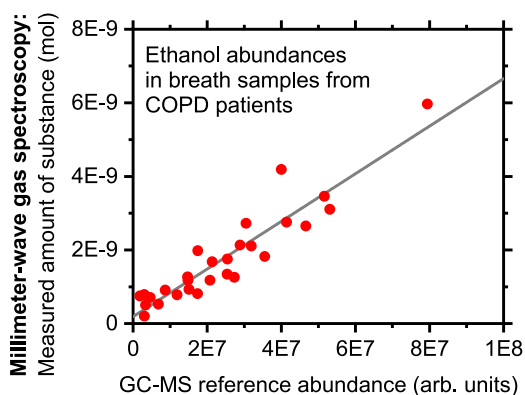


Figure 8: Comparison of ethanol abundances of 28 duplicate samples as measured by millimeter-wave gas spectroscopy and GC-MS. The results agree very well which validates the results from millimeter-wave gas spectroscopy for the analysis of exhaled human breath.

6 Conclusions

We have demonstrated a full-cycle breath gas sensor system based on terahertz/millimeter-wave spectroscopy. It is highly sensitive and allows for the detection of numerous compounds in human breath. So far, we have detected

more than 20 different compounds in human breath, but there will be much more to discover. The system is very easy to operate and the cycle times are adequate for practical use. Furthermore, most of the cycle time does not require any action of the operator. In conclusion, the system is suitable for on-site analyses of breath samples. For instance, it can be used by medical researchers or clinicians in diagnostic setups or screenings in medical laboratories, doctors' offices or hospitals. The ongoing development of silicon-based sources and detectors is a key factor for cost-efficient systems. Our next step will be to evaluate an extension of the frequency range to around 500 GHz. This is challenging with regard to the electronic circuits, but it will contain additional transitions, which increases sensitivity and selectivity. We will also use our system to demonstrate a medical study. This new method can be valuable for breath research and can help to establish the application of breath gas analysis in daily clinic life.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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