Gas recognition with terahertz time-domain spectroscopy and reference-free spectrum: a preliminary study

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***Abstract*—The ability to detect and recognise a variety of gases under certain environmental conditions has significant potential impact in many areas. Gas sensing has long received attention with microwave and infrared spectroscopy. With many molecular resonances occurring in the THz range leading to simple, unique spectral features, THz time domain spectroscopy (TDS) shows promise as a tool for gas detection and recognition. Our earlier work proposed a simple method that extracts the line positions from gas species without a reference pulse and classifies them by means of the minimum Euclidean distance classifier and the Submillimeter, Millimeter, and Microwave Spectral Line Catalog. This paper presents a preliminary investigation on a reference-free spectrum as an alternative classification feature for gas recognition.**

I. Introduction And Background

GAS sensing technologies have been widely reviewed in the literature with optical techniques such as Fourier transform microwave spectroscopy and Fourier transform infrared spectroscopy in general being the perfect trade-off between cost, robustness, and performance. However, on a fundamental level, microwaves and mid-infrared radiation has its own respective advantages and disadvantages for spectroscopy. Principally, heavy gas molecules tend to have rotational resonances at microwave frequencies, while light gas molecules have rotational resonances in the mid-infrared region. The absorption resonances in the mid-infrared region are generally congested with rotational and ro-vibrational modes, thus making the feature extraction process difficult. In contrast, the rotational transition modes in the microwave region are relatively lower, resulting in fewer available features. The THz region therefore presents an ideal trade-off between the two.

THz-TDS of polar gases has been extensively investigated in the literature [1-3] and given a sufficient concentration, they exhibit an ensemble of strong and sharp resonances at discrete frequencies due to quantised rotational energy transitions [4]. As the molecules differ in structure, resonance positions and relative strengths are unique to the gas species and therefore, can be used as classification features. Linear predictive codes have been successfully employed to capture these features efficiently [4]. The technique, however, does not take account of the phase information leading to inability in identifying gases with many absorption lines such as CH_3CN. Although the number of coefficients is fixed for each waveform, thereby making subsequent comparisons simple, choosing the optimal number is difficult. Fourier series coefficients have also been adopted, but it was found that more coefficients were required that lead only to minor performance improvement [5]. Our earlier work showed single gas species classification that compares locations of resonances from an existing spectral database with measured sample resonances [6], with the aid of recent work on reference pulse estimation [7]. Reference pulse estimation is necessary because, in a real-time gas sensing context, measurement of the reference pulse is not possible. Recent work by [8] exploited the almost-linear phase spectrum to determine the resonant locations from the reference-free spectrum. This paper therefore presents a preliminary application of the reference-free spectrum for gas recognition.

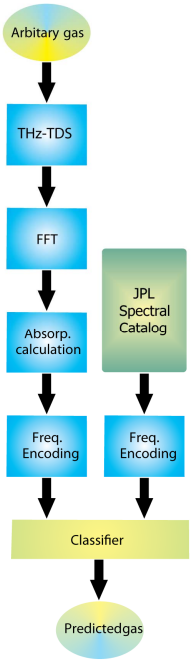

Figure 1 - Flow chart for the proposed approach

II. Results

Figures below compare the absorption coefficient and the reference-free phase spectrum for water vapor and ammonia gas respectively. In the water vapor measurement, the resonant locations in the reference-free phase spectrum appear to coincide well with that computed from the absorption coefficient. In contrast, ammonia gas measurement from our existing Picometrix 2000 spectrometer provides a less than satisfactory result. Closer examination of systems dynamic range [9] reveals that only for resonant locations below 1.2THz are should be investigated. The reference-free phase spectrum therefore picks up the resonant peak at approximately 0.6 THz that coincides well with the absorption coefficient. Common to both measurements is the strong

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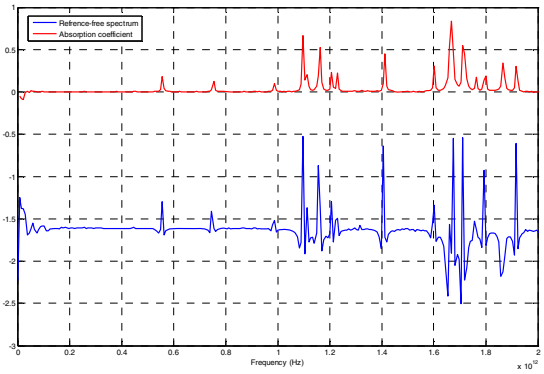
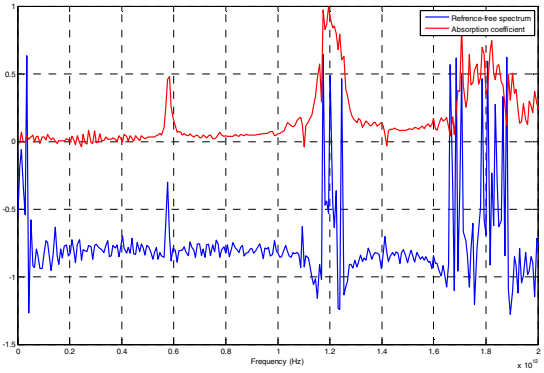
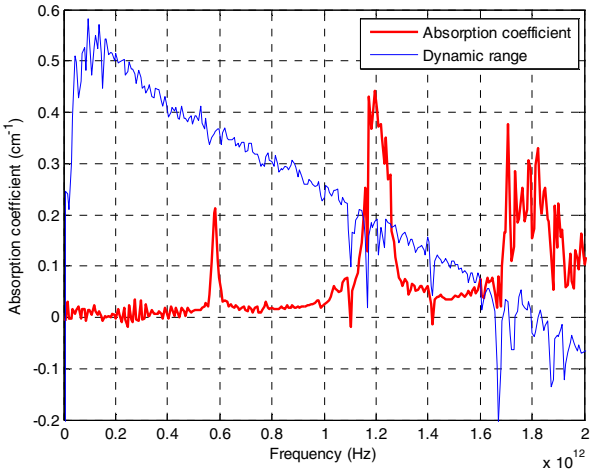
resonance in the frequency range below 0.2 THz in the reference-free phase spectrum. These peaks will need to be cropped for out for subsequent processing. Future work will compare reference-free phase spectrum and reference estimation techniques [7] for gas recognition.







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