Remote Detection of Gases and Liquids by Imaging Fourier Transform Spectrometry Using a Focal Plane Array Detector: First Results

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ABSTRACT

Infrared spectrometry allows detection and identification of gases in the atmosphere as well as analysis of solids and liquids from long distances. An application of the method which has received increased attention over the last years is the detection of hazardous compounds. These may be present in the gas phase in the atmosphere but also as liquid droplets on surfaces. In this study, imaging Fourier transform spectrometry (IFTS) was applied to detect both liquids and gases. Measurements were performed with an imaging Fourier transform spectrometer developed at TUHH. The imaging spectrometer and first results of measurements are presented.

Keywords: remote sensing, FTIR, passive, imaging spectrometry, imaging Fourier-transform spectrometer, emergency response

1. INTRODUCTION

Passive remote sensing by infrared spectrometry allows detection and identification of toxic clouds from long distances. Typical applications of the method are automatic surveillance of industrial facilities and identification of potentially hazardous clouds after chemical accidents. Conventional remote sensing Fourier transform infrared spectrometers are based on interferometers with a single detector element. The output of the system is usually a yes/no decision by an automatic identification algorithm that analyses the measured spectrum for presence of compounds of interest. The analysis of the measured spectrum by the operator alone is complicated and time consuming and thus this task would require an expert operator. Hence even if a scanning system is used for surveillance of a large area, under normal circumstances the operator is still dependent on the decision of the identification algorithm.

In contrast, imaging systems allow both automatic identification and intuitive interpretation, directly from the images generated during the analysis. An imaging spectrometer with such capabilities is the scanning infrared gas imaging system1 (SIGIS). This system is also based on an interferometer with a single detector element, in combination with a telescope and a synchronised scanning mirror. The results of the analyses of the spectra are displayed by an overlay of a false-colour image (the “hazardous chemical image”) on a video image.

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However, the temporal resolution of the system is limited by the sequential measurement of all fields of view within the field of regard. In order to measure a complete image with a single scan of the interferometer with all fields of view measured simultaneously, an imaging Fourier-transform spectrometer (IFTS) using a detector array instead of a single detector element has been developed at TUHH.

Another application of infrared spectrometry is the analysis of liquids and solids. Hazardous compounds may be present as liquid droplets on surfaces. Previous studies showed that infrared spectrometry allows detection and identification of liquid contaminants on surfaces. These studies were performed with conventional spectrometers, i.e. instruments with a single detector element. One problem associated with the use of a spectrometer with a single detector element to detect liquids on surfaces is the choice of the field of view of the spectrometer. If a large field of view is chosen, it may not be filled by the liquid which may be present in the form of small droplets. This results in high limits of detection. If a small field of view is chosen, the investigation of an extended area is time-consuming. In contrast, imaging spectrometry allows the inspection of extended areas (large field of view of the array) with a small instantaneous field of view (field of view of each pixel), resulting in low limits of detection.

In this preliminary study, an imaging Fourier-transform spectrometer is applied to detect gases in the atmosphere as well as liquids on surfaces.

## 2. IMAGING FOURIER-TRANSFORM SPECTROMETER

The system is based on the combination of a modified Michelson interferometer and a detector array (focal plane array).

### 2.1 Interferometer

The interferometer of the IFTS is a modified Michelson interferometer with cube-corner mirrors (Bruker Daltonics, Leipzig, Germany). The interferometer block is mounted on an aluminium base plate. The maximum optical path difference of the interferometer is 1.8 cm for two-sided interferograms. This corresponds to a width of the instrument line shape \( \Delta \sigma_{\text{FWHM}} \) of \( \Delta \sigma_{\text{FWHM}} = 0.33 \, \text{cm}^{-1} \). In this work, an optical path difference that corresponds to a spectral resolution of \( \Delta \sigma_{\text{FWHM}} = 5 \, \text{cm}^{-1} \) is used. The choice of resolution is a trade-off between the goals of a low limit of detection and a short measurement time on the one hand, and the goal of high selectivity on the other hand. The signal-to-noise ratio improves with decreasing spectral resolution for constant measurement time; while higher resolution yields greater selectivity.

### 2.2 Focal plane array

In the configuration used in this work, a focal plane array (FPA) consisting of 16384 pixels (128 × 128 pixels) is used (AIM 128 LW, AIM Infrarot-Module, Heilbronn, Germany). The detector material of the focal plane array is HgCdTe. The array is cooled by a Stirling cooler. The spectral range is 960 - 1330 cm\(^{-1}\). The size of the detector elements is 40 µm × 40 µm (pitch).
2.3 Data processing

2.3.1 Calculation of brightness temperature spectra

The first step of processing is the calculation of the spectra by application of a Fourier-transform to the interferograms. The next step is the calculation of the radiance spectra using the results of a radiometric calibration. The radiometric calibration is performed by measurement of spectra of black body reference sources at two temperatures. Finally, the brightness temperature spectrum of each pixel is calculated using the inverse of Planck’s function for the spectrum of the black body with respect to temperature.

2.3.2 Spatial filtering

The pixel pitch of current HgCdTe focal plane arrays in the spectral range 800 - 1250 cm⁻¹ (8 - 12.5 µm) is in the range 25 - 40 µm. The size of the detector element of a conventional remote sensing Fourier-transform spectrometer is of the order of 1 mm². Due to the small area of each pixel of an array, the power incident on each detector element is small compared to the power incident on the single detector element of a conventional remote sensing Fourier-transform spectrometer. Thus, longer integration times are necessary to achieve signal-to-noise ratios of the same order of magnitude as the signal-to-noise ratio of a conventional system. This may be realised by calculation of the mean of replicate measurements but this procedure degrades the temporal resolution and therefore reduces the benefit of an imaging system over a scanning system.

Another way to improve the signal-to-noise ratio of an imaging system is spatial filtering. By convolution of the image with a weighting function the signal-to-noise ratio may be improved. However, this method results in a degradation of the spatial resolution. The software of the IFTS system allows the application of various weighting functions. In this work, a two-dimensional rectangular function is employed. The result of the application of this function is equivalent to the calculation of the mean signal of adjacent pixels. If random errors dominate, the signal-to-noise ratio may be improved by a factor given by the square root of the number of pixels that were taken into account in the calculation.

2.4 Performance of the IFTS: Noise equivalent spectral radiance NESR

In order to measure the noise equivalent temperature difference NE∆T and the noise equivalent spectral radiance NESR, measurements of a black body calibration source were performed. The radiometric calibration was performed by measurements of spectra (image cubes) of a black body at two temperatures. The noise equivalent spectral radiance NESR was determined under the assumption that the data are ergodic. An image cube of an extended black body source at 310 K was measured. For each pixel the brightness temperature spectrum was calculated. In order to remove baseline shifts in the resulting spectra, which may be caused by various effects, such as a temperature drift of the interferometer⁵,⁶, a baseline correction by linear regression was applied. The noise equivalent temperature difference NE∆T was determined by calculation of the standard deviation of the resulting spectrum in the range 1100 - 1200 cm⁻¹. The noise equivalent spectral radiance NESR was calculated using the NE∆T and the derivative of Planck’s law with respect to temperature. In order to specify the NESR of the system, the median of the NESR of the central 64×64 pixels was calculated.

The specifications of the IFTS are shown in Table 1.
### Table 1: Specifications of the imaging Fourier transform spectrometer.

<table>
<thead>
<tr>
<th>Interferometer</th>
<th>Michelson interferometer with cube-corner retroreflectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral range (focal plane array)</td>
<td>960 - 1330 cm⁻¹</td>
</tr>
<tr>
<td>Spectral resolution ($\Delta \sigma_{\text{FWHM}}$)</td>
<td>5 cm⁻¹</td>
</tr>
<tr>
<td>NESR (single pixel, 310 K black body, single scan, $\Delta \sigma=5$ cm⁻¹, triangular apodisation, 1100 - 1200 cm⁻¹, median of 4096 pixels)</td>
<td>$3 \times 10^{-8}$ W/(cm² sr cm⁻¹)</td>
</tr>
<tr>
<td>Focal plane array</td>
<td>AIM 128 LW (128 × 128 pixels)</td>
</tr>
<tr>
<td>Size of detector elements (pitch)</td>
<td>40 µm × 40 µm</td>
</tr>
<tr>
<td>Focal length</td>
<td>50 mm</td>
</tr>
<tr>
<td>Instantaneous FOV (single pixel)</td>
<td>0.8 mrad</td>
</tr>
<tr>
<td>Display</td>
<td>Overlay of false colour image on video image</td>
</tr>
<tr>
<td>Dimensions</td>
<td>$610 \times 380 \times 300$ mm³</td>
</tr>
</tbody>
</table>

### 3. IDENTIFICATION ALGORITHM

In this work, an identification algorithm that was originally developed for remote detection of gases is applied to identify both gases and liquids. In the following paragraphs, a short description of the algorithm is given. The algorithm has been described in references 7, 8, and 9 and the reader is directed to these articles for further detail.

The identification method is based on the approximation of a measured spectrum with reference spectra. First, the spectrum of the brightness temperature $T_{Br}(\sigma)$ is calculated. The spectrum is analysed sequentially for a variable number of target compounds - which are contained in a spectral library - with different reference matrices. Each matrix contains spectral data of one target compound, atmospheric gases (e.g. H₂O), and it may also contain the signatures of potential interferents. Moreover, it contains functions for the approximation of the baseline. The frequency dependence of the brightness temperature of the background and thermal effects inside the spectrometer may cause baseline shifts that exceed the signal of the target compound.

The identification is performed in three steps. In the first step, the mean brightness temperature is subtracted and the signatures contained in the matrix are fitted to the resulting spectrum. In the next step, the contributions of all fitted signatures (i.e. interferents, atmospheric species, and baseline) except the signature of the target compound are subtracted from the measured spectrum.

Then, in order to decide if the target compound is present, the coefficient of correlation between the corrected spectrum, i.e. the result of the subtraction, and a reference spectrum is calculated in a compound-specific number of spectral windows. Moreover, the coefficient of correlation between the fitted spectrum and the measured spectrum is calculated. The signal-to-noise ratio is calculated by division of the maximum brightness temperature difference caused by the
target compound (determined by the least squares fitting procedure) by the noise equivalent temperature difference of the spectrum. If all coefficients of correlation and the signal-to-noise ratio are greater than compound-specific threshold values, the target compound is identified.

4. MEASUREMENT OF LIQUIDS ON SURFACES

4.1 Experimental

In order to examine the feasibility of imaging Fourier transform spectrometry for the detection of liquids on surfaces, a measurement set-up was implemented employing an artificial source of radiation. In this work, a radiant heater (600 W) was used as radiation source. The radiation source was positioned next to the IFTS. This configuration is illustrated in Fig. 1. The distance between the IFTS and the surface under examination was 1 m. The materials used as background surfaces were clay, wood, pressboard, polymethyl methacrylate (acrylic glass), and steel.

![Fig. 1: Set-up with an artificial source of radiation.](image)

Prior to all measurements, a radiometric calibration using a black body at two different temperatures was performed.

4.2 Results and discussion

As an example, results of measurements of 0.05 mL methyl salicylate applied to a clay tile are presented and discussed. Measurements were performed using the set-up shown in Fig. 1. Fig. 2 shows a video image of the tile and the liquid on the surface of the tile.
**Fig. 2:** Clay tile with methyl salicylate applied to the surface.

**Fig. 3:** Right: Image of the brightness temperature at 1300 cm\(^{-1}\). The area covered by methyl salicylate is clearly observable. Left: Brightness temperature spectra of an area covered with methyl salicylate (a, solid line) and an area not covered by methyl salicylate (b, dotted line).

Fig. 3 shows a false colour image of the brightness temperature at 1300 cm\(^{-1}\) as well as spectra of different areas of the tile. The area covered by methyl salicylate is clearly observable. Spectrum (a) is the brightness temperature spectrum of an area covered with methyl salicylate. Spectrum (b) is a brightness temperature spectrum of an area which is not covered by methyl salicylate. The emissivity of the clay surface is high and almost constant in the spectral range of the IFTS. Thus, in contrast to spectrum a, the brightness temperature spectrum b exhibits little structure \((T_B \approx \text{const.})\).

The measurements of methyl salicylate on pressboard and wood resulted in similar spectra as shown in Fig. 3. Based on these spectra, a reference spectrum was created. This reference spectrum was used as a target spectrum in the automatic identification algorithm described in section 3. Fig. 4 shows the result of the automatic identification algorithm applied to the measurement shown in Fig. 3. Spatial filtering with a weighting function of 3×3 pixels was applied. The identification result (yes/no decision) is visualised by an overlay of a false colour image on a video image. Fig. 5
depicts a false colour image of the signal of methyl salicylate, which was determined using the coefficient of the methyl salicylate signature of the least squares fit (see section 3).

**Fig. 4:** Identification of methyl salicylate.

Fig. 5 and Fig. 7 show results of a measurement of 0.15 mL methyl salicylate on a steel plate. Because of the high reflectivity of the steel surface, the strong absorption bands of methyl salicylate in the range 1200 - 1300 cm$^{-1}$ cause a
saturated signal; instead, the analysis was performed in the range 1000 - 1160 cm\(^{-1}\). A gas phase spectrum was used as reference spectrum. Spatial filtering with a weighting function of 3×3 pixels was applied.

**Fig. 6:** Identification of methyl salicylate on a steel plate. The background video image was recorded without methyl salicylate.

**Fig. 7:** Signal of methyl salicylate (coefficient of the methyl salicylate signature of the least squares fit, see section 3). The background video image was recorded without methyl salicylate.
The results demonstrate the feasibility of detection and identification of liquids on surfaces by imaging Fourier transform spectrometry and also suggest some of the areas requiring further work. The strong influence of the surface material and the influence of the thickness of the liquid film have to be considered in the development of a system for automatic identification of liquids.

5. MEASUREMENT OF GASES

5.1 Experimental

The experimental set-up for the detection and identification of gases is shown in Fig. 8. Prior to all measurements, a radiometric calibration was performed using a black body reference source at two different temperatures.

![Fig. 8: Measurement set-up for gas measurements.](image)

5.2 Results and discussion

As an example, results of measurements of methanol evaporating from a cup are presented. Measurements were performed using the set-up shown in Fig. 8. The distance between the system and the position of the release was 2 m. The temperature of the black surface was 313 K; the temperature of the methanol vapour was 297 K. A small flow of nitrogen gas was directed into the liquid methanol to increase the amount of methanol evaporating from the cup before the measurement was performed. Fig. 9 shows a video image of the scene.
Fig. 9: Video image of cup containing methanol in front of a black surface.

Fig. 10 depicts a false colour image of the signal of methanol, which was determined using the coefficient of the methanol signature of the least squares fit (see section 3). Spatial filtering with a weighting function of 5×5 pixels was applied. The analysis was performed in the range 1000 - 1150 cm⁻¹. Fig. 11 shows the result of the automatic identification algorithm applied to the measurement shown in Fig. 10. The identification result (yes/no decision) is visualised by an overlay of a false colour image on a video image.

Fig. 10: Signal of methanol (coefficient of the methanol signature of the least squares fit, see section 3).
6. SUMMARY AND CONCLUSIONS

Imaging Fourier transform infrared spectrometry was applied to detect, identify, and visualise liquids on surfaces from a distance of 1 m. The application of an imaging spectrometer results in a major improvement regarding the practicability of measurements because the technique allows the inspection of an extended area within a measurement time on the order of a second.

It is planned to modify the automatic identification algorithm in order to identify liquids automatically based on liquid phase reference spectra. Future work will also include field studies and further investigation of illumination geometries and sources.

The imaging Fourier-transform spectrometer also allows identification and visualisation of gases. In this work, laboratory measurements were presented. Future work will include field measurements of gases.

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8. REFERENCES


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