LWIR Multispectral Imaging Chemical Sensor

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ABSTRACT

Physical Sciences Inc. (PSI) has developed an Adaptive InfraRed Imaging Spectroradiometer (AIRIS), comprised of a low-order tunable Fabry-Pérot étalon coupled to an HgCdTe detector array, for passive, stand-off detection of chemical vapor plumes. The tunable étalon allows coverage of the 9.5 to 14 µm spectral region with a resolution of ~7 cm⁻¹ and provides the capability to obtain monochromatic images (λ/Δλ > 100) of a scene at only those wavelengths needed for chemical species identification and quantification. The adaptive sampling capability of the étalon allows suppression of background clutter and minimization of data volume. The tuning time between transmission wavelengths is typically ~10 ms, however the mirror tuning system may be operated to obtain tuning times as short as 1.3 ms. We present results using a brassboard imaging system for stand-off detection and visualization of chemical vapor plumes against near ambient temperature backgrounds. This data shows detection limits of 22 ppmv • m and 0.6 ppmv • m for DMMP and SF₆ respectively against a ΔT of 6 K. The reported detection limits are consistent with the measured system noise-equivalent spectral radiance, approximately 2 µW cm⁻² sr⁻¹ µm⁻¹.

Keywords: remote sensing, hyperspectral, imaging, chemical agent, Fabry-Perot, interferometer

1. INTRODUCTION

Imaging spectrometry is a field of increasing interest to the remote sensing community as it enables passive, stand-off analysis of the physical and chemical composition of wide areas. Remote monitoring of localized chemical vapor releases is a logical extension of existing visible and near-IR imaging spectrometer technology. The long-wavelength infrared (LWIR) is the spectral region of choice for monitoring chemical plume releases because most organic chemical vapors have their strongest identifying spectral signatures in the 8 to 14 µm atmospheric transmission window. An additional benefit of LWIR imaging is that the scene under study does not require external illumination. Thermal radiation provides the signature necessary to extract characteristic absorption and emission spectra of target chemical compounds. Chemical plume visualization requires exploitation of both the spectral signatures of the target compounds as well as the effective temperature difference between the vapor plume and the background scene. The integration of a spectral filter into an IR focal plane array (FPA) based sensor provides the resolution requisite to identify the spectral signatures of specific chemical compounds and the throughput to achieve high detection sensitivity.

Previous efforts to provide imaging capability for chemical vapors¹⁻⁴ focussed largely on the use of filter wheels in conjunction with forward-looking IR (FLIR) sensors. In contrast to filter wheel-based imagers, the number of wavelengths available to the tunable étalon based imaging system is not limited by considerations such as the number of slots available in a filter wheel. In its simplest configuration, the low-order tunable étalon replaces a filter wheel assembly with a more compact, frequency agile system offering considerable improvement in data acquisition capability. In contrast to imaging FTIR spectrometers such as the Livermore Imaging Fourier Transform Infrared Spectrometer⁵ (LIFTIRS) and dispersive imagers such as the Spectrally Enhanced Broadband Array Spectrograph System⁶ (SEBASS), the adaptive sampling capability of the tunable étalon provides computational simplicity and higher throughput. It allows the user to minimize data volume and simplifies data processing by imaging a scene at only those wavelengths needed for target identification and clutter suppression. The imaging spectroradiometer utilized in this paper has common pixel registry for all wavelengths and does not require significant image processing to generate a radiometrically calibrated image of the scene.
2. EXPERIMENTAL SYSTEM

2.1 Interferometer

The LWIR hyperspectral imaging system described here consists of an IR detector array which views the far field through a tunable, piezoelectric-actuated Fabry-Pérot etalon placed in the afocal region of the imaging system. A digital capacitance micrometry system is used to measure mirror spacing and alignment. A closed loop control system is used to position and align the interferometer to the desired wavelength in times as short as 1.3 ms. The basic concept is shown in Figure 1. The interferometer operates as a tunable interference filter which selects the wavelength viewed by the detector array.

Figure 1. LWIR imager optical configuration employing the off-axis parabolic reflectors as focusing elements.

The theoretical basis for the development of the tunable etalon based imaging spectroradiometer, as well as the consequences and advantages of low-order operation, are evident from the mathematical description of etalon transmission. Transmitted wavelengths fulfill the resonance condition:

$$2\ell \cdot \cos \theta = \left[ m + \frac{\phi(\lambda)}{\pi} \right] \cdot \lambda$$

where $\ell$ is the mirror spacing, $\theta$ is the angle of incidence of the light with respect to the optical axis of the etalon, $m$ is the order of interference, and $\phi(\lambda)$ is the phase change upon reflection from the mirror coating.\(^7\)

The wavelength dependent filter transmission is described by an Airy function:

$$\frac{I(\lambda)}{I_0(\lambda)} = \left\{ \frac{t(\lambda)}{1-r(\lambda)} \right\}^2 \times \left\{ 1 + \left[ \frac{2F(\lambda)}{\pi} \right]^2 \sin^2 \left( \frac{2\pi t(\lambda) \cos \theta}{\lambda} + \phi(\lambda) \right) \right\}^{-1}$$

where $t(\lambda)$ and $r(\lambda)$ are the wavelength dependent mirror coating transmission and reflectivity and $F(\lambda)$ is the interferometer finesse. The interferometer is equipped with nominal 94% reflectivity mirrors spanning the range 9.5 to 14.5 $\mu$m. Figure 2 provides an expanded view of the third order transmission band of the etalon near 10.55 $\mu$m. Peak transmission is >60% and includes slight attenuation by the two anti-reflection coated Ge windows which provide optical access to the etalon in its hermetically sealed housing. A detailed examination of the lineshape shows a good fit to the expected Airy function with a FWHM of 6.9 cm\(^{-1}\).

The etalon’s spectral resolution (finesse) is governed not only by mirror reflectivity, but also by surface roughness, collimation of light incident on the filter, and degree of mirror parallelism.\(^7\) For practical operation in the infrared, the substrate surface roughness is the limiting factor in determining total finesse. The limiting spectral resolution is seldom greater than $\Delta\lambda_{\text{FSR}}$/40, finesse = 40, due to this limitation. The observed resolution corresponds to a finesse ~25 and is better than 1% of $\lambda$ over the entire tuning range of the device. The free spectral range (FSR) of the etalon is defined as the wavelength spacing between adjacent transmission orders. For an ideal Fabry-Perot etalon, $\phi(\lambda)$=1, this expression simplifies to:

$$\Delta\lambda_{\text{FSR}} = \frac{\lambda_{\text{max}}}{m + 1}$$
where \( m \) is the operating order of the interferometer and \( \lambda_{\text{max}} \) is the longest transmitted wavelength when operating in order \( m \). A wide bandpass filter, matched to the etalon FSR, is placed in front of the detector array to select a single transmission order. Reflected phase dispersion in the dielectric mirror coating, \( \varphi_3 \) in Eqs. (1) and (2), contracts the observed FSR relative to that predicted by Eq. (3). In principle, a tunable etalon can cover the 8 to 12 \( \mu \text{m} \) spectral region in third order (\( m = 3 \)), however the observed FSR of our LWIR etalon in \( m = 3 \) is \( \approx 2 \mu \text{m} \). The effective FSR of the system is demonstrated in Figure 3 where we show a transmission spectrum of the interferometer recorded with an open path FTIR spectrometer.

An additional benefit of utilizing the tunable etalon with a cryogenic focal plane array is that it has low self radiance and may be operated at ambient temperature. System self-radiance not only reduces the effective detector dynamic range but also increases photon statistical noise, thereby reducing detection sensitivity. The etalon is reflective where it is not transmitting and, in the configuration depicted in Figure 1, system self-radiance arises from the weak emission of the high reflective mirror coating and mirror substrates, as well as radiation from the liquid nitrogen-cooled focal plane array reflected back by the first etalon mirror (Narcissus effect). The contribution of the latter two sources to the overall system self-radiance is negligible. The emissivity of the etalon may be calculated from first principles knowing that reflection, transmission, and emission sum to unity:

\[
t(\lambda) + r(\lambda) + \varepsilon(\lambda) = 1
\]  

Figure 4 depicts the calculated transmission, reflection, and emissivity as a function of wavelength for an idealized, \( \varepsilon(\lambda) = 0 \), Fabry-Perot etalon with 94% reflecting and 0.5% absorbing mirror coatings. In contrast to an absorbing or scattering filter, e.g., a LWIR AOTF (Ref. 8), the tunable etalon has extremely low self-radiance at ambient temperature. We calculate the field temperature required to produce a transmitted radiance equal to the emitted radiance of the etalon, i.e. the field temperature, \( T_{\text{field}} \), at which:

\[
\int_{\lambda_0}^{\lambda_1} \varepsilon(\lambda) \cdot N(\lambda, 300K) \, d\lambda = \int_{\lambda_0}^{\lambda_1} t(\lambda) \cdot N(\lambda, T_{\text{field}}) \, d\lambda
\]

Figure 5 depicts calculated equivalent field temperature as a function of mirror reflectivity for four different values of coating absorption.
The conclusion drawn from Figure 5 is that while it is desirable to minimize coating absorption, maximizing coating reflectivity does not necessarily maximize detection sensitivity. This is because etalon self-radiance scales with coating absorption while the integrated transmitted radiance scales with the width of the etalon’s transmission fringe, which is inversely proportional to coating reflectivity. Therefore, when specifying a mirror coating, efforts should be made to minimize absorption but reflectivity need only be increased to the point of meeting the out-of-band rejection requirements of the system. Spectral features of chemical warfare agents are broad, typically 50 to 100 cm⁻¹, so a modest reflectivity coating may be suitable for many CW agent release monitoring applications.

2.2 Optical configuration

There are four key elements to the imaging system shown in Figure 1: 1) an eight element (2 x 4 format) photoconductive HgCdTe detector array in an LN₂ cooled dewar; 2) the computer controlled tunable etalon; 3) a rotating wheel mechanical chopper used to modulate the far field radiation; and 4) a computer controlled galvo-driven two-axis scanning mirror system to provide a wide Field-of-Regard. The IR emission from the far field is sampled with the scan mirrors, brought to an intermediate focus by an off-axis parabolic reflector (OAP), modulated by the mechanical chopper (2870 Hz), recollimated by a matched OAP, and directed through the tunable etalon. The radiation transmitted by the etalon is directed into the detector array through a 10.0 to 11.5 µm transmitting cold filter chosen to closely match the etalon’s free spectral range. The tunable etalon is typically scanned from 10.1 to 11.4 µm during chemical vapor plume imaging experiments. A three-dimensional “data cube”, 2D-spatial by 1-D spectral, is produced by positioning the interferometer to transmit a chosen wavelength, scanning the galvo mirrors through 288 discrete positions to produce a 48 x 48 pixel image of the field, and repeating the process for all desired wavelengths. Two channels of D/A enable the computer to automatically scan the galvo mirror positions to build the 48 x 48 pixel scene using the 2 x 4 element array. Each 48 x 48 pixel spatial element in the data cube comprises a 40 by 40 deg FOV (14 mrad/pixel). Each data cube generated in the chemical plume imaging experiments consisted of 14 spectral elements. The galvo mirror scan is the rate-limiting step of the data acquisition and takes ~9 seconds (per wavelength) to complete.

The eight HgCdTe detector array elements are 0.5 mm square. Each element is biased and amplified using an eight-channel, custom-built amplifier board. The use of the mechanical chopper in conjunction with an eight-channel lock-in
3. CHEMICAL DETECTION EXPERIMENTS

The chemical imaging system was characterized using both direct absorption and passive IR emission measurements. Initial experiments were conducted utilizing the system to view an extended blackbody source through a 10 cm path absorption cell. Gas mixtures could be produced and flowed through the cell using a manifold of mass flow controllers coupled to vapor generators as well as pure target and diluent gases. An example of an absorption spectrum taken with the imaging system is shown in Figure 4 for a mixture of 7 ppmv • m SF₆ and 76 ppmv • m dimethyl methyphosphonate (DMMP). The data is compared with high resolution reference spectra, calculated for the same column density and convolved with the imaging system spectral resolution, as shown in Figure 2. The SF₆ and DMMP absorption coefficients were obtained from laboratory spectra recorded at 0.5 cm⁻¹ resolution with an FTIR spectrometer. The SF₆ absorption spectra were recorded in an atmospheric pressure flow cell (10 ppmv SF₆ in dry N₂). The calculated SF₆ absorption coefficient was scaled by ~10% to match the published value of the integrated absorption coefficient of the ν₃-fundamental band. This scaling correction is consistent with the calibration uncertainty in the SF₆ mass flow system. The DMMP absorption spectra were recorded in a sealed cell containing the saturation vapor pressure of the liquid. The individual components of the calculation and the combined spectra are shown in Figure 6. The data agree quite well with the calculations, indicating that the spectral resolution of the system as well as the absorption coefficients of the target gases are both well understood. It should be noted that the mirror coating used in the brassboard system was initially developed to detect chlorinated hydrocarbon gases at short range. Hence, the coating was designed for longer wavelengths than are optimal for the detection of chemical agents and their simulants, such as DMMP. As a result of this constraint, we are forced to use a weaker band of DMMP (10.85 µm peak) than is used in most other studies of chemical agent detection. The detection sensitivity, in the optically thin limit, scales with the absorption coefficient. Thus, we expect that detection sensitivities for DMMP could be improved by a factor of three if the stronger band at 9.4 µm were used in these measurements.

The passive detection of chemical vapors requires both high radiance contrast as well as good spectral resolution. A chemical vapor plume may appear in either emission or absorption depending upon the temperature and emissivity differences between the plume and the background. We calculate the plume spectral signature using a simplified three layer radiative transfer model, as shown in Figure 7. The model has been used previously by Flanigan and is an excellent approximation when the temperature variation within the plume is small in comparison to the temperature difference between the plume and the background. The total infrared radiance incident upon the sensor at a given wavelength (W cm⁻² sr⁻¹ µm⁻¹) is the sum of the contributions from each layer and is given by:

\[
N_{\text{sen}}(\lambda) = \tau_3 \tau_2 N_1(\lambda, T_1) + \tau_2 [1-\tau_2] N_2(\lambda, T_2) + [1-\tau_2] N_3(\lambda, T_3)
\]  

Figure 6. Observed and calculated transmission through an absorption cell containing 8 ppmv•m SF₆ and 80 ppmv•m DMMP in dry N₂. The reference blackbody is at 308 K and the gas temperature is 298 K. The data represent a six scan co-average.
Figure 7. Schematic diagram of three-layer model for quantitative analysis of scene radiance levels and plume concentration determination.

where $N_i$ is the Planck radiance of layer $i$ at its apparent temperature for that wavelength. The quantities $t_2$ and $t_1$ are the spectral transmission of the plume and the atmosphere between the plume and the sensor, respectively. The first term in Eq. (6) is the radiance from the background as attenuated by the chemical plume and intervening atmosphere. The second term is the radiance of the chemical species in the plume as attenuated by the atmosphere between the plume and the sensor. The third term is the radiance of the atmosphere between the plume and the sensor. For the short path between the sensor and the plume in these experiments we approximate $t_1$ to be unity. In our experiments, the background radiance, $N_1$, is assumed to be characteristic of a unit emissivity blackbody at temperature, $T_1$. The transmission of the plume, layer 2, is computed from the spectral properties of the chemical species contained therein:

$$t_2(\lambda) = \exp[-\Sigma k_i(\lambda) C_i L]$$  

where $C_i$ is the average concentration of the chemical compound over the path length $L$ and $k_i(\lambda)$ is the wavelength-dependent absorption coefficient. The sum over index $i$ in Eq. (7) is over all spectrally relevant chemical species.

It is essential to note that if there is no temperature difference between the background and the plume then no spectral signature of the chemical plume is observed. For a single species present in an optically thin plume, the uncertainty in the calculated column density is well approximated as inversely proportional to the absorption coefficient of the chemical species and the temperature difference between the plume and the background:

$$\delta[C_i L] \approx \frac{N_{ESR}}{k(\lambda) \cdot \frac{\partial N}{\partial T} [T_{plume} - T_{bb}]}$$  

The quantity NESR is the measured noise equivalent spectral radiance of the system. We combine absolute radiance calibration of the sensor with absolute measurements of a chemical compound’s absorption coefficient to predict the detection limit for that species. The calculated detection limits for SF$_6$ and DMMP are 0.6 and 22 ppmv·m against a ΔT of 6 K for the bands used in these measurements. As previously noted, use of the stronger DMMP band at 9.4 μm would improve the sensitivity by approximately a factor of three.

Initial imaging experiments involved viewing the absorption cell containing 20 ppmv·m SF$_6$ held at 298 K against a 308 K reference blackbody. The location of the SF$_6$ cell in the scene is independently determined by the two-band correlation analysis shown in Figure 8. Figure 8 depicts the measured radiance at 10.55 μm, the peak of the SF$_6$ absorption band, plotted versus the measured radiance at 10.85 μm, which is outside the SF$_6$ absorption band. This approach captures differences in apparent emissivity of the scene from pixel to pixel independent of variations in absolute radiance across the scene. The presence of a structured gas absorption feature, which is quite different from the more slowly varying background spectrum, is observed as pixels lying outside the primary vector defined by the majority of the scene pixels. Points falling above the primary vector would indicate SF$_6$ emission, whereas points lying below the primary vector indicate absorption. Because the cell is colder than the blackbody background, only absorption is evident. The pixels corresponding to those points falling $>$3σ below the primary vector locate the absorption cell in the scene. Figure 9 shows the pixels identified by two-band correlation analysis highlighted in black. We use the three layer radiative transfer model to calculate the SF$_6$ column density.
Figure 8. Two-band correlation plot of narrowband scene images at 10.55 and 10.85 µm. See text for details.

Figure 9. False black and white image of absorption cell recorded at 10.55 µm. The location of SF₆ absorption, as identified by two-band correlation analysis, is highlighted in black.

Figure 10. Calculated SF₆ column density in the absorption cell containing scene as determined using the three-layer radiative transfer model.

at the highlighted pixels and find good agreement with the concentration injected into the cell. Figure 10 depicts calculated column density as a function of position in the image. The calculated peak column density from the optical measurement, 18 ± 3 ppmv • m, is in excellent agreement with the 20 ppmv • m determined from calibrated mass flow measurements. Spectral data acquired from these measurements were subsequently used in spectrally matched filter analysis of SF₆ plumes released in an outdoor setting.

We have also tested the system sensitivity against controlled, calibrated plume releases of DMMP. Instrument sensitivity to DMMP is of greater interest than SF₆, as DMMP is more widely recognized as a simulant for toxic organophosphate vapors. The DMMP plume releases were performed at the Analytical Chemistry Laboratory at Argonne National Laboratory (ANL). The laboratory at ANL possesses an apparatus to vaporize and release low concentration plumes of CW agent simulants. The simulant release concentrations ranged from ~30 to ~220 ppmv·m and a NIST traceable blackbody was placed in back of the plume at its release point so that it is viewed against a calibrated background. The plume generating apparatus was contained in a laboratory hood and the LWIR imager was positioned outside the hood at ~1.5 m standoff distance during data acquisition. In this configuration the calibrated background occupies only a few pixels in the scene and the imagery is of little interest.
The spectra of the DMMP releases is analyzed by a least-squares fit of experimental data to Eq. (6). The background blackbody temperature, $T_1$, and plume release temperature, $T_2$, were continuously monitored and controlled during the measurements and therefore held could be fixed during the fit to the data. (The plume release temperature was 307 K and the calibrated background temperature was 313 K.) Figure 11 depicts the comparison of spectroradiometer data to Eq. (6). The data is taken from a point in the image corresponding to the center of the reference blackbody. The released DMMP column density is 141 ppmv • m based on the liquid flow rate into plume generating apparatus. The column density determined from the optical data is $163 \pm 29$ ppmv • m. Figure 12 shows optically determined DMMP column density plotted versus liquid flow rate determined concentration for the full range of release concentrations covered in the test series. Perfect correlation between the calculated and released column density would be indicated by all points falling on the dashed line. The error bars shown correspond to $\pm 1\sigma$ for a fit of experimental data between 10.4 and 11.2 µm to Eq. (6). Statistical analysis of the data in Figure 12 yields a correlation of 1.01 ppmv • m measured per ppmv • m DMMP released (1\(\sigma\) uncertainty: ±0.19) and a detection limit of ±22 ppmv • m. The latter figure is in very good agreement with the detection limit anticipated from the measured system NESR. When the region of comparison is extended to cover the full 10.1 to 11.4 µm spectral region stored in the data cube, the $1\sigma$ uncertainties in correlation and detection limits increase, but neither the slope nor intercept of the data plot changes appreciably. This increase occurs because the system NESR is greater near the long wavelength and short wavelength limits of the operating range than in the center of the range.

Finally, the system was tested against an outdoor plume release where a known flow rate of SF$_6$ was diluted in N$_2$ and released from a pipe of known cross section. This arrangement is depicted in Figure 13. Gas is released from the black pipe slightly below the center of the scene. The location of the SF$_6$ plume in the scene was identified using both two-band correlation analysis and a spectrally matched filter (SMF) algorithm$^{12-14}$ targeted on the SF$_6$ absorption feature at 10.55 µm. The results of the SMF analysis is shown in Figure 14. The SMF analysis locates a larger plume than does the two-band correlation analysis. In addition, the SMF analysis appears to yield fewer false alarms, albeit through the use of data in the entire spectral data cube. The SF$_6$ column density in the plume at the pixels identified by two-band correlation ($>3\sigma$ below the primary vector as for the absorption cell image analysis) was calculated using the three-layer radiative transfer model described previously and is
depicted in Figure 15. Unfortunately, the outdoor plume images were recorded on a windy afternoon and the SF₆ plume was rapidly dispersed in the atmosphere. Because of the rapid dispersion and fact that the opening of the release pipe was less than one pixel wide in the LWIR image, it is not possible to accurately model the actual SF₆ plume signature at the pipe exit. The building wall, which served as the background, was considerably warmer than ambient temperature, 313 to 315 K as opposed to 298 K, and the plume is observed most clearly there. The calculated column density using the radiative transfer model serves as a good cross check for both the two-band correlation and the SMF analyses. False alarms occurring in each analysis correspond to column densities very near or below the anticipated detection limits for the species. The radiative transfer model indicates an SF₆ column density of 5 ppmv • m at the apparent ΔT of 15 K. The SNR of the data is approximately 5:1 and is consistent with detection limits determined using Eq. (9) with the SF₆ absorption coefficient appropriate for the system spectral resolution.

4. CONCLUSIONS AND FUTURE WORK

The objective of this effort was the development of a LWIR hyperspectral imaging system specifically designed for imaging of gaseous chemical species in air. We have demonstrated that the tunable Fabry-Perot etalon provides sufficient spectral resolution, tuning range, and tuning rate to detect and identify vapor plumes of the two tested hazardous vapor simulants, SF₆ and DMMP. The current mirror set and capacitance micrometry system may be improved to extend the spectral tuning range and reduce the tuning time between spectral resolution elements to nearer the limit imposed by the mechanical tuning limit of the mirror actuators.

The NESR of the LWIR spectroradiometer is sufficient to allow detection of optically thin chemical vapor plumes against near ambient temperature backgrounds. Our experimentally determined detection limit of ±22 ppmv-m for DMMP against a temperature drop of 6 K is in excellent agreement with the value predicted using a simple radiative transfer model and the measured noise characteristics of the system detection electronics. In future efforts we will be replacing the scanned 2 x 4 element HgCdTe array with a 64 x 64 pixel format, 61 µm square pixel staring FPA. In addition to improving spatial resolution by approximately a factor of 10, system models indicate that the system NESR can be improved to approximately 0.5 μW cm⁻² sr⁻¹ μm⁻¹. We expect that, with the use of the improved focal plane array and the stronger 9.4 µm band of DMMP, we can improve our detection sensitivity by a factor of 10, to approximately 2 ppmv • m for DMMP against a 6K temperature differential.

The brassboard Fabry-Perot imaging spectroradiometer has provided hyperspectral imagery of sufficient quality to allow quantitative analysis of chemical vapor plume releases. Data is currently processed off-line, however we continue to upgrade
system hardware and data processing algorithms with the goal of providing a stand-off imaging sensor with real-time analysis of the scene chemical composition.

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6. REFERENCES