Visualization and tomographic analysis of chemical vapor plumes via LWIR imaging Fabry-Perot spectrometry

Bogdan R. Cosofret
Christopher M. Gittins
William J. Marinelli


Copyright © 2004 Society of Photo-Optical Instrumentation Engineers.

This paper was published in SPIE Optics East Chemical and Biological Standoff Detection II, and is made available as an electronic reprint (preprint) with permission of SPIE. One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper are prohibited.

Visualization and tomographic analysis of chemical vapor plumes via LWIR imaging Fabry-Perot spectrometry

Bogdan R. Cosofret*, Christopher M. Gittins and William J. Marinelli
Physical Sciences Inc., 20 New England Business Center, Andover, MA, USA 01810-1077

ABSTRACT

Physical Sciences Inc. (PSI) has recently demonstrated near real-time visualization of chemical vapor plumes via LWIR imaging Fabry-Perot Spectrometry. Simultaneous viewing of the plume from orthogonal lines-of-sight enables estimation of the 3-D plume concentration profile via tomographic analysis of the 2-D ‘chemical images’ produced by each spectrometer. This paper describes results of field experiments where a controlled release of sulfur hexafluoride (SF₆) was viewed by two Adaptive Infrared Imaging Spectroradiometers (AIRIS) located ~1 km from the plume release point. The PSI tomographic algorithm is capable of generating 3-D density distributions of the chemical cloud that are consistent with atmospheric model predictions even in the extreme limitation of using only two sensors viewing the chemical plume. Each AIRIS unit provides a 64 pixel x 64 pixel image with an angular resolution of ~5.5 mrad/pixel. Each AIRIS was configured to provide continuous coverage of the 10.0-10.8 µm spectral region at 6-8 cm⁻¹ spectral resolution and exhibits a noise equivalent spectral radiance of ~2 µW/(cm² sr µm).

Keywords: Infrared spectroscopy, computed tomography, chemical warfare detection, cloud tracking, multispectral imaging

1. INTRODUCTION

In this paper we describe the results of chemical imaging experiments conducted during the spring and summer of 2004 involving two LWIR imaging Fabry-Perot spectrometers developed by Physical Sciences Inc. (PSI). (The instrument is known as an Adaptive InfraRed Imaging Spectroradiometer, AIRIS™, U.S. Patent 5,461,477). The experiments involved imaging a series of controlled chemical vapor releases at Dugway Proving Grounds (DPG). The field study was focused on the dissemination of sulfur hexafluoride viewed from two fixed locations approximately 1.2 km away from the plume release point.

Passive sensing of chemical vapor plumes requires exploitation of both the spectral signatures of the target species as well as the radiance contrast between the vapor and the background scene. PSI’s imaging spectrometers are comprised of an LWIR focal plane array-based camera which views the far field through a low-order, tunable Fabry-Perot etalon [1,2]. The tunable etalon provides the spectral resolution necessary to resolve structured absorption and emission from molecular vapors. The focal plane array (FPA) enables radiance measurements of sufficient accuracy that chemical vapors may be selectively detected with only several degrees effective temperature difference between the vapor and the background.

In this paper we describe the implementation of the AIRIS technology to detect and track chemical clouds via computed tomography. Data acquired from the two sensors fielded at Dugway Proving Grounds has been used to construct a three dimensional representation of the chemical cloud density function from line density measurements. We present a synopsis of the development of the PSI tomographic algorithm by first describing results obtained from synthetic data. This exercise has allowed us to better understand the absolute capability of the algorithm in the case of limited projection views (only two sensors). Finally, we present the results obtained from the tomographic analysis of the infrared imagery from the DPG dissemination.

*cosofret@psicorp.com; phone 1 978 689-0003; fax 1 978 689-3232; http://www.psicorp.com
2. EXPERIMENTAL SETUP AND TECHNICAL BASIS OF THE DETECTION APPROACH

The basic AIRIS optical configuration is shown in Figure 1. The concept is based on the insertion of a tunable Fabry-Perot interferometer (etalon) into the field-of-view of an infrared focal plane array (FPA). The IR FPA views the far field through the piezoelectric-actuated etalon placed in an afocal region of the optical train. The tunable etalon is operated in low order (mirror spacing comparable to the wavelength of the light transmitted) and functions as an interference filter which selects the wavelength viewed by the FPA. The optical configuration depicted in Figure 1 affords a wide field of view, high optical throughput, and broad wavelength coverage at high spectral resolution.

The interferometer tuning time is 10-15 ms between transmission wavelengths. Fore-optics and integrated blackbody calibration sources, not depicted in Figure 1, enable control of each sensor’s field-of-regard and absolute radiometric calibration of AIRIS data. The AIRIS units operated in the study provide 64 pixel x 64 pixel imagery at 5.5 x 5.5 mrad IFOV per pixel. This configuration results in a 20 degree x 20 degree field of regard.

The two AIRIS units were configured to acquire imagery between 10.0 and 10.8 µm at 8 cm\(^{-1}\) spectral resolution. The FPA integration time was set to 1.5 ms and the sensor cameras acquired imagery at 20 Hz. The sensors acquired eight images at each detection wavelength. The images were averaged during data processing. Radiometric calibration of the data was accomplished using a two point gain and offset correction. The median noise equivalent spectral radiance in the data is \(\sim 1.5\ \mu\text{W cm}^{-2}\ \text{sr}^{-1}\ \mu\text{m}^{-1}\) at 10.5 µm. The spectral radiance of ambient temperature objects was typically \(\sim 800\ \mu\text{W cm}^{-2}\ \text{sr}^{-1}\ \mu\text{m}^{-1}\) over the sensor operating range and the change in radiance with temperature is \(\sim 15\ \mu\text{W cm}^{-2}\ \text{sr}^{-1}\ \mu\text{m}^{-1}\) per K. Figure 2 shows the vapor plume viewing geometry. The sensors were positioned 1.15 km south and 1.15 km east of the plume release point. The wind direction was primarily from the south with a speed of approximately 2 m/s. The purpose of choosing the sensors’ line of sight parallel and orthogonal to the plume propagation direction was to enable tomographic reconstruction of the 3-D SF\(_6\) concentration. When observations are limited to two sensors, the optimum lines of sight for tomographic reconstruction are parallel to and orthogonal to the plume propagation axis.

The physical principle of the approach is based on the change in passive infrared radiation received by a spectrally resolving sensor due to the presence of a chemical cloud. The basic process can be described by a three layer model, as shown by Flannigan [3] and it is illustrated in Figure 3.

The total infrared radiance incident on the sensor at a given wavelength is the sum of the contributions from each layer and is given by:

\[
N_{\text{sensor}}(\lambda) = t_1 \cdot t_2 \cdot N_1(\lambda, T_1) + t_3 \cdot [1 - t_2] \cdot N_2(\lambda, T_2) + [1 - t_3] \cdot N_3(\lambda, T_3)
\] (1)
where $N_1$ is the Planck radiance of the background, $N_2$ is the radiance of the chemical cloud, and $N_3$ is the atmospheric radiance. The quantities $t_2$ and $t_3$ are the spectral transmission of the plume and the atmosphere between the plume and the sensor, respectively. The first term in Eq. (1) is the radiance from the background as attenuated by the chemical cloud and intervening atmosphere. The second term is the radiance of the chemical species in the cloud as attenuated by the atmosphere between the cloud and the sensor. Finally, the third term in Eq. (1) is the radiance of the atmosphere between the cloud and the sensor. The transmission of the cloud, layer 2, is computed from the spectral properties of the chemical species contained therein:

$$t_2(\lambda) = \exp[-\sum k_i(\lambda)C_i\ell]$$  \hspace{1cm} (2)

where $C_i$ is the average concentration of the chemical compound over the path length $\ell$ and $k_i(\lambda)$ is the wavelength-dependent absorption coefficient. The sum over index $i$ in Eq. (2) is over all spectrally relevant chemical species. The differential radiance observed by the sensor as a result of the presence of the chemical cloud can be approximated as:

$$\Delta N(\lambda) = k(\lambda) \cdot \Psi \cdot \left[ \frac{\partial N}{\partial T} \right] \cdot \Delta T$$  \hspace{1cm} (3)

where,

$$\Psi \approx \rho \cdot 1$$  \hspace{1cm} (4)

and where $\Delta T$ is the temperature difference between background and chemical cloud ($T_2-T_1$), and $\rho$ is the column density of the chemical of interest. This approach has been applied to the detection of chemical agents and their simulants by all passive chemical agent sensors.

Figure 4 shows the detection of the chemical agent simulant SF$_6$ from each of the sensors. The purpose of acquiring imagery between 10.0 and 10.8 $\mu$m was to exploit the strong SF$_6$ absorption feature at 10.5 $\mu$m. When the SF$_6$ plume is warmer than the background, as in the case when viewed against the sky, it appears in emission. When the plume is cooler than the background it appears in absorption. When little thermal contrast exists between the plume and the background, it cannot be detected using such a passive IR method. The PSI detection algorithm has been described in detail elsewhere [4]. The algorithm performs a statistical estimate of the background, which is then subtracted from the data. The correlation between the

**Fig. 3.** Schematic diagram of three layer radiative transfer model.

**Fig. 4.** AIRIS data product. Red pixels indicate detected location of SF$_6$ plume.
differential radiance spectrum and the reference spectrum of the species in the plume is determined. The pixels in the image which meet the user defined correlation criteria are marked. Yellow pixels indicate a possible SF₆ detection; red indicated a high probability of SF₆ detection at that particular pixel.

The detection of the chemical agent simulant SF₆ during the March, 2004 Dugway tests, shown in Figure 2 using the formalism defined above, is a demonstration of the approach. The primary focus of this work is to use the AIRIS data product in order to provide information about the spatial and temporal composition of the chemical plume. Having such knowledge would permit understanding of the fate and transport of the chemical releases as well as provide ground truth for other sensor system evaluations. The AIRIS data product information about the chemical agent column density from each sensor can be used in a tomographic analysis of the chemical cloud in order to estimate its 3D concentration profile.

3. TOMOGRAPHY ALGORITHM AND ANALYSIS

AIRIS data can produce 2D measurements of the column density for individual components of a chemical plume. The column density, \( \psi(x,y) \) is the product of the density at that particular pixel location, \( \rho(x,y) \) and the viewing path length. The sensor measures the differential radiance from which the column density can be inferred, as defined by Eq. (3). Computed Tomography (CT) allows for the 3D reconstruction of an object from 2D line density measurements, thus inverting the column density function in order to obtain the concentration distribution function:

\[
\psi(x,y) = \int_0^L \rho(x,y,z)dz
\]  

The most difficult problem for optical tomography is the lack of sufficient projection data for reconstruction. The ability to provide a good tomographic reconstruction of a chemical cloud is dependent on the number of sensors used as well as the geometric positioning of the sensors. The quality of the reconstruction as a function of these parameters was a primary focus in deciding the tomographic method used and in the development of the algorithm. Based on our analysis, the algebraic reconstruction technique (ART) is best suited for this problem, i.e., limited projection field. PSI has developed analysis software, which is ART based, in order to perform this function. PSI’s algorithm is capable of generating a 2D column density distribution for each horizontal plane intersected by the image, as illustrated in Figure 5. The column density inferred from the IR measurement along a viewing projection is defined as a summation of all density values for all cells that are intersected by that projection. Each horizontal plane has 4096 cell elements. The full 3D distribution can then be generated by stacking each of the 2D distributions obtained in each plane (height).

The algorithm solves a set of linear algebraic equations, such that the reconstruction can be expressed in simple matrix form, \( \psi = WO \):
\[
\begin{bmatrix}
\Psi_p \\
O_p
\end{bmatrix} = \begin{bmatrix} W_j \end{bmatrix}
\]

Where: \( \Psi = \) Measurement Vector
\( W = \) Projection Matrix
\( O = \) Object Vector

- \( \Psi \) is a 128 element measurement vector corresponding to two 64 pixel measurements of the optical density in a plane for each of the orthogonal views (64 elements per view)
- \( O \) is the 4096 element object vector, corresponding to each pixel density value, \( \rho \) - the actual density in each pixel cell within the plane
- \( W \) is the (4096,128) projection array

The solution to the matrix equation is established through an iterative process, in which, an initial estimate of \( \rho \) for each cell in a single plane is given, followed by a calculation of the column density, \( \Psi \), which is compared to the measured value for the projection. A correction to the initial value of \( \rho \) is then performed, and the process is repeated until a given convergence criteria is achieved. PSI has conducted systematic investigations of synthetic data in order to better understand the effects of viewing geometry and number of sensors on the accuracy of the tomographic reconstruction. A set of data consisting of two 4096 element (64 pixel x 64 pixel) projections can be processed on a 1.8 GHz Pentium 4 with 480 MB RAM in approximately 10 minutes.

In order to better understand the capabilities of the algorithm under the circumstance of extreme limited number of views, we considered sample objects of increasing spatial complexity, and compared the reconstructed functions with the original analytical functions. We define the metric for the goodness of reconstruction as the nearness (the lower the nearness values, the better the reconstruction):

\[
\text{Nearness} = \frac{\sum_{j}^{N} (O_{j}^{*} - O_{j})^2}{\sum_{j}^{N} (O_{j}^{*} - O_{avg}^{*})^2}
\]

Where:
- \( O_{j}^{*} \) = original function value of jth cell
- \( O_{j} \) = reconstructed function value of jth cell
- \( O_{avg}^{*} \) = original function average value

We first evaluated the algorithm for N projections in two orthogonal projection views. As an example, we considered a 2D Cosine Function shown in Figure 6. In the case of only two projection views (0,90) with 19 projections per view, a nearness value of 0.08 is achieved. The overall shape and maximum values are still very well reproduced with an average error of 1.4%. The reconstruction result is shown in Figure 7.

For cases where synthetic data was used, we also investigated the accuracy of the reproduction as the number of projections per each orthogonal view increased. We observed little improvement beyond 19 projections per view, as illustrated in Figure 8, and therefore all synthetic data tomographic reproductions were investigated with 19 projection per view.
In order to increase the complexity of the synthetic data, we then considered a weighted superposition of the 2D Cosine Function and two Gaussian Peaks, as shown in Figure 9. In the case of only two projection views (0,90), a nearness value of 0.17 is achieved. The overall shape and maximum values are still well reproduced. There is however, a clear decrease in fidelity at higher spatial frequency. The reconstruction from the two orthogonal projections along with the error function is shown in Figure 10. However, when a third sensor (view) is added (0,45,90), a nearness value of 0.02 is obtained, resulting in a higher fidelity reconstruction, as clearly shown in Figure 11. However, the need for a third view becomes even more evident when the chemical plume directionality across the 2D grid is to be mapped accurately. In the case of only two sensors, plume propagation which is not parallel to one of the viewing axis can only be interpreted as increased dispersion. An additional instrument viewing along an axis which makes a 45 degree angle with respect to an existing sensor viewing centerline would allow independent analysis of the plume directionality and dispersion.

If we consider a plume described by a Gaussian dispersion function and the plume direction not along one of the two orthogonal projection views, then the reconstruction using only two views (sensors) does not map out well the original plume function, since the geometry does not permit sampling of the function’s width. However, an additional view significantly increases the fidelity of the reconstruction, as can be seen in Figure 12. In the case of only 2 orthogonal views (0,90), the algorithm produces a reconstruction in which the density function spreads across the entire grid, as a result of the inability to identify the directionality of the plume. A viewing geometry with 3 sensors (0,45,90) allows a reconstruction in which the width of the original function is well reproduced.
Our simulations lead us to conclude that the algorithm cannot accurately reproduce spatially complex plumes when only two orthogonal views are used for the plume reconstruction. However, for plumes approximately described by a single Gaussian dispersion function or smooth varying functions with propagation along one of the viewing centerlines, estimated plume concentrations were accurate to within 10% or less, even when only 2 projections views are used. The addition of a third view significantly increases the fidelity of the reconstruction, for both spatially complex plumes as well as plumes described by a single Gaussian distribution function.

4. DPG FIELD DATA TOMOGRAPHIC RESULTS

An additional source of uncertainty in the ability to reconstruct an accurate concentration map of the chemical cloud is that the data does not generate path-integrated column density, but rather a (column density) x (temperature differential) product. As a result of the fact that we do not have direct measurements of the temperature of the chemical cloud and the background temperature, the column density must be inferred using an indirect temperature measurement. The PSI detection algorithm determines a statistical estimate of the background radiance for each pixel. The radiometric values can be converted into temperature values at each pixel. The temperature differential is then approximated based on the ambient temperature and the temperature value calculated for each pixel. We believe uncertainty associated with column density estimates is on the order of 10 to 30%. Bearing these issues in mind, the tomographic results of the SF₆ dissemination study are described below.

As indicated in Figure 2, each AIRIS unit was located 1.1 km from the release stack. One sensor was set up to view the downwind direction. The other sensor was viewing the crosswind direction and was able to view approximately 400 m downwind of the release point. Figure 4 shows one example of AIRIS data products generated using data acquired simultaneously by the two sensors. Each pixel in the image maps to a plane ~6.0 m x 6.0 m along the plume propagation.
centerline. The red (dark) pixels indicate the location at which SF₆ was detected. Prior to tomographic analysis the data is corrected for the non-linear dependence of the absorption coefficient with column density. In the downwind view, since we are observing 300 m or more of the optical path containing the plume beyond the release stack, we are susceptible to growth of the voxel size. At the release point each pixel maps to ~6.0 m x 6.0 m, however beyond that point, the pixel size maps a greater area. However, bearing this issue in mind, the tomographic algorithm is setup to interpret the voxel size to be the same along the entire optical path.

Figure 13 shows the concentration estimated via tomographic analysis as a function of both the crosswind and downwind direction for various heights above the ground.

![Concentration profile](image)

Fig. 13. SF₆ concentration profile as a function of height as recovered via tomographic analysis of the chemical images shown in Figure 11.

The concentration profile estimated from our analysis is consistent with model predictions assuming Gaussian plume dispersion, a slightly unstable atmosphere, a wind speed of 2 m/s, and a release rate for SF₆ of 35 kg/hr. An example of a Gaussian model simulation, run under the above conditions is illustrated in Figure 14. Note that the derived SF₆ concentrations correspond to less than 1 ppmv. The line-of-sight integrated column densities are generally significantly lower than the value for which SF₆ becomes optically thick, ~30 ppmv-m. In several simultaneous AIRIS acquisitions the sensor viewing the downwind direction registered asymmetric plume propagation with respect to the downwind centerline axis, as illustrated in Figure 15.
Due to the limited number of projections used in the tomographic analysis as a result of only 2 sensors present, this asymmetric display is only modeled as an increased width of the density distribution function across the viewing area, as illustrated in Figure 16 which shows the tomographic analysis of the data set in Figure 15 at 21 meters above the ground. It is very possible that the wind direction shifted during the duration of the 2 hour release, propagating the plume at an angle with respect to the downwind centerline. This behavior however cannot be detected by the tomographic algorithm given only 2 projections. An additional instrument viewing along an axis which makes a 45 degree angle with respect to an existing sensor viewing centerline would allow independent analysis of the plume directionality and dispersion, as described in the previous section. The algorithm is currently capable of generating 3-D density functions from three sensors that can provide line density measurements.

Systematic errors in the estimated concentration are therefore attributable to using only two sensor views for reconstruction and the fact that the plume is optically thick along several lines of sight. The results shown in Figure 13 demonstrate that even in the limited case when only two orthogonal projection views are used, the calculated density values within the plume dispersion area are still consistent with atmospheric model predictions.
5. CONCLUSIONS

We have demonstrated that ability to use passive infrared multispectral imaging to track and quantify chemical clouds via computed tomography. The system employed is capable of imaging in the 8-11 micron region with a spectral resolution of 8-10 cm\(^{-1}\), and an NESR of 1-2 \(\mu\)W cm\(^{-2}\) sr\(^{-1}\) \(\mu\)m\(^{-1}\). The system is capable of detecting the chemical cloud from a standoff distance of 1.1 km, and to beyond 300 m downwind of the plume release point with a spatial resolution of 6 meters per pixel. We have shown that the PSI tomographic algorithm is capable of generating 3-D density distributions of the chemical cloud that are consistent with atmospheric model prediction even in the extreme limitation of using only two sensors viewing the chemical plume. The addition of a third sensor would significantly improve the fidelity of the reconstruction of the concentration profile as well as allow for an independent analysis of the plume directionality and dispersion.

ACKNOWLEDGMENTS

This work is supported by the U.S. Army Edgewood Chemical Biological Center. The authors acknowledge Dave Rossi, Teoman Ustun, and Mike Hinds for their efforts in developing the AIRIS units used in this work, and the DPG staff for their on-site support.

REFERENCES