Detection and Characterization of Chemical Vapor
Fugitive Emissions from Hyperspectral Infrared Imagery by
Nonlinear Optimal Estimation

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ABSTRACT

The clutter-matched filter (CMF) and the Adaptive Cosine Estimator (ACE) have become established metrics for
detecting chemical vapor plumes from hyperspectral infrared imagery. Both metrics follow from the presumption of a
linear additive signal model. However, examination of the underlying radiative transfer equation (RTE) indicates that
while the use of a linear additive signal model is a reasonable approximation when considering an optically-thin plume
viewed against blackbody background the RTE is in fact nonlinear. Unfortunately, presumption of a linear additive
signal model can significantly degrade plume detection statistics and results in significant errors in estimated chemical
column density when plumes are not optically-thin or are viewed against spectrally-complex backgrounds. This
paper describes a nonlinear estimation approach which integrates a parameterized signal model based on the RTE with a
statistical model for the infrared background. We show results obtained by applying the nonlinear estimation approach
to background-only hyperspectral imagery augmented with synthetic chemical vapor plumes and compare them with
results obtained presuming a linear additive signal model. As plumes become optically-thick, nonlinear estimation
yields significantly more accurate estimates of chemical vapor column density and significantly more favorable plume
detection statistics than clutter-matched-filter-based and adaptive-subspace-detector-based plume characterization and
detection.

Keywords: nonlinear estimation, hyperspectral, remote sensing, spectroscopy, Gauss-Newton

1. INTRODUCTION

This paper addresses detection and characterization of chemical vapor fugitive emissions in a non-scattering atmosphere
by processing of LWIR hyperspectral imagery. It is an abridged and edited version of paper published in August 2009
[1]. Readers should consult that publication for additional detail. (Readers may also be interested in a paper by Heasler
and co-workers [2] which describes a different nonlinear estimation approach.) The clutter-matched filter (CMF), a
measure of the ratio of signal power to noise power, and the Adaptive Cosine Estimator (ACE), a measure of correlation
between the test spectrum and a reference spectrum, have become established metrics for detecting chemical vapor
plumes from hyperspectral infrared imagery [3-7]. Both metrics follow from the presumption of a linear additive signal
model. However, examination of the underlying radiative transfer equation (RTE) indicates that while the use of a linear
additive signal model is a reasonable approximation when in certain cases, i.e. for an optically-thin plume viewed
against blackbody background, the RTE is in fact nonlinear.

We demonstrate that the presumption of a linear additive signal model can significantly degrade plume detection
statistics and results in significant errors in estimated chemical vapor column density when plumes are not optically-thin.
In order to address the ‘non-thin’ plume scenario, we introduce a nonlinear estimation approach which integrates a
parameterized signal model based on the RTE with a statistical model for the infrared background. For algorithm
assessment and comparison against CMF- and ACE-based plume detection and characterization, we simulate
observation of fugitive emissions by augmenting plume-free (background only) hyperspectral datacubes with synthetic
plume signatures using a process which preserves the noise characteristics of the original data. As plumes become
optically-thick, the nonlinear estimation algorithm yields significantly more accurate estimates of chemical vapor
column density the CMF and significantly more favorable plume detection statistics than ACE-based detection.

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2. DETECTION ALGORITHM FORMULATION

2.1 Radiative Transfer Model

The radiative transfer model which underlies our analysis approach follows from the stratified atmosphere approximation: the atmosphere along the sensor’s line-of-sight is modeled as n layers with each layer having uniform temperature, pressure, and chemical composition [8]. For this work, we consider the case where the atmosphere along the line-of-sight between the sensor and plume has uniform temperature and composition. The concept is shown schematically in Figure 1. After some algebraic manipulation of the RTE which describes the scenario depicted in Figure 1, for a non-scattering atmosphere the change in at-sensor spectral radiance due to the presence of a vapor plume may be reasonably approximated as:

\[
x_p - x_0 = \left[ 1 - \tau_p \right] \left[ L(T_a) - x_0 \right] + \tau_a \left[ L(T_p) - L(T_a) \right]
\]

(1)

where \(x_p\) is the at-sensor radiance with the plume present, \(x_0\) is the at-sensor radiance with the plume absent, \(L(T)\) is the Planck function evaluated at temperature \(T\), \(T_a\) is the temperature of the air, \(T_p\) is the temperature of the plume, \(\tau_a\) is the atmospheric transmission between the sensor and the plume, and \(\tau_p\) is the transmission of the plume. (The wavelength dependence of the terms in Eq. (1) have been suppressed for clarity.) In this paper we consider the further simplified case where the plume and atmosphere are at the same temperature so that the at-sensor spectral radiance with the plume present is

\[
x_p = x_0 + \left[ 1 - \tau_p \right] \left[ L(T_a) - x_0 \right] \quad (2)
\]

Equation (2) has formed the basis for multiple fugitive emissions detection and characterization approaches, see, e.g., [3-7,9-11]. Plume transmission is presume to follow Beer’s Law

\[
\tau_p = \exp(-\rho \cdot \kappa)
\]

(3)

where \(\rho\) is the chemical vapor column density and \(\kappa(\lambda)\) is the vapor absorption cross-section, convolved with the instrument lineshape. Note from Eq. (2) that if the background is a blackbody at the same temperature as the vapor/air then the presence of the vapor has no effect on the observed spectrum.

Figure 1. Stratified atmosphere model. Each layer defined to have uniform temperature (\(T_i\)), pressure, and chemical composition; layer transmission is \(\tau_i\). Chemical vapor plume of interest is Layer \(p\).

Matched-filter-based vapor detection and characterization algorithms follow from the assumption of an optically-thin plume, \(\tau_p \approx 1 - \rho \cdot \kappa\), and a blackbody background so that \(L(T_a) - x_0 \approx \left[ \partial L / \partial T \right]_{T_a} \Delta T_{eff} \), where \(\left[ \partial L / \partial T \right]_{T_a}\) is the derivative of the Planck function with respect to temperature evaluated at the air temperature and \(\Delta T_{eff} = T_a - T_{bkg}\) is the effective thermal contrast between the air (plume) and the background. Following these assumptions, the approximate RTE is linear in chemical vapor column density

\[
x_p \approx x_0 + \rho \cdot \kappa \left[ \frac{\partial L}{\partial T} \right]_{T_a} \Delta T_{eff}
\]

(4)
As \( \rho \cdot \kappa \rightarrow 0 \), the righthand sides of Eqs. (2) and (4) approach the same result; however, Eq. (4) is generally a poor approximation when \( \max \{ \rho \cdot \kappa(\lambda) \} > 1 \) and \( \Delta T_{\text{eff}} \neq 0 \).

Keeping in mind the ‘exact’ RTE in Eq. (2) and its approximation in Eq. (4), this paper has three primary goals:

1. Provide an algorithm for estimating \( \rho \) in cases where the thin plume approximation, \( \tau_p = 1 - \rho \cdot \kappa \), is a poor approximation
2. Characterize the effect of the thin plume approximation on plume detection statistics as \( \max \{ \rho \cdot \kappa(\lambda) \} \) increases and
3. Characterize the error in estimated \( \rho \) resulting from the thin plume approximation as \( \max \{ \rho \cdot \kappa(\lambda) \} \) increases.

Our model for background spectra follows below.

### 2.2 Sensor Signal and Background Model

Our detection algorithms treat as \( k \)-dimensional random vectors, \( \tilde{x} \), where \( k \) is the number of bands in the measured spectrum. Measured spectra are presumed to be sum of a noise-free spectral radiance and a noise vector:

\[
\tilde{x} = x + e
\]  

(5)

where \( x \) denotes the noise-free spectrum and \( e \) denotes measurement noise. With respect to Eq. (3), the vector representations of the plume transmission and chemical vapor absorption coefficient are \( \tau_e \) and \( \kappa \), respectively. Our analysis approach further presumes that the measurement noise is normally-distributed with zero mean and is uncorrelated from band to band, \( e \sim N(0, D) \) where \( D \) is a diagonal matrix, \( D = \text{diag} \{ \sigma_1^2, \sigma_2^2, ..., \sigma_k^2 \} \), where \( \sigma_i \) is the standard error of the measured spectral radiance in band \( i \).

We also presume that background spectra may be described by a linear mixing model:

\[
x_0 = \mu + B\beta
\]  

(6)

where \( \mu \) is the mean background spectrum, \( B \) is the \( k \times m \) dimensional matrix whose columns are the basis vectors used to span the data space and \( \beta \) is an \( m \times 1 \) vector of weight coefficients. We further presume that the basis vectors in Eq. (6) that the \( B \) matrix follow from a Principal Components decomposition of the sample covariance matrix, \( \Sigma \). Specifically, the \( B \) matrix follows from a regularization approximation of \( \Sigma \): \( \hat{\Sigma} = BB^T + D \) where \( \text{trace} \{ \Sigma \} = \text{trace} \{ \hat{\Sigma} \} \) [12]. This model is similar to the Probabilistic Principal Components model described by Tipping and Bishop [13].

### 2.3 Model Parameter Estimation

Combining Eqs. (2), (3), and (6), the signal model parameters are the chemical vapor column density, the weight coefficients for the basis vectors for the background (i.e., the elements of the \( \beta \) vector), and the plume/atmospheric temperature. For convenience, we define a reference column density, \( \rho_0 = 1/\max \{ \kappa(\lambda) \} \), and corresponding unitless quantity, \( \alpha = \rho/\rho_0 \), which corresponds to the peak optical density of the chemical vapor. In the interest of simplifying the algebra associated with the algorithm derivation below, we consider the case where the air temperature is known, i.e. does not need to be treated as a free parameter, and each model spectrum is characterized by a vector of model parameters, \( \theta = [\alpha, \beta] \).

Following Eq. (2), the model spectrum corresponding to the exact RTE is:

\[
f(\theta) = \tau_e \circ x_0 + \left[1 - \tau_e \right] \circ L_\lambda
\]  

(7)

where the vector \( x_0 \) is the estimated noise-free background spectrum given by Eq. (6), \( 1 \) is a \( k \)-element vector of ones, \( \tau_e \) is the plume transmission, the vector \( L_\lambda \) consists the Planck function evaluated at the plume temperature, \( T_\alpha \), and the appropriate wavelength, and \( u \circ v \) denotes the element-by-element product of the vectors \( u \) and \( v \).
For a given measured spectrum, there exist maximum likelihood model parameter values, \( \hat{\theta} = [\hat{\alpha}, \hat{\beta}] \). We take a Bayesian approach to estimating \( \hat{\theta} \). Given an observation, \( \tilde{x} \), the probability that the parameter values are \( \theta \) is

\[
p(\theta | \tilde{x}) = \frac{p(\tilde{x} | \theta)p(\theta)}{p(\tilde{x})}
\]

where \( p(\tilde{x} | \theta) \) is the conditional probability of observing \( \tilde{x} \) given \( \theta \), \( p(\theta) \) is the prior probability of the parameter values being \( \theta \), and \( p(\tilde{x}) \) is the prior probability of observing \( \tilde{x} \). The maximum likelihood parameter values are those which maximize \( p(\tilde{x} | \theta) \) or, equivalently, those which minimize \( -\ln p(\tilde{x} | \theta) \).

The background model Specifically, \( p(\theta) \) follows from the assumption that, given all pixels which constitute the background, \( \beta \) values have zero mean and are normally-distributed, \( \beta \sim N(0, I_m) \). Following this presumption, the maximum likelihood model parameters are those which minimize a cost function:

\[
C(\theta | \tilde{x}) = \frac{1}{2} [\tilde{x} - f(\theta)]^T D^{-1} [\tilde{x} - f(\theta)] + \frac{1}{2} \beta^T \beta
\]

As the cost function is nonlinear in \( \theta \), direction solution to obtain \( \hat{\theta} \) is not possible. (By ‘direct solution’, we mean solution of the system of equations which results from the \( \nabla C = 0 \) condition when \( C(\theta | \tilde{x}) \) is minimized.) Because the cost function is only weakly nonlinear in \( \theta \), the maximum likelihood model parameter values may be estimated using a Gauss-Newton algorithm. The Gauss-Newton algorithm updates parameter values iteratively as

\[
\theta_{i+1} = \theta_i - (J_i^T J_i)^{-1} J_i^T r_i
\]

where \( \theta \) indicates iteration number, \( r \equiv [D^{-1/2} [\tilde{x} - f(\theta)] \beta] \) is the Jacobian of the \( r \) vector, and \( J_i = \partial r_i / \partial \theta \). Eq. (10) is a general result. Analytic expressions for the elements of the Jacobian follow from Eqs. (7) and (9).

The formulation of Eq. (10) ensures that \( J_i^T J_i \) is invertible under virtually all physically plausible detection scenarios and thereby makes the Gauss-Newton algorithm extremely stable. When the atmospheric temperature is treated as a fixed parameter, the only scenario where \( J_i^T J_i \) is guaranteed not to be invertible, and therefore Eq. (10) cannot produce an accurate estimate of plume column density, is when the plume is opaque at all wavelengths, i.e., \( \tau_e = 0 \).

The Gauss-Newton algorithm requires an initial guess at the maximum likelihood model parameter values. The approximate RTE which follows from the thin plume assumption facilitates a reasonable initial guess. Following Eq. (4), the analogue of Eq. (7) is:

\[
g(\theta) = x_0 + \alpha' s
\]

where the vector \( s \) is

\[
s = \rho_o \kappa \left[ \frac{dL_a}{dT} \right]_{T_e} \Delta T_0
\]

The quantity \( [dL_a / dT]_{T_e} \) is the derivative of the blackbody function with respect to temperature evaluated at the air temperature, \( \Delta T_0 \) is a reference thermal contrast, nominally 1 K, and \( \alpha' = \alpha \cdot (\Delta T_{\text{eff}} / \Delta T_0) \) where \( \Delta T_{\text{eff}} \) is effective thermal contrast between the air temperature and the background:

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\[ \Delta T_{\text{eff}} = \Delta T_0 \cdot \frac{s^T \left[ \rho_0 \kappa \circ (L_w - x_0) \right]}{s^T s} \]  \hspace{1cm} (13) \]

Equation (11) leads to the CMF result [4,5]:

\[ \hat{\alpha} = \frac{s^T \Sigma^{-1} (\bar{x} - \mu)}{s^T \Sigma^{-1} s} \]  \hspace{1cm} (14) \]

For direct comparison of the nonlinear estimation result with the CMF result, we evaluate Eq. (14) using \( \Sigma = \hat{\Sigma} = BB^T + D \), the regularized sample covariance matrix.

### 2.4 Detection Decision Formulation

For some standoff detection applications, making the correct “plume absent”/“plume present” detection decision can be more important than accurate estimation of the chemical vapor column density. The cost function in Eq. (9) facilitates detection decisions on the basis of a statistical F-test. Under the nonlinear estimation approach, the F value associated with the measured spectrum, \( \bar{x} \), is

\[ F(\bar{x}) = (k - 1) \cdot \frac{C(\bar{x}, \hat{\theta}_0)}{C(\bar{x}, \theta)} - 1 \]  \hspace{1cm} (15) \]

where \( C(\bar{x}, \hat{\theta}_0) \) is the cost function evaluated using the Gauss-Newton algorithm allowing all parameter values to vary and \( C(\bar{x}, \theta) \) is cost function evaluated with \( \alpha \) fixed at zero, i.e., only \( \beta \) is allow to vary. “Plume present” is decided when the F value exceeds a user-specified threshold.

For the linear signal model given by Eq. (11), the analogue to the F test is an adaptive subspace detector, the Adaptive Cosine Estimator (ACE) [14,15]. The ACE value associated with the measured spectrum \( \bar{x} \) is

\[ A(\bar{x}) = \frac{\left( s^T \hat{\Sigma}^{-1} [\bar{x} - \mu] \right)^2}{s^T \Sigma^{-1} s} \left( \bar{x} - \mu \right)^T \left( \hat{\Sigma}^{-1} \bar{x} - \mu \right) \]  \hspace{1cm} (16) \]

The ACE statistic can be regarded as cosine-squared of the angle between the test spectrum and the reference spectrum in noise-whitened, mean-subtracted signal space. The ACE value calculated in Eq. (16) may be converted into an equivalent F value for direct comparison with the value calculated in Eq. (15), \( F_{\text{ACE}} = (k - 1)A / (1 - A) \).

### 3. TEST DATA

For algorithm performance evaluation we simulated observations of fugitive emissions by augmenting plume-free measured spectra with synthetic plume signatures. The plume-free spectra were collected using an Adaptive Infrared Imaging Spectroradiometer-Wide Area Detector (AIRIS-WAD) [16,17]. The AIRIS-WAD sensor is an imaging Fabry-Perot spectrometer comprised of a 256×256 pixel LWIR focalplane array (FPA) which views the far field through a rapidly-tunable LWIR etalon. The sensor’s optical system is configured to provide a 32 deg x 32 deg field-of-regard (2.2 mrad per pixel IFOV). Spectra are recorded band-sequentially and consist of measurements at twenty (20) user-specified wavelengths in the 8 to 11 \( \mu \)m spectral region. The instrument’s spectral resolution is \( \approx 0.08 \) \( \mu \)m, i.e., \( \approx 8 \) cm\(^{-1}\) FWHM at \( \nu=1000 \) cm\(^{-1}\), and its lineshape is well-described by a Lorentzian function. The sensor is equipped with an internal blackbody source to facilitate real-time radiometric calibration of the sensor data.

We augmented AIRIS-WAD data with synthetic 1,1,1,2-tetrafluoroethane (R-134a) spectra. R-134a is a freon widely-used in refrigeration systems and as a propellant for domestic and industrial applications. Data was augmented using the equation

\[ x_p = \left[ 1 - \tau_p \right] \circ L_w + \tau_p \circ \bar{x}_0 + \bar{e} \]  \hspace{1cm} (17) \]
where \( \hat{x}_0 \) is estimated noise-free background spectrum and \( \hat{e} \) is defined as the difference between the measured background spectrum and the estimated noise-free background spectrum, \( \hat{e} \equiv \bar{x} - \hat{x}_0 \). In order to exercise Eq. (17), the background spectrum was calculated by applying a linear filter function to the spectrum from the datacube

\[
\hat{x}_0 = \left[ D^{1/2} U_m \left( I_m - \varepsilon A_m^{-1} \right) U_m^T D^{-1/2} \right] \xi - \mu + \mu
\]  

(18)

where \( U_m \) is the \( k \times m \) matrix whose columns are the leading eigenvectors of the noise-whitened sample covariance matrix, \( D^{-1/2} \Sigma D^{-1/2} \), \( A_m \) is a diagonal matrix whose elements are the largest \( m \) eigenvalues of \( D^{-1/2} \Sigma D^{-1/2} \), \( I_m \) is the \( m \times m \) identity matrix, and \( \varepsilon \) is the average of the smallest \( (k-m) \) eigenvalues of \( D^{-1/2} \Sigma D^{-1/2} \).

A useful characteristic of Eq. (18) is that it preserves the noise in the original data as plume becomes optically thick and thereby provides more realistic spectra for testing estimation algorithms than fully synthetic data with added Gaussian noise. As the plume transmission goes zero \( x_p \rightarrow L_\mu + \hat{e} \), i.e., as the plume becomes opaque the pixel spectrum becomes a noisy blackbody spectrum rather than a noise-free blackbody spectrum. Conversely, as the plume column density goes to zero its effective transmission goes to unity and \( x_p = x_0 \), i.e., the output spectrum is equal to the original data if no plume is present.

The plume transmission was calculated using Eq. (3) but by first convolving a high resolution absorption spectrum of R-134a [18] with the AIRIS-WAD instrument lineshape. We exercised Eq. (17) to create synthetic R-134a plume signatures with peak optical density (OD) ranging from 0 to 3.0 (base e). For reference, a 197 ppmv-m R-134a plume corresponds to OD=1.0 at 8.42 \( \mu \)m, the wavelength of strongest absorption in the R-134a spectrum. The plume temperature was set equal to the local air temperature, 298.0 K, for this simulation. Synthetic plumes were added to 64 pixel (horizontal) \( \times \) 5 pixel (vertical) regions in the scene and the column density was the same at each pixel where the plume signature was added.

4. RESULTS AND DISCUSSION

4.1 General

In this Section we compare the results obtained by applying the Gauss-Newton solver for detection and column density estimation with those obtained and the linear model given by Eq. (11). The plume-augmented AIRIS-WAD data was processed on a quadrant-by-quadrant basis and the Huber-type M-estimator [19] was used to calculate the background covariance matrix of each quadrant. The motivation for using the M-estimator is that it de-weights the contribution of statistically-anomalous spectra to the estimated covariance. Pixels where the plume signature is statistically-significant generally constitute statistical anomalies so the M-estimator generally provides a more accurate estimate of the true background covariance matrix. In the interest of comparing algorithm performance in favorable and unfavorable detection regions, we present results obtained by processing data with synthetic plumes added to the regions shown in Figure 2. The effective thermal contrast in Region 1 is \( 2.6 \pm 0.5 \) K and the effective contrast in Region 2 is \( 5.9 \pm 0.6 \) K. (The variation is the 1\( \sigma \) standard deviation in \( \Delta T \) over the plume region, not the uncertainty in \( \Delta T \).)
Figure 2. Locations where synthetic R-134a plumes were added to AIRIS-WAD data. The effective thermal contrast in Region 1 is 2.6 ± 0.5 K and the effective contrast in Region 2 is 5.9 ± 0.6 K.

4.2 Column Density Estimation

In order to evaluate the accuracy and precision of the Gauss-Newton and linear model estimates of peak optical density, we calculated the median, $\text{median} [\hat{\alpha}_i]$, and the normalized median absolute deviation, $\hat{\sigma}_\alpha = \text{median} |\hat{\alpha}_i - \text{median} [\hat{\alpha}_i]|/0.6745$, of the estimated OD values in the plume-augmented region. We report $\text{median} [\hat{\alpha}_i]$ and $\hat{\sigma}_\alpha$ rather than the mean and standard deviation because we found that $\text{median} [\hat{\alpha}_i] \pm 2\hat{\sigma}_\alpha$ generally yields a more accurate estimate of the range which incorporates 95% of the sample values than does $\text{mean} [\hat{\alpha}_i] \pm 2\sigma$.

Figure 3 depicts the R-134a optical densities estimated in Region 1 using the Gauss-Newton solver and the CMF, Eq. (14). The error bars in each figure correspond to $\pm 1\hat{\sigma}_\alpha$. The solid symbols indicate the median OD estimated using the Gauss-Newton algorithm. The crossed open symbols indicate the median OD estimated using the clutter-matched filter. The black dashed line indicates perfect agreement between the actual and estimated OD values. As expected, in Region 2 the calculated $\text{median} [\hat{\alpha}_i]$ values were essentially identical to those in Region 1; however, $\hat{\sigma}_\alpha$ values were less than half that in Region 1 because the effective thermal contrast between the air and the background was >2x larger.

The Gauss-Newton algorithm provides a more accurate estimate of column density than the linear model in all cases. As expected, the accuracy of the CMF estimate degrades with increasing optical density. The systematic deviation of the Gauss-Newton-estimated optical densities from the “Ideal” line is due entirely to instrument effects, i.e., effects resulting from convolution of the high resolution absorption spectrum with the instrument lineshape.
4.3 Plume Detection Statistics

Figures 4-6 show the receiver operator characteristic (ROC) curves calculated for Regions 1 and 2 augmented with OD=0.3, 1.0, and 2.0 plumes. (We do not report results for OD<0.3 because detection statistics are generally unfavorable in both Region 1 and Region 2.) Each ROC curve is a plot of detection rate (DR) as a function of false alarm rate (FAR). For a given detection threshold, the DR is the fraction of pixels within the plume-augmented region which exceed the threshold; the FAR is the fraction of pixels outside the plume-augmented region which exceed the detection threshold. The ROC curve is created by varying the detection threshold (F-value) from zero to the maximum F-value observed in the plume-augmented region. In Figures 4-6 the solid symbols correspond to points resulting from application of the Gauss-Newton algorithm. The crossed open symbols correspond to points results for application of the ACE algorithm. The ROC curves in Figure 4 indicate that, as the plume is optically-thin for peak OD=0.3, the both nonlinear estimation and ACE-based detection generate nearly identical ROC curves. Some separation between the two curves is observed but the differences are modest. The difference in detection statistics between the Region 1 and Region 2 is consistent the difference in \( \Delta T_{\text{eff}} \) between the two regions.
Figure 4. ROC curves for OD=0.3 R-134a plumes added to Regions 1 and 2: ■ = Gauss-Newton solver applied to Region 2, □ = ACE applied to Region 2, ● = Gauss-Newton solver applied to Region 1, ○ = ACE applied to Region 1.

Figure 5. ROC curves for OD=1.0 R-134a plumes added to Regions 1 and 2: ■ = Gauss-Newton solver applied to Region 2, □ = ACE applied to Region 2, ● = Gauss-Newton solver applied to Region 1, ○ = ACE applied to Region 1.
The ROC curves in Figure 6, OD=1.0, show significantly better detection statistics for the Gauss-Newton algorithm than the ACE algorithm in both Region 1 and Region 2. The thin plume assumption is not valid at the wavelengths of strongest absorption and the nonlinear estimator is expected to outperform ACE-based detection. As is true at lower OD values, the detection statistics are significantly more favorable in Region 2 than in Region 1 because of greater thermal contrast between the plume and the background. Comparing the ROC curves for Gauss-Newton-based detection in Regions 1 with ACE-based detection in Region 2, while the degradation introduced by the thin plume approximation is apparent, it is less significant than the effect of enhanced thermal contrast in going from Region 1 to Region 2. Although the linear model which underlies the ACE detector is not precisely matched to the data, the ROC curve obtained by applying ACE to Region 2 is still more favorable than the ROC curve obtained by applying the Gauss-Newton algorithm to Region 1.

The ROC curves in Figure 6, OD=2.0, show an even greater improvement in detection statistics for the Gauss-Newton algorithm relative to the ACE algorithm as the thin plume approximation is poor near the wavelengths of strongest absorption. Comparing the ROC curve for Gauss-Newton detection in Regions 1 with ACE-based detection in Region 2, the degradation introduced by the thin plume approximation is more significant than the effect of enhanced thermal contrast in going from Region 1 to Region 2. With the OD increased to 2.0, the detection statistics in Region 1 become relatively favorable and for a detection rate of 80% the Gauss-Newton algorithm reduces the false positive rate by a factor of ~15 relative to ACE-based detection. The reduction in false alarm rate is even more pronounced in Region 2. One can also examine the differences in detection rate for a fixed false alarm rate. For FAR=1·10⁻⁴, use of the Gauss-Newton algorithm increases the detection rate from ~10% to nearly 80% in Region 1. For FAR=1·10⁻⁵, use of the Gauss-Newton algorithm increases the detection rate from ~70% to ~99% in Region 2.

4.4 Algorithm Convergence

As the Gauss-Newton algorithm is iterative, it is necessary to define a termination criterion. Our termination criterion is the fractional change in the cost function given by Eq. (9). The algorithm terminates when the fractional change falls below a user-specified value, δ:

\[
0 \leq 1 - \frac{C_{i+1}}{C_i} \leq \delta
\]  

(17)
The results presented in the preceding section were obtained using $\delta=0.01$. In the event that the cost function increases from the $i$-th to $(i+1)$-th iteration the parameter values are restored to those from the $i$-th iteration and the algorithm terminates. In the absence of any added plume signature, in Region 1 the algorithm terminated after one iteration for ~55% of the pixels and after the second iteration for ~45% of the pixels. Results were similar in Region 2 as well as the rest of the scene, i.e., the vast majority of pixels to which no plume signature was added. The number of iterations required for algorithm convergence increased as the plume OD increases. For spectra augmented with a OD=1.0 plumes, all pixels required at least two iterations to converge; ~80% of the pixels require two iterations and ~20% required three iterations. When the plume OD is increased to 2.0, the algorithm required three iterations to converge for almost all pixels. A similar result was obtained for OD=3.0.

Reducing the convergence criterion $\delta$ from 0.01 to 0.0001 increased the number of iterations for convergence; however, there was no significant effect on the estimated column density values. The observed differences in OD at algorithm termination were on the order of 0.1% of the estimated values. For comparison, the uncertainties in the estimated values were typically several orders of magnitude larger than the differences observed by making the convergence threshold more stringent.

5. SUMMARY AND CONCLUSIONS

We have presented a nonlinear optimal estimation method for detecting and characterizing chemical vapor fugitive emissions in a non-scattering atmosphere using passively-sensed LWIR spectra. The method integrates a parameterized signal model based on the RTE with a parameterized representation of covariance of the infrared background to create a probability-based cost function. The maximum likelihood model parameters are defined as those which minimize the cost function and are estimated using a Gauss-Newton algorithm. The algorithm formulation presented here presumes that the plume and air are in thermal equilibrium and that the air temperature is known; however, the algorithm may be easily modified to handle scenarios where the air temperature is not known.

For algorithm performance evaluation we simulated observation of fugitive emissions by augmenting plume-free spectra measured by an AIRIS-WAD sensor with synthetic R-134a plume signatures. The peak optical density of the synthetic plumes varied from OD=0.0 to OD=3.0. Results obtained by processing the simulated data indicate that the nonlinear estimator provides significantly more accurate estimates of chemical vapor column density and significantly more favorable detection statistics than matched-filter-based estimation when the vapor plume is optically-thick at one or more of the sensor observation wavelengths. This is because the signal model used for nonlinear estimation is based on the full clear air RTE, not an approximation which follows from the presumption of an optically-thin plume as do the clutter-matched filter and adaptive subspace detector. We note that while the nonlinear estimator provides significantly better results for optically-thick plumes, it produces the same result as a clutter-matched filter/adaptive subspace detector as the plume optical density approaches zero.

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7. REFERENCES


