



AN UNCERTAINTY PROPAGATIONS ANALYSIS FOR AN INFRARED BAND MODEL TECHNIQUE FOR COMBUSTION GAS DIAGNOSTICS

**ENGINE TEST FACILITY
ARNOLD ENGINEERING DEVELOPMENT CENTER
AIR FORCE SYSTEMS COMMAND
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April 1977

Final Report for Period January 1975 — June 1976

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Prepared for

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AEDC-TR-76-155	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) AN UNCERTAINTY PROPAGATIONS ANALYSIS FOR AN INFRARED BAND MODEL TECHNIQUE FOR COMBUSTION GAS DIAGNOSTICS		5. TYPE OF REPORT & PERIOD COVERED Final Report - January 1975 - June 1976
7. AUTHOR(s) C. C. Limbaugh - ARO, Inc.		6. PERFORMING ORG. REPORT NUMBER
9. PERFORMING ORGANIZATION NAME AND ADDRESS Arnold Engineering Development Center (DY) Air Force Systems Command Arnold Air Force Station, Tennessee 37389		8. CONTRACT OR GRANT NUMBER(s)
11. CONTROLLING OFFICE NAME AND ADDRESS Arnold Engineering Development Center (DYFS) Arnold Air Force Station Tennessee 37389		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Program Element 65807F
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		12. REPORT DATE April 1977
		13. NUMBER OF PAGES 25
		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE N/A
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Available in DDC		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) combustion products emission gases absorption diagnostic equipment mathematical analyses infrared spectroscopy		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The development of matrix equations for an uncertainty propagations analysis for the emission-absorption band model technique are described. The emission-absorption technique is used for the determination of local values of temperature and species concentration from measurements of radiance and transmittance on axisymmetric gas flows. The approach used depends on linearization of the original nonlinear system of		

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20. ABSTRACT (Continued)

equations comprising the solution to the radiative transfer problem for an emitting-absorbing source such as a turbojet or rocket engine exhaust plume. The resultant linear transformation matrix provides a means for determination of the variance-covariance matrix for inverted temperature and partial pressure, based on the experimentally determined variance-covariance matrix of the measured radiance and transmittances. The diagonal elements of the propagated variance-covariance matrix yield the square of the standard deviation of the temperature and partial pressure. Although the equations are developed for the uncertainty propagations analysis for the emission-absorption band model technique, the results are, in fact, a general property of linear transformations. They are thus applicable to any situation in which the dependence of analysis on measurements can be expressed by a linear relationship. The results of the analysis are applied to two illustrative sets of data.

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PREFACE

The research reported herein was conducted by the Arnold Engineering Development Center (AEDC) Air Force Systems Command (AFSC), under Program Element 65807F. The results of this research program were obtained by ARO, Inc., AEDC Division (a Sverdrup Corporation Company), operating contractor for AEDC, AFSC, Arnold Air Force Station, Tennessee. The work was accomplished in the Engine Test Facility (ETF) under ARO Project Numbers R32I-01A and R32S-06A. The author of this report was C. C. Limbaugh, ARO, Inc. The manuscript (ARO Control No. ARO-ETF-TR-76-118) was submitted for publication on October 8, 1976.

The author of this report expresses appreciation to K. R. Kneile, ARO, Inc., for valuable technical discussions of statistical theory, and to W. T. Bertrand, ARO, Inc., for making available radiance and transmittance data from the flat flame burner.

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1.0 INTRODUCTION

The emission-absorption (E/A) technique (Ref. 1) for determining spatial profiles of temperature and partial pressure of selected species in exhaust plumes of combustion sources has been utilized in several applications at the AEDC. The E/A technique develops by applying band model theory (Ref. 2) to the solution of the radiative transfer problem for the spatial distribution of the projected radiance and transmittance from a cylindrically symmetric radiating/absorbing medium. These radiance and transmittance data are then used in a radial inversion technique, based on the aforementioned band model theory, to provide radial profiles of the temperature and partial pressure of the radiating species (Ref. 1).

The data necessary for the determination of the temperature and partial pressure profiles consist of experimental infrared radiance and transmittance measurements, which are subject to normal experimental errors. Because the analytic approach for the technique is of necessity complex, the determination of uncertainties in the resultant temperature and partial pressure profiles, because of these experimental errors, is not straightforward. The complexity of the problem is compounded by the fact that any calculated temperature and partial pressure inside the plume is dependent on, or correlated to, the calculated temperature and partial pressure in the outer portions of the plume. However, since the emission-absorption technique is an important diagnostic tool for rocket and jet engine exhausts, knowledge of the uncertainty in the temperature and partial pressures due to the experimental uncertainties is required. There are two elements to the error and the random uncertainty. It is possible to determine bias error propagation by single application of the data reduction process, but the determination of random error propagations is not so straightforward. Propagation of these random uncertainties is the subject of this subject.

There is a variety of ways in which propagated experimental random uncertainty bounds may be assigned to the determined temperature and partial pressure, most of which are heuristic in nature. For example, the analysis of a certain set of data may be repetitively performed, with each set of measured data being randomly varied within the observed experimental bounds. Observation of the variation in the resulting temperature and pressure profiles provides an uncertainty estimate. However, such an approach generally requires many computations, and the cost can become unreasonable.

There is an analytic approach to determining the uncertainties which provides an estimate of the propagated random uncertainty without recourse to repetitive or heuristic techniques. Although it provides an a priori estimate of the uncertainty, dependent only on

the observed data characteristics and an analytic approximation, it is considerably more difficult analytically than the repetitive approach. The analytic determination of uncertainties has additional merit in that the formulation and development of the fundamental equations allows for straightforward extension to account for variations in parameters other than the direct experimental measurements.

In the following discussion, the equations describing this analytic approach for the random uncertainty propagation based on the variational dependence of the physical parameters are developed in convenient functional form for subsequent analysis. Certain definitions from statistical theory are introduced, and their implications to the present work are described. The method is applied to two illustrative examples, an analytic and experimentally obtained set of data, to demonstrate typical results.

2.0 ANALYTIC APPROACH

The functional considerations leading to the description of the emission-absorption problem in terms of a linearized system of equations are described in this section. The detailed equations, including description of a systematic accounting system used in the computer code are described in Appendix A. Subsequent to the linearization of the emission-absorption problem, the approach by which a variance-covariance matrix of the measurements is propagated through the linear transformation to yield the variance-covariance matrix of the results is presented.

The propagation of the variance-covariance matrix represents, in principle, the solution to the uncertainty propagation problem since the elements of the resultant matrix are related to the desired uncertainties. The diagonal elements of the variance-covariance matrix represent the variances which are the second moment about the mean of the probability distribution function of the parameters being measured or computed. The off-diagonal elements represent the covariances which are the joint moment about the mean of two parameters. Since experimental data are usually independent, the variance-covariance matrix for the experimental data is usually one with the principal diagonal being the square of the observed standard deviations of the corresponding measurements and the off-diagonal elements set to zero. Thus, with the determination of a linear transformation between the experimental measurement and the inverted temperature and pressure, the determination of the variance-covariance matrix of the temperature and partial pressure is immediate.

It should be pointed out that the results presented herein, although developed for the E/A problem, are a general property of linear transformations, and are thus not restricted to the determination of uncertainties in temperature and pressure in the E/A problem. Rather, the same fundamental approach can be used for determination of uncertainties in radiance and transmittance because of uncertainty in temperature and pressure or because of uncertainty in any of the parameters in the analytic model. The general results of the analysis can further be applied to any situation in which an analysis of data can be described by a linear transformation. Thus, when data are preconditioned by a smoothing process which is linear, e.g., linear least squares fitting, the variance-covariance matrix of the smoothed data can be obtained by application of the results of this section.

2.1 EMISSION-ABSORPTION TRANSFORMATION MATRIX

As described in Ref. 1, the measurements required for the emission-absorption technique consist of a series of radiance and transmittance measurements (experimentally the absorptance) spatially scanning the combustion (e.g., a turbojet or rocket exhaust plume). The plume is assumed to be formed from concentric isothermal, isobaric cylinders. By examining, for example, the k^{th} measurement of the radiance (N_k), and transmissivity (τ_k) (Fig. 1), each of the parameters is described and defined by the contribution of the properties (partial pressure and temperature) of the emitting-absorbing specie from each of the zones along the optical path.

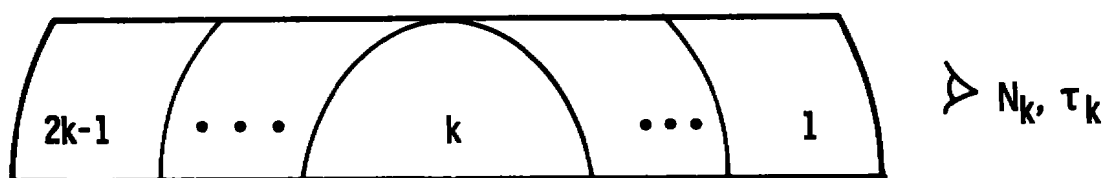


Figure 1. Diagram of cylindrically symmetric zones contributing to the k^{th} measurement of radiance and transmittance.

Functionally, one can write (with the cylindrical symmetry assumption)

$$\begin{aligned} N_k &= N_k(T_1, \dots, T_k; P_1, \dots, P_k) \\ \tau_k &= \tau_k(T_1, \dots, T_k; P_1, \dots, P_k) \end{aligned} \quad (1)$$

Expanding each term in a Taylor series, truncating after the linear terms, and rearranging, one can write

$$\delta N_k = \sum_{i=1}^{2k-1} \frac{\partial N_k}{\partial T_i} \delta T_i + \sum_{i=1}^{2k-1} \frac{\partial N_k}{\partial P_i} \delta P_i \quad (2)$$

$$\delta r_k = \sum_{i=1}^{2k-1} \frac{\partial r_k}{\partial T_i} \delta T_i + \sum_{i=1}^{2k-1} \frac{\partial r_k}{\partial P_i} \delta P_i$$

where the variational " δ " notation is utilized for the differences normally expressed in the Taylor series expansions and i is a dummy index identifying the location of a particular zone in the series. As is usual in the Taylor series expansion, Eq. (2) is strictly valid only for small δT and δP , or where the higher derivatives are much smaller than the first derivatives.

This linearization approximation represents the major analytic assumption in this work but is common in the analysis of nonlinear problems.

Note that although the emission-absorption source is assumed to be cylindrically symmetric,

$$\begin{aligned} T_{k+j} &= T_{k-j} \\ j &= 0, 1, \dots, k-1 \\ P_{k+j} &= P_{k-j} \end{aligned} \quad (3)$$

the summations in Eq. (2) are through $2k-1$. This is because, in Eq. (1), the functional dependence on the temperatures and pressures is in fact implicit, and the contribution to the measured radiance and transmittance from the $k+j$ zone is different than the $k-j$ zone. This implicit relationship makes Eq. (2) deceptively simple in that the partial derivatives must be obtained through successive applications of the chain rule. Hence, the contributions for each of the $2k-1$ zones must be calculated separately in the summations. The development of the detailed terms for expressing δN and δr in Eq. (1) are indicated in Appendix A.

If equations similar to those in Eq. (1) are written for each measurement and expanded by Eq. (2), the result can be symbolically expressed by the matrix equation,

$$\begin{bmatrix} \frac{\partial N}{\partial T} & \frac{\partial N}{\partial P} \\ \hline \frac{\partial r}{\partial T} & \frac{\partial r}{\partial P} \end{bmatrix} \begin{bmatrix} \delta T \\ \delta P \end{bmatrix} = \begin{bmatrix} \delta N \\ \delta r \end{bmatrix} \quad (4)$$

in which the unsubscripted symbols represents a submatrix or vector of appropriate terms obtained by proper arrangement and collection of similar terms in the system of equations, Eq. (2). Equation (4) is the form of linear equations

$$AX = D \quad (5)$$

with formal solution

$$X = A^{-1} D \quad (6)$$

where the identifications

$$X = \begin{bmatrix} \delta T \\ \hline \delta P \end{bmatrix} \quad D = \begin{bmatrix} \delta N \\ \hline \delta r \end{bmatrix} \quad A = \begin{bmatrix} \frac{\partial N}{\partial T} & \frac{\partial N}{\partial P} \\ \hline \frac{\partial r}{\partial T} & \frac{\partial r}{\partial P} \end{bmatrix} \quad (7)$$

are obvious. The X and D vectors each have 2k elements and represent the variations of the temperature and pressure and of the radiances and transmittances, respectively. The matrix A^{-1} is a 2k x 2k matrix and can be thought of as the transformation matrix from the data (N,r) space to the properties (T,P) space. It is a linear transformation with certain convenient properties for variance analysis as is described below.

2.2 VARIANCE-COVARIANCE MATRIX PROPAGATION

From elementary statistical theory (Ref. 3), the variance is defined as the second moment about the mean for a single observable. The covariance is the joint moment about the means of two observables. The covariance thus involves integration over the joint probability function, and if the observables are independent, the covariance is zero.

In the matrix notation, the variance-covariance matrix may be expressed

$$\Sigma_D = \langle (D - \mu_D) (D - \mu_D)^T \rangle \quad (8)$$

where D is the column vector of the observable, μ_D is the vector of the mean value for each of the D , Σ_D is the variance-covariance matrix, and the T superscript indicates the transposed matrix. The bracket notation expresses the expected value of the enclosed quantities and, for a matrix, is the matrix of the expected values of the elements. Σ_D is a symmetric matrix in which the diagonal elements are the variances of the data and the off-diagonal elements express the covariances.

If the D values are used in a linear transformation

$$X = CD \quad (9)$$

where C is the rectangular transformation matrix and X is a vector, then also

$$\mu_X = C\mu_D \quad (10)$$

for the mean value vector in the transformed space. The variance-covariance matrix for the X is formed analogous to the definition above, or:

$$\Sigma_X = \langle (X - \mu_X) (X - \mu_X)^T \rangle \quad (11)$$

Using the transformations (Eqs. (9) and (10)) gives

$$\Sigma_X = \langle C(D - \mu_D) (D - \mu_D)^T C^T \rangle \quad (12)$$

The expected value is a linear operator, thus

$$\Sigma_X = C \langle (D - \mu_D) (D - \mu_D)^T \rangle C^T \quad (13)$$

and the central term is just the variance-covariance matrix of the D observables (Eq. (10)) or

$$\Sigma_X = C \Sigma_D C^T \quad (14)$$

Thus, if the variance-covariance matrix (Σ_D) of a set of data (D) and the linear transformation (C) from D to X are known, then the variance-covariance matrix in the

transformed space (Σ_X) is immediately determinate. The transformation matrix (C) in Eq. (14) is to be identified with the partial derivative matrix (A^{-1}) in Eq. (9). Although this identification is not immediately obvious, it can be seen readily by noting that Eq. (9) also expresses the linearization of a Taylor series expansion of the (N, τ) data. Thus, Eq. (14) becomes the means by which the variance-covariance matrix of the k radiances and transmissivities is propagated through the inversion technique to the variance-covariance matrix of the temperatures and pressures.

Equation (14) is not restricted to the analysis of the E/A problem, however. Any analysis or experimental operation which can be cast into a form such as Eq. (9) responds to the foregoing treatment. Least-squares curve fitting represents a large class of commonly used data smoothing techniques which are amenable to the foregoing analysis.

2.3 APPLICATION

In order to utilize Eq. (14), it is necessary to determine the variance-covariance matrix for the radiance and transmissivity measurements (Σ_D). When the data are independent and uncorrelated, as is usually the case for raw experimental data, the off-diagonal elements, the covariances, can be taken as zero. The diagonal elements, the variances, are generally taken to be the square of the standard deviation of the raw data.

However, raw data are usually smoothed in some manner, say with linear least-squares curve fitting techniques or with Fourier filtering. If the smoothing technique is linear, as it is in each of the two aforementioned numerical techniques, then one can write an equation similar to Eq. (9) describing the technique for smoothing. The diagonal variance-covariance matrix for the independent raw data measurements can then be propagated through the smoothing technique by use of Eq. (14). That resultant symmetric variance-covariance matrix for the fitted data is then propagated through the inversion technique to yield the final variance-covariance matrix for the temperature and pressure.

3.0 RESULTS

The considerations described above have been applied to the emission-absorption radial inversion technique, and a computer program has been written to effect the calculations. The calculation procedure has been applied to two sets of data described below. These data are to be considered as indicative of typical results rather than yielding definitive bounds.

The first sample case to be described is purely a numerical model. The calculations were performed using the radiance and transmissivity of water-vapor at a wavelength of

2.5 μ . The radiance and transmittance were calculated for an imagined water vapor temperature and partial pressure profile. These data were then perturbed randomly about the calculated values using a uniform probability distribution function. The magnitude of the perturbation for each datum was constrained to be no greater in absolute value than 5 percent of the centerline value of the quantity. These simulated raw data were then least-squares curve fit to a 4th-degree polynomial evaluated at the same positions as the data, and the variance-covariance matrix for the fitted data was determined.

The radiances are plotted in Fig. 2, and transmittances are plotted in Fig. 3. The rectangles on each plot illustrate the original theoretical profile and geometry. The symbols are the values resulting from the curve fit used for subsequent analysis, and the bars are the uncertainty limit to be applied at each data point. In this manner, an experimental situation is simulated in which the data are assumed to be randomly distributed about some unknown function (the rectangles), and with a known error bound (the bars) on the experimental data. The raw data are smoothed, and these results (the points) are used for subsequent analysis.

For these determinations, the original data variance-covariance matrix was diagonal, with the elements being the square of the observed uncertainties. The least-squares polynomial fitting equations were cast into a form consistent with Eq. (9), and the resultant variance-covariance matrix, because of propagation through the curve fit, was calculated according to Eq. (14). This symmetric variance-covariance matrix was then propagated through the inversion procedure according to Eq. (14). Only the values of the elements of the matrix C and Σ_D vary from application to application.

These data were then inverted for water vapor temperature and partial pressure, and the propagated variance-covariance matrix was determined. These results for temperature are shown in Fig. 4 and for partial pressure in Fig. 5. The inverted results are denoted by symbols and the propagated uncertainty by the bars. The magnitude of the uncertainties is the square root of the diagonal elements of the variance-covariance matrix. For comparison purposes, the original profiles are shown by the rectangles.

The results show that, for the initial 5-percent centerline uncertainty on the original data, the centerline temperature is determinate within a 10-percent uncertainty and the centerline partial pressure is determinate to within 23-percent uncertainty. These uncertainties are more or less typical for this calculation except in the outer zones of the plume. As can be seen in Figs. 2 and 3, however, the signal-to-noise ratio in these outer zones is near one or less; therefore, the large uncertainty in that data is to be expected. As final comment on this first case, it should be noted that the choice of fitting function will affect the final error propagation result through the effect on the appropriate transformation matrix C . Some other choice of fitting function may easily change the propagated errors reported here.

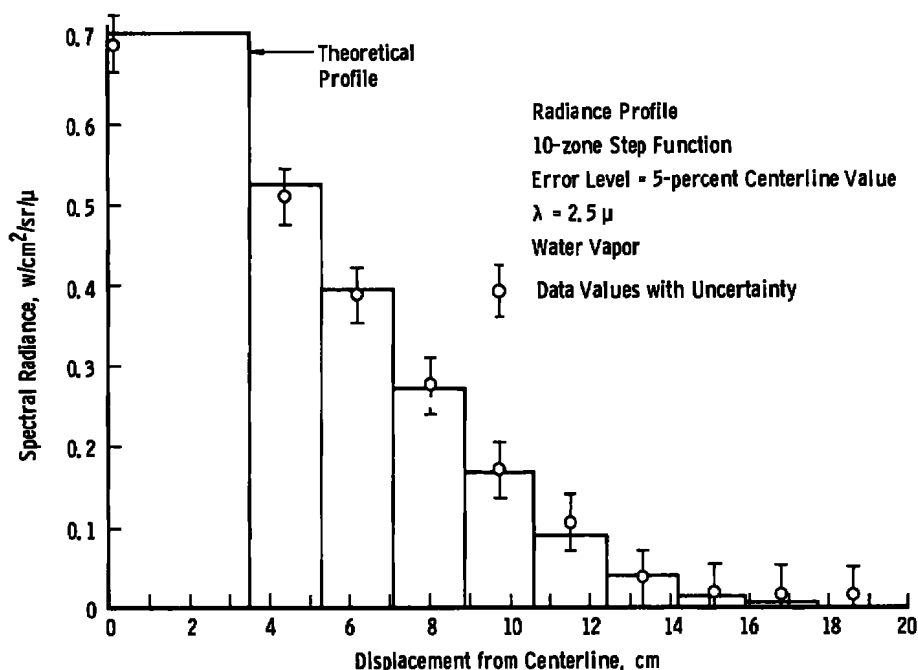


Figure 2. Theoretical and perturbed water vapor radiance profile.

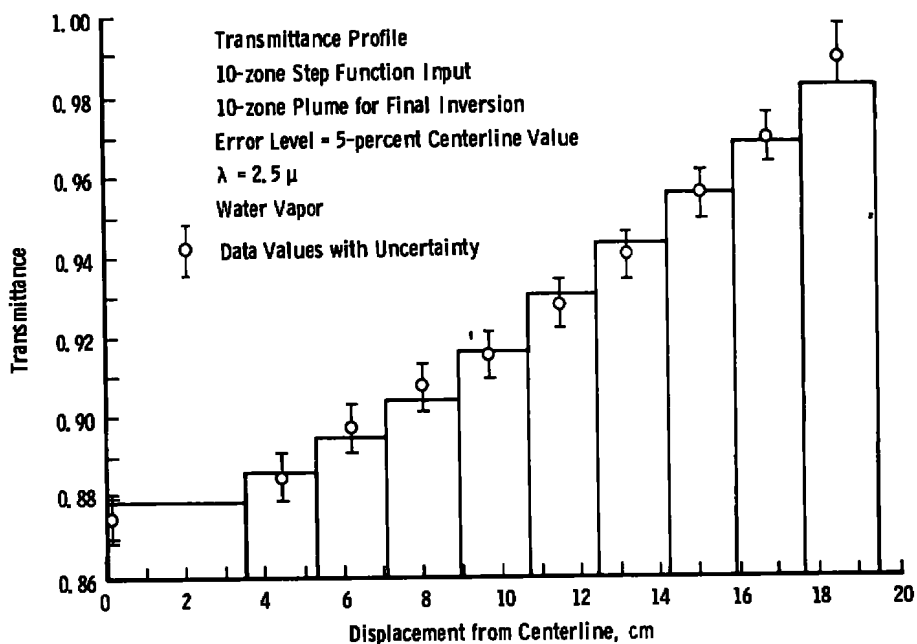


Figure 3. Theoretical and perturbed water vapor transmittance profile.

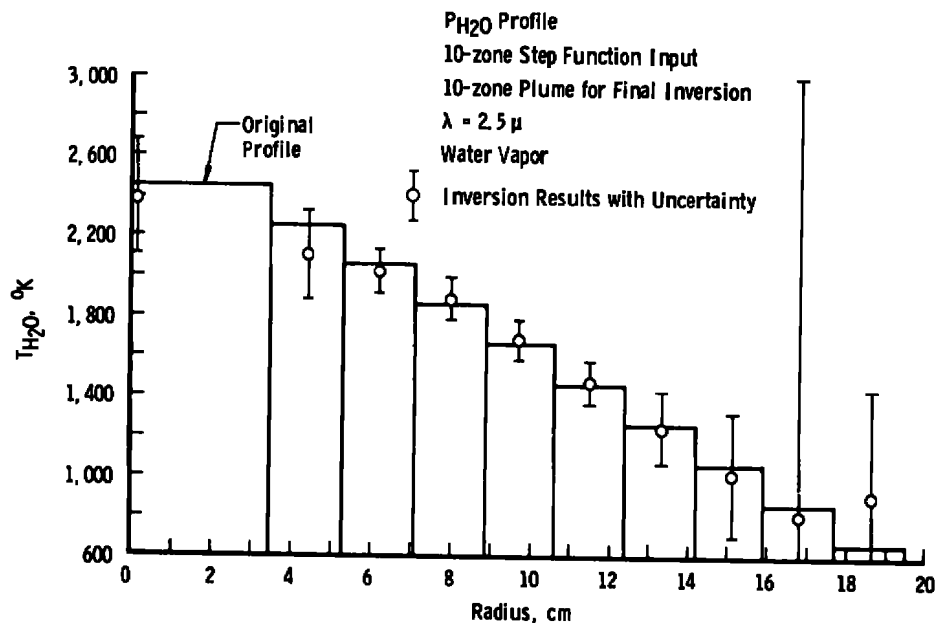


Figure 4. Original and inverted water vapor temperature profile.

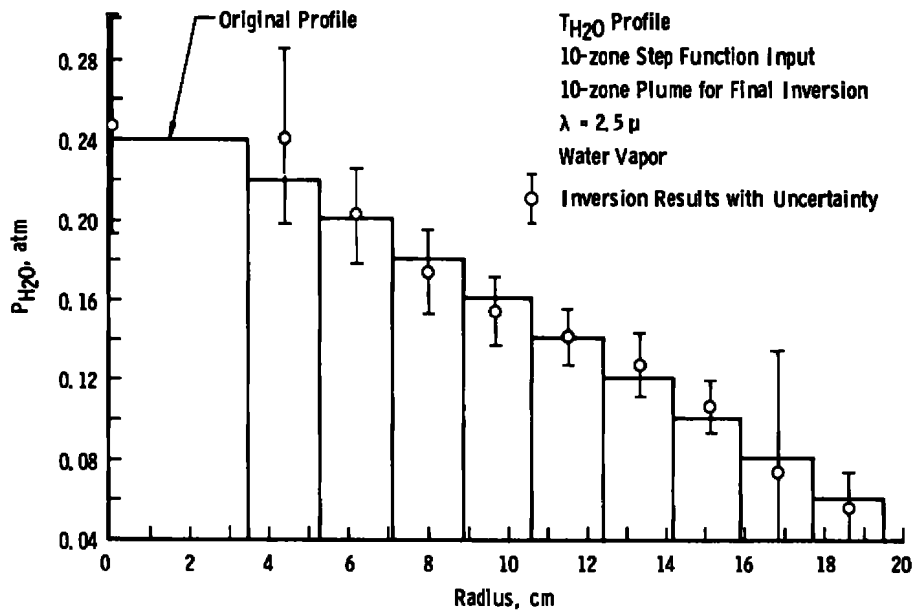


Figure 5. Original and inverted water vapor partial pressure profile.

The second case to be described is representative of typical measurements obtained from a laboratory flat flame burner burning methane and air. The emitting and absorbing specie in this experiment was carbon dioxide at a wavelength of $4.5\ \mu$. The raw data were least-squares curve fit to a polynomial function of displacement, and the spectral radiance and transmissivity were reevaluated at positions convenient to analysis. The raw data and results of the curve fit are shown in Fig. 6. In this figure, the raw data are represented by the points, and the curve fit used to generate the data for subsequent analysis is represented by the solid line. The symbol size indicates the maximum observed experimental uncertainty in these raw data, typically 3 percent of the maximum value, which can be taken as a 3σ bound. As before, the original data variance-covariance matrix is diagonal with the nonzero elements the square of the observed uncertainties. This diagonal matrix is then propagated successively through the curve-fit procedure and the inversion procedure according to repeated applications of Eq. (14). The uncertainties reported on the succeeding analysis plots are the square roots of the elements on the principal diagonal of the final symmetric variance-covariance matrix and thus represent the propagated 3σ bound.

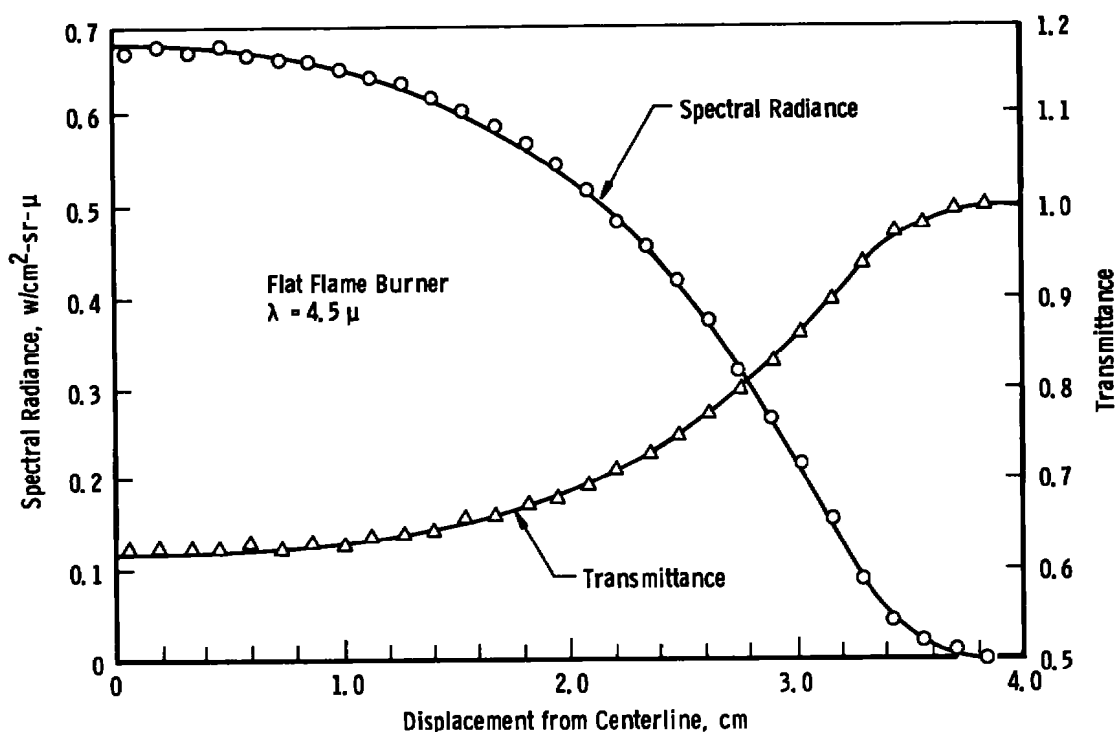


Figure 6. Spectral radiance and transmittance data versus displacement at $4.5\ \mu$.

The results of the inversion of these data and the propagated error bound are shown in Figs. 7 and 8. The CO_2 temperature (Fig. 7) shows approximately 5-percent uncertainty on the centerline, while the partial pressure (Fig. 8) shows approximately 15-percent uncertainty on the centerline. Further, as is seen in Figs. 7 and 8, the error propagation characteristics away from the centerline are improved over the centerline characteristics. This behavior is attributed to the geometry and uniform property profile of the flat flame burner. The central portions of the flame do not contribute materially to the observed spectral radiance and transmissivity (see Fig. 5). Hence, large variations in either or both the specie temperature or pressure can be allowed, provided there remains insignificant contribution to the centerline values of the data.

Extension of these representative results to the general case must be approached cautiously. These data were not chosen for any particular characteristics, and the assumed standard deviations are not necessarily consistent with any quantitative physical evidence. Further, the way any particular set of data is handled with respect to linear least-squares curve fitting, Fourier filtering, or other data smoothing technique will change the final result. Each set of data must be analyzed on its own merits and characteristics.

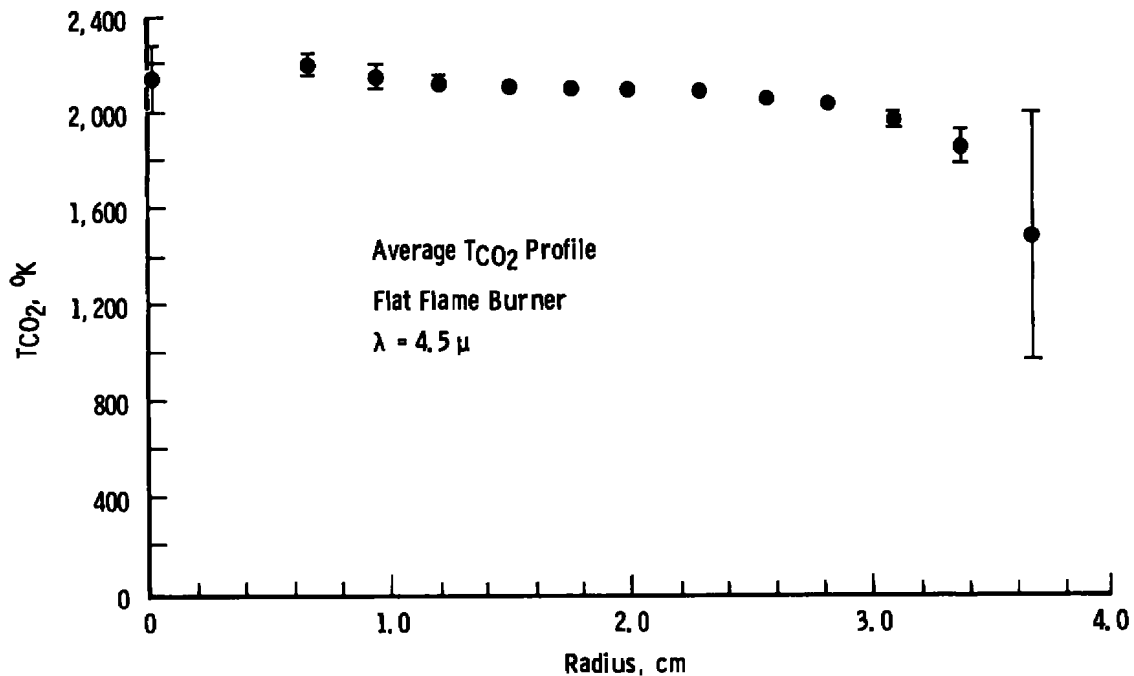


Figure 7. Radial CO_2 temperature profile obtained from 4.5μ data.

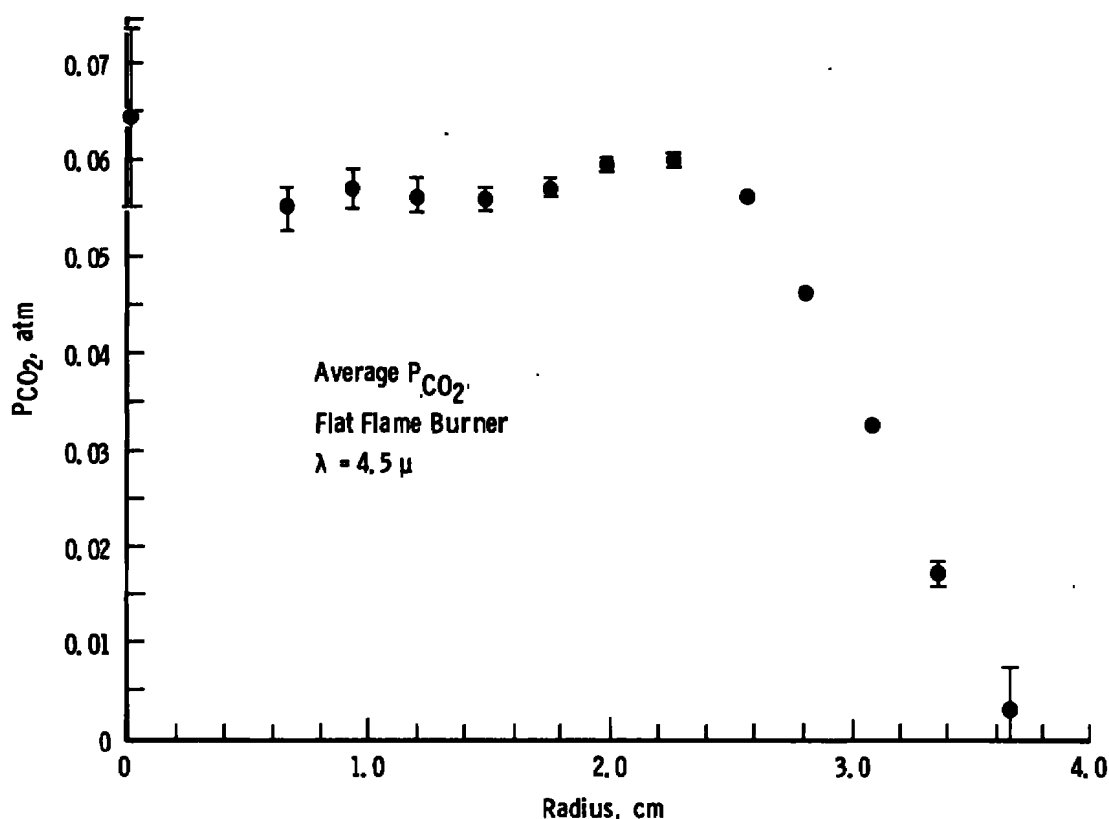


Figure 8. Radial CO_2 partial pressure profiles obtained from 4.5μ data.

4.0 CONCLUDING REMARKS

A method of determining the propagation of errors in the E/A technique was developed and described functionally. The E/A technique, used to determine temperature and partial pressure profiles, results from applying band model theory to the solution of the radiative transfer problem for the spatial distribution of the projected radiance and transmittance from a cylindrically symmetric radiating/absorbing medium. The method provides a means by which uncertainties in the determined temperature and partial pressure profiles, represented by a variance-covariance matrix, can be determined by direct calculations based on the uncertainties (variance-covariance matrix) of the experimental data. The development of the detailed equations describing the necessary terms in the analytic description of the propagation is indicated in Appendix A.

A computer program to perform the calculations described herein has been coded and was used to provide illustrative calculations for two typical emission-absorption

profiles. The results, which must be considered unique to those profiles shown, suggest that the propagated temperature uncertainty is generally slightly larger than the data uncertainty while the partial pressure uncertainty is considerably larger.

The analytic approach presented here can be extended straightforwardly to provide descriptions of the variational dependence of the radiance and transmittance on other parameters, and indeed should be. The work does not address the uncertainty of the results based on the uncertainty of the band model parameters but can be adapted for such a study. Another possible useful adaptation of the approach here would be to determine the uncertainty of the experimental measurements because of fluctuations in the temperature and partial pressure profiles induced by plume flicker and turbulence at selected positions along the line of sight. Each of the aforementioned studies, although detailed, develop straightforwardly from the approach and equations described in this report and Appendix A.

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APPENDIX A

DETAILED EQUATIONS FOR PARTIAL DERIVATIVES OF EMISSION/ABSORPTION EQUATIONS

The emission/absorption (E/A) technique is used for determining the temperature and pressure profiles in exhaust plumes from combustion sources (e.g., turbojet or rocket engine exhaust plumes). The E/A technique develops by applying band model theory to the solution to the radiative transfer problem for the spatial distribution of the projected radiance and transmittance from a cylindrically symmetric radiating/absorbing medium. Because the technique is used for the analysis of experimental data, a means of assessing the effect of the experimental uncertainties on the result is needed. The functional approach for this error propagation analysis is contained in the body of the report.

The major task in providing the analytic approach to performing the emission absorption uncertainty propagation analysis is the development of the detailed algebraic equations consistent with a meaningful accounting system for relating the mathematical symbols to identifiable physical parameters. These equations and the accounting system are described in this appendix.

The plume, shown schematically in Fig. A-1, is modeled by a series of concentric cylinders, within each of which the species temperature and partial pressure is constant. Measurements of radiance and transmittance are taken along a line of sight through each succeeding ring. With this geometrical model, the solution to the radiative transfer problem can be approximately expressed as

$$N_{xk} = \sum_{i=1}^{2k-1} N_b(T_{i,k}) (r_{i-1,k} - r_{i,k}) \quad (A-1)$$

where

$$\ln r_{j,k} = 2\pi \left(\frac{\gamma}{d} \right)_{j,k} f(X_{j,k}) \quad (A-2)$$

$$N_b(T_{j,k}) = \frac{2h c^2 \bar{\nu}^5}{\exp\left(\frac{hc\bar{\nu}}{kT_{j,k}}\right) - 1} \quad (A-3)$$

In the above equations, the subscript k identifies a particular measurement which in turn identifies a particular line of sight. For the double subscripted parameters, it is seen that the trailing subscript identifies this particular line of sight, whereas the leading subscript identifies a particular zone in the plume along the line of sight. This leading subscript starts with one on the measurement side of the plume and increments

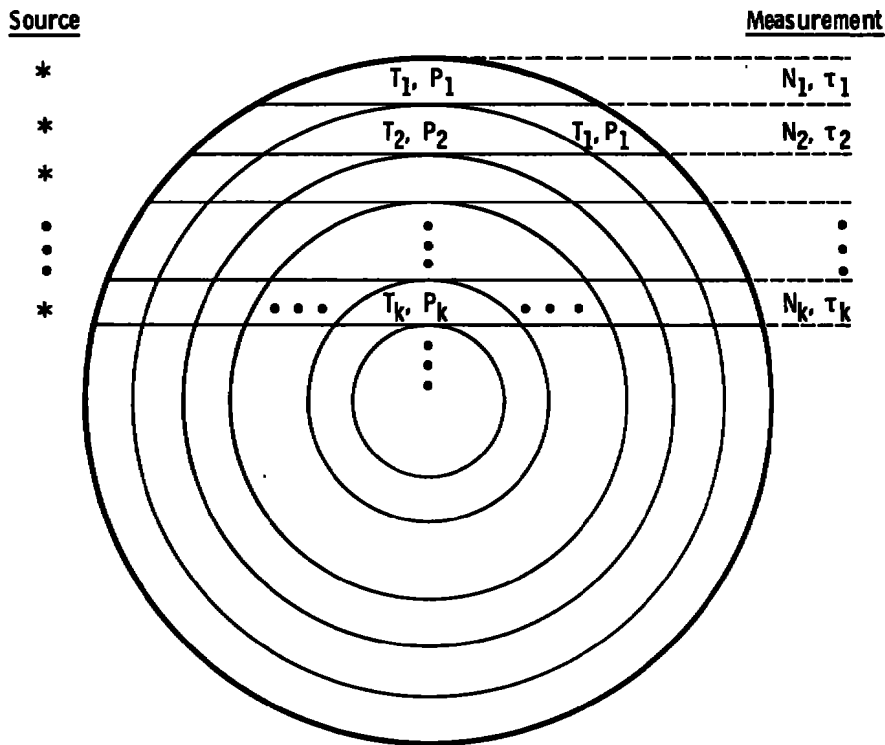


Figure A-1. Cross-sectional schematic diagram of inhomogeneous cylindrically symmetric source.

sequentially to the source side of the plume with a final value $2k-1$. The temperature and partial pressure of the central zone ($T_{k,k}$ and $P_{k,k}$) are the unknown parameters. Note that, with this accounting system, the transmittance measurement (τ_{xk}) can be expressed:

$$\tau_{xk} = \tau_{2k-1,k} \quad (\text{A-4})$$

Use of the Curtis-Godsen approximation (Ref. 1) provides the definitions

$$\left(\frac{\Gamma}{d}\right)_{j,k} = \frac{\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} (y/d)_{i,k}}{\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k}} \quad (\text{A-5})$$

$$X_{j,k} = \frac{\left[\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} \right]^2}{2\pi \sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} (y/d)_{i,k}} \quad (\text{A-6})$$

In Eqs. (A-5) and (A-6), $(s/d)_{i,k}$ and $(\gamma/d)_{i,k}$ are known specific functions of the temperature and partial pressure of the i^{th} zone along the k^{th} line of sight.

The development of the error propagation analysis equations described in the body require the partial derivatives of the radiance and transmittance with respect to the temperature and partial pressure in order to determine the elements of the propagated variance-covariance matrix. For the temperature,

$$\frac{\partial N_{xk}}{\partial T_{m,k}} = \sum_{i=1}^{2k-1} \left\{ \frac{\partial N_b(T_{i,k})}{\partial T_{m,k}} (r_{i-1,k} - r_{i,k}) + N_b(T_{i,k}) \left[\frac{\partial r_{i-1,k}}{\partial T_{m,k}} - \frac{\partial r_{i,k}}{\partial T_{m,k}} \right] \right\} \quad (\text{A-7})$$

$$\frac{\partial r_{j,k}}{\partial T_{m,k}} = -2\pi r_{j,k} \left\{ f(X_{j,k}) \frac{\partial(\Gamma/d)_{j,k}}{\partial T_{m,k}} + \left(\frac{\Gamma}{d} \right)_{j,k} \frac{\partial f}{\partial X_{j,m}} \frac{\partial X_{j,k}}{\partial T_{m,k}} \right\} \quad (\text{A-8})$$

$$\begin{aligned} \frac{\partial(\Gamma/d)_{j,k}}{\partial T_{m,k}} = & \frac{\ell_{m,k} \left[(s/d)_{m,k} \frac{\partial(\gamma/d)_{m,k}}{\partial T_{m,k}} + (\gamma/d)_{m,k} \frac{\partial(s/d)_{m,k}}{\partial T_{m,k}} \right]}{\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k}} \\ & - \frac{\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} (\gamma/d)_{i,k}}{\left[\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} \right]^2} \ell_{m,k} \frac{\partial(s/d)_{m,k}}{\partial T_{m,k}} \end{aligned} \quad (\text{A-9})$$

$$\begin{aligned} \frac{\partial X_{j,k}}{\partial T_{m,k}} = & \frac{2 \left[\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} \right] \ell_{m,k} \frac{\partial(s/d)_{m,k}}{\partial T_{m,k}}}{\sum_{i=1}^j 2\pi \ell_{i,k} (\gamma/d)_{i,k} (s/d)_{i,k}} \\ & \frac{\left[\sum_{i=1}^j \ell_{i,k} (s/d)_{i,k} \right]^2}{\left[\sum_{i=1}^j 2\pi \ell_{i,k} (\gamma/d)_{i,k} (s/d)_{i,k} \right]^2} \left\{ 2\pi \ell_{m,k} \left(\frac{\gamma}{d} \right)_{m,k} \frac{\partial(s/d)_{m,k}}{\partial T_{m,k}} + \left(\frac{s}{d} \right)_{m,k} \frac{\partial(\gamma/d)_{m,k}}{\partial T_{m,k}} \right\} \end{aligned} \quad (\text{A-10})$$

There are similar expressions for the partials derivatives with respect to pressure which are not repeated here. Their form is similar to Eqs. (A-7) through (A-10), replacing the symbol T by the symbol P.

The remaining functions not specifically defined to this point are the (s/d) , (γ/d) , and $f(X)$. Each of these depends on the particular form assumed for the absorption coefficient, line broadening parameter, and the specific form assumed for the band model. A description of the various options is included in Ref. 4. As a specific example, let

$$\left(\frac{s}{d}\right)_i = K_i \frac{T_o}{T_i} \frac{P_i}{P_o} \quad (A-11)$$

$$\left(\frac{\gamma}{d}\right)_i = \left(\frac{1}{d}\right)_i C \frac{T_o}{T_i} \frac{P_i}{P_o} \quad (A-12)$$

where K_i and $(1/d)_i$ are tabulated functions of temperature and wavelength, determined experimentally, and C is a constant. In this case, since $\partial T_i / \partial T_j = 0$ for $i \neq j$,

$$\frac{\partial (s/d)_i}{\partial T_i} = \frac{T_o}{T_i} \frac{P_i}{P_o} \frac{\partial K_i}{\partial T_i} - K_i \frac{P_i}{P_o} \frac{T_o}{T_i^2} \quad (A-13)$$

and

$$\frac{\partial (\gamma/d)_i}{\partial T_i} = C \frac{T_o}{T_i} \frac{P_i}{P_o} \frac{\partial (1/d)_i}{\partial T_i} - C \left(\frac{1}{d}\right)_i \frac{P_i}{P_o} \frac{T_o}{T_i^2} \quad (A-14)$$

and the similar concomitant expressions for the partial derivatives with respect to partial pressure.

If the random band model and an exponential line strength distribution are assumed, the resultant curve of growth is

$$f(X) = (1 + X)^{-1/2} \quad (A-15)$$

and the derivative

$$\frac{\partial f}{\partial X} = -\frac{1}{2} (1 + X)^{-3/2} \quad (A-16)$$

is immediate.

Thus, one has at hand the specific detailed expressions for determining the terms comprising the partial derivatives in Eq. (4). The necessary equations for the partial derivative with respect to temperature are formed by substituting Eqs. (A-8) through (A-16) into Eq. (A-2) for the partial derivative of N_{xk} with respect to temperature, keeping the appropriate subscripts compatible. There are comparable expressions for the partial derivative with respect to partial pressure, requiring only to change the symbol T with the symbol P , except for the partial derivatives of the band model parameters (s/d) and (γ/d) . In this case,

$$\frac{\partial(s/d)_i}{\partial P_i} = K_i \frac{T_o}{T_i} \frac{1}{P_o} \quad (A-17)$$

$$\frac{\partial(\gamma/d)_i}{\partial D_i} = C \left(\frac{1}{d} \right)_i \frac{T_o}{T_i} \frac{1}{P_o} \quad (A-18)$$

since K_i and $(1/d)_i$ are independent of the partial pressure.

As final comment, it is to be noted that the partial derivative of N_{xk} also requires the partial derivatives of $\tau_{i,k}$. Thus, as the expansion is developed, the partial derivative of N_{xk} will include the term $(\partial\tau_{2k-1,k}/\partial\tau_{m,k})$ (note Eq. (A-7)). Hence, since $\tau_{xk} = \tau_{2k-1,k}$ (Eq. A-4), one has at hand immediately the terms necessary to complete the partial derivative description required by the uncertainty propagation analysis described in the body of the report.

NOMENCLATURE

A	Matrix of partial derivatives defined in Eq. (7)
C	Linear transformation matrix from observable space to transformed space, Eq. (9), Used to indicate a constant in the Appendix
c	Speed of light, 2.997925×10^{10} cm/sec
D	Vector of observable, or data, values
1/d	Line broadening parameter, cm^{-1}
f(X)	Band model curve-of-growth
h	Planck's constant, 6.626196×10^{-27} erg sec
K	Absorption coefficient
k	Boltzmann's constant, 1.38062×10^{-16} erg/ $^{\circ}\text{K}$
ℓ	Path length, cm
N	Spectral radiance, $\text{watts/sr/cm}^2/\mu$
P	Partial pressure, atm
s/d	Average line strength parameter, Eq. (A-11)
T	Temperature, $^{\circ}\text{K}$
X	Vector of transformed data, Eq. (9) and hand model function agreement, Eq. (A-6)
Γ/d	Equivalent average line width parameter, Eq. (A-5)
γ/d	Average line width parameter, Eq. (A-12)
λ	Wavelength, μ
μ	Column vector of mean values

π	3.14159265
Σ	Variance-covariance matrix
τ	Transmittance
$\bar{\nu}$	Wave number, cm^{-1}

SUBSCRIPTS

0	Indicates reference properties
b	Denotes Planck's blackbody function
D	Indicates the observable or data space
i	Dummy index used as a counter
k	Index indicating the central zone of a slice across the cylindrically symmetric combustion source, or, the corresponding measurement of projected radiance or transmittance.
m	Indicates an arbitrary zone in the k^{th} slice across the source
x	Indicates transformed space for variance-covariance matrix, or, represents experimentally determined quantity in the appendix