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Nonisothermal Band Model Theory

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Nonisothermal Band Model Theory

Chemistry and Physics Laboratory
Laboratory Operations
The Aerospace Corporation
El Segundo, Calif. 90245

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FOR THE COMMANDER

John R Doughty, LtCol, USAF

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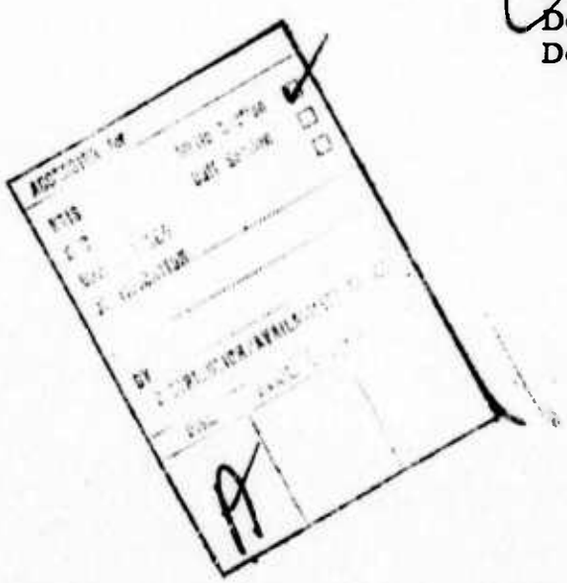

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Theoretical formulations of radiation band models for general nonuniform optical paths are presented. The models are framed within the statistical band model for an array of Lorentz lines and an inverse line strength distribution. Radiative transfer for an isolated line in a general nonuniform medium and the statistical model for a uniform optical path are reviewed in order to provide the foundation required for the band model formulations. Two approaches to the development of these models are taken. The first is based on making approximations to such radiative transfer functions as transmittance or equivalent

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width and yields models equivalent or similar to the traditional Curtis-Godson approximation. The second treats approximations to the spatial derivatives of these functions. From the standpoint of computing line or band radiance, the spatial derivatives are more fundamental quantities than the transfer functions themselves; consequently, these latter "derivative approximations" are intrinsically more accurate than the Curtis-Godson type approximations.

All of the models are formulated to give the spatial derivative of the mean equivalent width function $\overline{W}(s)/\delta$ in the form

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)\, p(s)\, \overline{k}(s)\, y(s) \quad ,$$

where $c(s)$, $p(s)$, and $\overline{k}(s)$ are the concentration, total pressure, and absorption band model parameter, respectively, at the local path position s. The functional form of the derivative function $y(s)$ is derived for each of the models. In general, $y(s)$ is a function of both local and path-averaged (subscript e) band model parameters. These local and averaged parameters are used to define a dimensionless optical depth parameter $\underline{x}_e = u\overline{k}_e/\beta_e$ and three nonuniformity indexes $\rho = \overline{\gamma}/\overline{\gamma}_e$, $r = \beta/\beta_e$, and $q = \overline{\delta}_e/\overline{\delta}$ (γ is line width, $\overline{\delta}$ is the mean line spacing band model parameter, and $\beta = 2\pi\gamma/\delta$). The explicit manner in which these parameters enter into the various functional forms for $y(s)$ is derived and discussed. The introduction of the parameter q is an important aspect of the new models and is an explicit measure of nonisothermality along the optical path. In addition to the traditional Curtis-Godson definitions for the effective parameters $\overline{k}_e$ and β_e, new definitions for the path averages $\overline{\gamma}_e$ and $\overline{\delta}_e$ are derived. These new definitions are obtained from the fundamental properties of the assumed inverse line strength distribution.

A summary of all of the models is given as a table of relevant equations for use in practical calculations.

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I. INTRODUCTION

The calculation of low-resolution radiance and transmittance spectra of molecular gases by narrow band model methods has widespread applicability in quantitative spectroscopy. Two particularly important areas of application are the calculation of heat transfer in the earth's atmosphere[1] and the calculation of infrared radiance signatures of hot combustion gases.[2] The latter spans the range from small laboratory flames to exhaust plumes of jet aircraft and rocket-propelled missiles.

Most practical applications of band model methods must treat nonuniform optical paths. In atmospheric applications, inhomogeneities result from the variation of pressure and mixing ratio of active species with altitude. Temperature variations also occur in the atmosphere, but for many applications, these variations may be neglected and the atmosphere treated as isothermal. In combustion gas applications, however, very strong thermal gradients may be encountered. This is particularly true for exhaust plume problems in which shock structure and the mixing and afterburning of unburned fuels with atmospheric oxygen are considered. An important problem that combines aspects of atmospheric and combustion gas methods is the propagation of radiation from a hot gas source through a long cool absorbing atmosphere. If the same molecular species is responsible for both emission and absorption, the high degree of line position correlation between the emission and absorption spectra may preclude the decoupling of the optical path into isolated emitter and absorber regions and multiplying the source band radiance by the absorber band transmittance in order to arrive at the transmitted radiance spectrum. The entire optical path through both the absorbing and emitting path segments must be treated as a single nonuniform optical path.

Radiative transfer along nonuniform optical paths for both isolated lines and bands of lines has a long and varied history of theoretical study. These studies can be conveniently grouped into three categories corresponding to

a priori assumptions concerning the type of optical path considered. The first category includes those solutions and approximations that make no prior assumptions concerning the variations along the path and are thus applicable (but not necessarily accurate) to any general nonuniform path. The most significant entries into this category include the Curtis-Godson (CG) approximation,[3-10] the Lindquist-Simmons (LS) approximation,[11-13] the derivative model of Lindquist et al.,[14] the intuitive method of Weinreb and Neundorffer,[15] and the exact solution for an isolated Lorentz line of Plass and Fivel.[16] The formulation discussed and applied by Simmons and others[17-21] can also be considered as a general path approximation, but requires the selection of parameters or functions that fit the model to specific types of nonuniform paths. The work of Boughner[22] on shock-heated gas also fits into this restricted general path category.

The second category includes studies that consider optical paths along which the pressure is specifically assumed to vary exponentially. Application to atmospheric slant paths is evident. Significant contributions in this category include the works of Plass and Fivel,[23] Yamamoto and Aida,[24] and Yamamoto et al.[25]

The third category of studies are most applicable to the problem of flame radiation through an absorbing atmosphere. The a priori path modeling here is the consideration of two uniform path segments in series. Treatment of line radiation for this case has been made by Sakai and Stauffer[26,27] [with comments by Plass[28]] and by Goody.[29] Sakai and Stauffer considered the general problem of two arbitrarily overlapping Lorentz lines. For zero separation, their analysis is applicable to the two-cell problem. Treatment of band radiation for two path segments in series has been given by Plass[30,31] and Rodgers.[32]

Despite the extensive work reflected in this short review, no band model has been developed that adequately handles general optical paths along which high degrees of inhomogeneity and, particularly, nonisothermality occur. The most often used of these approximations is the CG approximation. Generally speaking, this approximation is adequate for application to

atmospheric problems and even to combustion gas problems that display moderately strong temperature gradients.[2, 10, 22, 33] For very strong thermal gradients, and for the case of viewing hot gas sources through intervening cool absorption paths, the CG approximation as well as the remaining general path formulations often fail to yield adequate results.

The concern of the present paper is the formulation of improved band radiance models that can be applied efficiently to general nonuniform optical paths and that account for large nonuniformities better than previous models. Spectra generated with these models and experimental spectra are compared in a companion paper.* The models are formulated within the confines of the statistical band model for Lorentz line shape and inverse line strength distribution. Three works are of particular importance in establishing the groundwork for these formulations: (1) the work of Godson[5] contains the original derivation of the statistical model for the inverse line strength distribution and the most thorough treatment of the traditional CG approximation as applied to the statistical model; (2) the work of Lindquist and Simmons[11] rationalizes the approach of approximating the derivatives of such transfer functions as mean transmittance and equivalent width rather than approximating these functions directly; and (3) the recently reported work of Lindquist et al.[14] provides the intuitive direction for the formulations.

In this paper, radiative transfer for an isolated Lorentz line is reviewed in Section II, and the statistical band model for uniform optical paths is reviewed in Section III. Both discussions are restricted to topics required in subsequent developments, but are presented in some detail. The foundations established in these two sections are used in the formulations given in Sections IV and V. In Section IV, the CG approximation as given by Godson is discussed, and an alternative formulation of this approximation is considered. This alternative formulation establishes interpretations and

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*Stephen J. Young, "Evaluation of Nonisothermal Band Models for H_2O," J. Quant. Spectr. Radiative Transfer (to be published).

functional relations necessary to the formulation of the various derivative approximations made in Section V. The latter part of Section IV and Section V comprise the significant new work of this paper. The models are reviewed and summarized in Section VI.

II. ISOLATED LORENTZ LINE

A. GENERAL RELATIONS

In the statistical band model used in subsequent formulations, the average transmittance for a spectral interval $\Delta\nu$ is expressed in terms of the integrated absorptance (equivalent width) of the individual lines in $\Delta\nu$. In this section, the radiative transfer effects of an isolated Lorentz line are reviewed to the extent required for these subsequent formulations.

Consider an optical path that extends from the geometric position $s = 0$ to $s = S$. The concentration (mole fraction) of active gas $c(s)$, total gas pressure $p(s)$, and temperature $T(s)$ are considered as general, but known, functions of s. The gas is assumed to be in a state of local thermodynamic equilibrium. The spectral absorption coefficient for the Lorentz (dispersion) line shape is

$$k(\nu, s) = \frac{S(s)}{\pi} \frac{\gamma(s)}{\nu^2 + \gamma^2(s)} \quad ,$$

where $S(s)$ is the line strength and $\gamma(s)$ is the line width parameter. The reference of spectral position is the line center. $S(s)$ is assumed to be a function of temperature only, whereas $\gamma(s)$ may be a function of all three of the path variables. The variations of $S(s)$ and $\gamma(s)$ with $c(s)$, $p(s)$, and $T(s)$ are presumed known.

The two fundamental quantities of line radiation that are important here are the line radiance and the line absorptance. The former is defined by

$$N = \int_0^S N^*(s) \frac{dW(s)}{ds} \, ds \quad , \tag{1}$$

where W(s) is the integrated absorptance of the line (equivalent width) for the path segment between s = 0 and the general position s and is defined by

$$W(s) = \int_{-\infty}^{\infty} \left\{ 1 - \exp\left[-\frac{1}{\pi} \int_0^s \frac{c(s')p(s')S(s')\gamma(s')}{\nu^2 + \gamma^2(s')} \, ds' \right] \right\} d\nu \quad . \qquad (2)$$

The line absorptance is the equivalent width evaluated for the whole path W(S). N*(s) is the Planck radiation function evaluated at the true spectral position ν_0 of the line center and at the temperature T(s). The form of equation (1) is based on the assumption that N*(s) changes negligibly over the spectral width of the line.

B. EXACT SOLUTIONS FOR W(s)

The prediction of either N or W(S) for the line reduces formally to the evaluation of W(s) for general s. For a uniform optical path along which c(s), p(s), T(s), and hence S(s) and $\gamma(s)$ are constants, the solution[34] to equation (2) is

$$W(s) = 2\pi\gamma L[x(s)] \quad , \qquad (3)$$

where $x(s) = u(s)S/2\pi\gamma$ is a dimensionless optical depth parameter, and $u(s) = cps$ is the optical depth between s = 0 and s. L(x) is the Ladenburg-Reiche function

$$L(x) = xe^{-x}[I_0(x) + I_1(x)] \quad , \qquad (4)$$

where $I_0(x)$ and $I_1(x)$ are modified Bessel functions. L(x) is shown in Fig. 1. The asymptotic limits of L(x) for weak ($x \to 0$) and strong ($x \to \infty$) absorption

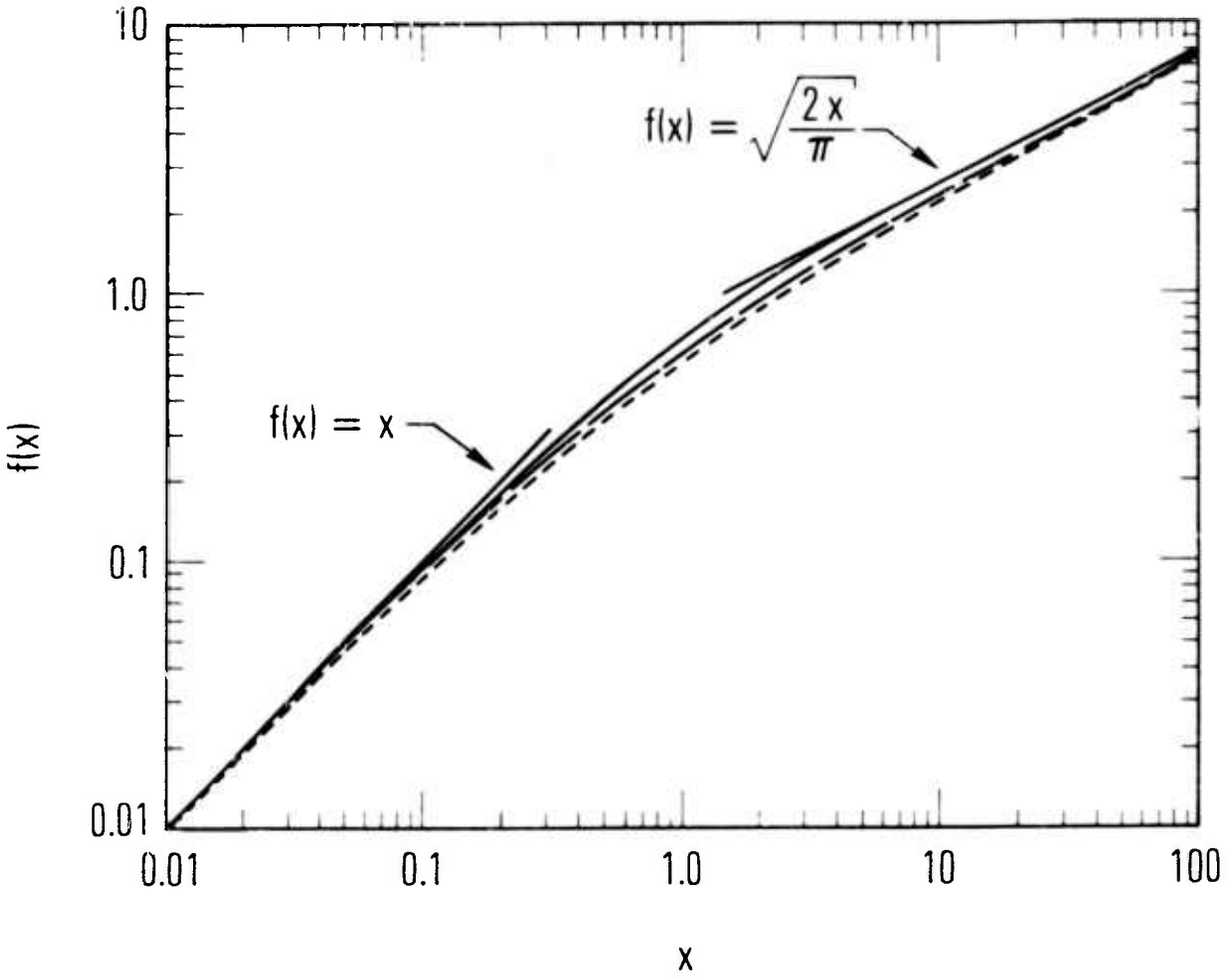

Figure 1. Curve-of-Growth Functions. — Landenburg-Reiche functions L(x); — — inverse distribution function I(4x)/4; ---- exponential-tailed inverse distribution function $I_e(\pi x)/\pi$.

are $L(x) \to x$ and $L(x) \to \sqrt{2x/\pi}$, respectively. The corresponding limits for $W(s)$ are

$$W(s) = \begin{cases} u(s)S = 2\pi\gamma x & \text{weak} \\ 2\sqrt{u(s)S\gamma} = 2\pi\gamma\sqrt{\frac{2x}{\pi}} & \text{strong} \end{cases} . \tag{5}$$

An exact solution for $W(s)$ for an arbitrary optical path has been given by Plass and Fivel.[16] The solution is a series expansion in terms of moments of $\gamma(s)$. The complexity of the solution and the fact that only the first three expansion coefficients have been evaluated preclude its use in most practical applications. This solution is not considered further here.

In the limits of weak and strong absorption, general solutions of equation (2) can be obtained in simple form. Familiar arguments[1] used to obtain the weak and strong limits for a uniform path are readily applied to a nonuniform path and yield

$$W(s) = \begin{cases} \int_0^s c(s')p(s')S(s')\,ds' & \text{weak} \\ 2\sqrt{\int_0^s c(s')p(s')S(s')\gamma(s')\,ds'} & \text{strong} \end{cases} .$$

At this point, it is convenient to introduce the concept of path-averaged line parameters. The path-averaged line strength $S_e(s)$ and line width $\gamma_e(s)$ are defined by

$$S_e(s) = \frac{1}{u(s)} \int_0^s c(s')p(s')S(s')\,ds' \tag{6}$$

and

$$\gamma_e(s) = \frac{1}{u(s)S_e(s)} \int_0^s c(s')p(s')S(s')\gamma(s')\,ds' \quad , \tag{7}$$

where u(s) is the optical depth

$$u(s) = \int_0^s c(s')p(s')\,ds' \quad . \tag{8}$$

A convenient dimensionless optical depth parameter is

$$x_e(s) = \frac{u(s)S_e(s)}{2\pi\gamma_e(s)} \quad . \tag{9}$$

In terms of these path-averaged parameters, the limiting solutions for W(s) may be written as

$$W(s) = \begin{cases} u(s)S_e(s) = 2\pi\gamma_e(s)x_e(s) & \text{weak} \\ 2\sqrt{u(s)S_e(s)\gamma_e(s)} = 2\pi\gamma_e(s)\sqrt{\dfrac{2x_e(s)}{\pi}} & \text{strong} \end{cases} \quad . \tag{10}$$

Comparison of equations (5) and (10) indicates that W(s) for a general path approaches the same limiting forms for weak and strong absorption as does W(s) for a uniform path. The difference is that the path averages $S_e(s)$ and $\gamma_e(s)$ replace the constants S and γ, respectively, and the general result for u(s) given by equation (8) replaces the quantity cps.

Considerations presented later require the spatial derivative of these exact limiting solutions. Straightforward differentiations yield

$$\frac{dW(s)}{ds} = \begin{cases} c(s)p(s)S(s) & \text{weak} \\ \dfrac{c(s)p(s)S(s)\gamma(s)}{\sqrt{u(s)S_e(s)\gamma_e(s)}} = \dfrac{c(s)p(s)S(s)}{\sqrt{2\pi x_e(s)}} \dfrac{\gamma(s)}{\gamma_e(s)} & \text{strong} \end{cases} . \qquad (11)$$

C. CURTIS-GODSON APPROXIMATION

The CG approximation was introduced by Curtis[3] and Godson[4, 5] in the context of isothermal band models used for computing heating rates in the atmosphere. An extensive literature exists on the application and interpretation of this approximation. The approximation can be formulated from several points of view. The conceptually simplest, and the one most in keeping with Curtis' original discussion, is that the path-integrated line-shape function [the exponential argument of W(s) in equation (2)] is replaced by a Lorentz line-shape function that depends on <u>effective</u> line parameters $\tilde{S}(s)$ and $\tilde{\gamma}(s)$. That is, W(s) is approximated by

$$W(s) = \int_{-\infty}^{\infty} \left\{ 1 - \exp\left[u(s) \frac{\tilde{S}(s)}{\pi} \frac{\tilde{\gamma}(s)}{\nu^2 + \tilde{\gamma}^2(s)} \right] \right\} d\nu \quad .$$

An immediate Ladenburg-Reiche integration can be made to give

$$W(s) = 2\pi\tilde{\gamma} L[\tilde{x}(s)] \quad ,$$

with

$$\tilde{x}(s) = \frac{u(s)\tilde{S}(s)}{2\pi\tilde{\gamma}(s)} \quad .$$

The effective parameters $\tilde{S}(s)$ and $\tilde{\gamma}(s)$ are determined by forcing the approximate solution for $W(s)$ to agree with the exact solutions [equation (10)] for weak and strong absorption. The result is that the effective parameters are best defined as the path-averaged parameters of equations (6) and (7), i.e., $\tilde{S}(s) = S_e(s)$ and $\tilde{\gamma}(s) = \gamma_e(s)$. The CG approximation for an isolated Lorentz line and general nonuniform optical path is, then,

$$W(s) = 2\pi\gamma_e(s)L[x_e(s)] \quad . \tag{12}$$

The functional form is the same as for a uniform path, but the constant parameters S and γ are replaced by the path averages $S_e(s)$ and $\gamma_e(s)$, respectively.

The calculation of line radiance according to equation (1) requires the derivative $dW(s)/ds$. Differentiation of equation (12) yields

$$\frac{dW(s)}{ds} = c(s)p(s)S(s)y[x_e(s), \rho(s)] \quad , \tag{13}$$

where

$$y(x, \rho) = (2 - \rho)\frac{dL(x)}{dx} + (\rho - 1)\frac{L(x)}{x} \quad , \tag{14}$$

with $dL(x)/dx = e^{-x}I_0(x)$. The parameter $\rho(s)$ is the ratio of the local value of line width to the path-averaged line width,

$$\rho(s) = \frac{\gamma(s)}{\gamma_e(s)} \tag{15}$$

and is the index that measures the degree of local path nonuniformity.

The asymptotic limits for the derivative function $y(x, \rho)$ given by equation (14) are readily verified to be $y(x, \rho) \to 1$ as $x \to 0$, and $y(x, \rho) \to \rho/\sqrt{2\pi x}$ as $x \to \infty$. Comparison of equation (13) with the exact solutions of equation (11) reveals that these limits for $y(x, \rho)$ are the correct limits. Although $y(x, \rho)$ approaches the correct limits for weak and strong absorption, spurious behavior may occur for intermediate values of x if the non-uniformity index $\rho(s)$ is large. A large value of $\rho(s)$ would occur, for example, if, along an isothermal path, there were a sudden pressure increase such that $\gamma(s) \gg \gamma_e(s)$. The derivative function is shown in Fig. 2 as a function of x for a few values of ρ. It can be shown that if $\rho \gtrsim 2$, there is a region of x values for which $y(x, \rho) > 1$. From equation (11), it is evident that this effect predicts that $W(s)$ grows at a rate faster than $\sqrt{x}$ does for weak absorption. This behavior is unacceptable and points out a fundamental flaw in the CG approximation.

D. LINDQUIST-SIMMONS APPROXIMATION

The approximation of Lindquist and Simmons[11] corrects the flaw in the CG approximation noted above. This approximation proceeds from the observation that the line radiance given by equation (1) is formulated in terms of the derivative $dW(s)/ds$ rather than $W(s)$ directly. The LS approximation thus considers a direct approximation to $dW(s)/ds$ rather than to $W(s)$. The spatial derivative of $W(s)$ from equation (2) is

$$\frac{dW(s)}{ds} = c(s)p(s)S(s)\frac{2}{\pi}\int_0^\infty \frac{\gamma(s)}{\nu^2 + \gamma^2(s)} \exp\left[-\frac{1}{\pi}\int_0^s \frac{c(s')p(s')S(s')\gamma(s')}{\nu^2 + \gamma^2(s')}\, ds'\right] d\nu \quad .$$

As in the CG approximation, the path-integrated line-shape function (the exponential argument) is replaced by a Lorentz line-shape function expressed in terms of effective line parameters $\tilde{S}(s)$ and $\tilde{\gamma}(s)$. The derivative may then be expressed as

$$\frac{dW(s)}{ds} = c(s)p(s)S(s)y[\tilde{x}(s), \tilde{\rho}(s)] \quad , \qquad (16)$$

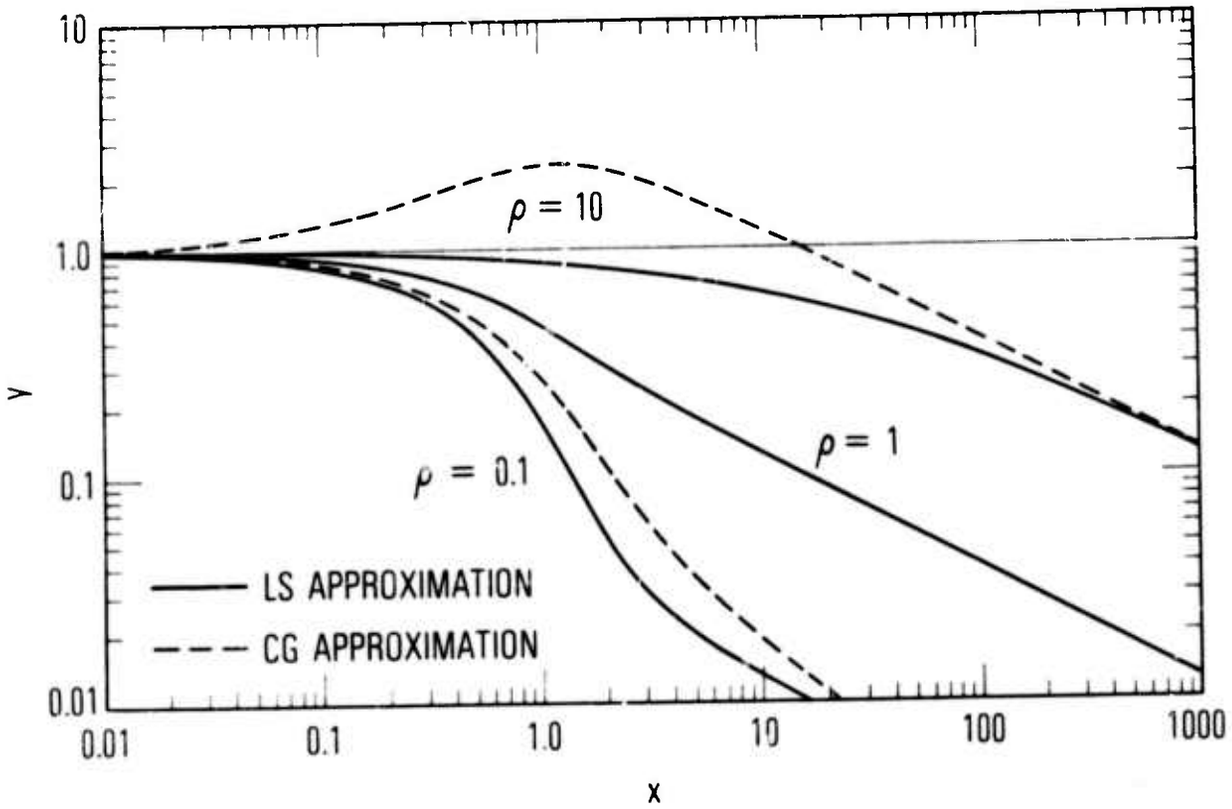

Figure 2. Derivative functions for an isolated Lorentz line.

where

$$\tilde{x}(s) = \frac{u(s)\tilde{S}(s)}{2\pi\tilde{\gamma}(s)} \quad ,$$

$$\tilde{\rho}(s) = \frac{\gamma(s)}{\tilde{\gamma}(s)} \quad ,$$

and

$$y(x,\rho) = \frac{2}{\pi}\int_0^\infty \exp\left\{-\frac{2x}{1+z^2\rho^2}\right\}\frac{dz}{1+z^2} \quad . \tag{17}$$

A simple analysis of equation (17) yields the asymptotic limits of $y(x,\rho)$ as $y(x,\rho) \to 1$ as $x \to 0$, and $y(x,\rho) \to \rho/\sqrt{2\pi x}$ as $x \to \infty$. Thus, the weak absorption limit of $dW(s)/ds$ given by equation (16) reduces to the correct limit given by equation (11) regardless of the choice of $\tilde{S}(s)$ and $\tilde{\gamma}(s)$. Agreement between equations (16) and (11) for strong absorption requires $\tilde{S}(s)\tilde{\gamma}(s) = S_e(s)\gamma_e(s)$, which can be satisfied with the intuitive choices $\tilde{S}(s) = S_e(s)$ and $\tilde{\gamma}(s) = \gamma_e(s)$.* The final result for the LS approximation is

$$\frac{dW(s)}{ds} = c(s)p(s)S(s)y[x_e(s),\rho(s)] \quad . \tag{18}$$

---

*An alternative approach to the CG approximation is to replace $\gamma(s')$ in only the denominator of the exponential argument of equation (2) by an effective width parameter $\tilde{\gamma}(s)$. A Ladenburg-Reiche integration and a forced fit between the approximate and exact solution for $W(s)$ in the weak absorption limit yields $\tilde{\gamma}(s) = \gamma_e(s)$ and, finally, the result of equation (12). If this same approach is used in the LS approximation, the correspondence $\tilde{\gamma}(s) = \gamma_e(s)$ is uniquely determined by the strong absorption fit of the approximate to exact solution for $dW(s)/ds$.

The derivative function of equation (17) is not expressible in terms of elementary functions. A tabulation and approximate solutions for extreme values of the arguments x and ρ have been given by Young.[12] The function is shown in Fig. 2 for comparison with the CG approximation. The function is well-behaved and never exceeds unity. Since the LS approximation treats dW(s)/ds, no solution for W(s) is given other than the formal solution

$$W(s) = \int_0^s \frac{dW(s')}{ds'}\, ds' \quad ,$$

which can, in application, be evaluated numerically.

III. STATISTICAL BAND MODEL

A. GENERAL RELATIONS

In this section, the radiative transfer effects are reviewed for an array (band) of many lines,* all with centers confined to a spectral interval $\Delta\nu$. The average radiance in $\Delta\nu$ due to these lines and for a general nonuniform optical path is

$$\overline{N} = -\int_0^S N^*(s) \frac{d\overline{\tau}(s)}{ds}\, ds \quad . \tag{19}$$

This form of the band radiance equation requires $\Delta\nu$ to be small enough that the Planck function $N^*(s)$ can be considered as sensibly constant across $\Delta\nu$. $\overline{\tau}(s)$ is the average spectral transmittance for $\Delta\nu$ and the path segment between $s = 0$ and general position s. The exact expression for $\overline{\tau}(s)$ is

$$\overline{\tau}(s) = \frac{1}{\Delta\nu}\int_{\Delta\nu} \tau(\nu, s)\, d\nu \quad , \tag{20}$$

where $\tau(\nu, s)$ is the spectral transmittance within $\Delta\nu$. If the number of lines N in $\Delta\nu$ is large, $\tau(\nu, s)$ is, in general, a rapidly fluctuating function of ν, and the evaluation of $\overline{\tau}(s)$ by equation (20) is quite tedious. In addition evaluation of $\overline{\tau}(s)$ by this method requires detailed knowledge of the spectral position, strength, and width of each of the N lines in $\Delta\nu$. In order to expedite the evaluation of $\overline{\tau}(s)$, band model techniques are used. The objective of

*All of these lines are assumed to arise from a single molecular gas species. Treatment of more than one species is trivially handled by invoking the multiplicative property of band transmittance for nonidentical species.

band model methods is to approximate $\bar{\tau}(s)$ by an expression that depends on only a few parameters. These band model parameters reflect average properties of the lines in $\Delta\nu$.

The statistical band model approximation of $\bar{\tau}(s)$ is developed from two fundamental assumptions. One is that the placement of lines in $\Delta\nu$ can be modeled by a random arrangement of equal width lines. The result of this assumption is that[1]*

$$\bar{\tau}(s) = \exp\left[-\frac{\overline{W}(s)}{\delta}\right] \quad , \tag{21}$$

where $\overline{W}(s)$ is the average value of $W(s)$ for the lines in $\Delta\nu$,

$$\overline{W}(s) = \frac{1}{N}\sum_{i=1}^{N} W(i, s) \quad , \tag{22}$$

and δ is a mean line spacing parameter $\delta = \Delta\nu/N$. This step in the formulation eases the difficulty in evaluating $\bar{\tau}(s)$ to the extent that the individual positions and widths of the lines in $\Delta\nu$ are no longer required. The strengths are still required for computation of $W(i, s)$.

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*This expression for $\bar{\tau}(s)$ is the limiting form for $N \to \infty$ and $\Delta\nu \to \infty$. The latter ensures that the absorption caused by each line in $\Delta\nu$ is confined to $\Delta\nu$. An additional note of importance is that $\bar{\tau}(s)$ derived in the statistical model is <u>not</u> a mean spectral transmittance in the sense of equation (20), but rather a spectral transmittance (for some position ν in $\Delta\nu$, generally the center of $\Delta\nu$) that has been averaged over all possible line arrangements. It can be established, however, for the condition $\Delta\nu \to \infty$ that equation (21) results for any choice of reference position ν in $\Delta\nu$. Thus, equation (21) is also an adequate representation for the average spectral transmittance.

The other modeling assumption is that the strengths of the lines in $\Delta\nu$ can be described by a continuous distribution function P(S). Then, rather than writing the average value of W(s) as a summation, as in equation (22), the integral expression

$$\overline{W}(s) = \int_0^\infty P(S)W(S, s)\, dS \tag{23}$$

is used. The use of this definition requires the selection of a plausible distribution function P(S) and the expression of W(s) for an isolated line in terms of a line strength parameter S. For an isothermal path (where S is a constant), this latter requirement is trivial. For a nonisothermal optical path, the expression of W(s) [and its derivative dW(s)/ds] in terms of an acceptable strength parameter is the basic problem considered in Sections IV through VI. For the remainder of this section, a uniform optical path is assumed.

B. INVERSE LINE STRENGTH DISTRIBUTION

P(S)dS is the probability that an arbitrarily selected line in $\Delta\nu$ will have strength S in the interval dS about S. Several distribution functions have been considered. Use of the dirac distribution $P(S) = \delta(S - \overline{S})$ is equivalent to the assumption that all lines in $\Delta\nu$ have a strength equal to the average line strength $\overline{S}$. The use of an exponential distribution $P(S) = \overline{S}^{-1} \exp(-S/\overline{S})$ yields the Mayer-Goody form of the statistical model.[35, 36] The distribution functions used here are the truncated inverse line strength distribution introduced by Godson[5, 37] and the exponential-tailed inverse distribution introduced by Malkmus.[38] The use of these two distributions yields nearly identical results for many applications. In the present work, the distributions are used interchangeably in the following manner: The formulation of models is made with the inverse distribution; the functions required to apply the models are derived with the exponential-tailed inverse distribution.

The form of the inverse distribution used here is

$$P(S) = \begin{cases} 0 & 0 \le S < S_M/R \\ \dfrac{1}{S \ln R} & S_M/R \le S \le S_M \\ 0 & S > S_M \end{cases} , \qquad (24)$$

where S_M and S_M/R are, respectively, the maximum and minimum line strengths allowed in the distribution and are introduced so that P(S) can be normalized. S_M and R are two independent parameters of the distribution. R is generally assumed to be large. The mean line strength for the distribution is

$$\overline{S} = \frac{R - 1}{R \ln R} S_M ,$$

with $\overline{S} \to S_M/\ln R$ for large R.

For application to nonisothermal paths, it is necessary to know in more explicit form how temperature enters into the distribution. In order to accomplish this, a functional relationship between line strength and temperature must be assumed. The form assumed here is

$$S(i, T) = S_M(i, T)\, e^{-\theta(i)/T} , \qquad (25)$$

where i is a line index, and $\theta(i)$ is the energy (expressed in temperature units) of the lower level of the quantum transition causing the line. This form for S(i, T) follows directly from the assumption that the strength in absorption is the product of the number of molecules in the lower level and an intrinsic oscillator strength $\sigma(i)$. A dominant factor that influences the magnitude of $\sigma(i)$ is the energy change in the transition causing the line.

lines confined to a small spectral interval $\Delta\nu$, this energy change is nearly constant. To a first approximation, then, $\sigma(i)$ can be considered independent of i. The preexponential factor $S_M(i, s)$ then, is also independent of i. This simplification is used and yields the final assumed form for the temperature variation as

$$S(i, T) = S_M(T)\, e^{-\theta(i)/T} \tag{26}$$

This form defines a unique relation (for fixed T) between the strength of a line and the energy of the lower level of the transition causing the line. A distribution of line strengths thus implies a distribution of energy levels. The use of the inverse strength distribution of equation (24), the relationship between S and θ given by equation (26), and the transformation relation $P(S)d(S) = P(\theta)d(\theta)$ gives the energy level distribution as

$$P(\theta) = \begin{cases} 0 & \theta < 0 \\ \dfrac{1}{T \ln R} & 0 < \theta \leq T \ln R \\ 0 & \theta > T \ln R \end{cases} .$$

Because the strongest lines in $\Delta\nu$ occur for absorption from (or emission to) the ground-level $\theta = 0$, $S_M(T)$ in equation (26) can be identified as the distribution parameters S_M in equation (24). The distribution $P(\theta)$ is constant in the variable θ up to a maximum value $\theta_m = T \ln R$. Since the distribution of energy levels within a molecule is an intrinsic property of the molecule, we must insist that θ_m be independent of temperature. This consideration thus yields an explicit form for the temperature dependence of the distribution parameter R as

$$R(T) = e^{\theta_m/T} .$$

The assumption that R is large implies that θ_m is large. The final form of the inverse line strength distribution used here is* (with R and $\theta_m \to \infty$)

$$P(S, T) = \begin{cases} \dfrac{T}{\theta_m S} & 0 \leq S \leq S_M(T) \\ 0 & S > S_M(T) \end{cases} , \qquad (27)$$

where the explicit dependence on temperature is included, and where $S_M(T)$ and θ_m are considered as the two independent parameters of the distribution.

C. STATISTICAL MODEL FOR A UNIFORM PATH

For an isolated Lorentz line and a uniform optical path, W is given as a function of S through the Ladenburg-Reiche solution [equation (3)] $W = 2\pi\gamma L(x)$, $x = Su/2\pi\gamma$. From equations (23) and (27), the mean equivalent width function is approximated as (with the transformation $\eta = Su/2\pi\gamma$)

$$\frac{\overline{W}}{\delta} = 2\pi\gamma \frac{T}{\delta\theta_m} \int_0^{x_M} \frac{L(\eta)}{\eta}\, d\eta \quad ,$$

where

$$x_M = \frac{S_M u}{2\pi\gamma} \quad .$$

*When the distribution is written in this form, it can be readily verified that if the inverse distribution is assumed to hold for any temperature, then it holds for all temperatures.

The integral over η is easily evaluated by using equation (4) for $L(\eta)$ and standard tables of integrals for Bessel functions. The result for the integral is

$$I(x) = \int_0^x \frac{L(\eta)}{\eta}\, d\eta = 2xe^{-x}[I_o(x) + I_1(x)] + e^{-x}I_0(x) - 1 \quad . \tag{28}$$

Thus, the solution for $\overline{W}/\delta$ is

$$\frac{\overline{W}}{\delta} = 2\pi\gamma \frac{T}{\delta\theta_m} I(x_M) \quad .$$

Introduction of the parameters

$$\overline{k} = \frac{S_M T}{\delta\theta_m} = \frac{\overline{S}}{\delta} \quad , \tag{29}$$

$$\frac{1}{\overline{\delta}} = \frac{4T}{\delta\theta_m} \quad , \tag{30}$$

$$\beta = \frac{2\pi\gamma}{\overline{\delta}} \quad , \tag{31}$$

and

$$x = \frac{\overline{k}u}{\beta} \tag{32}$$

permits the result to be simplified to

$$\frac{\overline{W}}{\delta} = \frac{\beta}{4} I(4x) \quad . \tag{33}$$

Equations (28) and (33) constitute the result first obtained by Godson.[5, 37] The curve-of-growth function I(4x)/4 is shown in Fig. 1. The weak and strong absorption limits are the same as for the Ladenburg-Reiche function, but the range of x over which the transition occurs is broader. This phenomenon occurs because the strong absorption limit for a band of lines is not obtained until a sizable fraction of the weakest lines allowed by the line strength distribution display strong absorption behavior. The weak and strong absorption limits of $\overline{W}/\delta$ are

$$\frac{\overline{W}}{\delta} = \begin{cases} u\bar{k} & \text{weak} \\ \sqrt{\dfrac{u\bar{k}\beta}{2\pi}} & \text{strong} \end{cases} .$$

D. BAND MODEL PARAMETERS

Equations (29) through (31) relate the two parameters $\bar{k}$ and β to the line arrangement parameter δ and the strength distribution parameters S_M and θ_m. These latter three parameters have meaning only within the confines of the modeling assumptions that lead to the results of equation (33). The practical interpretation of band modeling procedures is that the results [equations (28) and (33) in this case] constitute a functional form for the variation of $\overline{\tau}(s)$ [by equation (21)] with optical depth u that depends on two band model parameters $\bar{k}$ and β that are to be determined empirically by fitting the functional form to experimental data.

Two general procedures are used to determine $\bar{k}$ and β. In one, experimental absorption measurements are made on a uniform gas sample at fixed temperature T with a spectrometer centered at the spectral position ν of interest and adjusted to a spectral resolution $\Delta\nu$. The optical thickness u of the sample is varied over a wide range such that both weak and strong absorption data are obtained. By fitting the weak absorption portion of the experimental curve $\overline{\tau}(u)$ to the model, $\bar{k}$ can be determined. By fitting the strong absorption data, the product $\bar{k}\beta$, and hence β, can be obtained. In

this manner, the parameters $\bar{k}$ and β can be obtained for all spectral intervals $\Delta\nu$ across an entire molecular absorption band and for a wide range of temperatures.

The other approach to the determination of $\bar{k}$ and β can be used if the line optical parameters S(i) and γ(i) are known for all of the lines in each interval $\Delta\nu$. The temperature dependence of S(i) and γ(i) must also be known. From equations (22) and (3), $\overline{W}/\delta$ for a uniform optical path may be written in terms of the line parameters S(i) and γ(i) as

$$\frac{\overline{W}}{\delta} = \frac{1}{\Delta\nu} \sum_{i=1}^{N} 2\pi\gamma(i) L\left[\frac{S(i)u}{2\pi\gamma(i)}\right] \quad . \tag{34}$$

Equation (33) represents this same quantity expressed in terms of the band model parameters $\bar{k}$ and β. By forcing equations (33) and (34) to be identical for weak and strong absorption,* the following definitions can be obtained:

$$\bar{k} = \frac{1}{\Delta\nu} \sum_{i=1}^{N} S(i) \quad , \tag{35}$$

$$\beta = \frac{2\pi}{\bar{k}}\left[\frac{1}{\Delta\nu} \sum_{i=1}^{N} \sqrt{S(i)\gamma(i)}\right]^2 \quad . \tag{36}$$

*In both this and the experimental absorption approach, $\bar{k}$ and β are determined by fitting the model in the limits $\bar{\tau} = 0$ and $\bar{\tau} = \infty$. Godson[5, 39] has indicated that, for some applications, fits at other transmittance values may be desirable. In his work on the atmospheric transmittance of H_2O, for example, he used fits at $\bar{\tau} = 0.45$ and 0.95 to obtain a best overall agreement between model and data.

Note that, by including $\gamma(i)$ in the definition for β as a parameter that depends on the line index i, the model approximation that all γ are constant has been lessened.

Although only the two parameters $\bar{k}$ and β are required for application of the isothermal band model, it is convenient (and necessary for some extensions of the band model formulation to nonisothermal paths) to consider β as a ratio of two parameters $\bar{\gamma}$ and $\bar{\delta}$ by a generalization of equation (31),

$$\beta = \frac{2\pi\bar{\gamma}}{\bar{\delta}} \quad , \tag{37}$$

where $\bar{\gamma}$ is a measure of the average line width for the lines in $\Delta\nu$, and $\bar{\delta}$ is a measure of the mean line spacing in $\Delta\nu$. The use of three parameters ($\bar{k}$, $\bar{\delta}$, and $\bar{\gamma}$) in a two-parameter model required auxiliary information on one of the parameters. This information is generally introduced by performing independent experimental measurements of $\bar{\gamma}$ or by making theoretical and empirical assumptions on $\bar{\gamma}$. When band model parameters are determined from individual line data [equations (35) and (36)], $\bar{\gamma}$ is conveniently defined by

$$\bar{\gamma} = \frac{1}{N} \sum_{i=1}^{N} \gamma(i) \quad .$$

An advantage of introducing the two parameters $\bar{\gamma}$ and $\bar{\delta}$ in place of β is that the variations of β with the composition of the gas, i.e., the ratio of active gas concentration to various foreign gas concentrations, can all be placed in $\bar{\gamma}$, which leaves $\bar{\delta}$ as a function of temperature (and spectral position) only. When the fundamental band model parameters $\bar{k}$, $\bar{\delta}$, and $\bar{\gamma}$ have been determined as a function of spectral position and temperature, it is possible to

define the modeling parameters S_M and the product $\delta\theta_m$. From equations (29) and (30), the following expressions can be obtained:

$$S_M(T) = 4\bar{k}(T)\bar{\delta}(T) \quad , \tag{38}$$

$$\delta\theta_m = 4T\bar{\delta}(T) \quad . \tag{39}$$

These two relations are particularly important in the formulation of non-isothermal band models in Sections IV and V. An interesting side aspect of equation (39) is that the line density parameter $D \equiv 1/\bar{\delta}$ is predicted to display a linear temperature dependence. This result offers an opportunity to experimentally determine the adequacy of the entire modeling procedure by examining the constancy of the product $T\bar{\delta}$ with temperature.

E. EXPONENTIAL-TAILED INVERSE LINE STRENGTH DISTRIBUTION

Same comments on the use of the exponential-tailed inverse line strength distribution rather than the inverse distribution are appropriate here. This distribution function is[38]

$$P(S) = \frac{1}{S \ln R}\left[e^{-S/S_M} - e^{-RS/S_M}\right] \quad ,$$

where S is allowed to assume all values $0 \le S \le \infty$. S_M is no longer interpreted as a maximum allowed line strength, but simply as a parameter of the distribution. The distribution results by use of the more general result of equation (25) over (26) for line strength and the assumption that $S_M(i, T)$ is distributed about $S_M(T)$ according to an exponential strength distribution. In a sense, it is more general than the purely inverse line strength distribution.

For a uniform optical path, the formulation of a band model with the exponential-tailed distribution parallels the formulation with the inverse distribution, except that the curve-of-growth function $I(4x)/4$ is replaced by $I_e(\pi x)/\pi$, where $I_e(x) = (1 + 2x)^{1/2} - 1$, and the factor 4 in equations (30), (33), (38), and (39) is replaced by π.

IV. CURTIS-GODSON APPROXIMATIONS

In this and Section V, the fundamentals reviewed in Sections II and III are used to formulate band models for general inhomogeneous, nonisothermal optical paths. Here, two approaches to the familiar CG approximation for bands of lines are considered: that originally given by Godson[5], and one that is based on the same assumptions used in Godson's approach, but that expands on the nature of the assumptions. The second approach also yeilds expressions that are essential to the formulations in Section V.

A. GODSON'S FORMULATION

In Godson's approach, we assume that the functional form of the curve of growth for a nonuniform path is the same as that for a uniform path. The expression for the mean equivalent width is written, from equation (33), as

$$\frac{\overline{W}(s)}{\delta} = \frac{\beta_e(s)}{4} I[4x_e(s)] \quad , \qquad (40)$$

$$x_e(s) = \frac{u(s)\overline{k}_e(s)}{\beta_e(s)} \quad ,$$

where $\overline{k}_e(s)$ and $\beta_e(s)$ are effective band model parameters to be determined, and the optical depth u(s) is given by equation (8). The effective parameters $\overline{k}_e(s)$ and $\beta_e(s)$ are determined by a procedure similar to that used to determine $\overline{k}$ and β in terms of line parameters for a uniform path. That is, the weak and strong absorption limits of equation (40) are forced to agree (as well as possible) with the weak and strong results obtained from $\overline{W}(s)/\delta$ given by equation (22) and the exact limiting solutions to W(i, s) given by equation (10). The resulting definitions for $\overline{k}_e(s)$ and $\beta_e(s)$ parallel the definitions of

equation (35) for $\bar{k}$ and equation (36) for β, except that they are written in terms of the path-averaged parameters $S_e(i, s)$ and $\gamma_e(i, s)$.* They are

$$\bar{k}_e(s) = \frac{1}{\Delta\nu} \sum_{i=1}^{N} S_e(i, s) \quad , \tag{41}$$

and

$$\beta_e(s) = \frac{2\pi}{\bar{k}_e(s)} \left[\frac{1}{\Delta\nu} \sum_{i=1}^{N} \sqrt{S_e(i, s)\gamma_e(i, s)} \right]^2 \quad . \tag{42}$$

These definitions are not particularly useful because they not only require a detailed knowledge of individual line parameters, but also require that the path averages of the strength and width of each line be recomputed for each nonuniform path considered. These relations can be used, however, to formulate definitions that are practical. The procedure is most easily shown for $\bar{k}_e(s)$. By interchanging the order of line summation and path integration implicit in the above definition for $\bar{k}_e(s)$, we obtain

$$\bar{k}_e(s) = \frac{1}{u(s)} \int_0^s c(s')p(s') \left[\frac{1}{\Delta\nu} \sum_{i=1}^{N} S(i, s') \right] ds' \quad .$$

From equation (35), the quantity in brackets can be identified as the parameter $\bar{k}$ that corresponds to an isothermal path at temperature $T(s')$. Consequently,

$$\bar{k}_e(s) = \frac{1}{u(s)} \int_0^s c(s')p(s')\bar{k}(s')\, ds' \quad , \tag{43}$$

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*$S_e(i, s)$ and $\gamma_e(i, s)$ are defined by trivial generalizations of equations (6) and (7), respectively, that include the line index i as an explicit argument to S and γ.

where $\bar{k}(s')$ denotes $\bar{k}[T(s')]$. The effective absorption band model parameter $\bar{k}_e(s)$ is thus the average value of $\bar{k}$ over the nonisothermal path. If $\bar{k}$ is known for all temperatures in the range that occurs along the path, $\bar{k}_e(s)$ can be computed for all path positions s.

In order to obtain a corresponding result for $\beta_e(s)$, an additional assumption must be made in order to permit the interchange of the order of integration and summation in equation (42). With the definitions of equations (6) and (7), $\beta_e(s)$ may be written as

$$\beta_e(s) = \frac{2\pi}{\bar{k}_e(s)}\left[\frac{1}{\Delta\nu}\sum_{i=1}^{N}\sqrt{\frac{1}{u(s)}\int_0^s c(s')p(s')S(i,s')\gamma(i,s')\,ds'}\right]^2 \quad .$$

The additional assumption made by Godson is that $S(i, s')$ and $\gamma(i, s')$ may be written in the functional product forms

$$S(i, s') = \sigma_1(i)\sigma_2(s') \quad , \tag{44}$$

and

$$\gamma(i, s') = g_1(i)g_2(s') \quad . \tag{45}$$

The use of these relations and an interchange of the order of summation and integration yields

$$\beta_e(s) = \frac{2\pi}{u(s)\bar{k}_e(s)}\int_0^s c(s')p(s')\left\{\frac{1}{\Delta\nu}\sum_{i=1}^{N}\sqrt{\sigma_1(i)\sigma_2(s')g_1(i)g_2(s')}\right\}^2 ds' \quad .$$

The quantity under the square root sign is identified, from equations (44) and (45), to be $S(i, s')\gamma(i, s')$. The entire squared quantity under the path integral can then be identified, from equation (36), to be $\beta(s')\bar{k}(s')/2\pi$. Thus, $\beta_e(s)$

can be written as a path average of the band model parameter β weighted by the absorption parameter $\bar{k}$*

$$\beta_e(s) = \frac{1}{u(s)\bar{k}_e(s)} \int_0^s c(s')p(s')\bar{k}(s')\beta(s')\,ds' \quad . \tag{46}$$

Equations (40), (43), and (46) constitute the traditional formulation of the CG approximation for a statistical band model.

B. ALTERNATIVE FORMULATION

We now consider an alternative approach to the CG approximation for a random array of lines that more nearly parallels the formulation of the band model for a uniform optical path. The starting point is the use of the CG approximation for an isolated line [equations (12) and (9)]

$$W(s) = 2\pi\gamma_e(s)L\left[\frac{u(s)S_e(s)}{2\pi\gamma_e(s)}\right] \quad . \tag{47}$$

As in the formulation for a uniform path, we average this expression over a line strength distribution function P(S). Since the path is assumed to be nonisothermal, no explicit line strength appears in equation (47); only the path-averaged line strength $S_e(s)$ appears. It becomes necessary, then, to consider a strength distribution function for S_e. An approximate distribution $P(S_e)$ can be established by invoking the separability approximation

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*By use of the Schwartz inequality for integrals, it can be established that if the separability approximations of equations (44) and (45) are not invoked, then the optimum choice for $\beta_e(s)$ is some value less than or equal to the path average given by equation (46).

[equation (44)] on line strength. The path average for the strength of the i^{th} line in $\Delta\nu$ is [equation (6)]

$$S_e(i, s) = \frac{1}{u(s)} \int_0^s c(s')p(s')S(i, s')\, ds' \quad .$$

The use of equation (26) for $S(i, s')$ yields

$$S_e(i, s) = \frac{1}{u(s)} \int_0^s c(s')p(s')S_M(s')\, e^{-\theta(i)/T(s')}\, ds' \quad . \tag{48}$$

The separability approximation is now introduced by assuming that $T(s')$ in the exponential argument of equation (48) can be replaced by a quantity $T_e(s)$ that is independent of s'. This replacement corresponds to the use of

$$\sigma_1(i) = e^{-\theta(i)/T_e(s)}$$

and

$$\sigma_2(s') = S_M(s')$$

in equation (44). Then,

$$S_e(i, s) = S_{eM}(s)\, e^{-\theta(i)/T_e(s)} \quad , \tag{49}$$

where

$$S_{eM}(s) = \frac{1}{u(s)} \int_0^s c(s')p(s')S_M(s')\, ds' \quad . \tag{50}$$

Regardless of the choice of $T_e(s)$, it is clear from equations (26) and (49) that $S_e(i, s)$ displays the same functional dependence with $T_e(s)$ that $S(i, s)$ does with T. Consequently, because the energy level distribution function $P(\vartheta)$ is independent of temperature, it is readily established that, within the separability approximation, S_e is distributed according to the inverse distribution

$$P(S_e) = \begin{cases} \dfrac{T_e(s)}{S_e \theta_m} & 0 \le S_e \le S_{eM}(s) \\ 0 & S_e > S_{eM}(s) \end{cases} .$$

The application of this distribution to $W(s)$ given by equation (47) completely parallels the formulation for a uniform path given in Section III and yields the result

$$\frac{W(s)}{\delta} = \frac{\tilde{\beta}(s)}{4} I[4\tilde{x}(s)] \quad , \tag{51}$$

$$\tilde{x}(s) = \frac{u(s)\tilde{k}(s)}{\tilde{\beta}(s)} \quad ,$$

where

$$\tilde{k}(s) = S_{eM}(s) \frac{T_e(s)}{\delta\theta_m} \quad , \tag{52}$$

$$\tilde{\beta}(s) = 2\pi\bar{\gamma}_e(s) \frac{4T_e(s)}{\delta\theta_m} \quad . \tag{53}$$

The parameter $\bar{\gamma}_e(s)$ in equation (53) for $\tilde{\beta}(s)$ is given by

$$\bar{\gamma}_e(s) = \frac{1}{u(s)S_{eM}(s)} \int_0^s c(s')p(s')S_M(s')\bar{\gamma}(s')\,ds' \tag{54}$$

and is obtained from equations (6), (7), and (26) by again replacing $T(s')$ with $T_e(s)$ and assuming $\gamma(i, s')$ to be independent of i and equal to the band model parameter $\bar{\gamma}(s')$.

Since equations (40) and (51) are identical in form, it is clear that the assumption of equation (40) as the curve-of-growth function in Godson's formulation is equivalent to the use of the separability approximation for line strength and the use of the CG approximation for an isolated line.

The significant departure of this alternative formulation of the CG approximation from Godson's formulation is the manner in which the effective parameters $\tilde{k}(s)$ and $\tilde{\beta}(s)$ are determined. In Godson's formulation, the effective parameters were introduced *a priori* as unknowns to be determined. The present formulation has established a direct link between the effective band model parameters $\tilde{k}$ and $\tilde{\beta}$ and the band model parameters for isothermal paths. More explicitly, equations (52), (53), and (54) together with equation (50) for $S_{eM}(s)$ give $\tilde{k}(s)$ and $\tilde{\beta}(s)$ in terms of the modeling parameters $S_M(s)$ and $\delta\theta_m$. These later parameters are, in turn, given in terms of the isothermal parameters $\bar{k}(s)$ and $\bar{\delta}(s)$ by equations (38) and (39). Carrying through the formulation with these relationships, we find that $\tilde{k}(s)$, $\tilde{\beta}(s)$, and $\bar{\gamma}_e(s)$ can be expressed as

$$\tilde{k}(s) = \bar{k}_e(s)\left[\frac{T_e(s)}{T(s)}\,\frac{\bar{\delta}_e(s)}{\bar{\delta}(s)}\right]$$

$$\tilde{\beta}(s) = \frac{2\pi\bar{\gamma}_e(s)}{\bar{\delta}_e(s)}\left[\frac{T_e(s)}{T(s)}\,\frac{\bar{\delta}_e(s)}{\bar{\delta}(s)}\right]$$

$$\bar{\gamma}_e(s) = \frac{1}{u(s)\bar{k}_e(s)\bar{\delta}_e(s)} \int_0^s c(s')p(s')\bar{k}(s')\bar{\delta}(s')\bar{\gamma}(s')\,ds' \quad , \tag{55}$$

where $\bar{\delta}_e(s)$ is a path average of the line spacing band model parameter given by

$$\bar{\delta}_e(s) = \frac{1}{u(s)\bar{k}_e(s)} \int_0^s c(s')p(s')\bar{k}(s')\bar{\delta}(s')\,ds' \quad , \tag{56}$$

and $\bar{k}_e(s)$ is given by equation (43).

The weak limit form for $\overline{W}(s)/\delta$ with this result for $\tilde{k}(s)$ is

$$\frac{\overline{W}(s)}{\delta} = u(s)\tilde{k}(s) = u(s)\bar{k}_e(s)\left[\frac{T_e(s)}{T(s)}\,\frac{\bar{\delta}_e(s)}{\bar{\delta}(s)}\right] \quad .$$

Inasmuch as it has been established (in Godson's formulation) that the correct weak limit form for $\overline{W}(s)/\delta$ is $u(s)\bar{k}_e(s)$, however, the quantity in brackets must be unity. Thus, a definition for $T_e(s)$ is established as

$$T_e(s) = T(s)\,\frac{\bar{\delta}(s)}{\bar{\delta}_e(s)} \quad . \tag{57}$$

Although $T_e(s)$ does not enter into the final result of this approach to the CG approximation, the definition of $T_e(s)$ by equation (57) plays an important role in the band model formulations presented in Section V.

The final result for this alternative formulation of the CG approximation is the same as Godson's formulation, except that $\beta_e(s)$ is not defined as a path average of $\beta(s)$ according to equation (46), but rather by

$$\beta_e(s) = \frac{2\pi\bar{\gamma}_e(s)}{\bar{\delta}_e(s)} \quad , \tag{58}$$

where $\bar{\gamma}_e(s)$ is a path-averaged line width given by equation (55), and $\bar{\delta}_e(s)$ is a path-averaged line spacing parameter given by equation (56).

C. DERIVATIVE FUNCTIONS

The computation of band radiance by use of equation (19) requires the transmittance derivative $d\bar{\tau}(s)/ds$. Differentiation of equation (21) yields

$$\frac{d\bar{\tau}(s)}{ds} = -\bar{\tau}(s)\,\frac{1}{\delta}\,\frac{d\overline{W}(s)}{ds} \quad . \tag{59}$$

The equivalent width derivative obtained by differentiating Godson's result for the CG approximation is

$$\frac{1}{\delta}\,\frac{d\overline{W}(s)}{ds} = c(s)p(s)\bar{k}(s)y[4x_e(s), r(s)] \quad , \tag{60}$$

where the derivative function $y(x, r)$ is

$$y(x, r) = (2 - r)\,\frac{dI(x)}{dx} + (r - 1)\,\frac{I(x)}{x} \tag{61}$$

with

$$\frac{dI(x)}{dx} = \frac{L(x)}{x} \quad . \tag{62}$$

The nonuniformity index $r(s)$ is

$$r(s) = \frac{\beta(s)}{\beta_e(s)} \quad , \tag{63}$$

where $\beta_e(s)$ is given by equation (46). This result is similar in form to that obtained for an isolated line [equations (13) and (14)]. In particular, this result can display the same spurious behavior of $y > 1$ for intermediate x if the nonuniformity index $r(s)$ is very large.

By differentiating the result for $\overline{W}(s)/\delta$ obtained in the alternative formulation for the CG approximation, we obtain

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\overline{k}(s)y[4x_e(s), \rho(s), q(s)] \quad , \tag{64}$$

where

$$y(x, \rho, q) = \left(\frac{2-\rho}{q}\right)\frac{dI(x)}{dx} + \left(1 - \frac{2-\rho}{q}\right)\frac{I(x)}{x} \quad . \tag{65}$$

Here, the arguments $\rho(s)$ and $q(s)$ are

$$\rho(s) = \frac{\overline{\gamma}(s)}{\overline{\gamma}_e(s)} \tag{66}$$

and

$$q(s) = \frac{\overline{\delta}_e(s)}{\overline{\delta}(s)} \quad . \tag{67}$$

In the alternative formulation, the index $\rho(s)$ measures primarily the local degree of inhomogeneity at path position s, and $q(s)$ measures primarily the local degree of nonisothermality. The parameter $r(s)$ in Godson's formulation measures the combined effects of inhomogeneity and nonisothermality. For an isothermal path, $q = 1$, $r = \rho$, and equations (61) and (65) become identical. Thus, the two approaches treat inhomogeneities along the path in the same manner. The significant difference between the two approaches is the manner in which nonisothermalities are treated. Consider a homogeneous

path for strong absorption. Then, $\rho \simeq 1$ and $r = q$. For large x, equations (61) and (65) yield, respectively,

$$y(4x, q) \rightarrow \frac{q}{(2\pi x)^{1/2}} \quad ,$$

and

$$y(4x, 1, q) \rightarrow \frac{2q - 1}{q} \frac{1}{(2\pi x)^{1/2}} \quad .$$

Godson's approach yields a linear increase of y with q for strong absorption. The alternative approach displays a much weaker increase with q through the function $(2q - 1)/q$.

The results for either formulation of the CG approximation with the exponential-tailed distribution are identical to all of the results in this section, except that all occurrences of I(x) are replaced by $I_e(x)$, and the factor 4 that appears with $x_e(s)$ is replaced by π. In addition, $dI_e(x)/dx = 1/(1 + 2x)^{1/2}$ replaces equation (62).

V. DERIVATIVE APPROXIMATIONS

A. INTRODUCTION

The approach to the band models formulated in this section is fundamentally similar to the approach of the LS approximation for an isolated line. The radiance equation [equation (19)] for band radiation is formulated in terms of the transmittance derivative $d\bar{\tau}(s)/ds$ rather than in terms of the transmittance $\bar{\tau}(s)$ directly. The CG approximations presented in Section IV are essentially approximations to $\bar{\tau}(s)$ in that they deal directly with the quantity $\overline{W}(s)/\delta \equiv -\ln \bar{\tau}(s)$. Expressions for $d\bar{\tau}(s)/ds$ are obtained by differentiating the approximations. In this section, direct approximations to $d\bar{\tau}(s)/ds$ are treated. More accurately, because [equation (59)]

$$\frac{d\bar{\tau}(s)}{ds} = -\bar{\tau}(s)\,\frac{1}{\delta}\,\frac{d\overline{W}(s)}{ds} \quad ,$$

approximations to the mean equivalent width derivative are considered. The approach is similar to the alternative formulation of the CG approximation in that we start with an approximate solution for an isolated line, average over a line strength distribution, and express the distribution parameters S_M and δ_m in terms of band model parameters for isothermal paths by the direct relations of equations (38) and (39). The results are thus expressed in terms of the nonuniformity parameters $\rho(s)$ and $q(s)$. However, intuitive models based on the parameter $r(s)$ are also considered.

B. DERIVATIVE APPROXIMATION

Where the alternative formulation of the CG approximation was based on the CG approximation to $W(s)$ for an isolated line, we begin here with the LS approximation to $dW(s)/ds$ [equations (9), (15), (17), and (18)]

$$\frac{dW(s)}{ds} = c(s)p(s)S(s)\,\frac{2}{\pi}\int_0^\infty \exp\left\{-\frac{2u(s)S_e(s)}{2\pi\gamma_e(s)}\,\frac{1}{1+z^2\rho^2(s)}\right\}\frac{dz}{1+z^2} \quad . \qquad (68)$$

In the CG formulation, the only line strength parameter in the equations was the path-averaged strength S_e. An average over line strength was performed by deriving an approximate distribution for S_e. In the present case, both the path-averaged and local line strength S(s) appear in the formulation. In order to perform an average over line strength, it is necessary to express S_e as a function of S, or vice versa. This is accomplished by introducing the line strength separability approximation, but only for S(s') as it appears in the path integral for $S_e(s)$. That is, equation (49) is used to express $S_e(i, s)$ as

$$S_e(i, s) = S_{eM}(s)\, e^{-\theta(i)/T_e(s)} \quad . \tag{69}$$

The local line strength parameter S(i, s) is not separated and is retained as given by equation (26),

$$S(i, s) = S_M(s)\, e^{-\theta(i)/T(s)} \quad . \tag{70}$$

Elimination of $\theta(i)$ between equations (69) and (70) gives the desired approximate relationship between $\bar{S}$ and S_e

$$S_e(s) = S_{eM}(s)\left[\frac{S(s)}{S_M(s)}\right]^{T(s)/T_e(s)} \quad .$$

From equations (57) and (67), the temperature ratio can be expressed as

$$\frac{T(s)}{T_e(s)} = \frac{\bar{\delta}_e(s)}{\bar{\delta}(s)} = q(s) \quad .$$

With the definition

$$\eta = \frac{S(s)}{S_M(s)} \quad , \tag{71}$$

$S_e(s)$ can be written

$$S_e(s) = S_{eM}(s)\eta^{q(s)} \quad . \tag{72}$$

Then, with equations (71) and (72), equation (68) becomes

$$\frac{dW(s)}{ds} = c(s)p(s)S_M(s)\eta \frac{2}{\pi}\int_0^\infty \exp\left\{-\frac{2x_M(s)\eta^{q(s)}}{1 + z^2\rho^2(s)}\right\}\frac{dz}{1 + z^2} \quad ,$$

where

$$x_M(s) = \frac{u(s)S_{eM}(s)}{2\pi\gamma_e(s)} \quad .$$

This expression can now be averaged over the line strength distribution function for the local strength S(s). In terms of the paramet η, the distribution [equation (27)] is

$$P(\eta) = \begin{cases} \dfrac{T(s)}{\eta\theta_m} & 0 \le \eta \le 1 \\ \\ 0 & \eta > 1 \end{cases} \quad .$$

The relation for the mean equivalent width is then*

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\left\{S_M(s)\frac{T(s)}{\delta\theta_m}\right\}$$

$$\times\frac{2}{\pi}\int_0^\infty\left[\int_0^1 \exp\left\{-\frac{2x_M(s)\eta^{q(s)}}{1+\rho^2(s)z^2}\right\}d\eta\right]\frac{dz}{1+z^2} \quad .$$

The preintegral factor in brackets can be identified from equation (29) as the local value of the absorption parameter $\overline{k}(s)$. With the relationships and procedures used in the alternative CG formulation, it can be established that $x_M(s) = 4x_e(s)$, where $x_e(s)$ is defined by equation (40), and $\beta_e(s)$ is given by equation (58). The final result for the derivative is then

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\overline{k}(s)y[4x_e(s), \rho(s), q(s)] \quad , \tag{73}$$

where

$$y(x,\rho,q) = \frac{2}{\pi}\int_0^\infty\left[\int_0^1 \exp\left\{-\frac{2x\eta^q}{1+\rho^2z^2}\right\}d\eta\right]\frac{dz}{1+z^2} \quad . \tag{74}$$

The form of equation (73) is the same as those obtained in the CG approximations, but the derivative function $y(x,\rho,q)$ is different. In particular, where the derivative functions in the CG approximations can assume values

*The application of $P(\eta)$ to $dW(s)/ds$ gives the mean value of the derivative. Clearly, the operations of differentiation with respect to s and averaging over line strengths (η) are independent operations. Thus, the mean value of the derivative is equal to the derivative of the mean value of W, i.e., $\overline{dW(s)/ds} = d\overline{W}(s)/ds$.

greater than unity for some values of the argument, that of equation (74) is well-behaved for all values of the arguments. A comparison of the two CG expressions for y [equations (61) and (65)] and an approximation (Appendix) to the present function is shown in Fig. 3 for the case $\rho = 2$, $q = 3$, and $r = 6$.

Some analysis of $y(x, \rho, q)$ as given by equation (74) has been made by Lindquist et al.,[14] and an approximate method of computing $y(x, \rho, q)$ is given here in the Appendix.* An interesting behavior of this function that is not predicted by the CG functions is the asymptotic form $y \sim \text{CONST}/x^{1/q}$ for large x when $q > 2$. For $q < 2$, the expected relation $y \sim \text{CONST}/x^{1/2}$ is obtained. This feature is evident in Fig. 4, where $y(x, \rho, q)$ is plotted as a function of x for several values of q and the fixed value $\rho = 1$. These curves were generated with the approximate procedure outline in the Appendix.

C. LINDQUIST-SIMMONS APPROXIMATION

Lindquist and Simmons[11] extended their approximation for an isolated line to the case of a random array of Lorentz lines with equal strengths. Young[12, 13] further extended the approximation to the case where the line strengths are distributed according to an exponential or exponential-tailed inverse distribution. These latter extensions were made with the assumption that S and S_e are directly related, and that the constant of proportionality is independent of the line index i. This assumption is clearly equivalent to the assumption that $q(s) \equiv 1$ in equation (72). The result obtained for the exponential-tailed inverse distribution was given as

$$\frac{d\overline{W}(s)}{ds} = c(s)p(s)\overline{k}(s)y[\pi x_e(s), r(s)] \quad , \tag{75}$$

*In this approximate procedure, the exponential-tailed inverse line strength distribution is used. If $y(x, \rho, q)$ is computed according to this approximation, the factor 4 in equations (73) and (78) should be replaced by π.

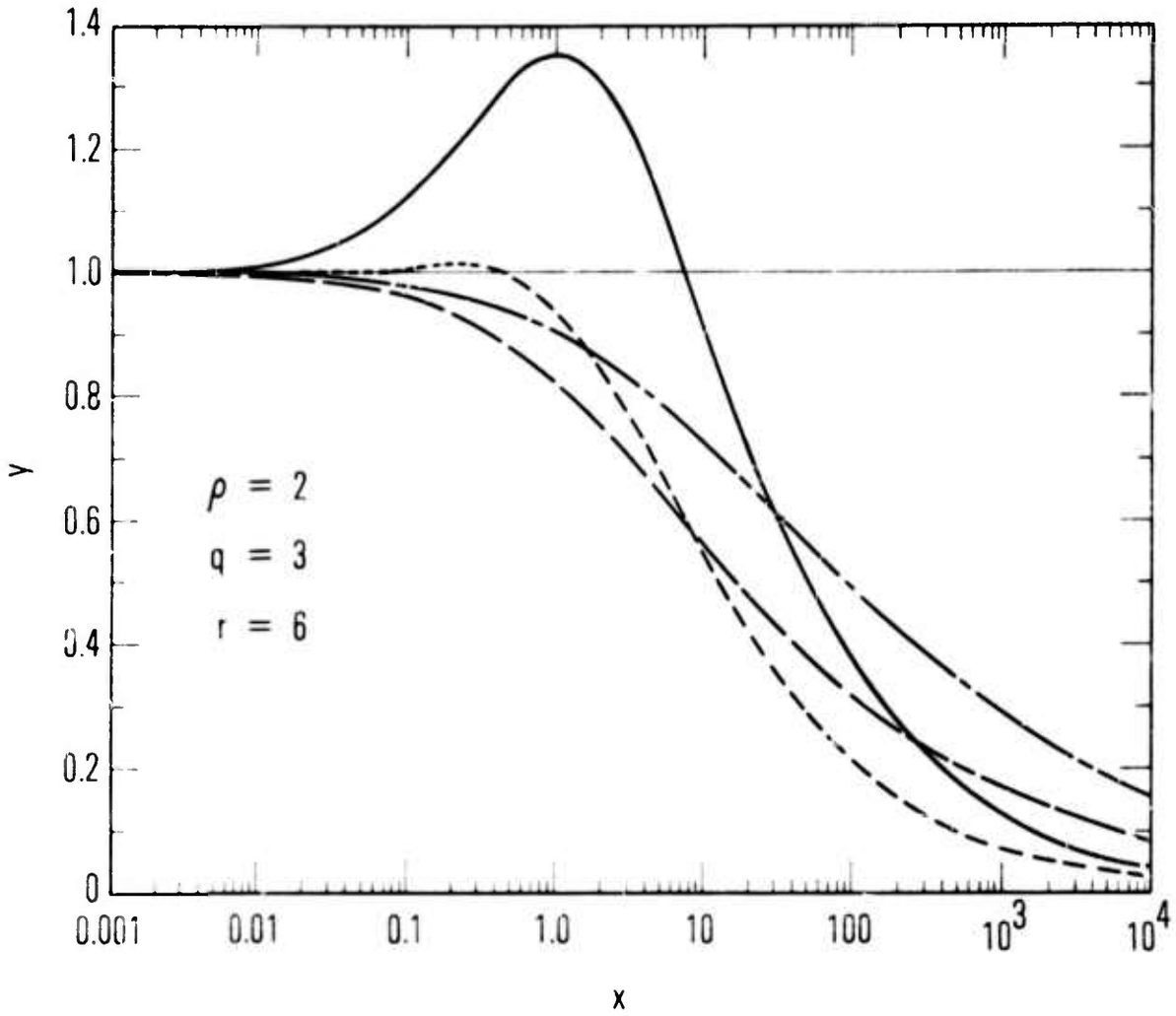

Figure 3. Intercomparison of Derivative Functions for Band Models. — CG approximation (Godson's method); ---- CG approximation (alternative formulation); – – formal derivative approximation [equation (73)]; ie, – - – intuitive derivative approximation [equation (78)].

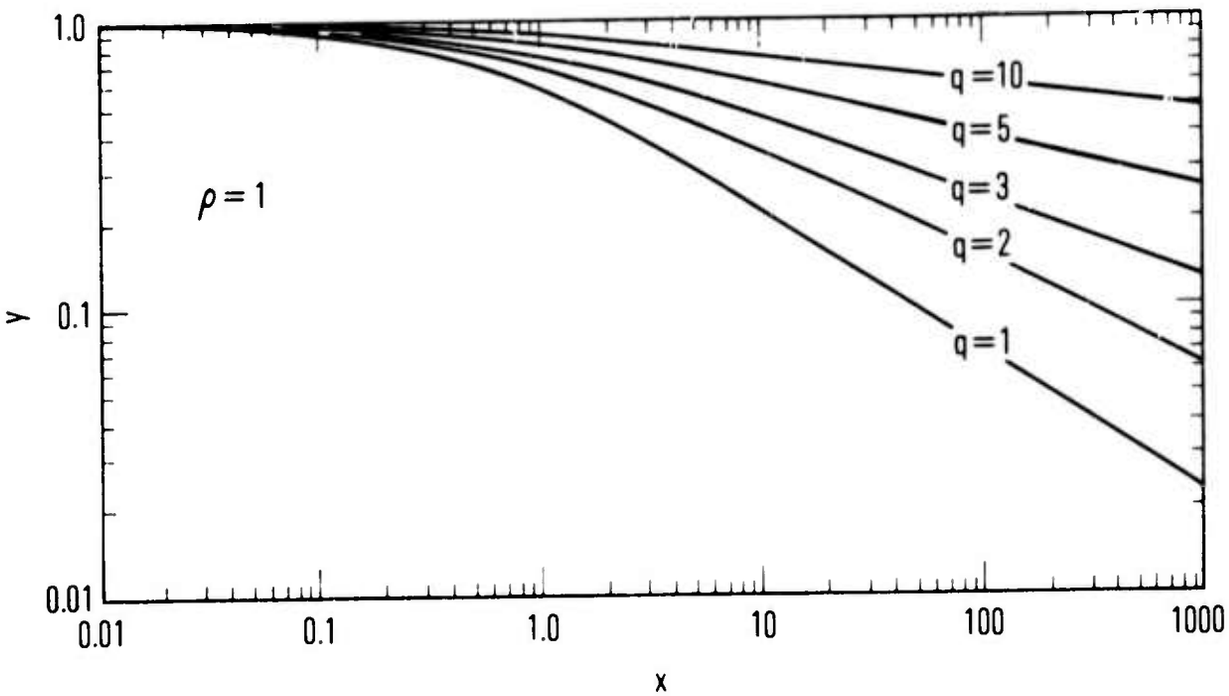

Figure 4. Derivative Function for the Derivative Approximation. $y(x, \rho, q)$ is computed according to the procedure given in the Appendix.

where $y(x, r)$ is the relatively simple expression

$$y(x, r) = \frac{2r(1 + x) + (1 + r^2)\sqrt{1 + 2x}}{\sqrt{1 + 2x}(r + \sqrt{1 + 2x})^2} \quad . \tag{76}$$

The arguments $x_e(s)$ and $r(s)$ were given in terms of $\beta_e(s)$ computed as a path average of β [equation (46)] as is used in Godson's formulation of the CG approximation. This choice for $\beta_e(s)$ was made intuitively so that the strong absorption limit ($x \to \infty$) of $y(x, r)$ given by equation (76) and $y(x, r)$ given by the CG result of equation (61) would agree. If the formulation for the exponential-tailed distribution is again carried out for $q(s) \equiv 1$, but without the intuitive use of $r(s)$, and with the direct relations of equations (38) and (39), the result is

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\overline{k}(s)y[\pi x_e(s), \rho(s)] \quad , \tag{77}$$

where $y(x, \rho)$ is still given by equation (76), but where t uniformity argument $\rho(s)$ is now given by equation (66). The result .. equation (75) is referred to herein as the intuitive LS approxima and that of equation (77) as the formal LS approximation.

The intuitive use of $r(s)$ instead of $\rho(s)$ in order to match the strong limit forms of the LS and CG approximations raises the possibility of intuitively replacing $\rho(s)$ by $r(s)$ in the derivative approximation of equation (73) also. If the result of equation (73) is referred to as the formal derivative approximation, then the form

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\overline{k}(s)y[4x_e(s), r(s), q(s)] \tag{78}$$

with $y(x, r, q)$ given by equation (74) is referred to as the intuitive derivative approximation.

D. MEAN-LINE APPROXIMATION

The following approximation is introduced to permit the use of the simple form of the derivative function given by equation (76), but to lessen the degree of approximation inherent in the assumption $q(s) \equiv 1$. If the line strength as given by equation (26) is averaged over the energy level distribution $P(\theta)$ of equation (27), the result is

$$\bar{S}(s) = S_M(s) \frac{T(s)}{\theta_m} \quad .$$

Consequently, the relationship between the mean line strengths at arbitrary path positions s and s′ is

$$\bar{S}(s') = \left[\frac{S_M(s')}{S_M(s)} \frac{T(s')}{T(s)}\right] \bar{S}(s) \quad . \tag{79}$$

The mean-line approximation assumes that this functional relationship holds for each line in $\Delta\nu$, thus,

$$S(i, s') = \left[\frac{S_M(s')}{S_M(s)} \frac{T(s')}{T(s)}\right] S(i, s) \quad . \tag{80}$$

Substitution of equation (80) into equation (6) for $S_e(i, s)$ and use of equations (38), (39), and (56) yield

$$S_e(i, s) = S_{eM}(s) \frac{\eta}{q(s)} \quad , \tag{81}$$

where η and $q(s)$ are defined by equations (71) and (67), respectively. This approximation retains the linearity of $S_e(i, s)$ with $S(i, s)$, but defines the constant of proportionality explicitly in terms of path properties. In particular,

an inverse dependence of $S_e(i, s)$ on $q(s)$ is predicted. Comparison of equation (81) with equation (72) shows that the former is obtained by factoring η^q as $\eta\eta^{q-1}$ and replacing η^{q-1} by its mean value in the interval $0 \leq \eta \leq 1$

$$\overline{\eta^{q-1}} = \int_0^1 \eta^{q-1}\, d\eta = \frac{1}{q} \quad .$$

The elimination of $S_{cM}(s)$ from equation (81) with equations (50) and (38) results in the final form for the formal mean-line approximation as

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\bar{k}(s)y\left[\frac{\pi x_e(s)}{q(s)},\ \rho(s)\right] \quad , \tag{82}$$

where $y(x, \rho)$ is given by equation (76). As for the previous two approximation, we can consider an intuitive mean-line approximation given by

$$\frac{1}{\delta}\frac{d\overline{W}(s)}{ds} = c(s)p(s)\bar{k}(s)y\left[\frac{\pi x_e(s)}{q(s)},\ r(s)\right] \quad . \tag{83}$$

VI. DISCUSSION AND SUMMARY OF BAND MODELS

A. SUMMARY OF FORMULATION PRINCIPLES

The formulation of band models for a random array of lines requires integrations over the spatial variable s', the spectral variable ν, and the line strength variable S. In a completely general formulation, these three variables are intimately interrelated in a complex manner. The heart of nearly all band model formulations for general optical paths is the introduction of approximations that separate the affects of the variables such that the orders of integrations can be interchanged. In the models discussed here, the variables s' and ν are separated with either the CG or LS approximations for a single line. The variables s' and S are effectively separated by using the line strength separability approximation.

The fundamental feature of the CG approximations is that they are approximations to the mean equivalent width function $\overline{W}(s)/\delta$. The various derivative approximations, on the other hand, attempt to make direct approximations to the derivative of the mean equivalent width function, which is the more fundamental of the two from the standpoint of calculating band radiance.

The CG approximation was formulated in two ways: (1) by defining the effective band model parameters $\overline{k}_e(s)$ and $\beta_e(s)$ according to Godson's procedure of fitting the model to exact weak and strong absorption limits (within the confines of the separability approximation), and (2) by defining these effective band model parameters directly in terms of isothermal band model parameters through relations that are derived from the properties of the assumed inverse line strength distribution function. The two approaches appear to be equivalent because they are based on the same assumptions. However, the results are somewhat different. The latter formulation depends more on the validity of the assumed line strength distribution model than does the former.

The derivative approximations were all derived in a manner similar to the second approach to the CG approximation. These formulations are, then, functions of the inhomogeneity index $\rho(s)$ and the nonisothermality index $q(s)$. In order to match the strong absorption limit of one of these derivative band models (LS) to the corresponding limit of the first approach to the CG approximation, an intuitive replacement of $\rho(s)$ with $r(s)$ was introduced. This replacement was extended to the remaining two derivative approaches.

In all of the models, temperature variations along an optical path are implicitly accounted for in the temperature variation of $\bar{k}(s)$ and $\bar{\delta}(s)$. Explicit account is made in all models, except the formal LS model, by the use of either the nonisothermality index $r(s)$ or $q(s)$. The intuitive models account most for local nonisothermalities by using both $r(s)$ and $q(s)$. Within the heirarchy of models, the degree of variation with thermal gradient increases in the order CG, LS, mean line, derivative approximation for the intuitive models, and LS, CG, mean line, derivative approximation for the formal models.

The results of the companion paper indicate that, for H_2O, the intuitive derivative approximation yields the best comparison between predicted and available experimentally measured radiance spectra.

B. SUMMARY OF MODELS

The eight models considered here are summarized below by extracting the relevant equations from the text and presenting them in groups that correspond to the inverse order in which they would be used in making an actual calculation. In all cases, the thermodynamic variables $c(s)$, $p(s)$, and $T(s)$ are presumed known along the general line of sight that extends from $s = 0$ to $s = S$. The band model parameters $\bar{k}(s)$, $\bar{\delta}(s)$, $\bar{\gamma}(s)$, and $\beta(s)$ are presumed known as a function of c, p, T, and thus s. All of the equations are written for the exponential-tailed inverse line strength distribution.

1. RADIANCE AND TRANSMITTANCE EQUATIONS

$$\bar{N} = -\int_0^S N^*(s)\,\frac{d\bar{\tau}(s)}{ds}\,ds \quad ,$$

$$\frac{d\bar{\tau}(s)}{ds} = -\bar{\tau}(s)\,\frac{1}{\delta}\,\frac{d\bar{W}(s)}{ds} \quad ,$$

$$\bar{\tau}(s) = \exp\left[-\frac{\bar{W}(s)}{\delta}\right] \quad ,$$

$$\frac{1}{\delta}\,\frac{d\bar{W}(s)}{ds} = c(s)\,p(s)\,\bar{k}(s)\,y(s) \quad ,$$

$$\frac{\bar{W}(s)}{\delta} = \begin{cases} \dfrac{\rho_e(s)}{\pi}\, I_e[\pi x_e(s)] & \text{CG approximations} \\ \displaystyle\int_0^s \frac{1}{\delta}\,\frac{d\bar{W}(s')}{ds'}\,ds' & \text{Derivative approximations} \end{cases}$$

2. DERIVATIVE FUNCTIONS

a. Godson's CG

$$y(s) = y[\pi x_e(s),\ r(s)] \quad ,$$

$$y(\bar{\tau}, r) = (2 - r)\,\frac{dI_e(\bar{\eta})}{d\bar{\eta}} + (r - 1)\,\frac{I_e(\bar{\eta})}{\bar{\eta}} \quad ,$$

$$I_e(\bar{\eta}) = \sqrt{1 + 2\bar{\eta}} - 1 \quad ,$$

$$\frac{dI_e(\bar{\eta})}{d\bar{\eta}} = \frac{1}{\sqrt{1 + 2\bar{\eta}}} \quad .$$

b. Alternative CG

$$y(s) = y[\pi x_e(s),\ \rho(s),\ q(s)] \ ,$$

$$y(\eta, \rho, q) = \left[\frac{2 - \rho}{q}\right] \frac{dI_e(\eta)}{d\eta} + \left[1 - \frac{2 - \rho}{q} \ \frac{I_e(\eta)}{\eta}\right] .$$

c. Formal LS

$$y(s) = y[\pi x_e(s),\ \rho(s)] \ ,$$

$$y(\eta, \rho) = \frac{2\rho(1 + \eta) + (1 + \rho^2)\sqrt{1 + 2\eta}}{\sqrt{1 + 2\eta}\ (\rho + \sqrt{1 + 2\eta})^2} \ .$$

d. Intuitive LS

The same as formal LS, except with $\rho(s)$ replaced by $r(s)$.

e. Formal Mean Line

$$y(s) = y\left[\frac{\pi x_e(s)}{q(s)} \ , \ \rho(s)\right] \ ,$$

$$y(\eta, \rho) = \text{same as formal LS.}$$

f. Intuitive Mean Line

The same as the formal mean line, except with $\rho(s)$ replaced by $r(s)$.

g. Formal Derivative

$$y(s) = y[\pi x_e(s),\ \rho(s),\ q(s)] \ ,$$

where $y(\eta, \rho, q)$ is from the Appendix.

h. Intuitive Derivative

The same as the formal derivative, except with $\rho(s)$ replaced by $r(s)$.

3. PATH AVERAGES

$$u(s) = \int_0^s c(s')\, p(s')\, ds' \ ,$$

$$\bar{k}_e(s) = \frac{1}{u(s)} \int_0^s c(s')\, p(s')\, \bar{k}(s')\, ds' \ ,$$

$$\bar{\delta}_e(s) = \frac{1}{u(s)\, \bar{k}_e(s)} \int_0^s c(s')\, p(s')\, \bar{k}(s')\, \bar{\delta}(s')\, ds' \ ,$$

$$\bar{\gamma}_e(s) = \frac{1}{u(s)\, \bar{k}_e(s)\, \bar{\delta}_e(s)} \int_0^s c(s')\, p(s')\, \bar{k}(s')\, \bar{\delta}(s')\, \bar{\gamma}(s')\, ds' \ ,$$

$$\hat{\beta}_e(s) = \begin{cases} \dfrac{1}{u(s)\, \bar{k}_e(s)} \displaystyle\int_0^s c(s')\, p(s')\, \bar{k}(s')\, \beta(s')\, ds' \\ \dfrac{2\pi \bar{\gamma}_e(s)}{\bar{\delta}_e(s)} \end{cases}$$

The first option for $\hat{\beta}_e(s)$ is used with Godson's formulation of the CG approximation and in the intuitive derivative approximations. The second option is used with the alternative formulation of the CG approximation and the formal derivative approximations

$$x_e(s) = \frac{u(s)\,\bar{k}_e(s)}{\beta_e(s)} \quad ,$$

$$\rho(s) = \bar{\gamma}(s)/\bar{\gamma}_e(s) \quad ,$$

$$q(s) = \bar{\delta}_e(s)/\bar{\delta}(s) \quad ,$$

$$r(s) = \beta(s)/\beta_e(s) \; [\beta_e(s) \text{ from option 1 above}] \quad .$$

APPENDIX

COMPUTATION OF $y(x, \rho, q)$ IN THE DERIVATIVE APPROXIMATION

Application of the derivative approximation band model requires the computation of the function

$$y(x,\rho,q) = \frac{2}{\pi}\int_0^\infty \left[\int_0^1 \exp\left\{-\frac{2x\eta^q}{1+\rho^2 z^2}\right\} d\eta\right] \frac{dz}{1+z^2} \qquad (A-1)$$

for arbitrary positive values of the arguments x, ρ, q. The inner integral may be expressed in terms of the incomplete gamma function

$$\gamma(a,\xi) = \int_0^\xi u^{a-1} e^{-u}\, du$$

by the transformation $u = 2x\eta^q/(1+\rho^2 z^2)$. Then, equation (A-1) becomes

$$y(x,\rho,q) = \frac{1}{q(2x)^{1/q}} \frac{2}{\pi}\int_0^\infty \frac{(1+\rho^2 z^2)^{1/q}}{1+z^2}\, \gamma\left(\frac{1}{q}, \frac{2x}{1+\rho^2 z^2}\right) dz \quad . \qquad (A-2)$$

Computation of $y(x, \rho, q)$ by numerical integration of equation (A-2) is complicated by the need to evaluate the incomplete gamma function and by the overall complex behavior of the integrand. In order to circumvent these difficulties, the following approximate method, which has been found to be both sufficiently accurate and efficiently applicable is used.

First, we write $y(x, \rho, q)$ in the form

$$y(x,\rho,q) = \frac{1}{q}\, y(x,\rho,1) + \frac{q-1}{q} \int_0^1 y(x\eta^q, \rho, 1)\, d\eta \quad , \qquad (A-3)$$

which expresses $y(x,\rho,q)$ in terms of its value at $q = 1$. This identity can be established as follows. For $q = 1$, the inner integration of equation (A-1) is easily performed and yields the result

$$y(x,\rho,1) = \frac{2}{\pi} \int_0^\infty \frac{1+\rho^2 z^2}{2x} \left[1 - \exp\left(-\frac{2x}{1+\rho^2 z^2}\right)\right] \frac{dz}{1+z^2} \quad . \qquad (A-4)$$

Replacement of x with $x\eta^q$ and integration of both sides over $0 \le \eta \le 1$ yields

$$\int_0^1 y(x\eta^q, \rho, 1)\, d\eta = \frac{2}{\pi} \int_0^\infty \left[\int_0^1 \frac{1+\rho^2 z^2}{2x\eta^q} \left\{1 - \exp\left(-\frac{2x\eta^q}{1+\rho^2 z^2}\right)\right\} d\eta\right] \frac{dz}{1+z^2} \quad .$$

If the inner integral is integrated by parts with

$$u = 1 - \exp\left(-\frac{2x\eta^q}{1+\rho^2 z^2}\right)$$

and

$$dv = \frac{1+\rho^2 z^2}{2x\eta^q}\, d\eta \quad ,$$

we obtain (for $q \neq 1$)

$$\int_0^1 y(x\eta^q, \rho, 1)\, d\eta = \frac{1}{1-q}\frac{2}{\pi}\int_0^\infty \frac{1+\rho^2 z^2}{2x}\left[1 - \exp\left(-\frac{2x}{1+\rho^2 z^2}\right)\right]\frac{dz}{1+z^2}$$

$$- \frac{q}{1-q}\frac{2}{\pi}\int_0^\infty \left[\int_0^1 \exp\left\{-\frac{2x\eta^q}{1+\rho^2 z^2}\right\} d\eta\right]\frac{dz}{1+z^2} \quad .$$

The integral in the first term is recognized from equation (A-4) to be $y(x, \rho, 1)$, whereas the double integral in the second term is recognized from equation (A-1) to be $y(x, \rho, q)$. Thus,

$$\int_0^1 y(x\eta^q, \rho, 1)\, d\eta = \frac{1}{1-q}\, y(x, \rho, 1) - \frac{q}{1-q}\, y(x, \rho, q) \quad ,$$

which, when inverted for $y(x, \rho, q)$, yields and establishes the validity of equation (A-3).

Next, we approximate $y(x, \rho, 1)$ by the function derived for the exponential-tailed inverse line strength distribution function.* This function has been derived by Young[13] and is

$$y(x, \rho, 1) = \frac{2\rho(1+x) + (1+\rho^2)\sqrt{1+2x}}{\sqrt{1+2x}\,[\rho + \sqrt{1+2x}]^2} \quad . \qquad \text{(A-5)}$$

*The equation that corresponds to equation (A-1) for the exponential-tailed distribution (with $R \to \infty$) is

$$y(x, \rho, q) = \frac{2}{\pi}\int_0^\infty \left[\int_0^\infty \exp\left\{-\eta - \frac{2x\eta^q}{1+\rho^2 z^2}\right\} d\eta\right]\frac{dz}{1+z^2} \quad .$$

Numerical evaluation of this integral is as difficult as the direct evaluation of equations (A-1) or (A-2). Moreover, an expression comparable to equation (A-3) cannot be written. Thus, use of the exponential-tailed distribution is delayed until equation (A-3) is established.

The approximate method involves the evaluation of $y(x, \rho, q)$ according to equation (A-3) with $y(x, \rho, 1)$ given by equation (A-5). The integral term of equation (A-3) is evaluated numerically as follows. The transformation $u = x\eta^q$ gives the integral term as

$$\int_0^1 y(x\eta^q, \rho, 1)\, d\eta = \frac{1}{qx^{1/q}} \int_0^x u^{(1/q)-1}\, y(u, \rho, 1)\, du \quad .$$

For $q > 1$, the integrand $u^{(1/q)-1}\, y(u, \rho, 1)$ is a decreasing function with u. The most rapid decrease occurs for small ρ [by inspection of equation (A-5)] and large q. In the limit $\rho \to 0$ and $q \to \infty$, the functional form of the integrand is

$$I \sim \frac{1}{u(1 + 2u)} \quad . \tag{A-6}$$

Thus, even in the worst case, the integrand decreases no faster than u^{-2}. Let I_1 be the value of the integrand at an arbitrary value u_1. The value of $u_2 > u_1$ for which the integrand has fallen to the value fI_1 $(0 < f < 1)$ is found from equation (A-6) to be

$$u_2 = \frac{1}{4}\left[\sqrt{\frac{1 + 8u_1\,(1 + 2u_1)}{f}} - 1\right] \quad . \tag{A-7}$$

The integration interval $0 \le u \le x$ is divided into a series of sequential intervals according to the algorithm of equation (A-7). The last interval is truncated at x if $u_2 > x$. A nonzero starting value of $u_1 = \varepsilon$ must be used. Thus, within each interval (except $0 \le u \le \varepsilon$), the integrand varies by less than the factor f. A two-point Gaussian quadrature is then used to evaluate the

integral over each interval.* The general form of each of these subintegrals is

$$\int_{u_1}^{u_2} u^{(1/q)-1}\, y(u, \rho, 1)\, du \quad .$$

With the transformation

$$\begin{aligned} z &= A + Bu \quad , \\ B &= 2/(u_2 - u_1) \quad , \\ A &= 1 - u_2 B \quad , \end{aligned} \tag{A-8}$$

the integral assumes the standard Gaussian form

$$\frac{1}{B} \int_{-1}^{1} u(z)^{(1/q)-1}\, y[u(z), \rho]\, dz \quad ,$$

with

$$u(z) = \frac{z - A}{B} \quad . \tag{A-9}$$

The two-point Gaussian quadrature approximation to the integral is

$$\frac{1}{B} \left\{ u(z_1)^{(1/q)-1}\, y[u(z_1), \rho] + u(z_2)^{(1/q)-1}\, y[u(z_2), \rho] \right\} \quad , \tag{A-10}$$

with $z_{1,2} = \pm 0.57735027$.

---

*With a starting value of $\epsilon = 0.01$, and with $t = 0.1$, only 15 intervals are needed to handle x as large as 2×10^6. This compares with hundreds (or more) of terms required in various exact series expansions of equation (A-1) and (A-2).

With f = 0.10, this procedure gives an accuracy of ~3% for the worst case of variation of the integrand, i.e., u^{-2}, and ~0.7% for a nominal variation of u^{-1}.

The contribution to the integral from the interval $0 \leq u \leq \epsilon$ is treated by a two-term series expansion. For small u, equation (A-5) gives

$$y(u, \rho, 1) \longrightarrow 1 - \frac{2u}{1 + \rho} \quad .$$

Thus,

$$\int_0^{\epsilon} u^{(1/q,-1} \, y(u, \rho, 1) \, du \longrightarrow q\epsilon^{(1/q)} \left[1 - \frac{2\epsilon}{(1 + \rho)(1 + q)}\right] . \qquad \text{(A-11)}$$

A nominal value $\epsilon = 0.01$ is used. If $x < 0.01$, this two-term expansion is used directly to evaluate the integral over $0 \leq u \leq x$.

A calculational flow diagram for the procedure is shown in Fig. A-1. Note that the routine treats only the case $q > 1$. A similar analysis could be made for $q < 1$, but this case is not as intrinsically important as the $q > 1$ case. If $q < 1$, we set $q = 1$.

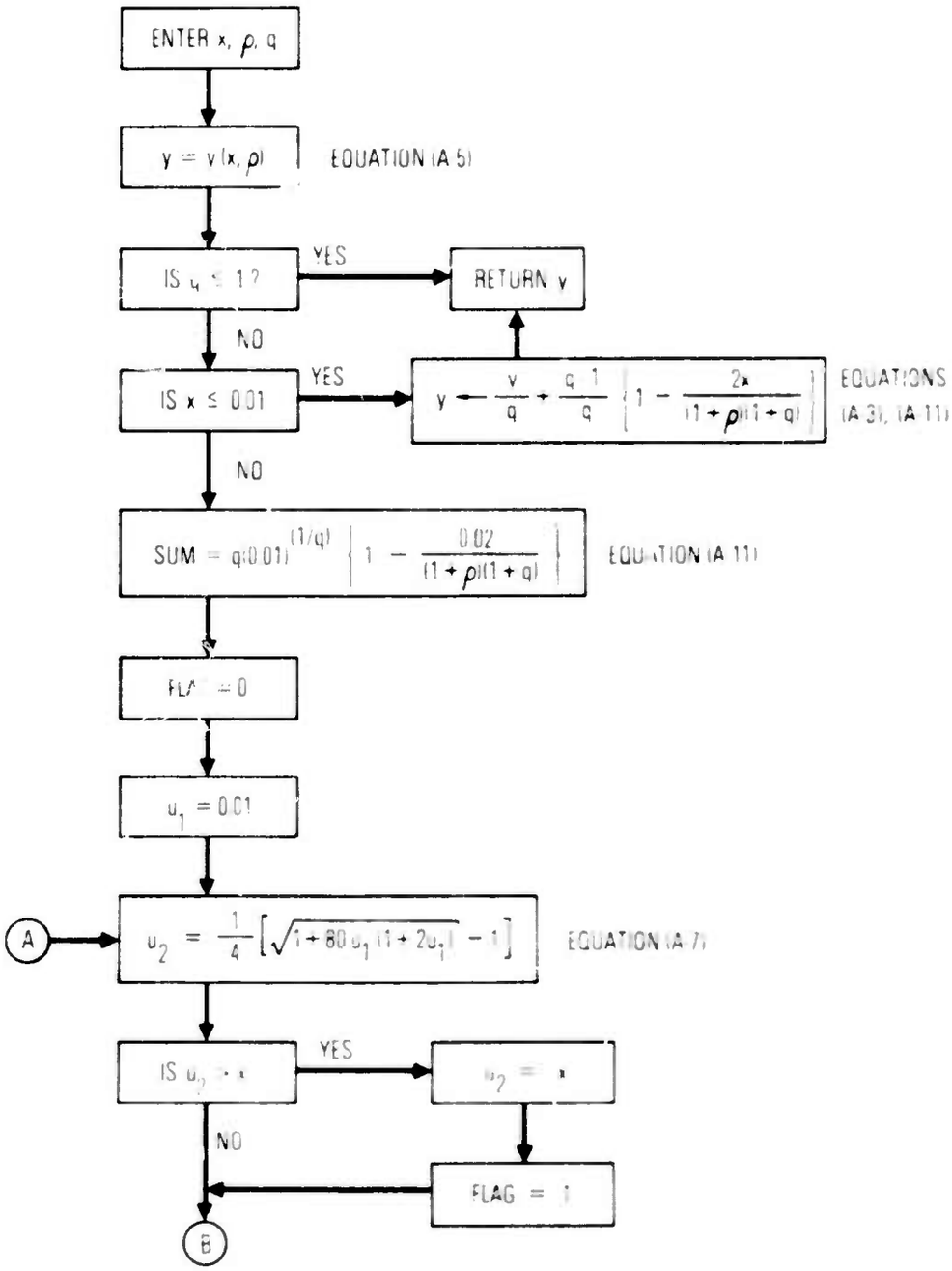

Figure A-1. Derivative Function Calculation Routine

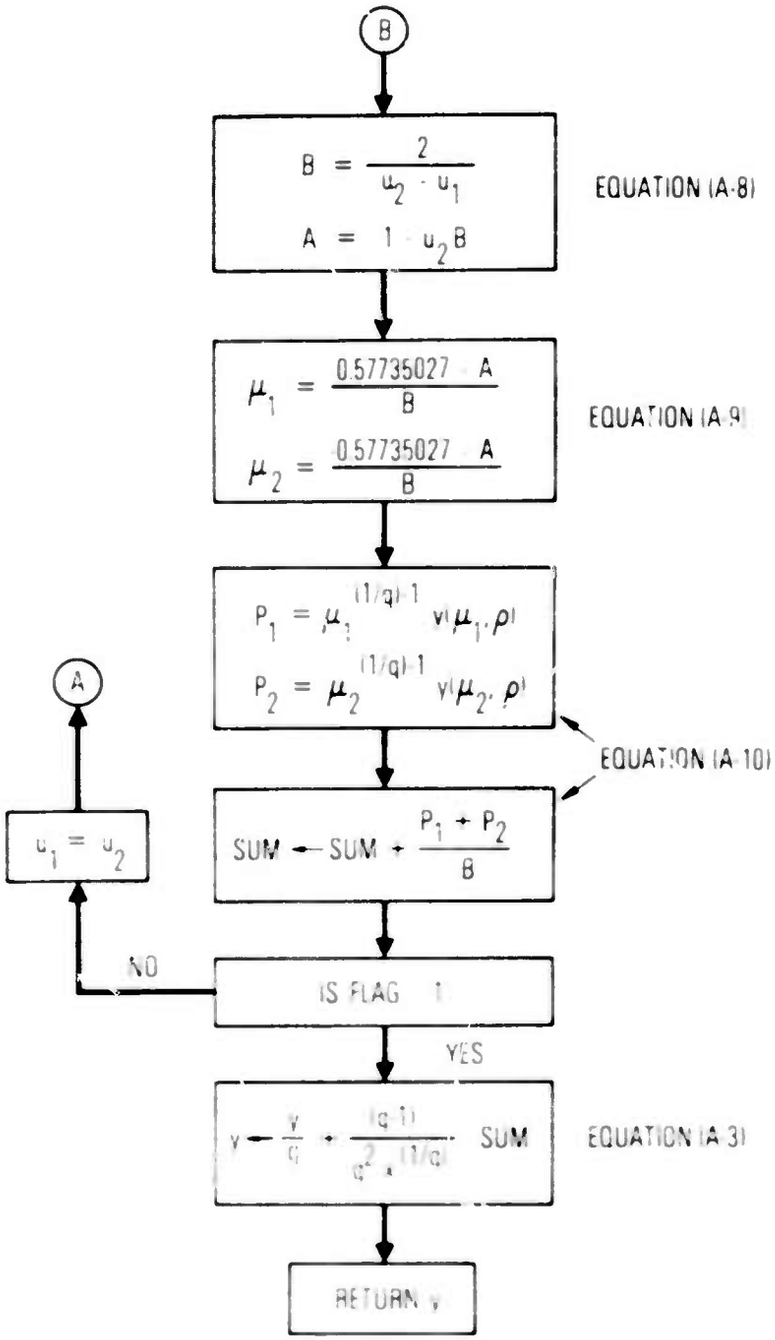

Figure A-1. Derivative Function Calculation Routine (Continued)

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