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A COMPUTATIONAL METHOD FOR SPECTRAL MOLECULAR ABSORPTION USING --ETC(U)
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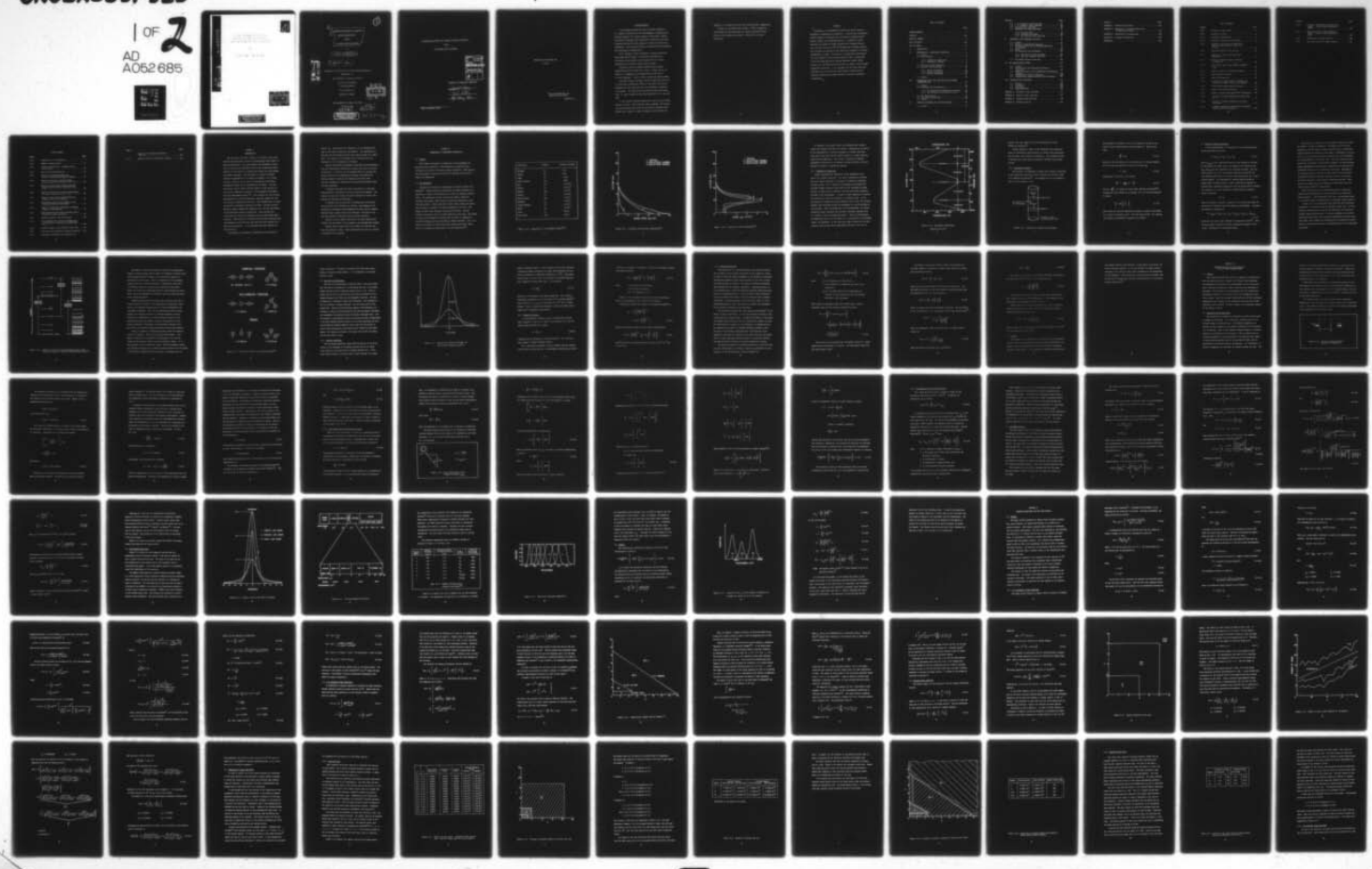

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A COMPUTATIONAL METHOD FOR SPECTRAL MOLECULAR ABSORPTION USING AN IMPROVED VOIGT ALGORITHM

BY

PETER CLARK VAN DERWOOD

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(6) A COMPUTATIONAL METHOD FOR SPECTRAL MOLECULAR ABSORPTION USING AN IMPROVED VOIGT ALGORITHM,

by

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A COMPUTATIONAL METHOD FOR SPECTRAL MOLECULAR ABSORPTION

USING

AN IMPROVED VOIGT ALGORITHM

APPROVED BY SUPERVISORY COMMITTEE:

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Yu-cheng Liu

DEAN OF GRADUATE SCHOOL

Dedicated to My Parents and

to John

"Be ye transformed by the
renewing of your mind"

Romans XII, 2

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ABSTRACT

Discussion of the fundamental elements and theory related to atmospheric transmittance is presented. A line-by-line transmission computer program is developed that utilizes the combined Doppler-Lorentz (Voigt) line broadening function. In addition a rapid algorithm to evaluate the Voigt function with a maximum relative error of about one part in 10^4 is described and a software package that processes the absorption line parameters necessary to calculate transmittance is given. The results of transmittance calculations for seven channels in the fifteen micrometer band, corresponding to the seven High Resolution Infrared Radiation Sounder (HIRS) channels, are furnished and the procedure to compute a band averaged transmission discussed. It is concluded that the Voigt algorithm developed here is an excellent computational procedure and the resulting transmittance program correctly calculates atmospheric transmission.

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CHAPTER I

INTRODUCTION

The thin film of gas that clings to the surface of the earth performs many functions, and has a correspondingly large number of important properties. To a meteorologist the atmosphere is basically a sink for solar radiation, and its most interesting characteristic is the ability to transform that energy into wind systems and rainfall averages. This phenomenon of radiative transfer through the atmosphere is too complex, in general, for a closed solution. However, if the scope of investigation is narrowed, mathematical models can be developed that are useful. One such application, that of energy transfer theory, is the retrieval of the vertical temperature structure of the atmosphere from remote satellite measurements [Kaplan[23]]. This requires not only accurate measurements and a stable mathematical inversion scheme, but also very accurate transmittance functions. This transmittance is easily calculated if atmospheric absorption is known. The most accurate method to predict atmospheric absorption is to add the contribution of each molecular species, line-by-line. These line-by-line calculations are very time consuming even with today's high speed computers. This document is concerned with molecular absorption and the mathematical functions that may reduce the time required for a given line calculation. It is organized into seven chapters as outlined below.

The equations of atmospheric transmittance are reviewed in

Chapter two. Additionally the composition of the atmosphere and some of its optical properties are examined. The constituents of interest and the processes by which they absorb energy are touched upon. The concept of an absorbing line is introduced and the phenomenom of line broadening is discussed.

Chapter three defines atmospheric absorption and transmittance. Then the transmittance differential equation this work is to solve is developed. A relation for the combined effects of Lorentz and Doppler spectral line broadening is obtained, and finally the frequency bands of interest for temperature retrieval from satellite soundings are defined and the molecular absorbers within the band identified.

In Chapter four begins the major contribution of this work. Three methods of evaluating the Voigt function are presented. The results of tests for accuracy and speed conducted for each of the methods are tabulated and discussed.

In Chapter five the data used in transmittance calculations and the units of all equations are covered. Some remarks on the derivation of absorption line parameters are given and the computer software used to handle the data is developed. The units of the data and necessary conversion factors are also presented.

Chapter six ties together the work of the other chapters and presents the end product of this research, the transmittance program.

Finally there is discussion of the results of this work and some conclusions are drawn. Where appropriate the work of a chapter is supported in an appendix.

CHAPTER II

FUNDAMENTALS OF ATMOSPHERIC ABSORPTION

2.1 Preface

This chapter discusses the composition of the atmosphere and molecular energy absorption. The atmosphere is presented first, followed by an outline of molecular energy transitions. Then spectral line broadening is treated and finally the important points of the chapter are summarized.

2.2 The Atmosphere

The gases that compose our atmosphere are listed in Table 2.2-1 [Hudson[18]]. Those who relative proportions are nearly constant up to altitudes in excess of 80 kilometers are called the permanent constituents. The atmosphere contains several other gases, called the variable constituents; their amounts varying with temperature, altitude and location. Chief among them is water vapor, which may constitute as much as 2 percent of a humid atmosphere at sea level. The amount of water vapor decreases rapidly with altitude. Another variable constituent ozone, is seldom observed at sea level. The amount of ozone in the atmosphere increases with altitude to a maximum at about 20 kilometers and then decreases at higher altitudes. Fig. 2.2-1 depicts the variance of water vapor with altitude and season, while Fig. 2.2-2 reflects the correlation for ozone [McClatchey[32]].

Constituent	Formula	Percent by Volume
Nitrogen	N_2	78.1
Oxygen	O_2	20.9
Argon	Ar	0.934
Carbon Dioxide	CO_2	0.032
Neon	Ne	$1.81 \cdot 10^{-3}$
Helium	He	$5.24 \cdot 10^{-4}$
Methane	CH_4	$2.0 \cdot 10^{-4}$
Krypton	Kr	$1.14 \cdot 10^{-4}$
Nitrous Oxide	N_2O	$5.0 \cdot 10^{-5}$
Hydrogen	H_2	$5.0 \cdot 10^{-5}$
Carbon Monoxide	CO	$2.0 \cdot 10^{-5}$
Xenon	Xe	$9.0 \cdot 10^{-6}$
Ozone	O_3	Varies
Water Vapor	H_2O	Varies

TABLE 2.2-1. Composition of the Atmosphere [Hudson[18]].

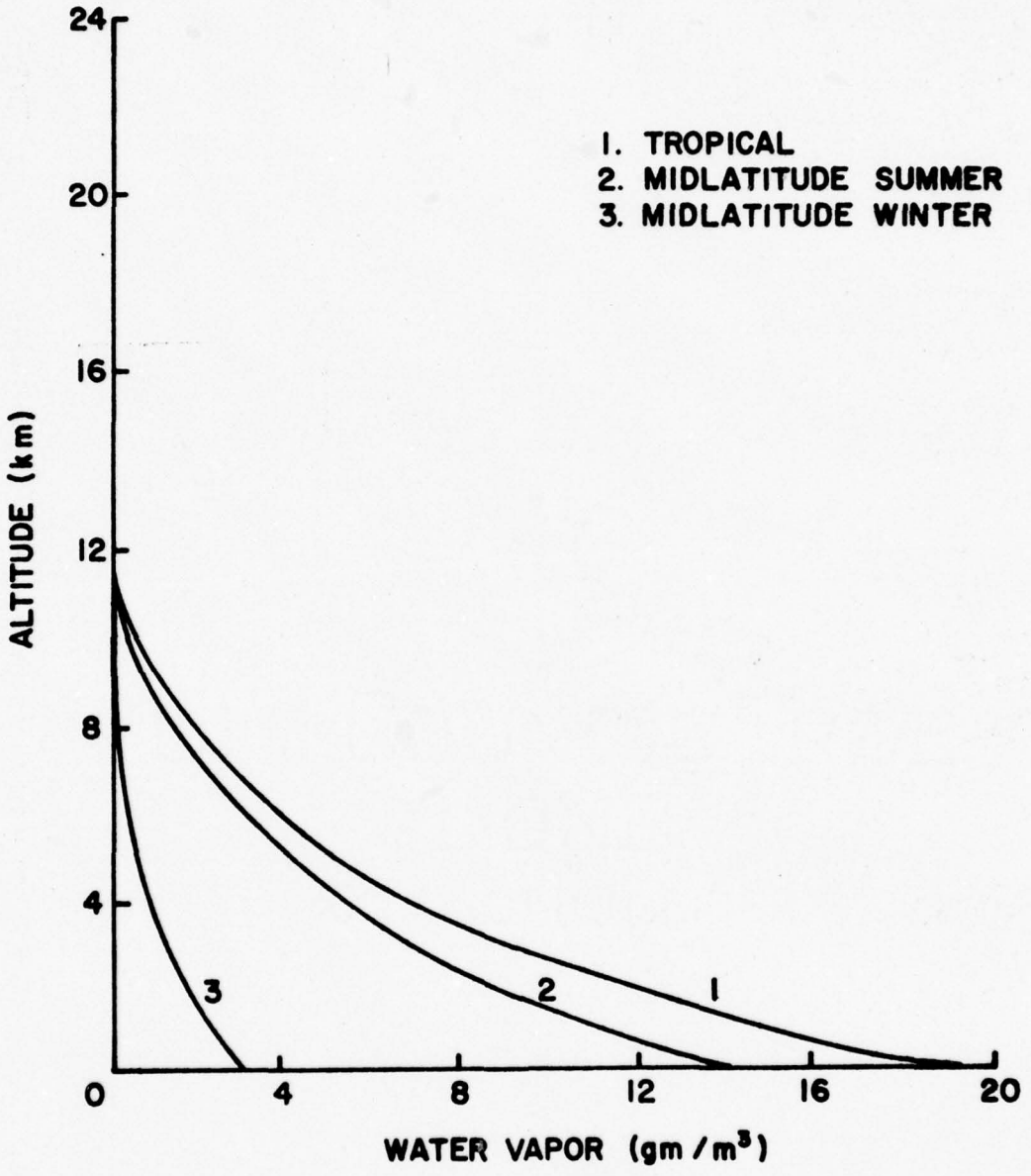


Figure 2.2-1. Variation of Water Vapor [McClatchey[32]].

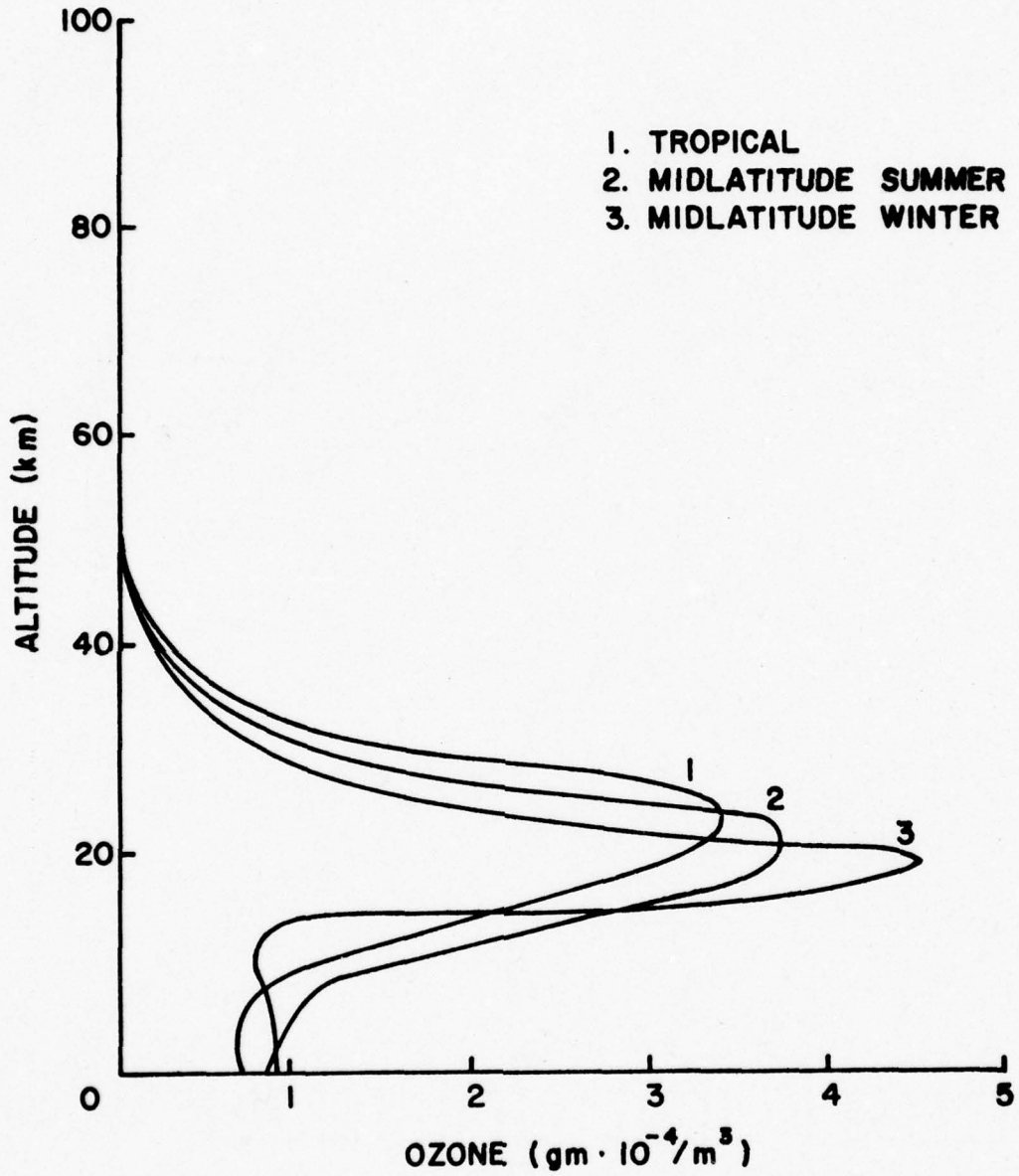


Figure 2.2-2. Variation of Ozone [McClatchey[32]].

In addition to the gases listed, the atmosphere may contain a variety of particles that may be of concern. Depending on the nature of the investigation it could be necessary to consider salt from ocean spray, fine dust from the earth's surface, or carbon particles resulting from combustion. Near cities or industrial complexes atmospheric pollutants such as ammonia, hydrogen sulfide, and sulfur dioxide are present in significant amounts.

2.2.1 Atmospheric Temperature

Having considered the composition of the atmosphere we now discuss its thermal properties. The earth's atmosphere is divided into four regions primarily on the basis of temperature gradients, as shown in Fig. 2.2-3. Typically the temperature decreases with altitude (termed a positive lapse rate) in the troposphere passing through a minimum at the tropopause, and then rises with increasing altitude in the stratosphere. A region in which temperature increases with altitude is termed an inversion, or inversion layer. At the stratopause the temperature passes through a more or less well defined maximum, then decreases through the mesosphere to a second minimum at the mesopause. Above the mesopause, in the thermosphere, the kinetic temperature again increases with altitude, reaching a maximum value at a height of several thousand kilometers. Above the thermosphere, and demarcated from it by the thermopause, is essentially an isothermal region, the exosphere. At any particular time or place the true temperature structure may differ appreciably from Fig. 2.2-3, but in

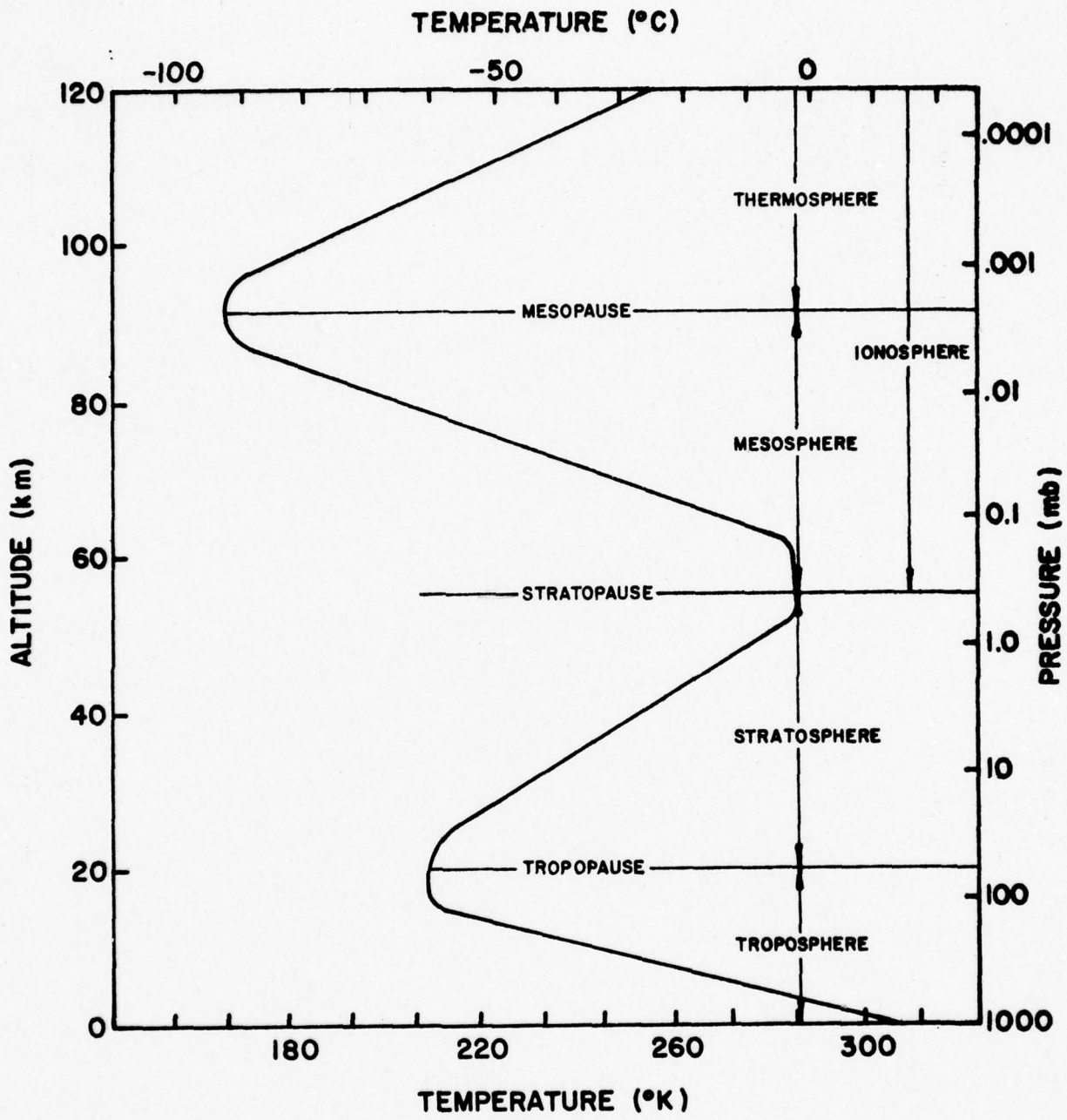


Figure 2.2-3. Atmospheric Nomenclature

(Adapted from [45])

general, the curve shown is at least qualitatively correct [McEwan and Phillips[34]].

Various regions or layers of the atmosphere have properties which are sufficiently characteristic to justify their being given special names, most notable the ionosphere. The ionosphere itself is divided into three regions according to altitude and electron density.

2.2.2 Atmospheric Pressure

The variation of atmospheric pressure with altitude is governed by the hydrostatic equation, which is derived with the aid of Fig. 2.2-4 [McEwan and Phillips[34]]. The pressure is P at an altitude Z, and P - ΔP at altitude Z + ΔZ.

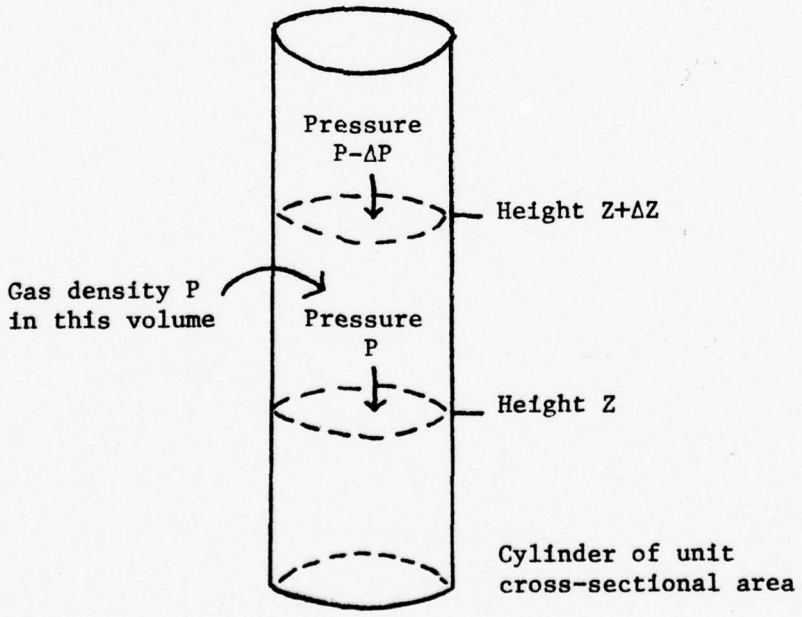


Figure 2.2-4. Variation of Pressure with Altitude.

The difference in pressure is due to the weight of the gas in the column of unit cross-sectional area and length ΔZ. Hence in the limit

$$\frac{dP}{dZ} = -\rho g, \tag{2.2-1}$$

where g is the acceleration due to gravity and ρ is the gas density. For air we use the equation of state for an ideal gas,

$$P = nkT. \tag{2.2-2}$$

Dividing Eq. 2.2-1 by Eq. 2.2-2 yields

$$\frac{dP}{P} = -\frac{\rho g}{nkT}\, dz = -\frac{dZ}{H}, \tag{2.2-3}$$

where $H = \frac{nkT}{\rho g}$, is termed the scale height [Whitten and Poppoff[52]]. Assuming the scale height to be constant, Eq. 2.2-3 can be integrated to obtain

$$\frac{P}{P_o} = \exp\left[-\frac{Z}{H}\right], \tag{2.2-4}$$

which shows the expected exponential decrease of pressure with height in a region of constant g and T. The left scale of Fig. 2.2-3 depicts the decrease of atmospheric pressure with altitude.

2.3 Molecular Energy Transitions

In first approximation, the energy (E) of an isolated molecule can be presented in the form

$$E = E_{trans} + E_{vib} + E_{ro} + E_{el} \qquad (2.3\text{-}1)$$

where E_{trans} is the translational motion, which depends on velocity and may assume any value, E_{el} is the energy of the electrons, and E_{vib} and E_{ro} are the vibrational and rotational energies. The last three terms in Eq. 2.3-1 are quantized [Weidner and Sells[50]] and take discrete values only, the values being specified by one or more quantum numbers. Any combination of quantum numbers defines an energy state or quantum state, or term. Radiation is absorbed or emitted when a transition takes place from one energy state to another. The frequency (ν) of the absorbed or emitted quantum is given by Planck's relation,

$$\Delta E = h\nu, \qquad (2.3\text{-}2)$$

where h is Planck's constant. Equation 2.3-1 is valid only when the interaction of different molecular motions is disregarded. In general, the energy of a molecule is

$$E = E_{trans} + E_{vib} + E_{ro} + E_{el} + E_{el\text{-}vib} + E_{el\text{-}ro} + E_{vib\text{-}ro} \qquad (2.3\text{-}3)$$

where the last three terms represent the interaction [Zuev[54]]. Thus, the most general transition involves simultaneous changes of electronic, vibrational, and rotational energy.

The electronic, vibrational, and rotational energies of a molecule differ in order of magnitude. The energy of an electronic transition is of the order of several electron volts, a vibrational energy transition is reckoned in the tenths or hundredths of an electron volt, and a rotational energy transition is in the thousandths or ten-thousandths of an electron volt. But, since a molecule has electronic, vibrational, and rotational energies, and these energies change simultaneously on emission or absorption, the electronic and vibrational spectra are not evidenced in pure form. Depending on the frequency range of interest we deal either with an electronic-vibrational-rotational molecular spectrum, or with a vibrational-rotational spectrum, or with purely a rotational spectrum. These spectra are referred to as the electronic, vibrational, and rotational spectra [Goody[15]], respectively.

Each electron state has a corresponding grid of vibrational energy levels characterized by certain values of the vibrational quantum number v. Each vibrational level has a corresponding series of rotational levels, characterized by a rotational quantum number j.

In Fig. 2.3-1 it is easily seen why electronic and vibrational transitions of a molecule cannot be observed in pure form. For each electronic transition of a molecule the vibrational and rotational energies change simultaneously. The entire aggregate of electronic transitions gives rise to the electronic-vibrational-rotational spectrum, whose line strengths are determined by the energy-level distributions of the molecules and by the probabilities of the corresponding transitions.

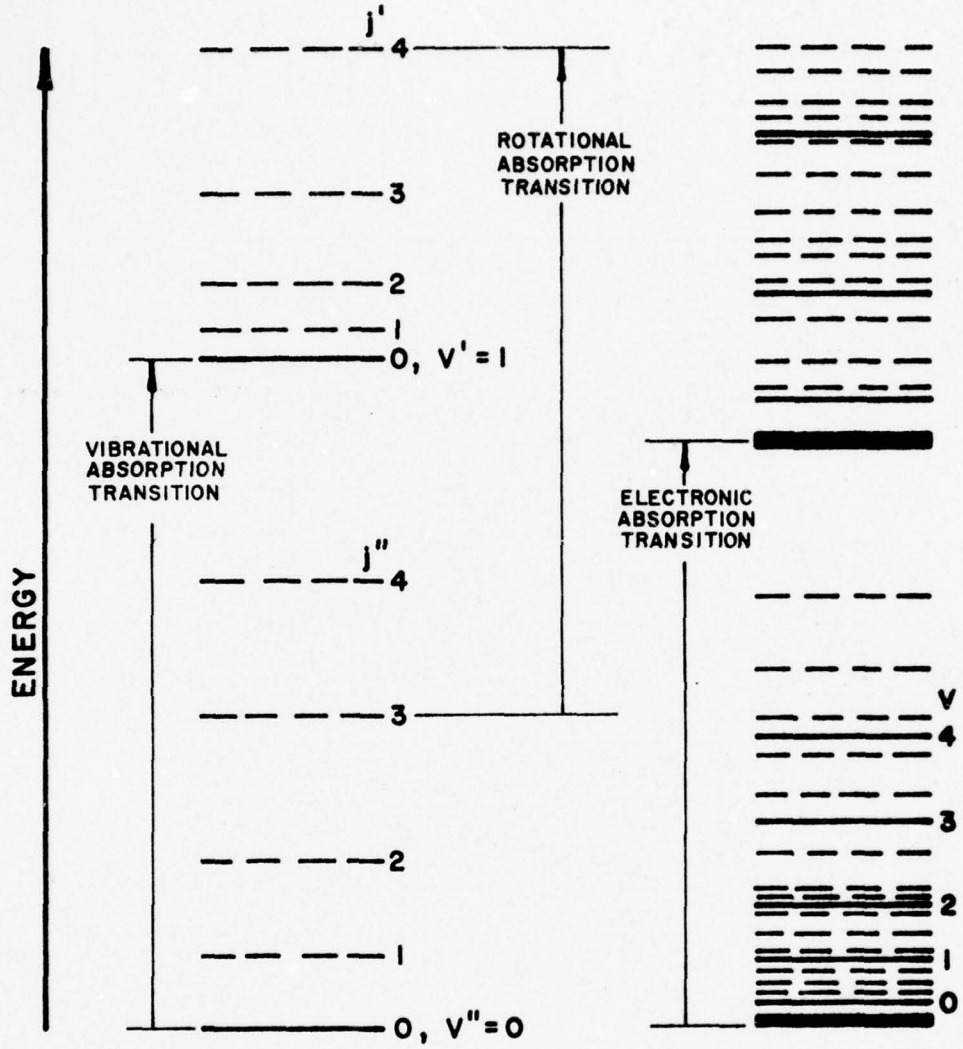


Figure 2.3-1. Diagram of Vibrational and Rotational Levels of Two Electronic States of a Molecule [Adapted from [Orchin[37]].

The number of different vibrational transitions accompanying a change in electron energy and the number of different rotational transitions associated with a change in the vibrational energy of a molecule may be very large. This is responsible for the extremely complex structure of molecular spectra. Additionally vibrational or rotational levels of a molecule may overlap with each other. Figure 2.3-2 shows the vibrational modes of carbon dioxide and water vapor, two of the atmospheric consituents that have absorption lines in the infrared spectrum.

Detailed discussion of the energy level selection rules may be found in Kroto[25] or Goody[15]. The interaction of electronic, vibrational, and rotational energies may, as a first approximation, be considered as additive. Thus, if the energies were strictly independent, the selection rules for a combined transition could be regarded as a combination of the three separate selection rules. Atoms and molecules can exhibit electronic line spectra, but the overall complexity, overlapping, and simultaneous changes of all three forms of quantized energy of molecules requires band systems.

Lastly, we consider a fundamental property under the classical theory of a molecule. That is the electric dipole moment. This moment is defined as the product of the magnitude of an electric charge and the distance between it and its opposite charge. It is this property by which absorption occurs. The electromagnetic radiation absorption happens when an electric field interacts with the motion of the molecule, changing the dipole moment and bringing about an

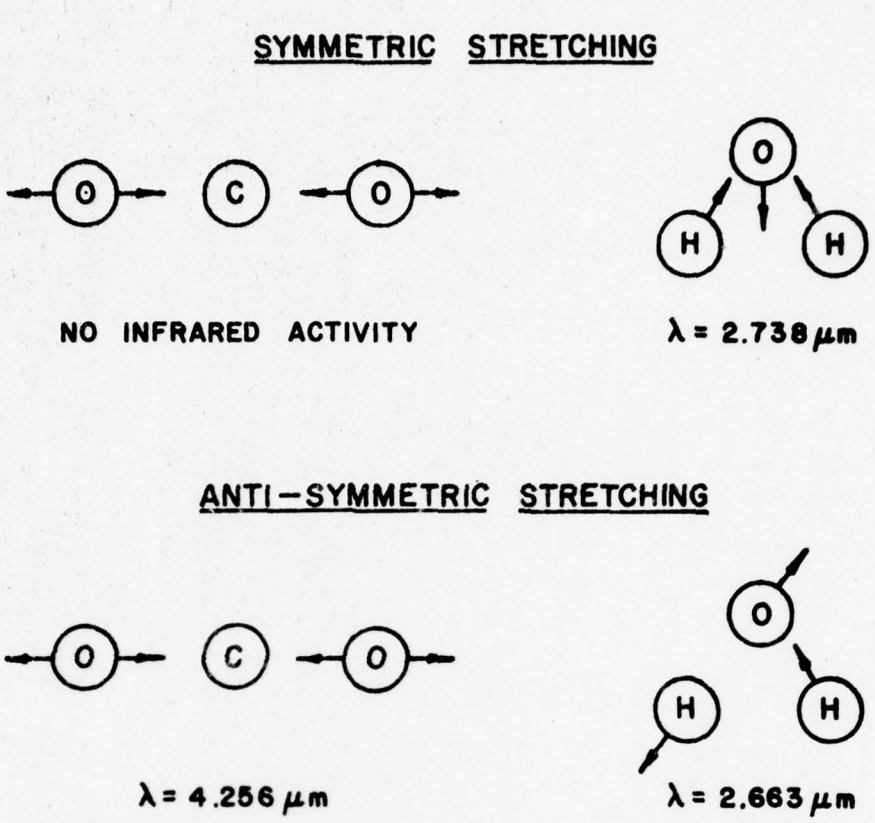


Figure 2.3-2. Vibrational Modes of CO_2 and H_2O [Hudson[18]].

energy transition. In symmetric molecules some vibrational modes produce no change in dipole moment. As a consequence, no infrared activity occurs.

2.4 Spectral Line Broadening

Thus far in the discussion of spectral lines it has been stated that the position (frequency) of an absorbing line due to an allowed energy transition may be predicted exactly by Eq. 2.3-2. While in theory this is true, in practice the line that is observed is not a singled frequency slit from the electromagnetic spectrum. The line is widened by a phenomenon termed line broadening. The expansion is due to a variety of reasons [Breene[4]], but only three will be discussed here. Natural line-broadening, Doppler line-broadening, and pressure or Lorentz line-broadening are the main mechanisms considered for atmospheric calculations and are therefore, developed below. The line breath is conventionally taken as the spectral width corresponding to the half maximum intensity points on the curve describing the line. The profiles are assumed symmetric hence, half the line breath is used in characterizing the line shape, and is termed the half width. Figure 2.4-1 depicts the Doppler line shape, the Lorentz line shape and the half width of each.

2.4.1 Natural Broadening

The uncertainty principle states that the product of the uncertainty of our knowledge of the energy and mean life of an atomic state cannot be less than Planck's constant divided by 4π. Since every excited state of a molecule has a finite lifetime, its energy

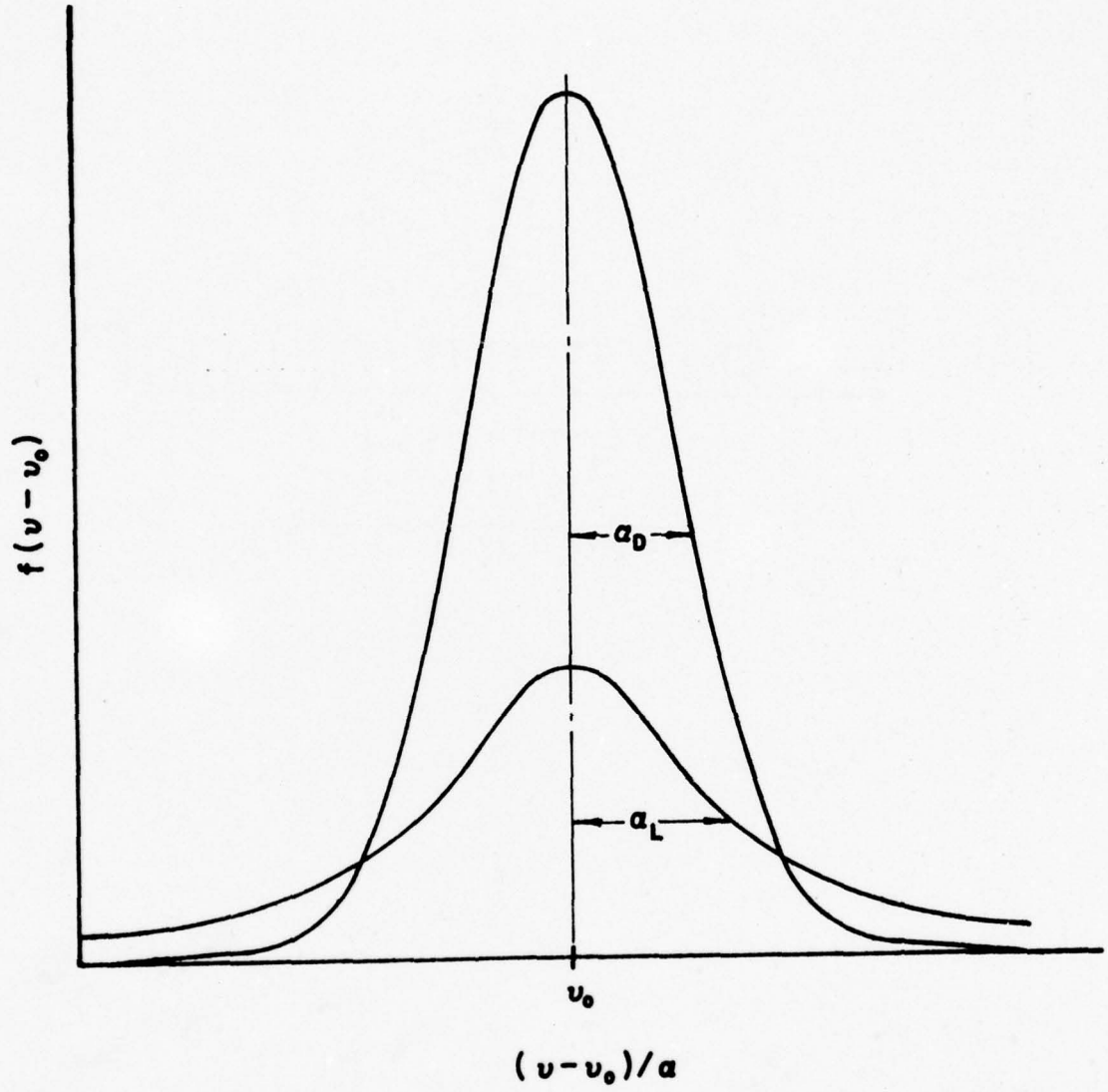


Figure 2.4-1. Doppler and Lorentz Line Shapes and Half Widths [Jaimeson, et al[22]].

cannot be measured exactly. Thus, because we do not know precisely a molecule's energy transition, we cannot know absolutely the frequency of emmission or absorption [Jamieson, et al[22]]. This uncertainty leads to a lower limit of the width of an observed spectral line, termed the natural width (α_N). It is given by

$$\alpha_N = \frac{1}{4\pi\phi_i} \quad , \tag{2.4-1}$$

where ϕ_i is the lifetime of an energy transition. For a typical vibrational transition ϕ_i is of the order of 0.1 seconds [Goody[15]]. Thus, from Eq. 2.4-1, α_N is of the order of $3 \cdot 10^{-11}$ cm^{-1}, in wave numbers. This is trivial when compared to other line widths and is neglected for atmospheric calculations.

2.4.2 Doppler Broadening

If a monochromatic radiation source is moving with velocity whose component in the line of sight to the observer is u, the frequency appears shifted by an amount

$$\Delta\nu = \frac{u}{c}\nu_o \quad , \tag{2.4-2}$$

compared with the frequency of the source when it is at rest (ν_o). This change is termed the Doppler Effect.

For a stratified atmosphere it may be assumed that the translational states of molecules are in thermodynamic equilibrium and their

velocity u, relative to an observer, is given by the Maxwell velocity distribution [Kuhn[26]]

$$p(u) = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mu^2}{2kT}\right), \qquad (2.4\text{-}3)$$

where m is the mass of the molecule,
k is Boltzman's constant,
and T is temperature in °K.

When u<<c this probability function for velocity manifests itself in a broadening of the spectral line observed.

Defining the doppler half width at half maximum [Anding[2]] as

$$\alpha_D = \frac{\nu_o}{c}\left(\frac{2kT\ln 2}{M}\right)^{1/2}$$

$$= 3.58\cdot 10^{-7}\left(\frac{T}{M}\right)^{1/2}\nu_o, \qquad (2.4\text{-}4)$$

where M is molecular weight, the line shape is predicted by

$$f(\nu-\nu_o) = \left(\frac{\ln 2}{\pi}\right)^{1/2}\frac{1}{\alpha_D}\exp\left\{-\frac{\nu-\nu_o}{\alpha_D}\right\}. \qquad (2.4\text{-}5)$$

Goody[15] gives the two extreme values for α_D as $3.3\cdot 10^{-2}$ cm^{-1} and $3.5\cdot 10^{-4}$ cm^{-1}.

2.4.3 Pressure Broadening

The interaction of a radiating particle with another particle has an effect on the spectral line which is very complex in nature. In order to make the problem manageable it is necessary to introduce simplifying assumptions whose justifications are not often obvious and whose validity is limited. The theory of pressure broadening has developed from two opposite viewpoints. Following Lorentz, it is considered that a collision breaks the otherwise unperturbed wave train of a radiating particle. The line width is then determined, not by the natural life time T, but by the shorter time T_c between collisions. A fourier analysis of the wave train leads to a line width proportional to $1/T_c$; the effect is a kinetic one, depending on the relative velocities of the molecules.

The statistical approach was first applied by Holtsmark[17] to the effect of ions on each other. It was later applied by others to the mutual effects of neutral atoms. It neglects the motion of the atoms and regards them as being at rest, but distributed randomly in space. The characteristic frequency of the radiating or absorbing molecule is changed by the presence of another molecule according to some function of the distance separating them. Each molecule can be regarded as emitting one frequency at any given time, but the random effect of many radiating molecules leads to a continuous intensity distribution whose calculation is purely statistical in nature.

The Fourier analysis of the emitted radiation of a particle that has been interrupted by a collision, leads to an expression for the intensity of the disturbed wave function [Breene[4]] of

$$I(\nu) \alpha R\left\{\int_{-\infty}^{\infty} dt \exp\left(2\pi i(\nu_o-\nu)t\right) \overline{\exp 2\pi i\, \eta(t)}\right\} \qquad (2.4\text{-}6)$$

where $I(\nu)$ is intensity as a function of ν,

R is the operation of taking the real part of the expression,

$\eta(t)$ is the phase shift due to interaction as a function of time, and the bar over the function indicates a time averaging.

Now if there is negligible phase shift before time t, then an encounter occurs and the integral terminates, we have

$$I(\nu) \alpha R\left\{\int_{o}^{t} dt' \exp(2\pi i(\nu_o-\nu)t')\right\}$$

$$= R\left\{\frac{1}{2\pi i(\nu_o-\nu)} \left[\exp(2\pi i\left\{(\nu_o-\nu)t\right\})-1\right]\right\}$$

$$= \frac{\sin 2\pi(\nu_o-\nu)t}{2\pi(\nu_o-\nu)} \cdot \qquad (2.4\text{-}7)$$

This result is now averaged over all possible values of t, while neglecting the time spent in collision. The interruption theory has now become impact theory.

According to the kinetic theory of gases, the distance (l) traveled between collisions by a molecule with velocity u follows the distribution function

$$p(l)\ dl = \frac{dl}{\bar{l}_u}\ \exp(-l/\bar{l}_u)\ , \qquad (2.4\text{-}8)$$

where $\bar{l}_u$ is the mean free-path for molecules of velocity u. The distribution function for the time between collisions follows from the substitution udl = dt, and is given by

$$p(t)\ dt = \frac{dt}{T_c}\ \exp\left(-\frac{t}{T_c}\right)\ , \qquad (2.4\text{-}9)$$

where T_c is again the mean time between collisions. Now the product of Eq. 2.4-9 and Eq. 2.4-7, integrated over all time yields [Goody[15]]

$$I(\nu,u) = \frac{1}{(\nu-\nu_o)^2 + \left(\frac{1}{2\pi T_c}\right)^2}\ ,$$

which if normalized so that its area for all ν is unity, may be written as

$$f(\nu,u) = \frac{1}{\pi}\ \frac{\alpha_L(u)}{(\nu-\nu_o)^2 + \alpha_L^2(u)}\ , \qquad (2.4\text{-}10)$$

where the Lorentz line width (α_L) is defined as

$$\alpha_L(u) = \frac{1}{2\pi T_c} \quad . \tag{2.4-11}$$

The Lorentz line width is very strongly dependent upon pressure and temperature [Zuev[54]] and is often approximated by

$$\alpha_L = \alpha_{L_o}\left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)^n \quad . \tag{2.4-12}$$

The subscript zero denotes some reference width calculated at the reference pressure P_o and temperature T_o. The exponent n is an empirically derived number, usually set to 0.5.

Having replaced the velocity dependence of α_L with a pressure, temperature relation, the common form of the Lorentz line shape (Pressure Broadening) is given as

$$f(\nu,\alpha_L) = \frac{1}{\pi} \frac{\alpha_L}{(\nu-\nu_o)^2 + \alpha_L^2} \quad . \tag{2.4-13}$$

Typical values for α_L range from 0.055 cm^{-1} for methane to 0.11 cm^{-1} for ozone [McClatchey, et. al[31]].

2.5 Summary

A knowledge of the composition and properties of the atmosphere, together with an understanding of molecular energy transitions, and spectral line broadening are the tools to be used for atmospheric absorption computations. It is possible to identify those molecules

that absorb radiation and determine, to some degree of accuracy, the center frequency absorbed. It is also possible to roughly predict the shape of the spectral line, given information on the composition of the atmosphere. This information, when calculated accurately, may be used for the temperature retrieval scheme alluded to in the introduction [McClatchey[33]].

CHAPTER III

TRANSMITTANCE AND THE VOIGT FUNCTION IN THE FIFTEEN MICROMETER BAND

3.1 Preface

This Chapter addresses the subject of atmospheric transmittance with the combined effects of Doppler and Pressure line broadening. The definitions of absorption and transmittance are first presented then a function including both types of spectral line spreading is developed. This function is then introduced into the transmittance differential equation and the final form of the transmittance relation is given. Next the frequency band used here is briefly discussed, together with the validity of the assumptions made that limit investigation to this interval. Finally a summary of the important aspects of the chapter is given.

3.2 Absorption and Transmittance

The interaction of radiation with matter can lead to three types of changes in the energy. (1) Reflection, in which a part of the incident energy is deflected back. The reflected radiation as a fraction of that incident is the power of reflection of the substance. (2) Scattering, a part of the radiation energy incident at a definite direction is scattered in all directions. This is caused by an interaction depending on the relationship of the radiation wave length to the scattering particle size or certain optical flaws, such as differences in refractive index in the material. (3) Absorption, by which is designated the conversion of radiation energy into heat. The

portion of the energy transformed, expressed as a fraction of the incident energy, is known as the power of absorption. Chapter two developed the molecular model used for this energy absorption and now the model to predict absorption not on a molecular level, but a quantitative level, is developed.

These three effects depend in a characteristic manner on the wave length of the radiation and also on the specific properties of the substance to be investigated. For the infrared region, only the last effect is important [La Rocca and Turner[28]]. Therefore it will be discussed exclusively.

The radiant energy of a definite monochromatic frequency ν passing into a body of length Δx, as shown in Fig. 3.2-1, is denoted $I_\nu(X_1)$. The emanating energy is reduced by some amount, proportional to the length Δx, and is denoted $I_\nu(X_2)$.

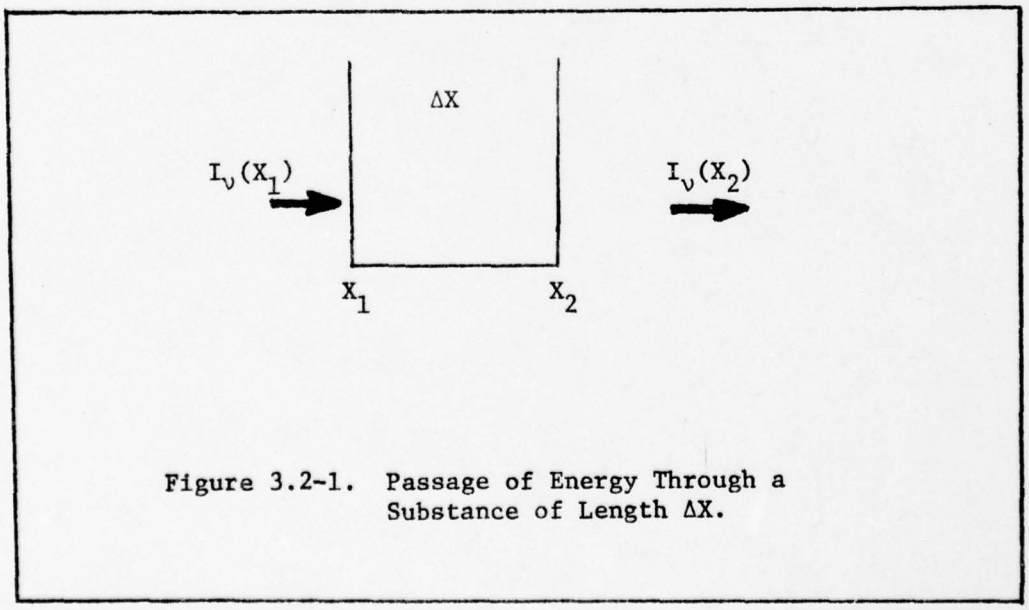


Figure 3.2-1. Passage of Energy Through a Substance of Length ΔX.

For atmospheric purposes it is recognized that the reduction in intensity of the radiation is due to the absorption of a portion of the energy by the molecules present in the path. Figure 3.2-1 is expressed mathematically as

$$I_\nu(X_2) = \alpha I_\nu(X_1)\ \Delta X$$

or in differential form

$$dI_\nu(X) = -I_\nu(X)\ \alpha dX. \qquad (3.2\text{-}1)$$

The constant of proportionality is termed α and is also called the extinction coefficient. The negative sign is due to the reduction in intensity. Equation 3.2-1 is integrated to obtain

$$\int_{I_\nu(o)}^{I_\nu(x)} \frac{d\ I_\nu(x)}{I_\nu(x)} = \int_o^x -\alpha dx,$$

$$\ln \frac{I_\nu(x)}{I_\nu(o)} = -\alpha x,$$

and finally

$$I_\nu(x) = I_\nu(o)\ \exp(-\alpha x). \qquad (3.2\text{-}2)$$

Equation 3.2-2 is known as the absorption law and is usually named after Lambert-Bouguer. The index αx is called the optical

density [Brugel[6]]. The optical density is an index of a power and must be dimensionless. The layer thickness x is usually measured in centimeters, thus the extinction coefficient is expressed in cm^{-1}.

A graphical representation of the optical density (αx), or the radiation energy transmitted ($I_\nu(x)$), both for a constant layer thickness (x); or the extinction coefficient (α) as a function of frequency, give the spectrum of the substance investigated. However, other quantities are usually used in the representation of spectra, namely the transmittance (τ) or the absorption (A), both given as a percentage of the incident radiation. The first is defined as the ratio of the energy passed to that which was incident. So from Eq. 3.2-2,

$$= \frac{I_\nu(x)}{I_\nu(o)} = \exp(-\alpha x). \qquad (3.2\text{-}3)$$

The absorption (A) is defined as

$$A = 1-\tau = 1-\exp(-\alpha x). \qquad (3.2\text{-}4)$$

Accordingly, the extinction (E) is defined

$$E = -\ln\tau = \ln\frac{1}{\tau} = \ln\frac{I_\nu(o)}{I_\nu(x)} \cdot \qquad (3.2\text{-}5)$$

The law of absorption (Eq. 3.2-2) gives a first quantitative unit for spectral measurements. Obviously, the absorption of a body is larger

the greater the thickness x, or the larger the extinction coefficient α, for the wavelength in question. In the last resort, however, the number of molecules absorbing in the volume is what is responsible for the absorption. Accordingly the extinction coefficient suffices completely for the description of the absorption power of a substance provided the number of molecules in the volume under consideration remains constant. Unfortunately this does not apply to the atmosphere where the number of molecules per unit volume is dependent upon the pressure. Therefore a relation must be derived between the concentration of a substance and the absorption it causes. Since in the atmosphere the number of molecules responsible for the absorption depends directly on the pressure, it is logical to write the extinction as a linear function of the concentration (or density) of the absorbing gas.

$$E = K \rho(x)dx \tag{3.2-6}$$

This equation is referred to as Beer's Law, in honor of its discoverer, A. Beer. Now from Eqs. 3.2-6 and 3.2-5 we obtain

$$\tau = \exp(-K\rho(x)dx). \tag{3.2-7}$$

This combined relationship of Eq. 3.2-6 and Eq. 3.2-5 is known as the Lambert-Beer Law.

For mixtures of absorbing materials the incremental absorption is additive in the absence of chemical interaction [Whiffen[51]]. Thus Eqs. 3.2-2 and 3.2-7 may be rewritten as

$$I_\nu(x) = I_\nu(o)\ \exp(\Sigma_j -\alpha_j x), \qquad (3.2\text{-}8)$$

and

$$\tau = \exp(-\Sigma_j K_j \rho_j(x)dx), \qquad (3.2\text{-}9)$$

where the sumation over j accounts for the different gases in the atmosphere. Equation 3.2-9 is the basis of the whole infrared spectral analysis. It is true in most cases for monochromatic radiation. However care must be taken when it is applied to a band, as must be done with any measurement instrument. Brugel[6] contains a discussion of the limits of Eq. 3.2-9.

3.2.1 The Transmittance Differential Equation

While Eq. 3.2-9 is correct, it is not in a convenient form for calculation of atmospheric transmittances from the top of the atmosphere to the bottom (ground level). Beginning with a form of Eq. 3.2-1 and utilizing Beer's Law the starting relation is given as

$$dI = -I\ K\rho(x)dx. \qquad (3.2\text{-}10)$$

The expressed dependence of intensity (I) and the absorption coefficient (K) on wavelength, temperature, and pressure is dropped, but still understood. Rearranging 3.2-10 we obtain

$$\frac{dI}{I} = -K\rho(x)dx.$$

The hydrostatic equation (2.2-1) relates density (ρ) to pressure (P) in the manner desired. It is restated below without the negative

sign. For atmospheric considerations we begin at altitude Z and pressure P and move down to altitude Z-ΔZ and pressure P+ΔP. Also the mixing ratio M(P) is introduced to reflect a relation between total pressure and the pressure of only one gas under consideration. Chapter five contains a detailed explanation of Eq. 3.2-11.

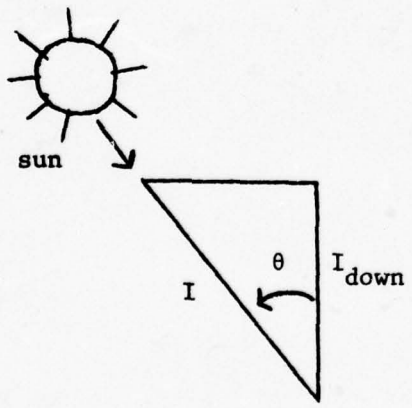
$$\frac{dP}{g} = \frac{1}{M(P)\rho(x)dx} \tag{3.2-11}$$

This yields

$$\frac{dI}{I} = -\frac{KM}{g}\,dP, \tag{3.2-12}$$

where the dependence of the mixing ratio on pressure is understood.

Instruments measure that portion of the intensity of radiation directed downward only and what needs to be considered is the total intensity. If θ is the solar zenith angle, from Fig. 3.2-2 Eq. 3.2-12 becomes



$$\cos\theta = \frac{I_{down}}{I}$$

$$I = I_{down}\sec\theta$$

Figure 3.2-2. Solar Zenith Angle θ And Downward Intensity I_{down}.

$$\frac{dI}{I} = -K \frac{M \sec \theta}{g} dP.$$

Integrating this equation from the top of the atmosphere (P=0, $I=I_o$) to a point where the pressure is P and the intensity I, yields,

$$\int_{I=I_o}^{I=I} \frac{dI}{I} = - \frac{\sec \theta}{g} \int_o^P MKdP,$$

$$\ln \frac{I}{I_o} = - \frac{\sec \theta}{g} \int_o^P MKdP,$$

or from the definition of transmittance,

$$\tau = \exp \left\{ - \frac{\sec \theta}{g} \int_o^P KMdP \right\}. \qquad (3.2\text{-}13)$$

Now at a reference point (T_o, P_o) calculate a reference transmittance τ_o and let

$$c = \frac{\sec \theta}{g}. \qquad (3.2\text{-}14)$$

Thus,

$$\tau_o = \exp \left\{ -c \int_o^{P_o} KMdP \right\},$$

and at any other position given by $P = P_o + \Delta P$, calculate

$$\tau = \exp\left\{ -c \int_{o}^{P=P_o+\Delta P} KMdp \right\} .$$

Dividing this expression by the reference transmittance gives

$$\frac{\tau}{\tau_o} = \exp\left\{ -c \left[\int_{o}^{P_o+\Delta P} KMdp - \int_{o}^{P_o} KMdP \right] \right\}$$

$$\frac{\tau}{\tau_o} = \exp\left\{ -c \int_{P_o}^{P_o+\Delta P} KMdP \right\} .$$

Now let $P_o = P_r$, a reference pressure

$\tau_o = \tau_r$, the associated reference transmittance

$P = P_o+\Delta P$, and

$$\tau = \tau_r \exp\left\{ -c \int_{P_r}^{P} KMdP \right\} . \qquad (3.2\text{-}15)$$

We may place this relation in differential equation form.

$$\frac{\tau}{\tau_r} = \exp\left\{ -c \int_{P_r}^{P} KMdP \right\}$$

$$\ln \frac{\tau}{\tau_r} = -c \int_{P_r}^{P} KMdP$$

$$\frac{d}{dP}\left\{ \ln \frac{\tau}{\tau_r} \right\} = \frac{d}{dP}\left\{ -c \int_{P_r}^{P} KMdP \right\}$$

$$\frac{\tau_r}{\tau} \cdot \frac{1}{\tau_r} \cdot \frac{d\tau}{dP} = \frac{d}{dP}\left\{ -c \int_{P_r}^{P} KMdP \right\}$$

Using Leibnitz's rule for differentiating an integral [Spiegel[44]],

$$\frac{1}{\tau}\frac{d\tau}{dP} = -c\left[\int_{P_r}^{P} \frac{d}{dP}(KM)dP + KM\frac{dP}{d\nu} - KM\frac{dP_r}{d\nu} \right].$$

Since K is a function of ν, the last two terms follow. Neither P nor P_r are functions of ν, so $\frac{dP}{d\nu} = \frac{dP_r}{d\nu} = 0$.

$$\frac{1}{\tau}\frac{d\tau}{dP} = -c\int_{P_r}^{P}\frac{d}{dP}(KM)dp$$

Using the fundamental theorm of calculus [Britten, et al[5]],

i.e.: if $f(x) = \frac{d}{dx}g(x)$

then $\int f(x)dx = \int \frac{d}{dx}g(x)dx = g(x)$,

subject to boundary conditions;

$$\frac{1}{\tau}\frac{d\tau}{dP} = -cKM.$$

Writing this expression to explicitly show the functional dependence upon frequency, temperature, and pressure and utilizing the knowledge that the extinction coefficient (K) of each gas may be superimposed (as in Eq. 3.2-9), the transmittance differential equation is obtained.

$$\frac{d\tau(\nu,T,P)}{dP} = \left\{-\frac{\sec\theta}{g}\sum_j K_j(\nu,T,P)M_j(P)\right\}\tau(\nu,T,P). \quad (3.2\text{-}16)$$

The iterative solution of this expression yields the desired transmittance values from the top of the atmosphere to ground level.

3.2.2 The Absorption Coefficient $K(\nu,T,P)$

For a given gas there exists a variety of forms for the absorption coefficient $K(\nu,T,P)$ [L'Vov[30]]. In general the coefficient can be written

$$K_j(\nu,T,P) = \sum_i S_{ij}\, f(\nu-\nu_{o_{ij}}). \qquad (3.2\text{-}17)$$

S_i represents the strength of the ith spectral line, ν_{o_i} is the center frequency of the line and the function $f(\nu-\nu_{o_i})$ defines the line shape of the ith line. In theory the contribution of each spectral line is added together (the summation over i) to obtain an absorption coefficient for a molecular species (gas type). Several authors give expressions for the line intensity (S_i) [Goody[15], Hertzberg[16]]. Miller, et al.[35] gives

$$S_{ij} = S_{o_{ij}}\, Q_j(T) \left(\frac{T_o}{T}\right)^{C_j} \exp\left\{\frac{E_{ij}}{kT_o}\left(1 - \frac{T_o}{T}\right)\right\}, \qquad (3.2\text{-}18)$$

where S_o is a reference strength calculated at (T_o,P_o),

E is the energy of the lower state involved in the molecular transition,

k is the Boltzman's constant,

T is temperature in degrees Kelvin, and

Q is the vibrational partition function.

This strength function is one that currently being used for atmospheric transmittance calculations and is adopted here.

What remains of Eq. 3.2-17 to be specified is the line shape function. Chapter two enumerated the three most important line broadening mechanisms. In practice the investigator must decide if the problem at hand can be resolved by a single broadening function or if a more complicated one is needed to accurately describe the absorption coefficient. There are several approaches to the problem and the interested individual is referred to Miller, et al.[35], Anding[2], or La Rocca and Turner[28]. For rapid line-by-line computation of transmittance at the sacrifice of some accuracy the Lorentz line shape function is generally used [Potter[40], Gibson[14]]. The shape function employed in this work is developed in the next section.

3.3 The Voigt Function

The first twenty years of the twentieth century were marked by considerable achievements in the field of atomic absorption theory. During this period the fundamental relationships between absorption and the atomic constants were established and, as was discussed in Chapter two, the theory for pressure broadening of lines was formulated [Lorentz[29]]. The theory of Natural and Doppler broadening had been already developed. While several individuals realized that line broadening phenomena could not be completely predicted unless all causes were accounted for, it was W. Voigt[48] who first proposed that the effects of Doppler and Collision broadening could be dealt with in a single line shape function. Today this relation bears his name.

The relation may be derived by assuming that the line shape function follows a Doppler profile near the center and Lorentz in the wings.

The Lorentz line shape was developed in Chapter two and is restated here.

$$f(\nu-\nu_o) = \frac{1}{\pi} \frac{\alpha_L}{(\nu-\nu_o)^2 + \alpha_L^2} . \tag{3.3-1}$$

The Doppler effect that causes a frequency shift of the monochromatic wavelength (ν_o), emitted by a molecule at rest, is written

$$\nu_o' = \nu_o(1 - \frac{u}{C}). \tag{3.3-2}$$

Again u is the line-of-sight velocity component of the molecule. From Eq. 3.3-2 two relations to be used later are obtained.

$$u^2 = \frac{C^2(\nu_o' - \nu_o)^2}{\nu_o^2} \tag{3.3-3}$$

$$du = \frac{C}{\nu_o} d\nu_o' \tag{3.3-4}$$

Now if the translational states of the molecules under consideration are in thermodynamic equilibrium, the fractional number of molecules with velocities between u and u + du is given by the Maxwell velocity distribution p(u).

$$p(u)du = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mu^2}{2kT}\right) du \tag{3.3-5}$$

Substituting Eq. 3.3-3 and 3.3-4 into 3.3-5 yields

$$p(u)du = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left[-\frac{mc^2(\nu_o' - \nu_o)^2}{2kT\nu_o^2}\right] \frac{C}{\nu_o} d\nu_o'. \tag{3.3-6}$$

The contribution to the shaping function from all Doppler shifted components will be the probability function p(u)du times the Lorentz line shape, integrated over all frequencies. It may be expressed as

$$f(\nu - \nu_o) = \int_{-\infty}^{\infty} p(u)\, f'(\nu - \nu_o)du. \qquad (3.3\text{-}7)$$

The function $f'(\nu - \nu_o)$ is given by Eq. 3.3-1 with the center frequency of absorption (ν_o) replaced by the Doppler shifted frequency (ν_o'). Thus,

$$f'(\nu - \nu_o) = \frac{1}{\pi} \frac{\alpha_L}{(\nu - \nu_o')^2 + \alpha_L^2}, \qquad (3.3\text{-}8)$$

and

$$\nu - \nu_o' = (\nu - \nu_o) - (\nu_o' - \nu_o). \qquad (3.3\text{-}9)$$

Now utilizing Eqs. 3.3-9, 3.3-8, 3.3-6 and 3.3-7 the combined Doppler-Lorentz function is obtained [Voigt[47]].

$$f(\nu-\nu_o) = \int_{\infty}^{\infty} \frac{1}{\pi} \frac{\alpha_L \exp - \left[\frac{mc^2(\nu_o'-\nu_o)^2}{2kT\nu_o^2}\right]}{[(\nu-\nu_o) - (\nu_o'-\nu_o)]^2 + \alpha_L^2} \left(\frac{m}{2\pi kT}\right)^{1/2} \frac{c}{\nu_o} d\nu_o' \qquad (3.3\text{-}10)$$

Defining the variable

$$t = \left(\frac{mc^2}{2kT}\right)^{1/2} \left(\frac{\nu_o' - \nu_o}{\nu_o}\right), \qquad (3.3\text{-}11)$$

we have immediately,

$$t^2 = \frac{mc^2}{2kT}\left(\frac{\nu_o' - \nu_o}{\nu_o}\right)^2 \tag{3.3-12}$$

and

$$dt = \left(\frac{mc^2}{2kT}\right)^{1/2} \frac{d\nu_o'}{\nu_o} \tag{3.3-13}$$

So now Eq. 3.3-10 becomes

$$f(\nu-\nu_o) = \frac{1}{\pi}\int_{\infty}^{\infty} \frac{\alpha_L \exp[-t^2]\nu_o\left(\frac{2kT}{mc^2}\right)^{1/2}}{[(\nu-\nu_o)-(\nu_o'-\nu_o)]^2 + \alpha_L^2}\left(\frac{mc^2}{2\pi kT}\right)^{1/2}\frac{1}{\nu_o}\,dt. \tag{3.3-14}$$

$$= \frac{1}{\pi}\left(\frac{mc^2}{2\pi kT\nu_o^2}\right)^{1/2}\alpha_L \int_{-\infty}^{\infty} \frac{\exp(-t^2)\,dt}{\frac{1}{\nu_o}\left(\frac{mc^2}{2kT}\right)^{1/2}\left\{[(\nu-\nu_o)-(\nu_o'-\nu_o)]^2 + \alpha_L^2\right\}}$$

$$= \frac{1}{\pi^{3/2}}\left(\frac{mc^2}{2kT\nu_o^2}\right)^{1/2}\alpha_L \int_{-\infty}^{\infty} \frac{\left(\frac{mc^2}{2kT\nu_o^2}\right)^{1/2}\exp(-t^2)\,dt}{\left[\left(\frac{\nu-\nu_o}{\nu_o}\right)\left(\frac{mc^2}{2kT}\right)^{1/2} - \left(\frac{\nu_o'-\nu_o}{\nu_o}\right)\left(\frac{mc^2}{2kT}\right)^{1/2}\right]^2 + \left(\frac{mc^2}{2kT\nu_o^2}\right)\alpha_L^2} \tag{3.3-15}$$

Now using Eq. 3.3-11 again and defining

$$\alpha_D = \left(\frac{2kT}{mc^2}\right)^{1/2} \nu_o, \tag{3.3-16}$$

$$\frac{\alpha_L}{\alpha_D} = y, \quad \text{and} \quad \frac{\nu-\nu_o}{\alpha_D} = x, \tag{3.3-17}$$
$$\tag{3.3-18}$$

where α_D is the Doppler half width, the relation becomes

$$f(\nu-\nu_o) = \left(\frac{mc^2}{2kT\nu_o^2}\right)^{1/2} \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} \frac{y \exp(-t^2)dt}{[x-t]^2 + y^2} . \tag{3.3-19}$$

The absorption coefficient for the mixed Doppler-Lorentz (Voigt) function is then given by Eq. 3.2-17 and the following new definition of strength

$$K_{o_{ij}} = \frac{S_{ij}}{\alpha_D} \left(\frac{1}{\pi}\right)^{1/2} , \tag{3.3-20}$$

where S_{ij} is defined in Eq. 3.2-18. Thus

$$K_j(\nu,T,P) = \sum_i \frac{K_{o_{ij}}}{\pi} \int_{-\infty}^{\infty} \frac{y \exp(-t^2)dt}{y^2 + (x-t)^2} . \tag{3.3-21}$$

Other derivations of this Voigt profile are given in Penner[38], Goody[15], or more recently Young[53].

Combining Eq. 3.3-21 and the transmittance differential equation (3.2-16) one obtains the relation for atmospheric transmittance considering the Voigt profile. Several authors assert that this function should be used if completely accurate results are to be obtained [LaRocca and Turner[28], Anding[2], and Rodgers[41]]. The summary of this chapter collects all the equations thus far derived that are needed. The evaluation of the Voigt profile is discussed in the next chapter.

Figure 3.3-1 shows the relation between the Doppler line shape, Lorentz line shape and the Voigt profile.

3.4 The Fifteen Micron Band

Figure 3.4-1 shows the electromagnetic spectrum and the nomenclature used for different regions. This work is limited to the so called fifteen micron band. The limits of the band are not well defined and in fact depend much on the instrument used to investigate the region. As the name implies however it is generally around the 15μm portion of the spectrum.

The NIMBUS 6 High Resolution Infrared Radiation Sounder (HIRS) is a third generation infrared radiation sounding satellite possessing many new features for greatly improved capability of sounding the earth's atmosphere. The investigations of this work used the specifications of the NIMBUS 6 to calculate the transmittances needed to provide correct temperature soundings. NIMBUS 6 uses seven channels in the fifteen micron band. The channels are monitored by a multichannel filter radiometer. The band provides better sensitivity to

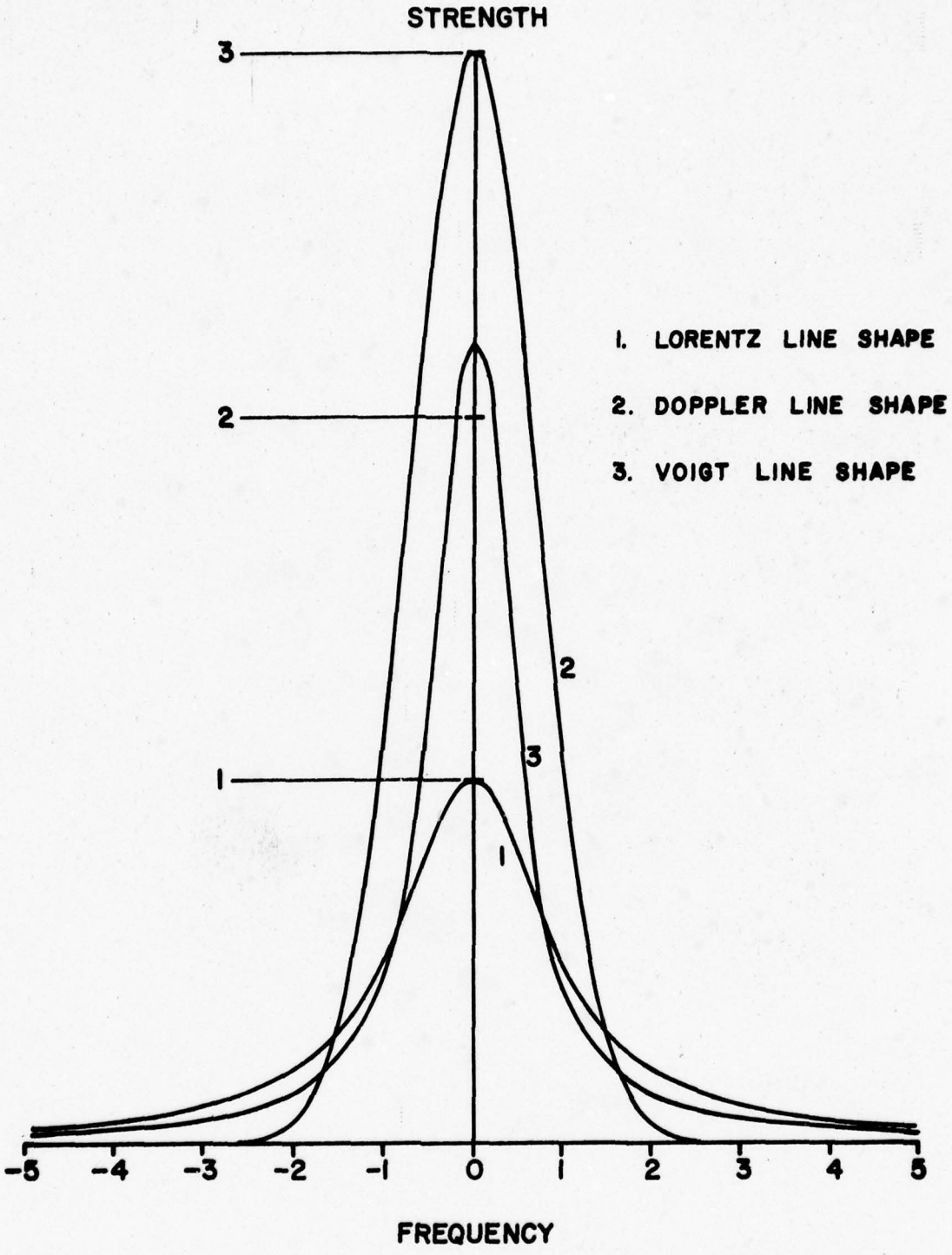


Figure 3.3-1. Doppler, Lorentz and Voigt line shapes.

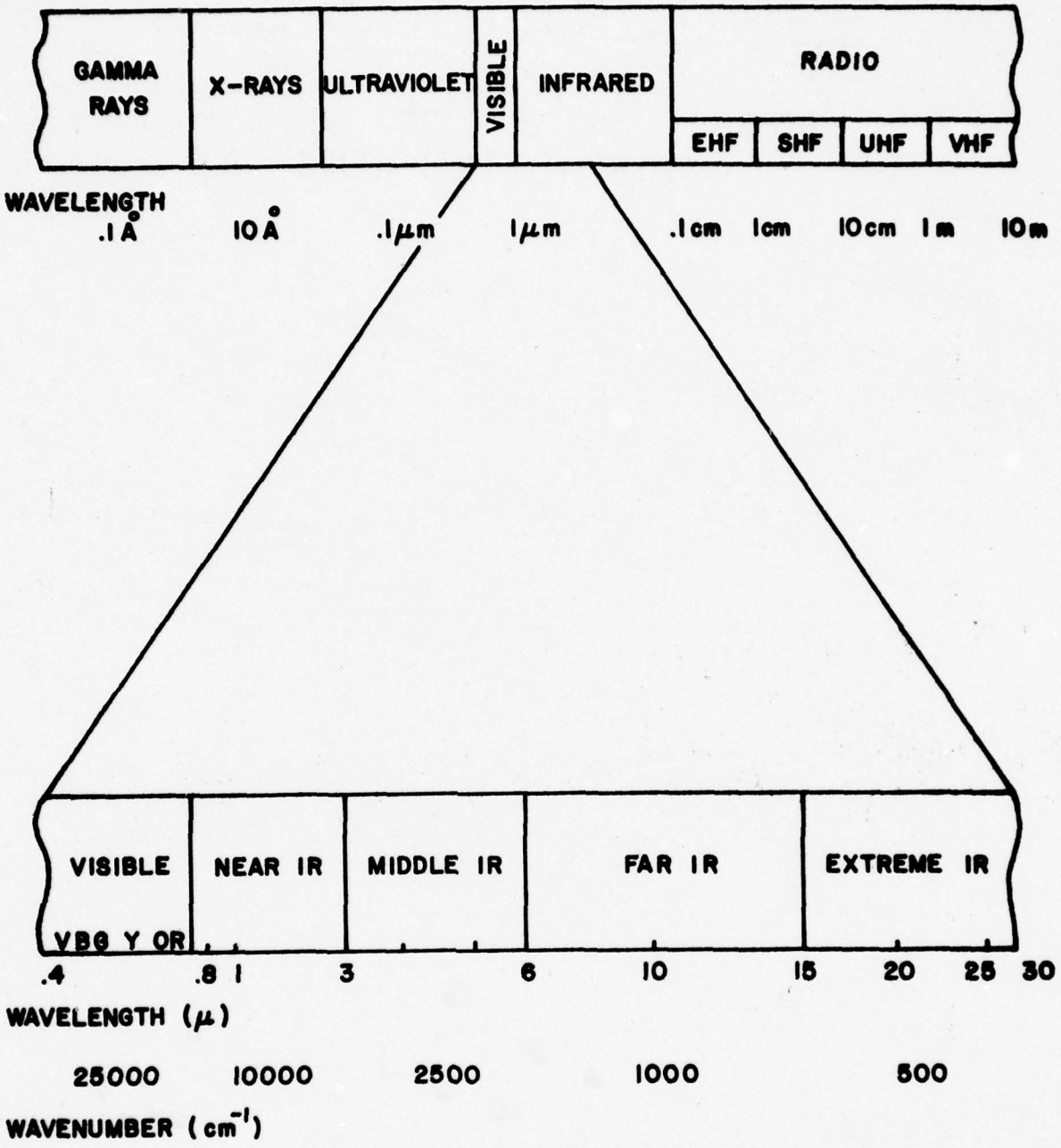


Figure 3.4-1. The Electromagnetic Spectrum.

the temperature of the relatively cold regions of the atmosphere [Sissala[43]] than can be achieved with the 4.3μm band channels. These cooler temperatures correspond to higher altitudes and lower pressures. At these levels the Lorentz line width is reduced and the Doppler line width is broadened. Therefore for most accurate transmittance calculations both line broadening schemes must be represented. For this reason the Voigt profile is used in calculations.

The important engineering aspects of NIMBUS 6 design are depicted in Table 3.4-1 and Fig. 3.4-2.

Channel Number	Central Wavenumber (cm^{-1})	Interval Between 50% Response Points (cm^{-1})	Primary Absorber	Level of Peak Energy Contribution
1	668	2.8	CO_2	30mb
2	679	13.7	CO_2	60mb
3	690	12.6	CO_2	100mb
4	702	15.9	CO_2	250mb
5	716	17.5	CO_2	500mb
6	733	17.6	CO_2/H_2O	750mb
7	749	18.4	CO_2/H_2O	900mb

Table 3.4-1. NIMBUS 6 Characteristics. (Adapted from Sissala[43])

Figure 3.4-2 depicts the filter responses for the seven channels of interest. For atmospheric calculations it is necessary to consider

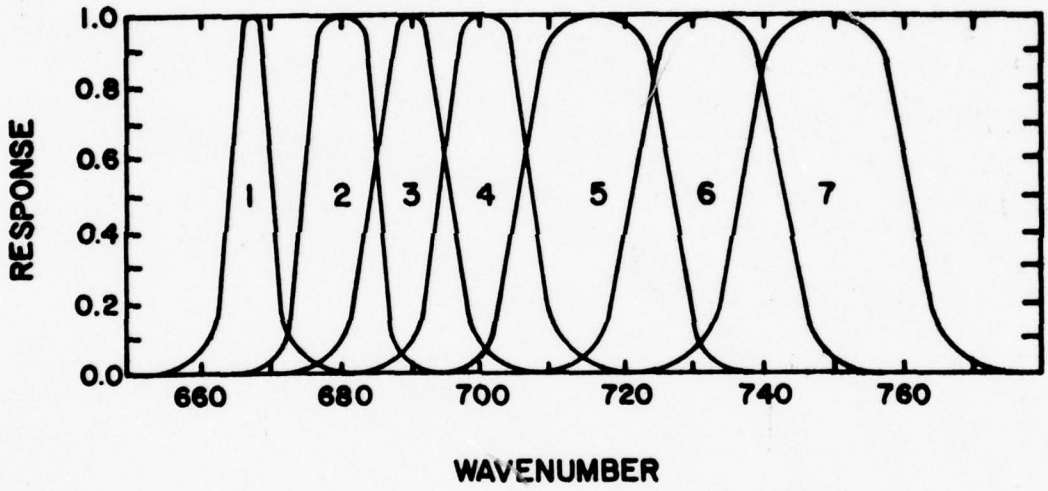


Figure 3.4-2. HIRS filter responses [Sissala[43]].

all lines whose center frequency (ν_o) is within a channel, for the transmittance of that channel. Thus, for example, the summation over i in Eq. 3.3-21 runs over those lines whose center frequency is between 665.2 cm^{-1} and 670.8 cm^{-1} for channel one. In addition it may be necessary to consider the wings of lines whose center frequency lies outside the channel interval. Figure 3.4-3 depicts such a line (wavenumber ν_{o_1}). Although the center frequency is outside the channel limits, the right wing of the line contributes to absorption within the channel.

3.5 Summary

The transmittance differential equation to be used in this investigation is given by

$$\frac{d\,\tau(\nu,T,P)}{dP} = \left\{ -\frac{\sec\theta}{g} \sum_j K_j(\nu,T,P)\, M_j(P) \right\} \tau(\nu,T,P). \qquad (3.2\text{-}16)$$

K_j is called the absorption coefficient and has different representations, depending upon the nature of the investigation. For instances where the combined effects of Doppler-Lorentz (Voigt) broadening are to be considered, the absorption coefficient is expressed by the Voigt profile,

$$K_j = \sum_i \frac{k_{o_{ij}}}{\pi} \int_{-\infty}^{\infty} \frac{y \exp(-t^2)\,dt}{y^2 + (x-t)^2} \qquad (3.3\text{-}21)$$

where

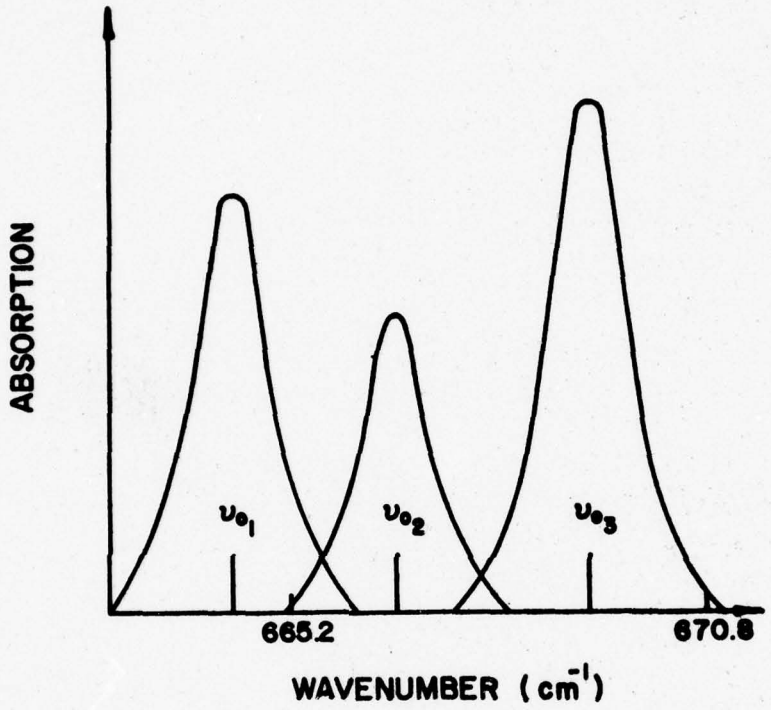


Figure 3.4-3. A spectral line (ν_{o_1}) that absorbs in channel one although its center is out of the channel.

$$K_{o_{ij}} = \frac{S_{ij}}{\alpha_D} \left(\frac{\ln 2}{\pi}\right)^{1/2} \qquad (3.3\text{-}20)$$

is the line strength,

$$y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2}, \qquad (3.3\text{-}17)$$

$$x = \frac{\nu - \nu_o}{\alpha_D} (\ln 2)^{1/2}, \qquad (3.3\text{-}18)$$

$$\alpha_L = \left(\frac{P}{P_o}\right)\left(\frac{T_o}{T}\right)^{1/2} \alpha_o , \qquad (2.4\text{-}12)$$

$$\alpha_D = 3.58 \cdot 10^{-7} \left(\frac{T}{M}\right)^{1/2} \nu_o , \qquad (2.4\text{-}4)$$

$$S_{ij} = S_{o_{ij}} Q_j(T) \left(\frac{T_o}{T}\right)^{C_j} \exp\left\{\frac{E_{ij}}{kT_o}\left(1 - \frac{T_o}{T}\right)\right\} . \qquad (3.2\text{-}18)$$

NOTE: The doppler width $\alpha_D(\ln 2)^{1/2}$ is used instead of α_D in all equations [Anding[2]].

M is the molecular weight, α_L the Lorentz half width, α_D the Doppler half width, Q the vibrational partition function (see Chapter six), E the energy of the lower state of a transition, and k Boltzman's constant. The subscript zero indicates a reference value calculated at (T_o, P_o), except when used with ν. Then it indicates the center frequency of absorption. The subscript j is for gas type and the

subscript i is for the absorbing lines. J runs for all molecular species of concern, while the i counter runs for all the lines that fall within a channel of the instrument used for measurements. The limits of the channel may have to be extended by some amount to account for the wings of lines whose center frequency is outside the channel. The channels used here and their filter responses are depicted in Table 3.4-1 and Fig. 3.4-2 respectively.

CHAPTER IV

COMPUTER ALGORITHMS FOR THE VOIGT PROFILE

4.1 Preface

The Voigt profile developed in chapter three is widely accepted but, until recently, not widely used because it is difficult to quickly evaluate. This chapter presents three methods of evaluation that are easily computerized. The first was developed by John Keilkopf, the second by S. R. Drayson and the last is a new method developed here. In searching for methods to compute the profile, speed and accuracy were the primary concerns. In a line-by-line transmittance model as much as 75% of the computional time may be used to evaluate the Voigt function. Any reduction in calculation time for the function would then obviously have a dramatic effect on the transmittance program execution time.

The accuracy required of any algorithm is about one part in 10^4. The uncertainty of absorption line parameters limit transmittance accuracy so that this degree of exactness is all that is needed. Function subprograms for each method are listed in appendices.

The results of tests for speed and accuracy of each method are presented last. The design of the examination is specified and the outcome is tabulated. The method selected for use in these transmittance calculations is specified and some comments on its applicability are given.

4.2 J. F. Kielkopf's Voigt Algorithm

The Voigt profile derived in chapter three is written in slightly

different form by Kielkopf[24]. Following the development of his algorithm the two forms will be related. Starting as Kielkopf, the Voigt profile may be written

$$V(\beta_\ell, \beta_g : \nu) = \int_{-\infty}^{\infty} \frac{\beta_\ell/\pi \exp[-(\nu'/\beta_g)^2] d\nu'}{[\beta_\ell^2 + (\nu-\nu')^2]} . \qquad (4.2\text{-}1)$$

A standardized form of the function that does not change its width or height as a function of parameters is given by

$$U(x) = \frac{V(\beta_\ell, \beta_g : \beta X)}{I(\beta_\ell, \beta_g)} , \qquad (4.2\text{-}2)$$

where $\nu = \beta x$ and the peak value of V is I. For large values of x the function may be approximated by

$$\eta = \frac{\ell}{\ell + g^2} , \qquad (4.2\text{-}3)$$

where

$$\ell = \beta_\ell/\beta , \qquad (4.2\text{-}4)$$

$$g = \beta_g/\beta . \qquad (4.2\text{-}5)$$

The letters g and ℓ represent the gaussian and lorentzian parts of the line shape respectively. Near the line core, gaussian properties appear in U and an approximation to the standardized function is

$$U(\eta : x) = (1-\eta)G(x) + \eta L(x), \qquad (4.2\text{-}6)$$

where

$$G(x) = \exp[-(\ell n2)x^2], \tag{4.2-7}$$

and

$$L(x) = \frac{1}{1+x^2}. \tag{4.2-8}$$

A function of the form of Eq. 4.2-6 has substantial errors in the limit as x grows large, however. Therefore corrections and adjustments are made to the relations used for ℓ, g, and U.

The graphs given by Van de Hulst and Reesnick[46] show that the gaussian and lorentzian portions of a line are related approximately by

$$g^2 = (1/\ln 2)(1-\ell). \tag{4.2-9}$$

A small quadratic correction results in a highly accurate relation.

$$g^2 = (1/\ln 2)[1-(1+\varepsilon\ln 2)\ell+(\varepsilon\ln 2)\ell^2] \tag{4.2-10}$$

$$\varepsilon = 0.0990$$

The lorentzian fraction is similarly

$$\ell = \frac{2}{[1+\varepsilon\ln 2+[(1-\varepsilon\ln 2)^2+(4\ln 2/a^2)]^{1/2}]} \tag{4.2-11}$$

Here a is called the Voigt parameter and is defined as

$$a = \beta_\ell/\beta_g = \frac{\ell}{g}. \tag{4.2-12}$$

From Eq. 4.2-4 we have

$$\beta = \beta_\ell / \ell \tag{4.2-13}$$

Next what is needed is the peak intensity I. It is given in terms of the complementary error function as

$$I(\beta_\ell, \beta_g) = \frac{a}{\pi^{1/2}\beta_\ell} \exp(a^2)\ \mathrm{erfc}(a). \tag{4.2-14}$$

There are a large number of methods to compute the complementary error function. The one chosen here is

$$\mathrm{erfc}(a) = f(a) \exp(-a^2) \tag{4.2-15}$$

where

$$f(a) = \frac{1}{\pi^{1/2}} (b_1 t + b_2 t^2 + b_3 t^3) \tag{4.2-16}$$

and

$$t = \frac{1}{1+b_0 a} \quad . \tag{4.2-17}$$

$b_0 = 0.47047$ $\qquad$ $b_1 = 0.61658$

$b_2 = -0.16994$ $\qquad$ $b_3 = 1.32554$

Combining Eqs. 4.2-14, 15 and 16,

$$I(\beta_\ell, \beta_g) = \frac{a}{\pi\beta_\ell} \left(b_1 t + b_2 t^2 + b_3 t^3 \right) \tag{4.2-18}$$

Beginning with Eq. 4.2-6 and adding a correction term, the final form of $U(\eta;x)$ was determined by Kielkopf[24] as

$$U(\eta;x) = (1-\eta)G(x)+\eta L(x)+\eta(1-\eta)E(x)[G(x)-L(x)]. \qquad (4.2\text{-}19)$$

The function $E(x)$ was determined empirically as

$$E(x) = \frac{0.8029 - 0.4207x^2}{1 + 0.2030x^2 + 0.07335x^4} \quad . \qquad (4.2\text{-}20)$$

Now the relation between the variables of Eq. 4.2-1 and the standard form of the Voigt profile is shown.

$$f(\nu-\nu_o) = y/\pi \int_{-\infty}^{\infty} \frac{e^{-t^2}}{y^2 + (x-t)^2}\, dt, \qquad (4.2\text{-}21)$$

where

$$x = \frac{\nu-\nu_o}{\alpha_D} (\ln 2)^{1/2}, \qquad (4.2\text{-}22)$$

$$y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2} \quad . \qquad (4.2\text{-}23)$$

Substituting these definitions in Eq. 4.2-21 yields

$$f(\nu-\nu_o) = \frac{1}{\pi} \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{\left(\frac{\alpha_L}{\alpha_D}\right)^2 \ln 2 + \left[\frac{\nu-\nu_o}{\alpha_D} (\ln 2)^{1/2} - t\right]^2}$$

$$= \frac{1}{\pi}\frac{\alpha_L}{\alpha_D}(\ln 2)^{1/2}\int_{-\infty}^{\infty}\frac{e^{-t^2}\,dt}{\frac{\ln 2}{\alpha_D^2}\left[\alpha_L^2 + [(\nu-\nu_o) - \frac{\alpha_D}{(\ln 2)^{1/2}}t]^2\right]} .$$

Now let

$$t = \nu'/\beta_g , \tag{4.2-24}$$

$$\nu-\nu_o = \nu , \tag{4.2-25}$$

$$\frac{\alpha_D}{(\ln 2)^{1/2}} = \beta_g , \tag{4.2-26}$$

$$\alpha_L = \beta_\ell , \tag{4.2-27}$$

so that

$$f(\nu-\nu_o) = \frac{1}{\pi}\frac{\beta_\ell}{\beta_g}\int_{-\infty}^{\infty}\frac{\exp\left[-\left(\frac{\nu'}{\beta_g}\right)^2\right]\frac{1}{\beta_g}\,d\nu'}{\left[\beta_\ell^2 + [\nu-\nu']^2\right]\left(\frac{1}{\beta_g}\right)^2} .$$

$$f(\nu-\nu_o) = \frac{\beta_\ell}{\pi}\int_{-\infty}^{\infty}\frac{\exp\left[-\left(\frac{\nu'}{\beta_g}\right)^2\right]d\nu'}{\beta_\ell^2 + (\nu-\nu')^2} \tag{4.2-28}$$

This is exactly the form given by Kielkopf[24], so the relations of Eqs. 4.2-24, 25, 26, and 27 are those desired.

Now in terms of the line parameters previously defined, the pro-

cedure for the algorithm is summarized.

(1) $$a = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2} \qquad (4.2\text{-}29)$$

(2) $$\ell = \frac{2}{\left\{1 + \varepsilon\ln 2 + \left[(1-\varepsilon\ln 2)^2 + (4\ln 2/a^2)\right]^{1/2}\right\}} \qquad (4.2\text{-}30)$$

$$\varepsilon = 0.0990$$

(3) $$g^2 = (1/\ln 2)[1-(1-\varepsilon\ln 2)\ell + (\varepsilon\ln 2)\ell^2] \qquad (4.2\text{-}31)$$

(4) $$\eta = \frac{\ell}{\ell+g^2}$$

(5) $$\beta = \frac{\alpha_L}{\ell} \qquad (4.2\text{-}32)$$

(6) $$x = \frac{\nu-\nu_o}{\beta} \qquad (4.2\text{-}33)$$

(7) $$I(\beta_\ell,\beta_g) = \frac{a}{\pi\alpha_L} (b_1 t + b_2 t^2 + b_3 t^3) \qquad (4.2\text{-}34)$$

$$t = \frac{1}{1+b_o a}$$

$$b_0 = 0.47047 \qquad b_1 = 0.61686$$

$$b_2 = -0.16994 \qquad b_3 = 1.32554$$

(8) $$G(x) = \exp[-(\ln 2)x^2] \qquad (4.2\text{-}35)$$

(9) $$L(x) = \frac{1}{1+x^2} \qquad (4.2\text{-}36)$$

(10) $$E(x) = \frac{0.8029 - 0.4207x^2}{1 + 0.203x^2 + 0.07335x^4} \qquad (4.2\text{-}37)$$

(11) $$U(\eta:x) = (1-\eta)G(x) + \eta L(x) + \eta(1-\eta)E(x)[G(x) - L(X)] \qquad (4.2\text{-}38)$$

(12) $$V(\beta_\ell\ \beta_g,\nu) = U(\eta:x)\ I(\beta_\ell,\beta_g) \qquad (4.2\text{-}39)$$

These twelve steps yield the desired value of the Voigt profile. The accuracy of this method is given [Kielkopf[24]] as 10^{-4} times the peak intensity. The FORTRAN IV function subprogram implementing this method is listed in Appendix A.

4.3 S. R. Drayson's Voigt Algorithm

In developing a computer algorithm to evaluate the Voigt function, Drayson required accuracy of about one part in 10^4. Beyond this the chief aim was rapid computation of the function, which is repeated here for clearity.

$$f(\nu-\nu_o) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)\ dt}{y^2 + (x-t)^2} \qquad (4.3\text{-}1)$$

$$x = \frac{\nu-\nu_o}{\alpha_D}\ (\ln 2)^{1/2} \qquad y = \frac{\alpha_L}{\alpha_D}\ (\ln 2)^{1/2}$$

It is easily seen from the definition of x that it can assume values that are both positive and negative. However since it is assumed that $f(\nu-\nu_o)$ is an even function in x, i.e. $f(x) = f(-x)$, only positive values of x are needed for line broadening problems. Similarly it is seen that y will assume only positive values as long as the Lorentz half-width (α_L) is included. For other applications negative values of y occur [Fried and Conte[13]]. Limiting x and y so that they are greater than or equal to zero defines the first quadrant of the xy plane.

Now consider the complex probability function defined as

$$w(Z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{Z-t}\, dt = e^{-Z^2} \left(1 + \frac{2i}{\pi} \int_0^Z e^{t^2} dt \right) , \qquad (4.3\text{-}2)$$

where $Z = x + iy$, $x \geq o$, $y > o$. Separating this function into real and imaginary parts yields

$$w(Z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{ie^{-t^2} dt}{(x+iy) - t}$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{ie^{-t^2} dt}{(x-t) + iy} \cdot \frac{(x-t) - iy}{(x-t) - iy}$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y\, e^{-t^2} + i(x-t)e^{-t^2}}{(x-t)^2 + y^2}\, dt$$

$$w(Z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y\, e^{-t^2}}{(x-t)^2 + y^2}\, dt + \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{(x-t) e^{-t^2}}{(x-t)^2 + y^2}\, dt \qquad (4.3\text{-}3)$$

It is thus shown that the Voigt profile is the real part of the complex probability function w(Z). Several authors have tabulated values of this function for both the real and imaginary parts, but the most complete account of its mathematical properties appears to be that of Faddeyeva and Terentév[12] or more recently, for atmospheric applications, Armstrong[3].

In order to evaluate the real part of w(Z) as rapidly as possible, the xy plane is partitioned as shown in Figure 4.3-1 [Drayson[11]] and different approximating functions are used in each region.

In Region I w(Z) may be rewritten as

$$\left.\begin{aligned} w(Z) &= e^{-Z^2} + \frac{2i}{\pi^{1/2}} F(Z) \\ F(Z) &= e^{-Z^2} \int_0^Z e^{-t^2} dt \end{aligned}\right\} . \qquad (4.3\text{-}4)$$

For real Z, the function F(Z) is known as Dawson's function. The coefficients (d_n) of a Taylor series expansion of F(Z) about any real point (x,o), have the relationships

$$d_o = F(x),\ d_1 = 1-2xd_o,\ d_{n+1} = -\frac{2}{n+1}(xd_n + d_{n-1}) \qquad (4.3\text{-}5)$$

for n = 1, 2, 3, ... [Dawson[10]].

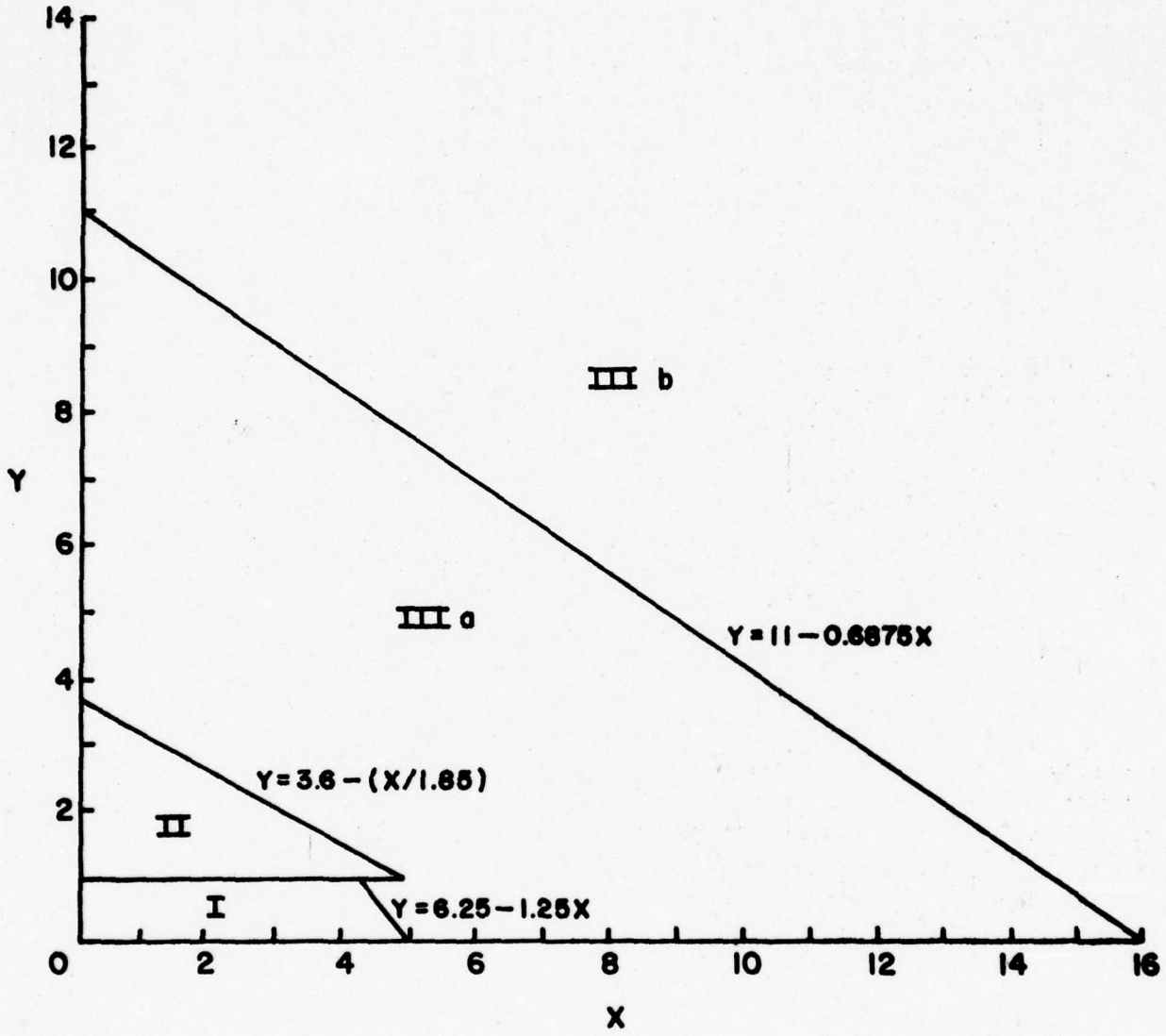


Figure 4.3-1. Computational regions used by Drayson [11].

Thus, for Region I, Dawson's function is first evaluated on the x-axis and a Taylor series is used to find the imaginary part of F(Z) and thus the real part of w(Z).

Dawson's function may be evaluated by series expansion, asymptotic expansion, or a Chebyshev expansion [Hummer[19]]. In the method developed for his program Drayson evaluates Dawson's function initially by Chebyshev expansion on the x-axis for x = 0.1, 0.3, 0.5, ..., 4.9. The coefficients d_1, d_2, d_3, d_4 are computed at each point using Eq. 4.3-5 and stored for later use. This process is required only once. Dawson's function is then evaluated for arbitrary x by a Taylor series expansion about the nearest tabulated point (x = 0.1, 0.3, ..., 4.9). The number of terms needed in the series expansion of F(Z) is a function of x and y. To avoid a test for convergence of the series, an empirical function was developed to determine the number of terms required.

For Region II first note that it has been shown by Chebyshev[9] and later K. A. Posse[39] that an integral of the type

$$\int_a^b \frac{p(t)}{Z-t}\,dt$$

can be represented by the continued fraction

$$\cfrac{\lambda_o}{Z - \alpha_1 - \cfrac{\lambda_1}{Z - \alpha_2 - \cfrac{\lambda_2}{Z - \alpha_3 - \cdots}}}\ ,$$

where λ_n and α_n are coefficients in a recurrence formula. Fried and Conte[13] applied this technique to the function w(Z) to obtain its fractional expansion.

$$w(Z) = \frac{1}{\pi^{1/2}} \cfrac{1}{Z + \cfrac{1/2}{Z + \cfrac{1}{Z + \cfrac{3/2}{Z+\ldots}}}}$$

$$w(Z) = \frac{1}{\pi^{1/2}} \cdot \frac{1}{Z +} \frac{1/2}{Z +} \frac{1}{Z +} \frac{3/2}{Z} \cdots \frac{n/2}{Z+} \cdots \qquad (4.3\text{-}6)$$

Along the line y = 1, which separates Region I and II, the Taylor series and the continued fraction require about the same computational time. The number of terms needed in the fractional expansion varies from n = 4 to n = 19 [Drayson[11]]. Again an empirical function was developed to determine the number of terms required and thus avoid a check for convergence.

For Region III the complex argument (Z) has a sufficiently large modulus, i.e. $|Z| = (x^2+y^2)^{1/2}$, so that Gauss-Hermite quadrature is effective [Faddeyeva and Terentév[12]]. The Voigt profile is approximated by a four-point quadrature in Region IIIa and a two-point quadrature in Region IIIb. The expressions used are

$$\frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{y^2 + (x-t)^2}\, dt \doteq \frac{y}{\pi} \sum_{i=0}^{3} W_i \frac{1}{y^2 + (x-t_i)^2} \qquad (4.3\text{-}7)$$

in Region IIIa, and

$$\frac{y}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{y^2+(x-t)^2}\,dt \doteq \frac{y}{\pi}\sum_{i=0}^{1} W_i \frac{1}{y^2+(x-t_i)^2} \qquad (4.3\text{-}8)$$

in Region IIIb. Here W_i are the weight factors and the t_i's are the roots of the Hermite polynomial of degree n+1. Carnahan, et al.[8] has an explanation of Gaussian Quadrature methods as well as tables of W_i and t_i for the Gauss-Hermite Quadrature method.

Utilizing the four regions of Fig. 4.3-1 and the three methods described to approximate the real part of Eq. 4.3-2, Drayson has written a FORTRAN IV function subprogram that he claims is accurate to about one part in 10^4 and much more rapid than any other currently available to evaluate the Voigt profile. A listing of the program is contained in Appendix B.

4.4 Proposed Voigt Algorithm

This method begins, as does Drayson's with the complex probability function

$$w(Z) = e^{-Z^2}\left(1+\frac{2i}{\pi^{1/2}}\int_0^Z e^{t^2}dt\right). \qquad (4.4\text{-}1)$$

Again, $Z = x + iy$ and $x, y \geq o$. It was shown in section 4.3 that the real part of this function is the Voigt profile. From the definition of the complementary error function of complex argument,

$$\operatorname{erfc}(-iZ) = \left(1+\frac{2i}{\pi^{1/2}}\int_0^Z e^{t^2}dt\right). \qquad (4.4\text{-}2)$$

Therefore

$$w(Z) = e^{-Z^2} \operatorname{erfc}(-iZ), \tag{4.4-3}$$

or in terms of the error function of complex argument

$$w(Z) = e^{-Z^2} \left[1 - \operatorname{erf}(-iZ)\right]. \tag{4.4-4}$$

It is possible to approximate w(Z) by utilizing Euler's formula for e^Z and a series expansion of the error function for complex argument. Euler's formula applied here is

$$e^{-Z^2} = \exp(-x^2 + y^2)\left[\cos(2xy) - i \sin(2xy)\right]. \tag{4.4-5}$$

The series expansion for the error function is [Salzer[42]]

$$\operatorname{erf}(-iZ) = \frac{2}{\pi^{1/2}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,(2n+1)} (-iZ)^{2n+1}. \tag{4.4-6}$$

Combining Eq. 4.4-5 and 4.4-6 into Eq. 4.4-4 yields the algorithm desired.

It was noted, however, that for large modulus the series expansion of the error function required upwards of 50 terms for convergence. Therefore, the xy plane was divided in a manner similar to that of Drayson. The difference is that there are only three regions and two approximating functions. Figure 4.4-1 depicts the three regions.

The series is used in Region I. In order to avoid testing for convergence a computer routine was developed to determine the number of terms of the series required for various values of x and y in the

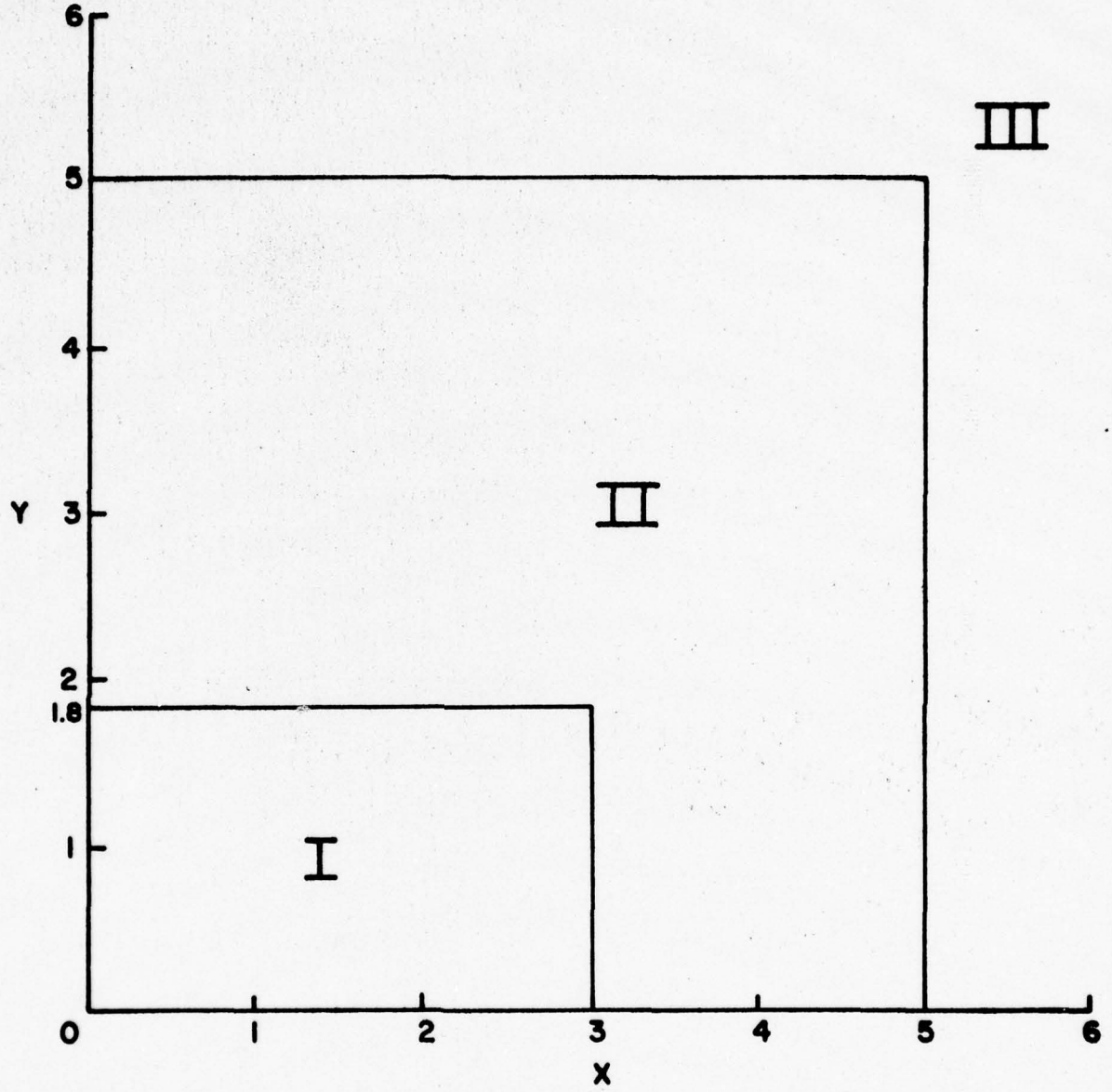


Figure 4.4-1. Regions proposed by this work.

region. The results of that routine are shown in Fig. 4.4-2. It was noticed that if the points of x = 0.1 and x = 2.0 are used (a rough linear fit), the lines for different values of y have the same slope. The line just moves up for increasing values of y. Therefore the relation used to fix the number of terms was chosen to be

$$N = 6.842\, x + 8. \tag{4.4-7}$$

The position of this line with respect to the test results is also shown in Fig. 4.2-2. In implementation the value of N is truncated to yield an integer. The minimum for N was set to 8 to assure convergence. The single exception is for x = o. Then the number of terms is set to 15.

The limits of the regions depicted in Fig. 4.4-1 were chosen after analyzing different approximations for w(Z). It was decided that a quadrature of the integral would be the simplest and most accurate for regions two and three. Using a modified Gauss-Laguerre quadrature, Abramowitz[1] obtains two approximations that are used for w(Z). The limits expressed by Abramowitz were modified since a reduced accuracy from that which he specified was acceptable. For Region II a three point formula yields

$$w(Z) = iZ\left(\frac{A_1}{Z^2-A_2} + \frac{A_3}{Z^2-A_4} + \frac{A_5}{Z^2-A_6}\right). \tag{4.4-8}$$

$A_1 = 0.4613135$ $\qquad$ $A_2 = 0.1901635$

$A_3 = 0.9999216$ $\qquad$ $A_4 = 1.7844927$

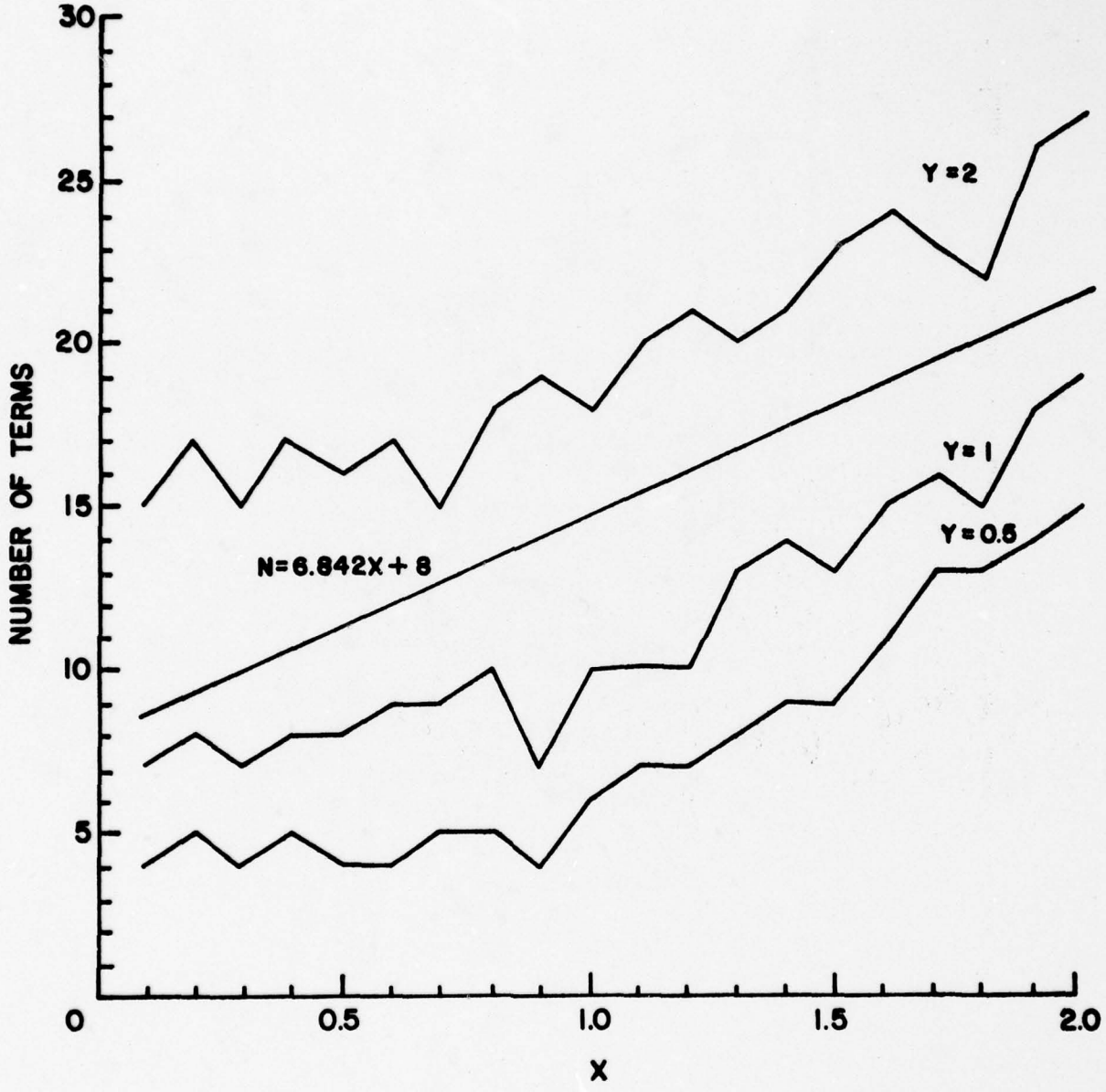


Figure 4.4-2. Number of series terms required for convergence.

$$A_5 = 0.002883894 \qquad A_6 = 5.5253437$$

Only the real part of equation 4.4-8 is required, so the relation is separated into real and imaginary parts.

$$w(Z) = iZ \left\{ \frac{A_1}{(x^2-y^2-A_2) + i2xy} + \frac{A_3}{(x^2-y^2-A_4) + i2xy} + \frac{A_5}{(x^2-y^2-A_6) + i2xy} \right\}$$

$$= iZ \left\{ \frac{A_1(x^2-y^2-A_2) - i2A_1xy}{(x^2-y^2-A_2)^2 + (2xy)^2} + \frac{A_3(x^2-y^2-A_4)-i2A_3xy}{(x^2-y^2-A_4)^2 + (2xy)^2} + \right.$$

$$\left. \frac{A_5(x^2-y^2-A_6) - i2A_5xy}{(x^2-y^2-A_6)^2 + (2xy)^2} \right\}$$

$$= iZ \left\{ \underbrace{\frac{A_1(x^2-y^2-A_2)}{(x^2-y^2-A_2)^2+(2xy)^2} + \frac{A_3(x^2-y^2-A_4)}{(x^2-y^2-A_4)^2+(2xy)^2} + \frac{A_5(x^2-y^2-A_6)}{(x^2-y^2-A_6)^2+(2xy)^2}}_{R} \right.$$

$$\left. -i \left(\underbrace{\frac{2A_1xy}{(x^2-y^2-A_2)^2+(2xy)^2} + \frac{2A_3xy}{(x^2-y^2-A_4)^2+(2xy)^2} + \frac{2A_5xy}{(x^2-y^2-A_6)^2+(2xy)^2}}_{I} \right) \right\}$$

$$= iZ(R-iI)$$

$$= (-y+ix)(R-iI)$$

The real part of this relation is

$$R\left\{w(Z)\right\} \doteq -yR + xI.$$

In terms of the constants and x and y

$$R\left\{w(Z)\right\} = A_1 \frac{2x^2y-(x^2-y^2-A_2)y}{(x^2-y^2-A_2)^2 + (2xy)^2} + A_3 \frac{2x^2y-(x^2-y^2-A_4)y}{(x^2-y^2-A_4)^2 + (2xy)^2} +$$

$$A_5 \frac{2x^2y-(x^2-y^2-A_6)y}{(x^2-y^2-A_6)^2 + (2xy)^2} . \qquad (4.4\text{-}9)$$

Equation 4.4-9 is the expression used in Region II. It is accurate to about two parts in 10^4 for any (x,y) in the region.

For Region III a two point Gauss-Laguerre quadradure formula gives

$$w(Z) = iZ \left(\frac{B_1}{Z^{2-}B_2'} + \frac{B_3}{Z^2-B_4} \right) \qquad (4.4\text{-}10)$$

$B_1 = 0.5124242$ $\qquad$ $B_2 = 0.2752551$

$B_3 = 0.05176536$ $\qquad$ $B_4 = 2.724745$

Following the same procedure as before, the real portion of the function can be acertained as

$$R\left\{w(Z)\right\} = B_1 \frac{2x^2y-(x^2-y^2-B_2)y}{(x^2-y^2-B_2)^2 + (2xy)^2} + B_3 \frac{2x^2y-(x^2-y^2-B_4)y}{(x^2-y^2-B_4)^2 + (2xy)^2} . \qquad (4.4\text{-}11)$$

This expression is accurate to about one part in 10^4 for (x,y) in Region III. The FORTRAN IV program implementing Eqs. 4.4-4, 4.4-9, and 4.4-11 is listed in Appendix C.

4.5 Comparison of Voigt Algorithms

In order to select one of the previous methods for evaluation of the Voigt function it was necessary to design computer programs to verify the accuracy of each method and establish some relative times for execution. Additionally the ease of implementation and program size of each method had to be considered.

It was assumed that any time savings in the computation of the parameters x and y would be as beneficial to one method as another. Therefore the execution time of a method is defined to be the time that expires from the issuance of a call statement to the return of a value by the subroutine. Compilation time of the program was not included nor was any input or output. Timing of the routines became a problem and several methods of time determination were tried. In the end it was decided to use the execution time returned by the operating system of the computer. That should account for all the time that a program has control of the central processing unit (CPU) and is probably as accurate as any timing routine.

Accuracy determinations were somewhat simpler. Faddeyeva and Terentév[12] have tabulated values for $\breve{w}(Z)$ when $0 < x < 5$ and $0 < y < 5$ to six decimal figures. For regions outside of that range Drayson's[11] method was used to set the true value of w(Z). It was assumed that since his work had been published it would be as accurate as he claimed.

All programs were processed by an IBM 360/65 computer.

4.5.1 Accuracy Tests

Three separate tests were conducted to determine the accuracy of each method. As an initial screening Kielkopf's method and the method proposed here were pitted against Drayson's method. A synopsis of the results are shown in Table 4.5-1.

This first test was conducted using double precision operations to increase accuracy in all measurements. The table does not show all the digits used, which is why entries such as the one for $x = 0.5$, $y = 4.0$ appear to have no error when actually there is a slight difference. As the table indicates, Kielkopf's method has accuracy errors that are relatively large. Examination of his values with true, tabulated values [Faddeyeva and Terentév[12]] revealed unacceptable margins of error. Thus the same conclusion drawn by Drayson in his search for an accurate Voigt Algorithm was reached. Kielkopf's method is not accurate enough for atmospheric work [Drayson[11]].

The second test was designed to verify the accuracy of both the proposed method and Drayson's method. The regions used by the proposed method were selected, one at a time, and one hundred values of the function were computed by each method. The computed values were compared to those tabulated by Faddeyeva and Terentév[12] for $o < x < 5$, $o < y < 5$. In Region III, where $x > 5$, $y > 5$ the values returned by the two methods were compared with each other, since no tabulated values were available.

Figure 4.5-1 depicts the regions used by the proposed method.

x	y	True Value (Drayson's)	Kielkopf's Value	Proposed Value	Percent Relative Error	
					Kielkopf	Proposed
0.1	1.0	.426050	.426182	.426042	$3.09 \cdot 10^{-4}$	$1.84 \cdot 10^{-3}$
0.3	1.0	.413984	.415461	.413989	$3.56 \cdot 10^{-3}$	$1.21 \cdot 10^{-3}$
0.5	1.0	.391218	.394833	.391236	$9.24 \cdot 10^{-3}$	$4.71 \cdot 10^{-3}$
0.1	2.0	.254974	.254805	.254970	$6.62 \cdot 10^{-4}$	$1.56 \cdot 10^{-5}$
0.3	2.0	.251677	.244411	.251692	$2.88 \cdot 10^{-2}$	$5.96 \cdot 10^{-5}$
0.5	2.0	.245279	.224884	.245226	$8.31 \cdot 10^{-2}$	$2.16 \cdot 10^{-4}$
0.1	3.0	.178842	.180084	.178841	$6.94 \cdot 10^{-3}$	$4.11 \cdot 10^{-4}$
0.3	3.0	.177581	.171631	.177581	$3.35 \cdot 10^{-2}$	$2.78 \cdot 10^{-4}$
0.5	3.0	.175105	.155897	.175105	$1.09 \cdot 10^{-1}$	$2.56 \cdot 10^{-5}$
0.1	4.0	.136923	.139572	.136924	$1.93 \cdot 10^{-2}$	$1.28 \cdot 10^{-3}$
0.3	4.0	.136329	.132635	.136330	$2.70 \cdot 10^{-2}$	$1.05 \cdot 10^{-3}$
0.5	4.0	.135155	.119779	.135155	$1.13 \cdot 10^{-1}$	$6.60 \cdot 10^{-4}$
0.1	5.0	.110663	.114381	.110664	$3.35 \cdot 10^{-2}$	$2.78 \cdot 10^{-4}$
0.3	5.0	.110341	.108533	.110342	$1.63 \cdot 10^{-2}$	$2.20 \cdot 10^{-4}$
0.5	5.0	.109702	.092719	.109703	$1.55 \cdot 10^{-1}$	$1.75 \cdot 10^{-4}$

Table 4.5-1. Initial accuracy tests. Drayson's values used as true. (Not all digits shown in value columns.)

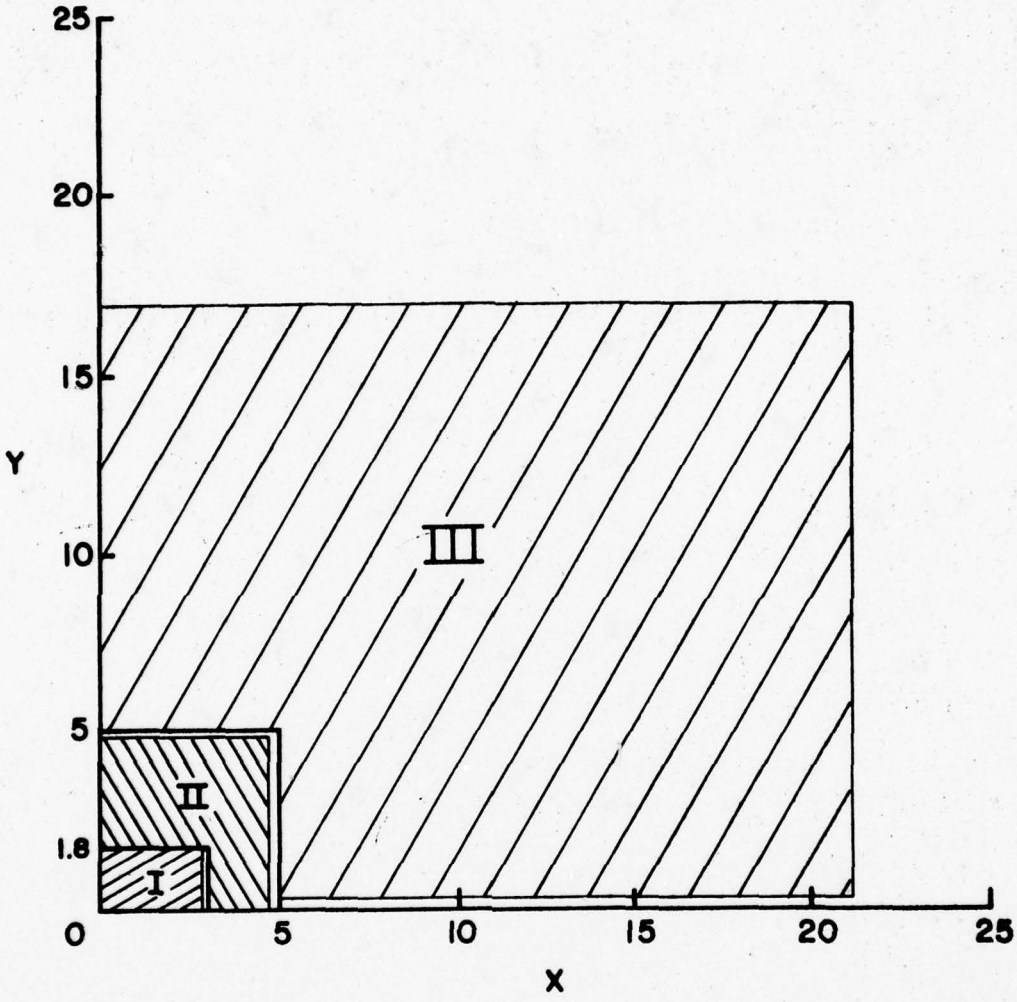


Figure 4.5-1. Coverage of proposed regions by accuracy test two.

The shaded areas are the range of the points used for comparison. The points were selected to include as much of the area of each region as possible. In Region I

$y = 0$ to 1.8 in increments of 0.2,

$x = 0$ to 2.7 in increments of 0.3.

In Region II

$y = 2$

$y = 2.5$ to 4.6 in increments of 0.3,

$x = 0$ to 4.5 in increments of 0.5,

and $y = 0$ to 3.5 in increments of 0.5,

$x = 3$ to 4.6 in increments of 0.4.

In Region III

$y = 5$ to 17 in increments of 3.0,

$x = 2$ to 11 in increments of 1.0,

and $y = 0.5$ to 5 in increments of 0.5,

$x = 5$ to 21 in increments of 4.0.

The results of this test are summarized in Table 4.5-2. The peak deviation in Region I for the proposed method is larger than the peak for Drayson, but the actual error for that single point was only three parts in 10^4. The root mean square error was well within acceptable limits.

For Region II the peak deviations were nearly the same, while the root mean square error for the proposed method was better than Dray-

Region	Drayson's Method		Proposed Method	
	Peak Deviation	RMS Deviation	Peak Deviation	RMS Deviation
I	$1.72504.10^{-5}$	$4.29676 \cdot 10^{-7}$	$3.89991 \cdot 10^{-4}$	$4.07495 \cdot 10^{-6}$
II	$1.41329 \cdot 10^{-3}$	$1.41402 \cdot 10^{-4}$	$1.41342 \cdot 10^{-3}$	$1.42011 \cdot 10^{-5}$
III	$*3.41969 \cdot 10^{-6}$	$*6.03836 \cdot 10^{-8}$	$*3.41969 \cdot 10^{-6}$	$*6.03836 \cdot 10^{-8}$

*Deviation of one method from another.

Table 4.5-2. Results of accuracy test two.

son's. In Region III the deviation of one method from the other is small, reflecting the two different quadrature techniques used.

The final accuracy test used the regions suggested by Drayson, one at a time. Figure 4.5-2 depicts the coverage of each area. Rather than using tabulated values, the results obtained with Drayson's method were compared to those obtained using the proposed method. Table 4.5-3 summarizes the results of the test.

It is clearly seen from Table 4.5-2 and Table 4.5-3 that the proposed method yields values of the Voigt profile that are accurate enough for atmospheric work. Root-mean-square errors indicate accuracies that normally exceed tabulated values of the profile.

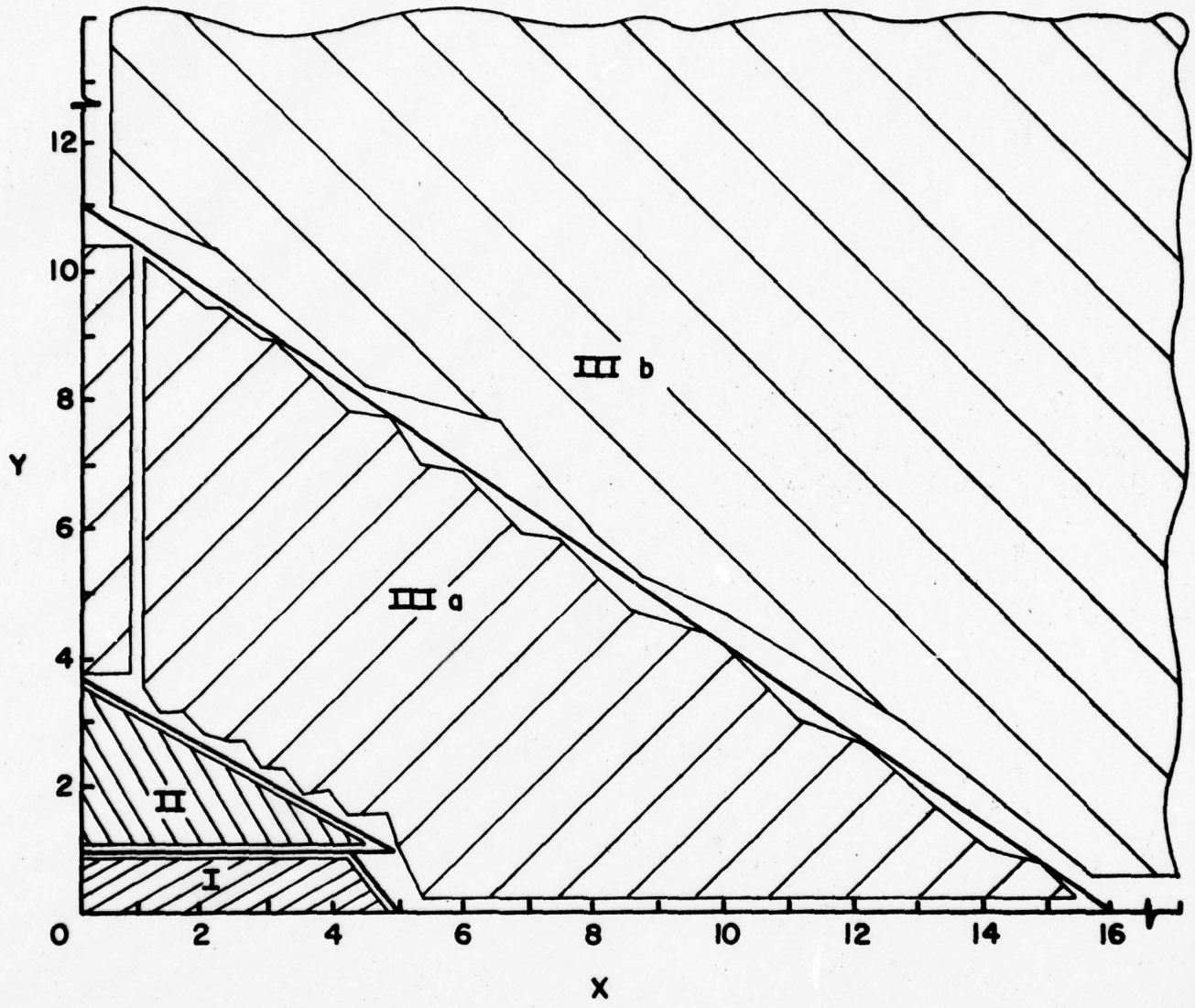


Figure 4.5-2. Coverage of Drayson's regions for accuracy test three.

Region	Peak Deviation	RMS Deviation	Number Points Used
I	$5.27915 \cdot 10^{-5}$	$2.46145 \cdot 10^{-7}$	452
II	$3.44067 \cdot 10^{-3}$	$1.34552 \cdot 10^{-5}$	283
IIIa	$6.92595 \cdot 10^{-6}$	$2.06357 \cdot 10^{-8}$	744
IIIb	$3.41969 \cdot 10^{-6}$	$1.99151 \cdot 10^{-8}$	420

Table 4.5-3. Deviations of Proposed method from Drayson's method using Drayson's regions.

4.5.2 Execution Time Tests

Four tests were conducted utilizing Drayson's method and the proposed method in an effort to determine which algorithm would save the most computer execution time. For each of the tests a small main routine was written that fixed the values of x and y and then called the routine being tested. The master program of some tests performed input/output or accuracy measurements. The other main routines performed no extraneous operations. The tests involved merely replacing that portion of the program implementing Drayson's method with the proposed method and resubmitting the job for execution.

The first test used the regions of the proposed method, selecting points from one region at a time. This is a slightly biased test since the proposed algorithm remained in one region while Drayson's algorithm jumped from region to region, depending on the value of the parameters. However Drayson contended that his method was the most rapid available, and placed no stipulations on how parameters were selected. The main routine for this test performed input and output as well as accuracy measurements for both methods. Therefore, the times were somewhat over true execution time, but reflected the relative speed of each method. Table 4.5-4 lists the results of this test. The method proposed in this work reduced the time to approximate the Voigt profile by an average of 26.6%.

A second test was conducted using the regions proposed by Drayson, selecting points from one region at a time. This has the same bias as the first test except that it is in Drayson's favor this time.

Region	Drayson's Method		Proposed Method	
	CPU Seconds	%	CPU Seconds	%
I	4.05	100	2.92	72.09
II	4.14	100	3.00	72.46
III	3.87	100	2.92	75.45

Table 4.5-4. Results of time tests conducted using regions and points indicated in Fig. 4.5-1.

One hundred points were selected from each region. The results of the test are shown in Table 4.5-5. The main routine for this test performed output operations as well as calling the method being tested. The method proposed by this work reduced the time to approximate the Voigt profile by an average of 27.5%.

An offshoot of the accuracy test conducted using the regions and points shown in Fig. 4.5-2 was that the times for execution were available. This comprised the third speed test. The main routine in this case performed output and deviation analysis in addition to calling the Voigt algorithm. Again the times were somewhat in excess of true execution time, but still reflected the relative speed of each method. Table 4.5-6 summarizes this test. The proposed method reduced the time to evaluate the Voigt profile by an average of 29.5%.

A final test was conducted that did not use regions. Ten-thousand points were selected as follows

$y = 0$ to 19.8 in increments of 0.2,

$x = 0$ to 24.75 in increments of 0.25.

The master routine performed no input or output and no other calculations. This was strictly comparing the time for Drayson's method and the proposed method to evaluate ten-thousand points. The results are enumerated in Table 4.5-7.

4.5.3 The Selected Voigt Algorithm

In view of the results of the time tests conducted the selection was not difficult. Both methods yield the accuracy necessary for good

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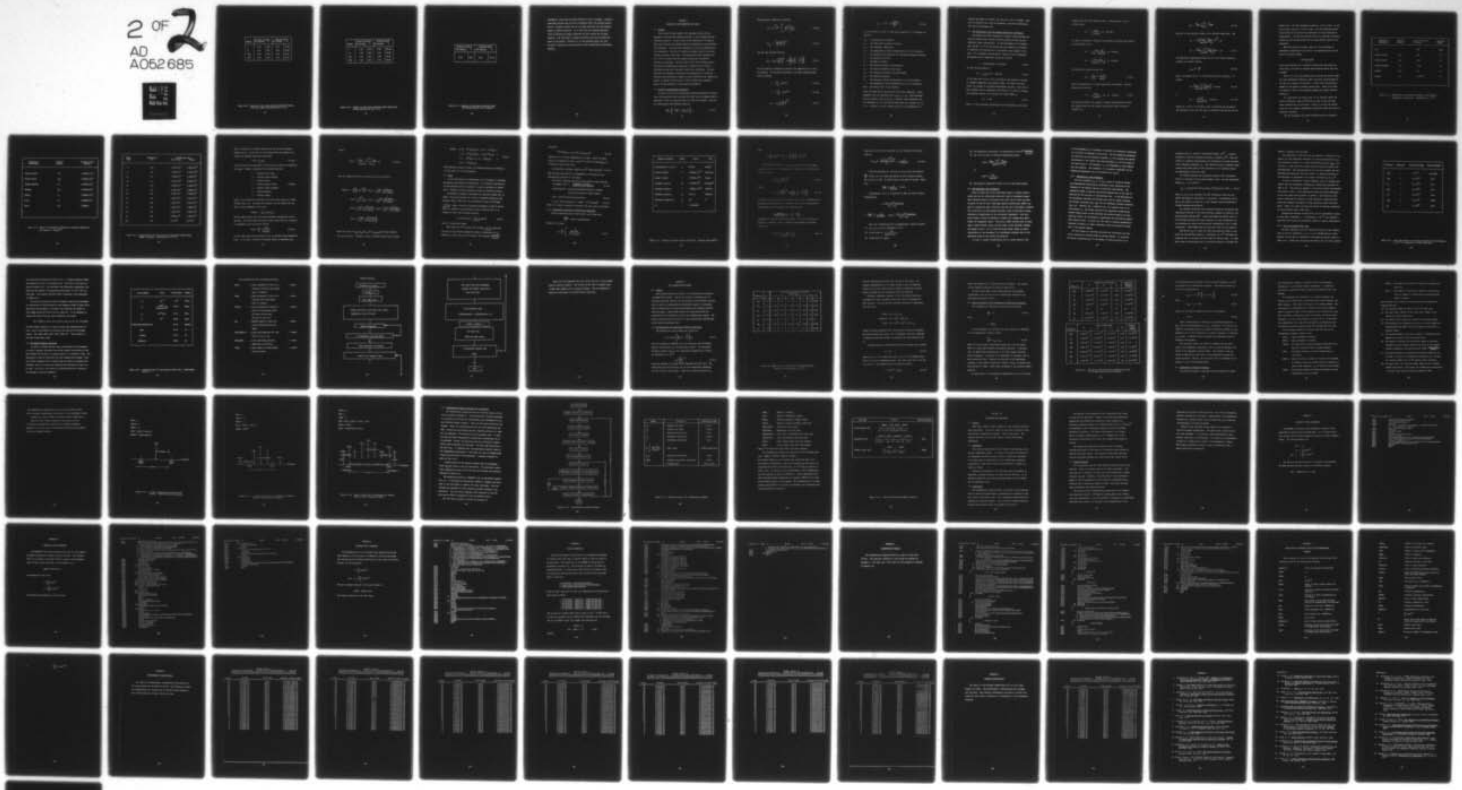

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Region	Drayson's Method CPU Seconds	%	Proposed Method CPU Seconds	%
I	3.30	100	2.37	71.81
II	3.22	100	2.52	78.26
IIIa	3.90	100	2.52	64.61
IIIb	3.59	100	2.70	75.21

Table 4.5-5. Results of time tests conducted using 100 points from each region indicated in Fig. 4.2-1.

Region	Drayson's Method CPU Seconds	%	Proposed Method CPU Seconds	%
I	3.45	100	2.29	66.38
II	3.12	100	2.49	79.80
IIIa	3.72	100	2.69	72.31
IIIb	3.69	100	2.42	65.58

Table 4.5-6. Results of time tests conducted using regions and points indicated in Fig. 4.5-2.

Drayson's Method		Proposed Method	
CPU Seconds	%	CPU Seconds	%
3.15	100	2.25	71.42

Table 4.5-7. Results of time tests conducted using ten-thousand points and no regions.

atmospheric calculation and both methods are easy to program. Drayson's algorithm contains some 64 source statements while the proposed method has 40. Drayson's method was run in single precision and the proposed method in double precision. It is felt that the proposed algorithm could be executed in single precision and still retain the accuracy required. The conversion to single precision would only increase the speed of the method. Therefore it is the proposed method that will be used to evaluate the Voigt profile in the transmittance differential equation.

CHAPTER V

ABSORPTION LINE PARAMETERS AND UNITS

5.1 Preface

This chapter brings together the remaining topics that are necessary to develop the computer solution to the transmittance differential equation. A brief review of the equations to be used is given and the known and unknown quantities appearing in the relations are identified. The input data necessary to solve the equations are also identified. The value of physical constants used in the calculations is given at this time. The mixing ratio M(P) introduced in Eq. 3.2-11 is derived and the combined extinction coefficient relation is developed. Then the units of all the relations used in this work are dimensionally analyzed to assure they are correct. Additionally some unit conversion factors are introduced. The data available as atmospheric absorption line parameters are presented together with some general remarks on their derivation and compilation. Finally a computer routine that is used to handle the tremendous amount of data available is developed and explained.

5.2 Review of Transmittance Equations

In order to solve the transmittance equation developed in chapter three the quantities that are known and those that are unknown must be specified. First all equations that are used are restated. They are the transmittance differential equation,

$$\frac{d\tau}{dP} = \left\{ - \frac{\sec \theta}{g} \sum_j K_j M_j(P) \right\} \tau. \qquad (5.2\text{-}1)$$

The absorption coefficient relations,

$$K_j = \sum_i \frac{K_{o_{ij}}}{\pi} \int_{-\infty}^{\infty} \frac{y\, e^{-t^2}\, dt}{y^2 + (x-t)^2}, \qquad (5.2\text{-}2)$$

$$K_{o_{ij}} = \frac{S_{ij}}{\alpha_D} \left(\frac{\ln 2}{\pi}\right)^{1/2}, \qquad (5.2\text{-}3)$$

and the line strength function

$$S_{ij} = S_{oij}\, Q_j \left(\frac{T_o}{T}\right)^{c_j} \exp\left\{\frac{E_{ij}}{kT_o}\left(1 - \frac{T_o}{T}\right)\right\} . \qquad (5.2\text{-}4)$$

For the purpose of dimensional analysis the summations over i and j are dropped. The variables appearing in the above equations must also be defined,

$$y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2} , \qquad (5.2\text{-}5)$$

$$x = \frac{\nu - \nu_o}{\alpha_D} (\ln 2)^{1/2} , \qquad (5.2\text{-}6)$$

$$\alpha_L = \alpha_o \frac{P}{P_o} \left(\frac{T_o}{T}\right)^{1/2} , \qquad (5.2\text{-}7)$$

$$\alpha_D = 3.58 \cdot 10^{-7} \left(\frac{T}{M}\right)^{1/2} \nu_o \cdot \qquad (5.2\text{-}8)$$

It is seen that in order to solve these equations it is necessary to specify:

S_o... a reference line strength,

Q ... the vibrational partition function,

T_o... the reference temperature,

T ... the temperature at which transmittance is to be calculated,

c ... the exponent that expresses the rotational partition function,

E ... the energy of the line,

k ... Boltzman's constant,

M ... The molecular weight of the absorber,

ν_o... the center wavenumber of the line,

α_o... the reference Lorentzian line half-width,

P_o... the reference pressure,

P ... the pressure at which transmittance is to be calculated,

ν ... the wavenumber at which transmittance is to be calculated,

M(P). the mixing ratio of the absorber.

These variables may be grouped into four broad catagories. Those dependent upon the absorbing line (S_o, E, ν_o, α_o), those dependent upon the absorber type or gas (Q, c,M,M(P)), those dependent upon the atmosphere (T, P), and finally those that are constant (T_o, P_o, k, ν). Actually ν is not constant since if the transmittance at

another wavenumber is desired, the value of ν must be changed. Data must be obtained then, from the atmosphere, from the abosrbing gas, and from the absorbing line.

5.3 The Mixing Ratio and The Combined Extinction Coefficient

The mixing ratio M(P) introduced in chapter three expresses the relation between total pressure and the pressure of only one gas (absorber) under consideration. In the development of the Lambert Beer law (Eq. 3.2-7) it was stated that the reduction in intensity of radiation was proportional to the amount of gas present in the path. If u represents the gas amount, then du is the incremental gas amount and the Lamber-Beer Law may be written

$$\tau = \exp(-K\rho(x)dx) = \exp(-Kdu). \qquad (5.3\text{-}1)$$

So that the gas amount is

$$du = \rho_{gas}(x)\, dx. \quad (gm/cm^2) \qquad (5.3\text{-}2)$$

If the right side of Eq. 5.3-2 is divided by the density of the gas at standard temperature and pressure (STP), the units of the gas amount are changed to centimeter-atmospheres (cm-atm). This unit is more commonly used in atmospheric work since it is easier to compute the equivalent amount of an absorber in a path length as

$$\Delta L = cRP \qquad (5.3\text{-}3)$$

where c is the fractional concentration of the absorber, R the path

length (cm), and P the pressure (atm). Converting Eq. 5.3-2 to cm-atm yields

$$du = \frac{\rho_{gas}}{\rho_{gas(STP)}} \, dx \quad \text{(cm-atm)}.$$

In order to introduce a mixing ratio multiply and divide the relation by the density of air.

$$du = \frac{\rho_{air} \; \rho_{gas}}{\rho_{air} \; \rho_{gas(STP)}} \, dx \quad \text{(cm-atm)}$$

$$du = \frac{\rho_{air} \; \rho_{gas}}{\rho_{gas(STP)} \; \rho_{air}} \, dx \quad \text{(cm-atm)}$$

Now define the density mixing ratio

$$M_d = \frac{\rho_{gas}}{\rho_{air}} \triangleq \frac{gm/cm^3}{gm/cm^3}, \qquad (5.3\text{-}4)$$

where the densities are at some temperature and pressure. Now gas amount may be written

$$du = \frac{\rho_{air}}{\rho_{gas(STP)}} \, M_d \, dx. \quad \text{(cm-atm)} \qquad (5.3\text{-}5)$$

The relation between the volumetric mixing ratio measured in parts per million (ppm) and the density mixing ratio (M_d) is given by [Weast[49]] as

$$M_d = \frac{M_{ppm} \cdot 10^{-6} \cdot Mt_{gas}}{Mt_{air}} , \qquad (5.3\text{-}6)$$

where Mt is the molecular weight of air and gas respectively. Now

$$du = \frac{\rho_{air} M_{ppm} \cdot Mt_{gas} \cdot 10^{-6}}{\rho_{gas(STP)} Mt_{air}} dx$$

$$du = \frac{M_{ppm} \cdot 10^{-6} Mt_{gas} \rho_{air}}{\rho_{gas(STP)} Mt_{air}} dx. \qquad (5.3\text{-}7)$$

The hydrostatic approximation given by Eq. 2.2-1 relates density to pressure in a manner desired,

$$\rho_{air} dx = \frac{dP}{g} , \qquad (5.3\text{-}8)$$

Here P is pressure and g. is the acceleration due to gravity. So finally

$$du = \frac{M_{ppm} \cdot 10^{-6} Mt_{gas}}{\rho_{gas(STP)} Mt_{air}} \frac{dP}{g} \quad (cm\text{-}atm) \qquad (5.3\text{-}9)$$

or

$$du = \frac{M_d \, dP}{\rho_{gas(STP)} \, g} \quad (cm\text{-}atm). \qquad (5.3\text{-}10)$$

Either Eq. 5.3-9 or 5.3-10 may be used to calculate the gas amount. The selection of one over the other is dependent upon the gas and the

mixing ratio. For most atmospheric gases Eq. 5.3-9 is used. In the case of water vapor Eq. 5.3-10 is used. The calculated gas amount is multiplied by the extinction coefficient in the calculation of transmittance. As might be expected there is a different extinction coefficient (K) and gas amount (du) for each absorber (gas) in the atmosphere.

When more than one absorber (gas) is to be considered in atmospheric transmittance the index of the exponential must be the sum of all optical depths.

$$\tau \exp(-\sum_{j} K_j M_j dP).$$

Since every absorber has a different mixing ratio and extinction coefficient, each must be computed and multiplied before they can be added.

Table 5.3-1 lists the mixing ratios in parts per million (ppm) for those atmospheric absorbers whose fractional concentrations do not vary as a function of altitude. It also lists the molecular weights of the gases of constant mixing ratio. Table 5.3-2 gives the density at STP of the atmospheric gases that absorb infrared radiation.

For cases where the mixing ratio is not constant (water and ozone) a different value of M(P) must be used at each altitude where Transmittance is calculated. Table 5.3-3 lists the mixing ratios for the variable atmospheric constituents water and ozone at different altitudes.

For the atmosphere only seven absorbers need be considered.

Atmospheric Constituent	Chemical Formula	Parts per Million by Volume	Molecular Weight
Air		10^6	28.97
Carbon Dioxide	CO_2	330	44
Nitrous Oxide	N_2O	0.28	44
Carbon Monoxide	CO	0.075	28
Methane	CH_4	1.6	16
Oxygen	O_2	$2.095 \cdot 10^5$	32

Table 5.3-1. Mixing Ratios and Molecular Weights of Non-Varying Atmospheric Constituents. [McClatchey, et al.[31]]

Atmospheric Constituent	Chemical Formula	Density at STP (gm/cm^3)
Carbon Dioxide	CO_2	$1.9768441 \cdot 10^{-3}$
Nitrous Oxide	N_2O	$1.9781371 \cdot 10^{-3}$
Carbon Monoxide	CO	$1.2510101 \cdot 10^{-3}$
Methane	CH_4	$7.1678376 \cdot 10^{-4}$
Oxygen	O_2	$1.4286545 \cdot 10^{-3}$
Ozone	O_3	$2.1436282 \cdot 10^{-3}$
Water	H_2O	1.0000010

Table 5.3-2 Density of Atmospheric Absorbers at Standard Temperature and Pressure. [Nelson[36]]

Height (Km)	Temperature (°K)	Mixing Ratio (M_d) Water Vapor	Ozone
0	294	$1.1754 \cdot 10^{-2}$	$5.0378 \cdot 10^{-8}$
5	267	$1.3867 \cdot 10^{-3}$	$9.1527 \cdot 10^{-8}$
10	235	$1.5388 \cdot 10^{-4}$	$2.1639 \cdot 10^{-7}$
15	216	$3.6122 \cdot 10^{-6}$	$9.0304 \cdot 10^{-7}$
20	218	$4.7604 \cdot 10^{-6}$	$3.5967 \cdot 10^{-6}$
25	224	$1.5625 \cdot 10^{-5}$	$6.9962 \cdot 10^{-6}$
30	234	$2.7231 \cdot 10^{-5}$	$1.5128 \cdot 10^{-5}$
35	245	$1.6873 \cdot 10^{-5}$	$1.4112 \cdot 10^{-5}$
40	258	$1.2913 \cdot 10^{-5}$	$1.2312 \cdot 10^{-5}$
45	270	$1.0814 \cdot 10^{-5}$	$7.3989 \cdot 10^{-6}$
50	276	$6.6232 \cdot 10^{-6}$	$4.5204 \cdot 10^{-6}$
70	218	$2.0876 \cdot 10^{-6}$	$1.2824 \cdot 10^{-6}$
100	210	$2.0 \cdot 10^{-6}$	$8.6 \cdot 10^{-8}$

Table 5.3-3. Mixing Ratios for Water Vapor and Ozone from A Midlatitude Summer Atmosphere. [McClatchey, et al.[32]]

Five of these have a constant mixing ratio and two have variable mixing ratios. In any case we are concerned with the product K du. Define the combined extinction coefficient

$$ABSK = \sum_j K_j du_j \qquad (5.3\text{-}11)$$

Let the value of the subscript j vary from one to seven to account for all gases. Further, establish the following relations

1 ... denotes water vapor,

2 ... denotes carbon dioxide,

3 ... denotes ozone,

4 ... denotes nitrous oxide, (5.3-12)

5 ... denotes carbon monoxide,

6 ... denotes methane,

7 ... denotes oxygen.

$K_1 du_1$ is the extinction coefficient for water vapor, $K_2 du_2$ for carbon dioxide, and so on. Defining the variable L as the counter for the level of the atmosphere we can write

$$ABSK(L) = \sum_{j=1}^{7} K_j(L) du_j(L)$$

The gas amount $du_j(L)$ will have seven different expressions; one for each gas. For water vapor and ozone the gas amount will be a function of atmospheric level and can be written

$$du(L) = \frac{dP}{g} \frac{M_d(L)}{\rho_{gas(STP)}} \qquad (5.3\text{-}13)$$

For the other gases the gas amount is not so dependent upon atmospheric level. It is only a function of pressure (which is dependent upon

level),

$$du(L) = \frac{M_{ppm} \cdot 10^{-6} \; Mt_{gas}}{\rho_{gas(STP)} \; Mt_{air} g} \, dP. \qquad (5.3\text{-}14)$$

Thus the combined extinction coefficient can be written as

$$ABSK(L) = \frac{dP}{g}\left\{ K_i(L) \frac{M_d(L)}{1.0} + K_2(L) \frac{(330 \cdot 10^{-6})(44)}{(1.97 \cdot 10^{-3})(28.97)} \right.$$

$$K_3(L) \frac{M_d(L)}{2.14 \cdot 10^{-3}} + K_4(L) \frac{(.28 \cdot 10^{-6})(44)}{(1.97 \cdot 10^{-3})(28.97)} +$$

$$K_5(L) \frac{(.075 \cdot 10^{-6})(28)}{(1.25 \cdot 10^{-3})(28.97)} + K_6(L) \frac{(1.6 \cdot 10^{-6})(16)}{(7.16 \cdot 10^{-4})(28.97)} +$$

$$\left. K_7(L) \frac{(2.095 \cdot 10^{-1})(32)}{(1.42 \cdot \cdot 10^{-3})(28.97)} \right\},$$

where the value of M_{ppm}, Mt_{gas}, Mt_{air} and $P_{gas(STP)}$ have been inserted into the equations. Assuming a value of 980.665 cm/sec^2 for g yields

$$\begin{aligned} ABSK(L) = [&1.02 \cdot 10^{-3} K_1(L) M_d(L) + 2.59 \cdot 10^{-4} K_2(L) + \\ &4.76 \cdot 10^{-1} K_3(L) M_d(L) + 2.19 \cdot 10^{-7} K_4(L) + \\ &5.9 \cdot 10^{-8} K_5(L) + 1.25 \cdot 10^{-6} K_6(L) + \\ &1.65 \cdot 10^{-1} K_7(L)] dp \end{aligned} \qquad (5.3\text{-}15)$$

This relation is used to obtain the combined extinction coefficient at each level (L) of the atmosphere.

5.4 Units

In the calculation of transmittance it is necessary to determine gas amounts and extinction coefficients. For different applications or when different data is available, it may be necessary to convert units. Therefore a brief treatise is given on conversion factors.

According to Avogadro's hypothesis the molecular weight (M), in grams, of any gas occupies 22.4 liters at standard temperature and pressure (STP). Hence one cubic centimeter of gas at STP weighs $\frac{M}{2.24 \cdot 10^4}$ grams. Since one centimeter-atmosphere at STP is equivalent to a length of one centimeter of gas at STP per cm^2, it is possible to write the following relation

$$1 \text{ cm-atm of gas} = \frac{M}{2.24 \cdot 10^4} \text{ gm-cm}^2, \qquad (5.4\text{-}1)$$

where M is molecular weight.

Also since one cm^3 of gas at STP contains $\frac{1}{2.24 \cdot 10^4}$ moles and one mole of gas contains Avogadro's number of molecules, it is possible to write that one cm^3 of gas at STP contains $\frac{6.02 \cdot 10^{23}}{2.24 \cdot 10^4}$

molecules,

$$1(\text{cm-atm})_{STP} = 2.69 \cdot 10^{19} \text{ molecules/cm}^2 \qquad (5.4\text{-}2)$$

Equation 5.4-1 is valid independent of the gas. Since for water vapor it is possible to write 1 gm-cm^2 in terms of $(\text{cm-atm})_{STP}$ it is shown for water vapor that

$$1 \text{ precipitable centimeter } (H_2O) = 3.34 \cdot 10^{22} \text{ (molecules/cm}^2\text{)} \qquad (5.4\text{-}3)$$

Thus the unit molecule/cm^2 is independent of the nature of the absorbing gas and basic to all gases.

Some other relations that have proven useful in this work are:

$$\text{wavenumber } (\text{cm}^{-1}) = \frac{\text{frequency (1/sec)}}{\text{speed of light (cm/sec)}} \qquad (5.4\text{-}4)$$

energy(joules) = energy (wavenumbers)·Planck's constant (joules-sec)·speed of light (cm/sec)

$$E(j) = [E(\text{cm}^{-1})][h(\text{j-sec})][c(\text{cm/sec})] \qquad (5.4\text{-}5)$$

$$1 \text{ atm} = 1013.25 \text{ milibars} = 1.01325 \cdot 10^5 \text{ newtons/m}^2 \qquad (5.4\text{-}6)$$

Table 5.4-1 lists the physical constants that were used in this work.

5.4.1 Dimensional Analysis of Transmittance Equations

From the equations used in this work it can be seen that

$\frac{KMdP}{g}$ must be dimensionless.

Equation 5.2-2 gives

$$K = \frac{K_o}{\pi} \int_{-\infty}^{\infty} \frac{ye^{-t^2}dt}{y^2 + (x-t)^2} , \qquad (5.4\text{-}7)$$

Physical Constant	Symbol	Value	Unit
Acceleration of gravity	g	980.665	cm/sec^2
Planck constant	h	$6.626196 \cdot 10^{-34}$	Joule-sec
Speed of light	c	$2.997925 \cdot 10^{10}$	cm/sec
Avogadro constant	Na	$6.022169 \cdot 10^{23}$	$molecule^{-1}$
Boltzman constant	k	$1.380622 \cdot 10^{-23}$	Joule/°K
Reference Pressure	P_o	1013.25	milibars
Reference Temperature	T_o	296	°K
Pi	π	3.141592654	

Table 5.4-1. Physical constants used in this work. (Adapted from Weast[49]).

with

$$y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2} \quad \text{and} \quad x = \left(\frac{\nu - \nu_o}{\alpha_D} \right) (\ln 2)^{1/2} .$$

Provided that $\alpha_L, \alpha_D, \nu, \nu_o$ all have units of cm^{-1} the integral portion of Eq. 5.4-7 is dimensionless. Therefore K will have units of K_o, given by

$$K_o = \frac{S}{\alpha_D} \left(\frac{\ln 2}{\pi} \right)^{1/2} , \tag{5.4-8}$$

where

$$S = S_o \, Q \left(\frac{T_o}{T} \right)^{C_j} \exp\left\{ \frac{E}{kT_o} \left(1 - \frac{T_o}{T} \right) \right\}. \tag{5.4-9}$$

As long as T_o and T have the same units their ratio is dimensionless. The partition function Q has a numerical value and is dimensionless and the index of the exponential is dimensionally

$$\frac{(\text{Joules})}{(\text{Joules}/^\circ K)(^\circ K)} \left(1 - \frac{^\circ K}{^\circ K} \right),$$

provided the energy E is given in joules. If it is not it must be converted. (See Eq. 5.4-5). Therefore the strength S will have units of S_o.

$$S \stackrel{d}{=} S_o \stackrel{d}{=} \frac{cm^{-1}}{\text{molecule} - cm^{-2}} \tag{5.4-10}$$

From Eq. 5.4-8 it can be seen that K_o, and therefore K will have units of

$$K \triangleq K_o \triangleq \frac{\frac{cm^{-1}}{molecule - cm^{-2}}}{cm^{-1}} = \frac{cm^2}{molecules} \cdot \qquad (5.4\text{-}11)$$

From the discussion of section 5.3 recall that the quantity $\frac{MdP}{g}$ of Eq. 5.4-7 is really gas amount du and is given by either Eq. 5.3-9 or 5.3-10. In either case it has units of cm-atm. Therefore

$$\frac{KMdP}{g} \triangleq \frac{cm^2}{molecule} \cdot cm\text{-}atm$$

Utilizing Eq. 5.4-2 it is possible to make the above relation dimensionless.

$$1 = \frac{2.69 \cdot 10^{19} \text{ molecules}}{cm^3 - atm}$$

$$1 \cdot \frac{KMdP}{g} \triangleq \frac{cm^2}{molecules} \cdot cm\text{-}atm \cdot \frac{2.69 \cdot 10^{19} \text{ molecules}}{cm^3 - atm}$$

Thus, all calculations will be dimensionally correct provided

(1) α_L, α_D, ν, ν_o are in wavenumbers (cm^{-1}),

(2) S_o has units of $\frac{cm^{-1}}{molecule\text{-}cm^{-2}}$,

(3) E has units of joules,

(4) The extinction coefficient K is multiplied by $2.69 \cdot 10^{19}$ $\frac{\text{molecules}}{\text{cm}^3\text{-atm}}$,

(5) Eq. 5.2-1 is used to calculate transmittance where

$$M_j(P) = \frac{M_{ppm} \cdot 10^{-6} \cdot Mt_{gas}}{\rho_{gas(STP)} \, Mt_{air}}$$

or

$$M_j(P) = \frac{M_d}{\rho_{gas(STP)}}$$

(6) The physical constants of Table 5.4-1 are used where needed.

5.5 The Absorption Line Parameters

About 10 years ago various individuals began to compile spectroscopic data on the vibrational-rotational lines of atmospheric gases. This continued mostly as individual work until about 5 years ago when an effort at the Air Force Cambridge Research Laboratories (AFCRL) was made to continue the data collection with the aim of providing a complete set of data for all vibrational-rotational lines of naturally occuring molecules of significance in the terrestrial atmosphere. With such data at hand it would be possible to compute the transmittance appropriate for atmospheric paths. The work at AFCRL includes data on water vapor, carbon dioxide, ozone, nitrous oxide, carbon monoxide, methane, and oxygen to date. All of these molecules except oxygen are minor constituents of the atmosphere, but nonetheless represent most of the absorption lines in the visible and infrared.

In order to compute transmittance due to a given spectral line

in the atmosphere it is necessary to describe the absorption coefficient as a function of frequency of each line. The four essential parameters for each line are the resonance frequency ν_o, the intensity per absorbing molecule S, the Lorentz line width parameter α_o, and the energy of the lower state E. The frequency, ν_o, is independent of both temperature and pressure. The intensity, S, is pressure indpendent and its temperature dependence can be calculated from ν and E.

5.5.1 Derivation of Line Parameters

The four parameters ν_o, E, S, and α_o must of course be derived from experimental observations, subjected to data reduction in the framework of the general theories of molecular spectroscopy. The complexity needed to approach the problem depends both on the type of molecule and the accuracy of observational data. In the derivation of the parameters, equations and methods were used for linear triatomic and diatomic molecules (CO_2, N_2O, CO) and nonlinear triatomic molecules (H_2O, O_3). Methane, CH_4, a spherical top, is a special case, as is the diatomic O_2. The energy states and the transition probabilities between energy states of the molecules are defined primarily by their numerical values, as established by experiments and the quantum numbers which identify them. In nearly all the cases of interest mathematical relations of greater or lesser complexity relate the numerical properties to the quantum numbers.

For both linear and nonlinear molecules the vibrational and rotational states may be characterized by quantum numbers. To calculate the purely vibrational part of the energy of linear molecules it is

necessary first to compute an unperturbed energy, G_v^{uup}. A similar procedure is used for nonlinear molecules to compute G_v^{uup}. Then the effects of resonance perturbations are incorporated to obtain the molecular vibrational energies, G_v. This method was used to generate those energy levels which have not been observed; for all observed states the experimental values were used.

For linear molecules the rotational energy of each vibrational state is a function of the quantum numbers J and l, and the vibrational energy, G_v. It is given by

$$E_{v,j} = G_v+B_v[J(J+1)-\ell^2]-D_v[J(J+1)-\ell^2]^2+H_v[J(J+1)-\ell^2]^3+.... \quad (5.5\text{-}1)$$

where B_v, D_v, H_v are constants for each vibrational state that are either determined by observation or calculated. The equations for B_v and D_v are similar to those for G_v and likewise require modification through resonance perturbation.

For nonlinear molecules the rotational levels are calculated from complicated functions of the three different moments of inertia of the molecule model [Hertzberg[16]]. Having determined the energy states of the different molecules and their isotopes, the line frequencies (ν_o) are determined by taking the differences corresponding to all allowed transitions. These depend upon the selection rules for the molecule.

Half-widths (α_o) of lines are taken from observed values or computed for each molecular species. McClatchey, et al.[31] discusses the procedure used to calculate the half width of each gas type. In cases where there is insufficient data to warrent inclusion of variable half

widths, a constant value was used.

The intensities of the lines are calculated as a function of frequency (ν), the vibrational intensity of a nonrotating molecule (S_v), the rotational intensity of a rigid nonvibrating molecule (S_{ROT}), and a factor, F, that takes into account that both forms of motion occur simultaneously. The respresentations of F are quite complex and very dependent upon molecular type and isotope. A complete discussion of the derivation of parameters can be found in McClatchey, et al.[31].

In order to establish a minimum intensity value, an extreme atmospheric path was considered, assuming gas concentration specified in Table 5.3-1. This path was tangent to the earth's surface and extended from space to space. Lines yielding less than 10 percent absorption at the line center would normally be omitted. This absolute cutoff was not maintained in regions of strong absorption (relatively weak lines were dropped) and regions of weak absorption (most lines were kept). Table 5.5-1 gives the mean half-widths and minimum intensities for each molecule used in this work.

Utilizing the methods outlined above and the experimental results of many other scientists, R. A. McClatchey, et al.[31], has complied a data tape that contains the parameters needed to compute transmittance.

5.5.2 The Line Parameter Data Tape

The data compilation thus far described resulted in the accumulation of the four quantities ν_o, S, E, α_o for 108,000 spectral lines between 1 μm and the far infrared for the molecular species listed in Table 5.5-1. Additional identifying information has also been supplied

Molecule	Identifier	Intensity Minimum	Mean Half-Width
H_2O	1	$3\ 10^{-27}$	not given
CO_2	2	$2.2\ 10^{-26}$	0.07
O_3	3	$3.5\ 10^{-24}$	0.11
N_2O	4	$3.0\ 10^{-23}$	0.08
CO	5	$8.3\ 10^{-23}$	0.06
CH_4	6	$3.3\ 10^{-24}$	0.055
O_2	7	$3.7\ 10^{-30}$	0.06

Table 5.5-1. Mean half-widths and intensity minimums used by McClatchey, et al.[31] in compilation of AFCRL data tape.

for each line as indicated in Table 5.5-2. A standard computer format was adopted for card or card-image input. The units of the data are given in Table 5.5-2. The rotational and vibrational identifiers, the date, and the isotope are explained by McClatchey, et al.[31], but not used here. The molecule (columns 78-80) correspond to the identifier of Table 5.5-1.

The data are frequency ordered on magnetic tape and are contained in records each of which contain 40 card images as shown in Table 5.5-2. Each record is preceded by a variable that indicates the number of card images within the record (in all cases 40). It is necessary to decode each record from the tape according to the format

I10, 40(F10.3, E10.3, F5.3, F10.3, 5A6, A5, I3, I4, I3) 23A30.

The last format (23A30) is to read the space that separates each record. End of file markers are placed on the tape at the following points: 500, 1000, 2000, 5000, 7500, 10000 cm^{-1}. This results in the tape having seven files.

5.6 The DATSET Computer Subroutine

In order to utilize the data tape of McClatchey it was necessary to write a computer subroutine that would transfer that portion of the data needed from the tape to computer memory or if desired to disk. The subroutine is used in conjuction with the transmittance program. Some job control language (JCL) is needed with the routine to identify the different files of the tape and establish the disk space if that is to be used. The flow of the routine is outlined below and a listing of the program is given in Appendix D.

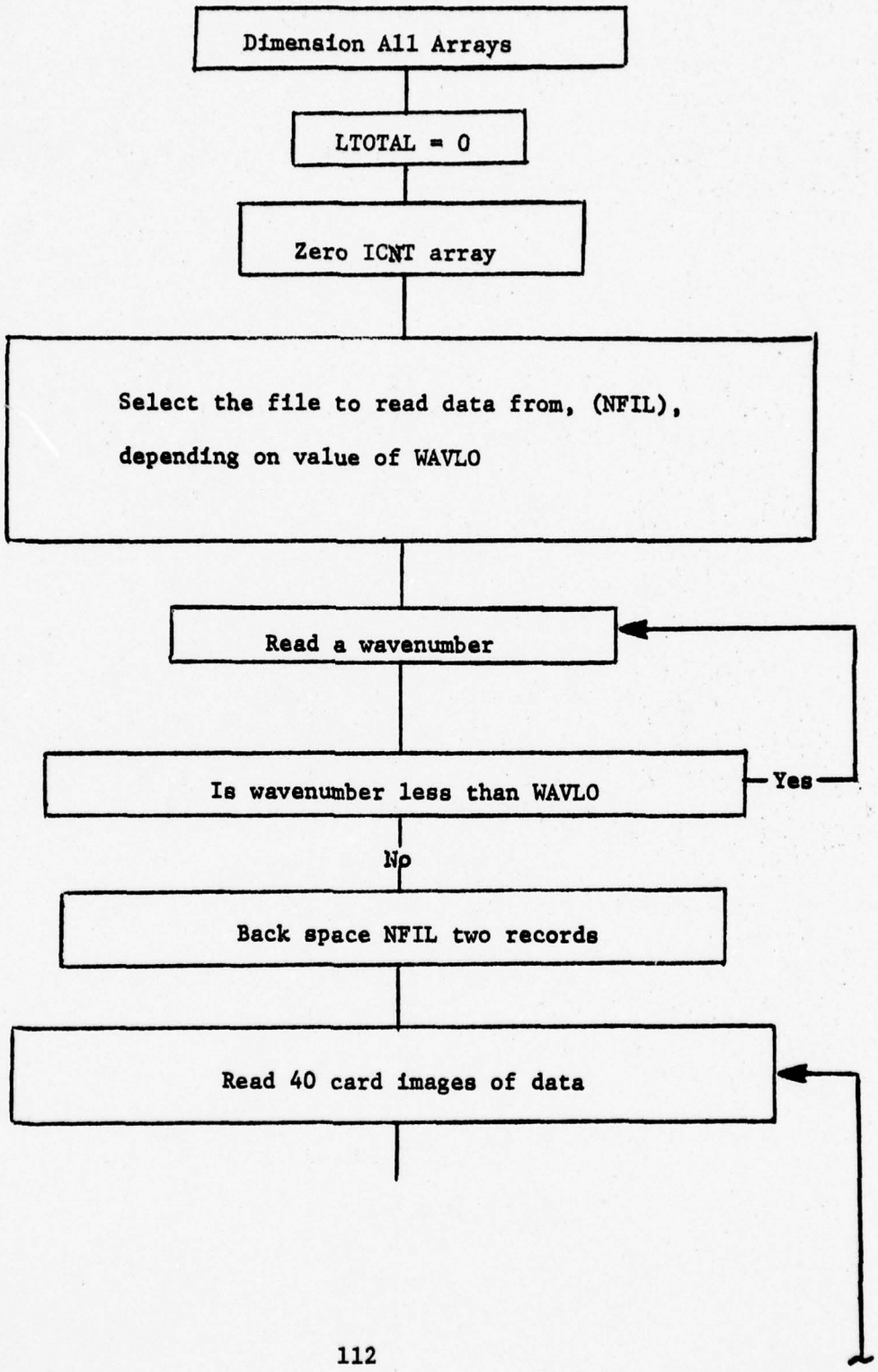
Data element	Units	Card Column	Format
ν_o	cm^{-1}	1-10	F10.3
S_o	$\frac{cm^{-1}}{molecule\text{-}cm^2}$	11-20	E10.3
α_o	cm^{-1}/atm	21,25	F5.3
E	cm^{-1}	26-35	F10.3
Rotational-Vibration ID		36-70	5A6,A5
Date		71-73	I3
Isotope		74-77	I4
Molecule		78-80	I3

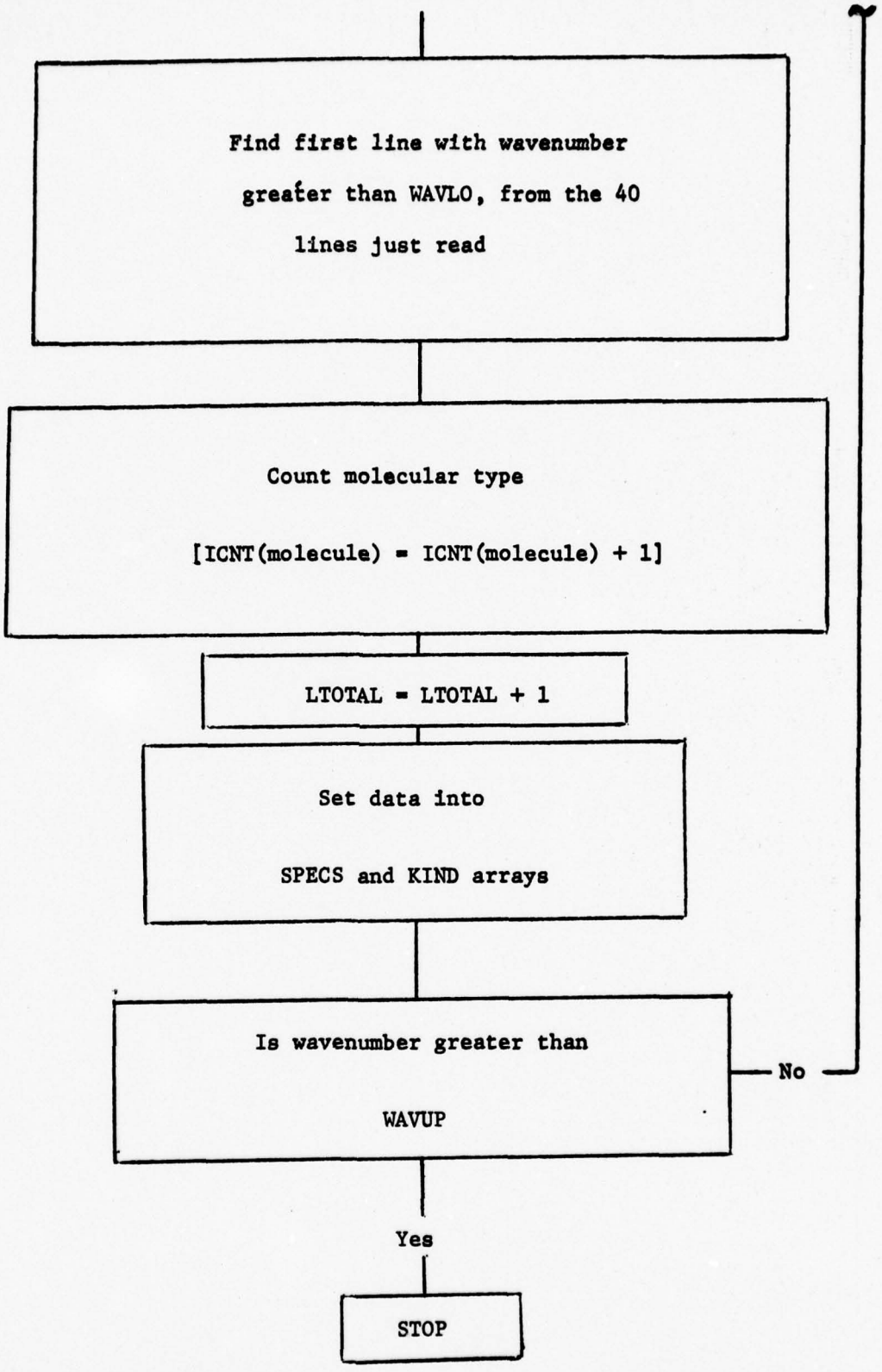
Table 5.5-2. Computer format of each spectral line's data. [McClatchey, et al.[31]]

The subroutine has the following parameters:

WAVLO	....lower wavenumber of data to be extracted from data tape (lower limit of channel)	....input
WAVUP	....upper wavenumber of data to be extracted from tape (upper limit of channel)	....input
ICNT(T)	....Array containing the number of spectral lines between wavlo and wavup, by gas type. (1= H_2O, 2= CO_2, etc.)	....output
MAX	....Maximum number of lines that can be transfered from tape (3000)	....input
SPECS(3000,4)	....Array containing data for each line (ν_o, S_o, E, α_o)	....output
KIND(3000)	....Array containing molecular identifier of each line	....output
LTOTAL	....Total number of lines between wavlo and wavup	....output

DATSET Flowchart




Find first line with wavenumber greater than WAVLO, from the 40 lines just read
Count molecular type
[ICNT(molecule) = ICNT(molecule) + 1]
LTOTAL = LTOTAL + 1
Set data into
SPECS and KIND arrays
Is wavenumber greater than
WAVUP
No
Yes
STOP

There are error messages that will inform the user if the program does not execute properly. The routine can be used to transfer data to disk (see comment card in program listing). The JCL necessary to define the files must be included before using disk.

CHAPTER VI

THE TRANSMITTANCE PROGRAM

6.1 Preface

This chapter presents the object of the previous five chapters, a transmittance program. Before the routine is presented the vibrational partition function (Q) is developed, the interative solution used to solve the transmittance differential equation is explained, and the methods used to compute monochromatic and averaged transmittance are given. These final details are incorporated with the equations thus far developed to yield the transmittance program. The chapter concludes with the results of some transmittance calculations in the fifteen micrometer band.

6.2 The Rotational and Vibrational Partition Functions

The equation for line strength may be given as

$$S = S_o \, Q_R \exp\left\{ \frac{E}{kT_o} \left(1 - \frac{T_o}{T}\right) \right\} Q_v \qquad (6.2\text{-}1)$$

The line strength is dependent upon the rotational and vibrational modes of the molecule in a characteristic manner. The rotational partition function (Q_R) is very temperature dependent and is given by [McClatchey, et al.[31]]

$$Q_R = \left(\frac{T_o}{T}\right)^{C_j}, \qquad (6.2\text{-}2)$$

where the exponent C_j assumes values dependent upon gas type. The vibrational partition function (Q_v) is also temperature dependent, but not in such a clear manner. Table 6.2-1 gives the value of C_j

Molecule	C_j	Vibrational Partition Function Temperature						
		175	200	225	250	275	296	325
H_2O	1.5	1.0	1.0	1.0	1.0	1.0	1.0	0.999
CO_2	1.0	1.082	1.072	1.058	1.041	1.019	1.0	0.970
O_3	1.5	1.042	1.038	1.033	1.024	1.013	1.0	0.981
N_2O	1.0	1.108	1.094	1.075	1.051	1.025	1.0	0.963
CO	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
CH_4	1.5	1.007	1.007	1.006	1.005	1.003	1.0	0.996
O_2	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.999

Table 6.2-1. Rotational and Vibrational Partition Functions.
(Adapted from McClatchey, et al.[31])

and the vibrational functions that are used in this work. For computer implementation it is simple enough to use the different values for C_j from a look-up array, however a speedy and accurate method is needed for the vibrational partition function.

Therefore regression analysis of the vibrational points was performed for linear, quadratic, and cubic fits to determine the best relation. For each gas the following functions of temperature (T) were tried.

$$\text{Linear...} Q_v = A_1 T + A_2$$

$$\text{Quadratic...} Q_v = B_1 T^2 + B_2 T + B_3$$

$$\text{Cubic...} Q_v = C_1 T^3 + C_2 T^2 + C_3 T + C_4$$

Linear fits were abandoned after the partition function was graphed and several lines were tried. For the quadratic and cubic relations a computer routine was written to determine the coefficients B_i and C_i.

In matrix form the vibrational partition functions can be written

$$Q_v = AT, \tag{6.2-3}$$

where Q_v is a (7 x 1) partition array, A is a (7 x 3) unknown array, and T is a (3 x 1) temperature array. For cubic fit A is (7 x 4) and T is (4 x 1). The unknown array A is given by [Burr[7]]

$$A = [T^t T]^{-1} [T^t Q_v], \tag{6.2-4}$$

where the superscript (t) indicates matrix transpose. The results of the regression analysis are given in Table 6.2-2.

In view of the small errors associated with the quadratic coefficients, they are used in the transmittance program for the vibrational partition function.

6.3 Euler's Solution of the Transmittance Differential Equation

The transmittance differential equation may be written

$$\frac{d\tau}{dP} = \sigma\tau, \qquad (6.3\text{-}1)$$

where

$$\sigma = \sum_j K_j M_j.$$

If the atmosphere is stratified and every layer has a different σ, the transmittance relation becomes

$$\frac{d\tau_\ell}{dP} = \sigma_{\ell+1}\ \tau_{\ell+1}, \qquad (6.3\text{-}2)$$

where dP is the pressure difference between the ℓ and ℓ+1 layers. This is a first-order ordinary differential equation. A solution, $\tau(P)$, is desired that satisfies Eq. 6.3-2 and a single specified initial condition. In general it is impossible to determine $\tau(P)$ in exact analytical form. Instead, the interval in the independent variable, P, over which a solution is desired, $[0,P_o]$, is divided into sub-intervals or steps. These steps correspond to the pressure differences dP.

An application of the Runge-Kutta algorithms to Eq. 6.3-2 results

Molecule	Quadratic Coefficients B_1	B_2	B_3	Error of Quadratic Formula
H_2O	$-9.88 \cdot 10^{-8}$	$4.49 \cdot 10^{-5}$	0.99	$9.6 \cdot 10^{-3}$%
O_3	$-2.16 \cdot 10^{-6}$	$6.77 \cdot 10^{-4}$	0.98	$2.1 \cdot 10^{-2}$%
CO_2	$-2.54 \cdot 10^{-6}$	$5.16 \cdot 10^{-4}$	1.07	$1.3 \cdot 10^{-2}$%
N_2O	$-2.81 \cdot 10^{-6}$	$4.28 \cdot 10^{-4}$	1.12	$2.5 \cdot 10^{-2}$%
CO	0.0	0.0	1.0	0.0 %
CH_4	$-6.00 \cdot 10^{-7}$	$2.28 \cdot 10^{-4}$	0.98	$1.3 \cdot 10^{-2}$%
O_2	$-9.89 \cdot 10^{-8}$	$4.49 \cdot 10^{-5}$	0.99	$9.6 \cdot 10^{-3}$%

Molecule	Cubic Coefficients C_1	C_2	C_3	C_4	Error of Cubic Formula
H_2O	$-1.68 \cdot 10^{-9}$	$1.16 \cdot 10^{-6}$	$-2.63 \cdot 10^{-4}$	1.02	$8.9 \cdot 10^{-3}$%
O_3	$1.08 \cdot 10^{-9}$	$-2.98 \cdot 10^{-6}$	$8.76 \cdot 10^{-4}$	0.97	$2.2 \cdot 10^{-2}$%
CO_2	$-1.67 \cdot 10^{-9}$	$1.16 \cdot 10^{-6}$	$-2.63 \cdot 10^{-4}$	1.02	3.9 %
N_2O	$8.85 \cdot 10^{-9}$	$-9.46 \cdot 10^{-6}$	$2.05 \cdot 10^{-3}$	0.99	$2.9 \cdot 10^{-2}$%
CO	$-6.38 \cdot 10^{-14}$	$4.77 \cdot 10^{-11}$	$-1.16 \cdot 10^{-7}$	1.00	$2.8 \cdot 10^{-8}$%
CH_4	$-6.91 \cdot 10^{-10}$	$-8.19 \cdot 10^{-8}$	$1.01 \cdot 10^{-4}$	0.99	$1.3 \cdot 10^{-2}$%
O_2	$-1.68 \cdot 10^{-9}$	$1.16 \cdot 10^{-6}$	$-2.63 \cdot 10^{-4}$	1.01	$8.9 \cdot 10^{-3}$%

Table 6.2-2. Regression coefficients for quadratic and cubic fit of Vibrational Partition Function.

in the improved Euler's method or Heun's method [Carnahan, et al.[8]] of solution of the differential equation. The desired solution of Eq. 6.3-2 is thus given as

$$\tau_{\ell+1} = \tau_{\ell} + \frac{dP}{2} \left\{ \sigma\tau_{\ell} + \sigma\bar{\tau}_{\ell+1} \right\} \tag{6.3-3}$$

where

$$\bar{\tau}_{\ell+1} = \tau_{\ell} + dP\sigma\tau_{\ell} \; ; \tag{6.3-4}$$

subject to the initial condition (top of the atmosphere)

$$\tau(o) = 1 \; . \tag{6.3-5}$$

Euler's algorithm may be viewed as a predicting equation for $\bar{\tau}^{1}_{\ell+1}$ (the first approximation to $\tau_{\ell+1}$), whereas Eq. 6.3-3 may be considered a correcting equation to produce an improved estimate of $\tau_{\ell}+1$. Equation 6.3-3 is used iteratively to produce a sequence of corrected $\tau_{\ell+1}$ values. A maximum of ten iterations per atmospheric layer is allowed in the program.

This procedure results in values of transmittance for every layer of the atmosphere, beginning at P=0, τ=1 and continuing to the bottom of the atmosphere (ground level). The variable σ must of course be computed for each layer of the atmosphere utilizing the proper equations. However, the calculation of σ is sovereign of the solution τ, and is done independently.

6.4 Transmittance Iteration Technique

This section explains a technique that was developed to enable

the transmittance program to calculate either a monochromatic transmission or an averaged channel transmission. In addition, the option to extend the channel limits was incorporated into the program.

In calculating the transmission at a single frequency the effects of all lines within a specified range of that frequency are added together. This range is denoted by the variable SEARCH. When calculating the transmittance of a channel, the distance BOUND is used to extend the limits of the channel and thus account for lines that contribute to absorption within the channel, but whose center frequency ν_o is out of the channel (see Fig. 3.4-3). To calculate the transmittance for a band the monochromatic transmittances are calculated at several frequencies and then averaged over the band.

The following variables are defined below and used in the transmittance program, iteration loop.

WAVLO... Lower wavenumber of channel.

WAVUP... Upper wavenumber of channel.

SEARCH... The range about a single frequency within which the effects of spectral lines are added together.

CNTR... The single frequency at which transmittance is calculated.

BOUND... Amount by which the limits of a channel are enlarged to consider lines that absorb within the channel, but whose center frequency, ν_o, is outside of the channel.

SPACE... The distance between the single frequencies at which transmittances are calculated.

INTVLS... The number of intervals the channel is divided into, minus one.

INCR... The number of intervals the channel is divided into. Also, the number of transmittance calculations made within a channel.

The increment loop proceeds as follows during the transmittance program execution:

(1) The variables BOUND and INTVLS are read as input data.

(2) The lower limit, WAVLO, and the upper limit, WAVUP, of the channel are read as input data.

(3) The limits of the channel are adjusted by the amount BOUND.

(4) The absorption line parameters (ν_o,S,E,α) of lines between the adjusted WAVLO and WAVUP limits are transferred from tape to computer memory.

(5) The variable SEARCH is set equal to BOUND. If BOUND was zero, SEARCH is set equal to half the channel width.

(6) The channel is divided into the desired number of intervals (INTVLS+1) and the variable SPACE is set equal to the distance between transmission calculation points, SPACE = $\frac{\text{WAVUP-WAVLO}}{\text{INTVLS}}$.

(7) The first frequency of transmission calculation, CNTR, is set to WAVLO. If only one transmittance calculation is to be made in a channel, CNTR is set to the channel center frequency.

(8) The upper limit, UP, and lower limit, DOWN, are set to CNTR $\pm$ SEARCH respectively. This causes the transmittance calculations to include lines within the distance SEARCH of CNTR.

(9) Transmission computations are made for the frequency CNTR.

(10) If another transmittance calculation is to be performed in this channel, the value of CNTR is changed to CNTR + SPACE (go to step 9) if not, another channel is done (go to step 2).

(11) After all channels are completed the program terminates.

Figures 6.4-1, 6.4-2, and 6.4-3 graphically display this procedure for three increment options.

INCR = 1

INTVLS = 0

BOUND = 0

CNTR = (WAVUP + WAVLO)/2

SEARCH = (WAVUP-WAVLO)/2

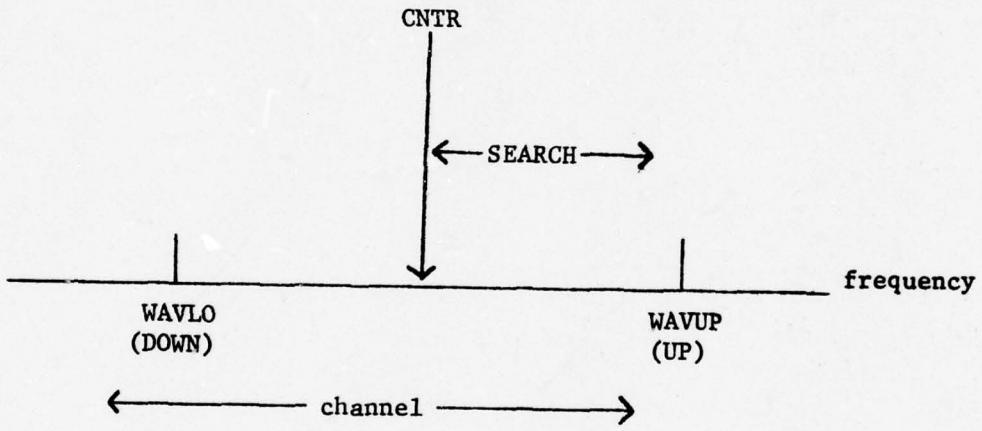


Figure 6.4-1. A single transmission calculation per channel. Channel limits not adjusted.

```
INCR = 1

INTVLS = 0

BOUND = 5

CNTR = (WAVUP + WAVLO)/2

SEARCH = BOUND
```

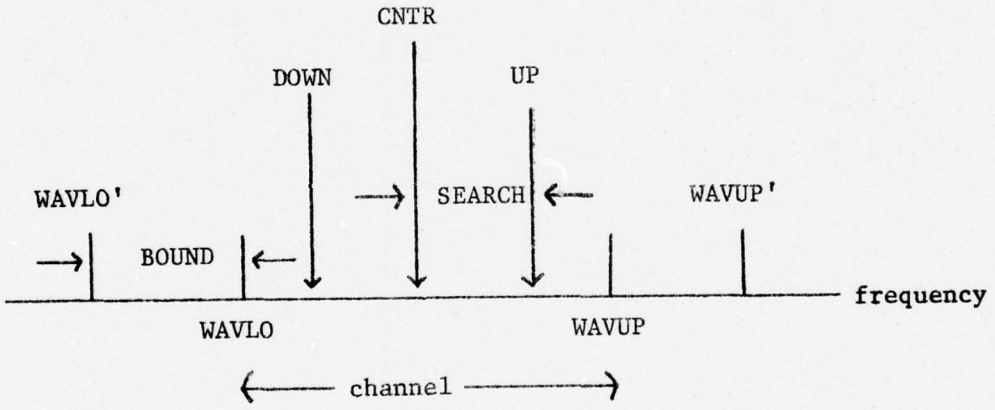


Figure 6.4-2. A single transmission calculation per channel. Channel limits adjusted by BOUND.

INTVLS = 2

INCR = 3

BOUND = 5

CNTR = WAVLO, WAVLO + SPACE, WAVUP

SEARCH = BOUND

SPACE = (WAVUP-WAVLO)/INTVLS

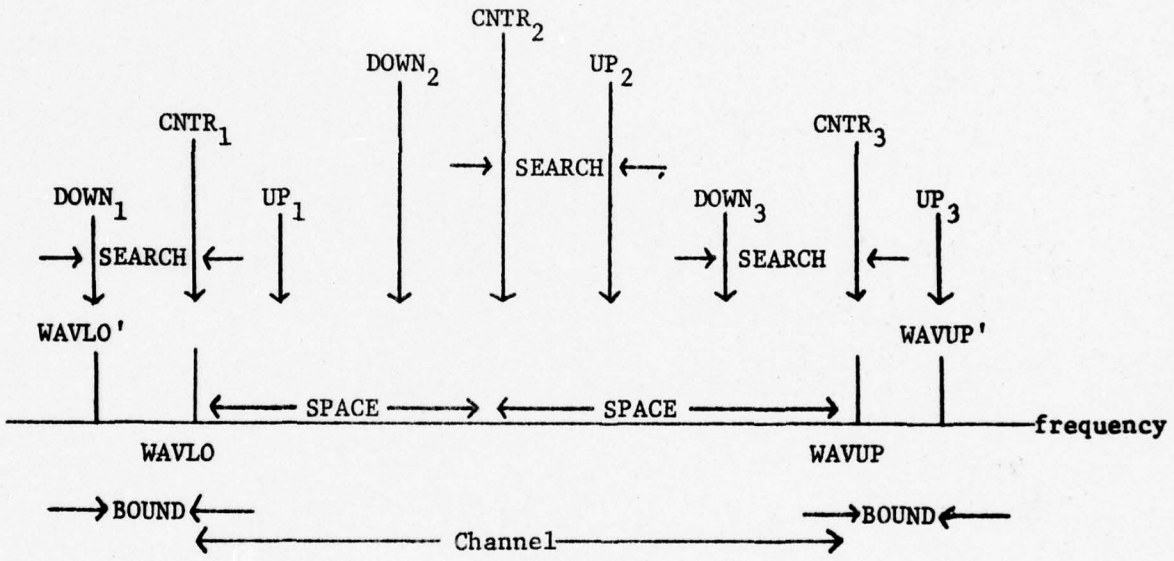


Figure 6.4-3. Three transmittance calculations per channel. Channel limits adjusted by BOUND.

6.5 Transmittance Program Flowchart and Utilization

The transmittance program written as the final product of this work is listed in Appendix E. The equations and relations necessary to calculate the line-by-line transmittance were implemented in the most efficient manner possible. There are five main portions of the program. First, all initializations and one-time computations are made. Second the calculations and data transfer peculiar to a channel are completed. The third step is the increment loop. It sets how many and where (frequencies) transmittance calculations are to be performed. Fourth, the equations that are a function of atmospheric level (altitude) are processed. The fifth and final step is the line loop. It considers only the appropriate spectral lines in the transmission calculations. The output is a set of transmittance values for each layer of the atmosphere. A general flowchart is given in Fig. 6.5-1.

A major portion of the program transfers data or determines which spectral lines to use in calculations. The absorption coefficient computation occurs in the line loop and utilizes the equations indicated in Table 6.5-1.

The program was written in FORTRAN IV for an IBM 360/65 computer [20, 21]. It utilizes two subroutines; DATSET to transfer data from tape to core and ZVOIGT to compute the voigt line shape. Both subroutines are explained in other sections and have listings in the appendices. The job control language (JCL) necessary to read the data tape is listed in Appendix D with the DATSET routine.

The card input required to execute the program is:

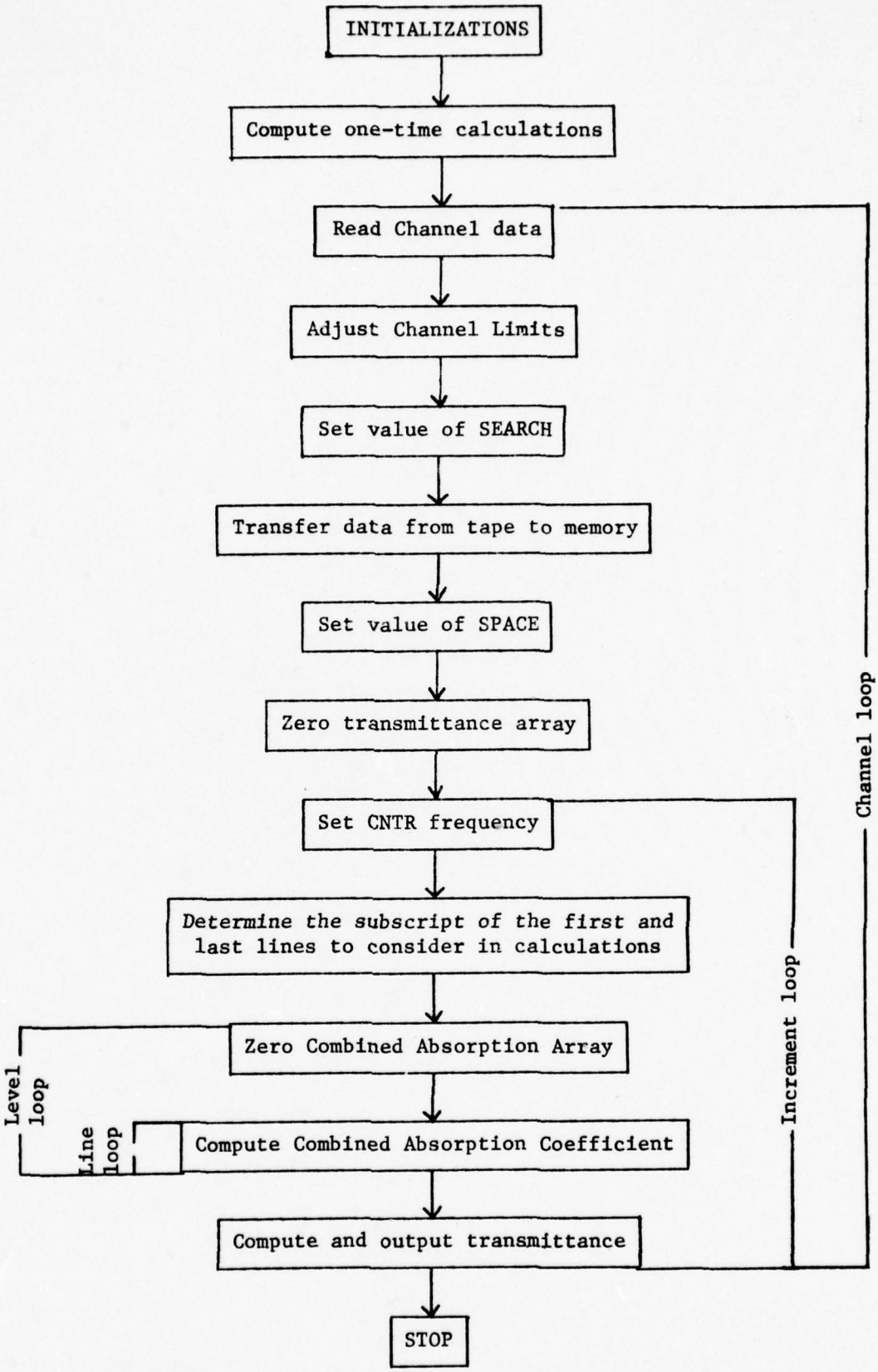


Figure 6.5-1. Transmittance Program Flowchart.

Symbol	Definition	Equation(s) Used
α_D	Doppler line width	2.4-4
α_L	Lorentz line width	2.4-12
y	Doppler-Lorentz ratio	4.3-1
K_o	Absorption coefficient	3.3-20
x	Wavenumber difference	4.3-1
$\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{ye^{-t^2}dt}{y^2+(x-t)^2}$	Voigt shape	ZVOIGT subroutine
$\sum_j K_j$	Extinction coefficient	3.2-21
ABSK	Combined extinction coefficient	5.3-15
τ	Transmittance	6.3-3, 6.3-4

Table 6.5-1. Equations used in the transmittance program.

NCHNL... Number of channels

LEVS... Number of atmospheric layers

BOUND... Extention amount of channel limits

INTVLS... Number of channel intervals, minus one

PRESS(LEVS)... Pressure for each layer

TEMP(LEVS)... Temperature for each layer

H2OMIX(LEVS)... Water vapor concentration for each layer

O3MIX(LEVS)... Ozone concentration for each layer

WAVLO... Lower channel limit (for each channel)

WAVUP... Upper channel limit (for each channel)

Figure 6.5-2 shows the input format and order required.

The transmittance program was executed for the following input data. NCHNL=7, LEVS=33, BOUND=0, INTVLS=0

The channel limits for each channel were taken from Table 3.4-1. The pressure, temperature, water vapor concentration and ozone concentration were taken from McClatchey, et al.[32] and are similar to Table 5.3-3. The results of this monochromatic layer transmittance for each channel are given in Appendix G. Other computations were made utilizing several frequencies per channel (INTVLS $\neq$ 0) to test the iteration portion of the program. The transmittance of a single channel using INTVLS = 10 is given in Appendix H for comparison with the monochromatic calculation.

Card Name	Format	Number Required
Level-Channel Data	NCHNL LEVS BOUND INTVLS 1X I3 1X I3 1X F10.3 1X I4	1
Atmosphere Data	PRESS(I) TEM(I) H2OMIX(I) O3MIX(I) 6X E9.3 F5.1 1X E9.3 1X E9.3	LEVS
Channel limits Data	WAVLO WAVUP 1X F10.3 1X F10.3	NCHNL

Figure 6.5-2. Input data format and number required.

CHAPTER VII

DISCUSSION AND CONCLUSION

7.1 Preface

This final chapter briefly comments on this research and draws some conclusions. It was the object of this work to develop a fast monochromatic transmittance program. That has been done. The chapter ends with a note on what future, related works might investigate.

7.2 Discussion

This work was approached with the intent of developing a line-by-line transmission model. To construct that model the physics of the atmosphere and some molecular theory of gases was introduced. It is hoped that the development of the transmittance algorithm proceeded in a fluid manner and with enough detail to enable the reader to follow.

During the development of the equations that were needed, an algorithm to quickly evaluate the Voigt function was born. It is sincerely hoped that this Voigt algorithm proves to be a valuable one for atmospheric work.

7.3 Conclusions

The transmittance program written as a result of this work was used to compute the monochromatic transmission for channels in both the 15 and 4.3 micrometer band. Also, averaged transmittances were computed for selected channels. In all cases the program executed properly and returned values that seemed to be correct.

The results of the program were not compared with any other, as they were not available. However, the extinction coefficients computed in the program were compared to those computed in a completely different manner; in a program written by Mr. T. Potter.[40] The agreement of the coefficients computed in the two different methods was excellent. From these coefficients it is a simple matter to compute transmittance, so it is assumed that if the extinction coefficients were correct the transmittances would be correct.

The single most important conclusion is that the Voigt algorithm developed in this work is a rapid and accurate method to evaluate the Voigt profile. The results of tests that were made with the algorithm surpassed all expectations (see chapter four).

7.4 Ongoing Research

It is my opinion that the Voigt algorithm developed here can be improved. First, the routine need not be double precision. I believe that it is possible to obtain very good results with a single precision routine. Secondly, the series used for the algorithm in Region I could be expanded to thirty terms and a Chebyshev economization used to reduce the number of terms. This would increase speed and maintain the desired accuracy.

The results of this transmittance program need to be compared with some other results. Although the values appear to be correct, they need confirmation. Once the validity of the method is established, additional data needs to be obtained so the transmittance of the

atmosphere can be more closely tabulated. For this the atmosphere should be divided into 100 layers. Additionally, the transmittance computed for a channel needs to be convolved with a slit function corresponding to the HIRS instrument.

Finally a more efficient routine needs to be developed to yield an averaged transmittance. The method used in this work is very time consuming. To calculate a single monochromatic transmittance takes about 15 CPU seconds. If a step of 0.01 wavenumbers is used for a channel with a width of 20 wavenumbers, it means 2000 single evaluations or about 8 hours of computation time. A better system must be developed.

APPENDIX A

KIELKOPF'S VOIGT ALGORITHM

The FORTRAN IV subroutine that implements Kielkopf's Voigt algorithm is listed on the following page. It is a double precision routine that has three parameter inputs and a single parameter output. The input parameters are

$$BL = \alpha_L$$

$$BG = \alpha_D/(1n2)^{1/2}$$

and $$V = \frac{\nu-\nu_0}{\alpha_D}(1n2)^{1/2}$$

The value of the *Voigt Function is returned* as the variable VGT when the main program contains the following statement

CALL COEFF(BL, BG, V, VGT).

```
FORTRAN IV G LEVEL  21                  COEF                    DATE = 77108          11/01/30

0001                  SUBROUTINE COEF(BL,BG,V,VGT)
0002                  IMPLICIT REAL*8(A-H,O-Z)
0003                  DATA TWO/2.00000000/
0004                  A=BL/BG
0005                  AL=2./(1.+.099*DLOG(TWO)+DSQRT((1.-.099*DLOG(TWO))**2+
                     1     ((4.*DLOG(TWO))/(A*A))))
0006                  G2=(1./DLOG(TWO))/(1.-AL)
0007                  B=BL/AL
0008                  ETA=AL/(AL+G2)
0009                  X=V/B
0010                  GX=DEXP(-(DLOG(TWO)*X*X))
0011                  ALX=1./(1.+X*X)
0012                  EX=(.8029-.4207*X*X)/(1.+.2030*X*X+.07335*X*X*X*X)
0013                  UX=(1.-ETA)*GX+ETA*ALX+ETA*(1.-ETA)*EX*(GX-ALX)
0014                  T=1./(1.+.47047*A)
0015                  XI=A*(.61686*T-.14994*T*T+1.32554*T*T*T)/(3.141592654*BL)
0016                  VGT=XI*UX*(1.772453851/(BL/BG))
0017                  RETURN
0018                  END
```

APPENDIX B

DRAYSON's VOIGT ALGORITHM

The FORTRAN IV function subprogram that uses the four regions proposed by Drayson is a single precision routine. The variable VOIGT is set equal to the Voigt function value in the subprogram when the main routine executes a call statement, i.e.,

SHAPE = VOIGT (X,Y).

The parameters X and Y are:

$$Y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2}$$

$$X = \frac{\nu - \nu_0}{\alpha_D} (\ln 2)^{1/2}$$

The program listing begins on the next page.

```
FORTRAN IV G LEVEL  21                VOIGT                DATE = 77108          11/01/30

0001                  FUNCTION VOIGT(X,Y)
0002                  REAL B(22)/0.,.7093602E-7/,RI(15),XN(15)/10.,9.,2*8.,7.,6.,5.,4.,
                     1  7*3./,YN(15)/3*.6,.5,2*.4,4*.3,1.,.9,.8,2*.7/,
                     2  D0(25),D1(25),D2(25),D3(25),D4(25),HN(25),
                     3  H/.201/,XX(3)/.5246476,1.65068,.7071068/,
                     3 HH(3)/.2562121,.2588268E-1,.2820948/,
                     4  NBY2(19)/9.5,9.,8.5,8.,7.5,7.,6.5,6.,5.5,5.,4.5,4.,3.5,3.,2.5,
                     5  2.,1.5,1.,.5/,
                     6  C(21)/.7093602E-7,-.2518434E-6,.8566874E-6,-.2787638E-5,
                     7  .866074E-5,-.2565551E-4,.7229775E-4,-.1933631E-3,.4899520E-3,
                     7  -.1173267E-2,.2648762E-2,-.5623190E-2,.1119601E-1,-.2084976E-1,
                     8  .3621573E-1,-.58514112E-1,.8770816E-1,-.121664,.15584,-.184,.2/
0003                  LOGICAL TRU/.FALSE./
0004                  IF(TRU) GO TO 104
0005                  TRU=.TRUE.
0006                  DO 101 I=1,15
0007             101  RI(I)=-I/2.
0008                  DO 103 I=1,25
0009                  HN(I)=H*(I-.5)
0010                  CO=4.*HN(I)*HN(I)/25.-2.
0011                  DO 102 J=2,21
0012             102  B(J+1)=CO*B(J)-B(J-1)+C(J)
0013                  D0(I)=HN(I)*(B(22)-B(21))/5.
0014                  D1(I)=1.-2.*HN(I)*D0(I)
0015                  D2(I)=(HN(I)*D1(I)+D0(I))/RI(2)
0016                  D3(I)=(HN(I)*D2(I)+D1(I))/RI(3)
0017             103  D4(I)=(HN(I)*D3(I)+D2(I))/RI(4)
0018             104  IF(X-5.) 105,112,112
0019             105  IF(Y-1.) 110,110,106
0020             106  IF(X.GT.1.85*(3.6-Y)) GO TO 112
0021                  IF(Y.LT.1.45) GO TO 107
0022                  I=Y+Y
0023                  GO TO 108
0024             107  I=11.*Y
0025             108  J=X+X+1.85
0026                  MAX=XN(J)*YN(I)+.46
0027                  MIN=MIN0(16,21-2*MAX)
0028                  UU=Y
0029                  VV=X
0030                  DO 109 J=MIN,19
0031                  U=NBY2(J)/(UU*UU+VV*VV)
0032                  UU=Y+U*UU
0033             109  VV=X-U*VV
0034                  VOIGT=UU/(UU*UU+VV*VV)/1.772454
0035                  RETURN
0036             110  Y2=Y*Y
0037                  IF(X+Y.GE.5.) GO TO 113
0038                  N=X/H
0039                  DX=X-HN(N+1)
0040                  U=(((D4(N+1)*DX+D3(N+1))*DX+D2(N+1))*DX+D1(N+1))*DX+D0(N+1)
0041                  V=1.-2.*X*U
0042                  VV=EXP(Y2-X*X)*COS(2.*X*Y)/1.128379-Y*V
0043                  UU=-Y
0044                  MAX=5.+(12.5-X)*.8*Y
0045                  DO 111 I=2,MAX,2
0046                  U=(X*V+U)/RI(I)
0047                  V=(X*U+V)/RI(I+1)
0048                  UU=-UU*Y2
```

```
0049          111 VV=VV+V*UU
0050              VOIGT=1.128379*VV
0051              RETURN
0052          112 Y2=Y*Y
0053              IF(Y.LT.11.-.6875*X) GO TO 113
0054              U=X-XX(3)
0055              V=X+XX(3)
0056              VOIGT=Y*(HH(3)/(Y2+U*U)+HH(3)/(Y2+V*V))
0057              RETURN
0058          113 U=X-XX(1)
0059              V=X+XX(1)
0060              UU=X-XX(2)
0061              VV=X+XX(2)
0062              VOIGT=Y*(HH(1)/(Y2+U*U)+HH(1)/(Y2+V*V)+HH(2)/(Y2+UU*UU)+
                 1  HH(2)/(Y2+VV*VV))
0063              RETURN
0064              END
```

APPENDIX C

PROPOSED VOIGT ALGORITHM

The implementation of the proposed Voigt algorithm utilizing three regions of the XY plane is a FORTRAN IV function subprogram. The routine sets the variable ZVOIGT equal to the value of the Voigt profile, for the parameters

$$Y = \frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2}$$

and $$X = \frac{\nu - \nu_0}{\alpha_D} (\ln 2)^{1/2} .$$

The call statement required in the main program is

SHAPE = ZVOIGT (X,Y).

The program listing is on the next page.

```
0001                FUNCTION ZVOIGT(X,Y)
0002                IMPLICIT REAL*8(A-H,O-Z)
0003                REAL*8 AN(30)/1.00000000,-.33333333,.10000000,-.238095238E-1,
                   1  4.629629639E-3,-7.57575757E-4,1.068376069E-4,-1.322751323E-5,
                   2  1.458916916E-6,-1.450385222E-7,1.312253296E-8,-1.089222104E-9,
                   3  8.350702795E-11,-5.947794014E-12,3.955429516E-13,
                   4  -2.466827016E-14,1.448326465E-15,-8.032735012E-17,
                   5  4.221407289E-18,-2.107855192E-19,
                   +  1.002516493E-20,-4.551846759E-22,1.977064754E-23,
                   +-8.230149299E-25,3.289260349E-26,-1.264107899E-27,4.67848352E-29,
                   +  -1.669751793E-30,5.754191644E-32,-1.916942862E-33/,
                   +  A1/.46131350/,
                   6   A2/.19016350/,A3/.09999216/,A4/1.78449270/,A5/.002883894/,
                   7  A6/5.52334370/,B1/.51242424/,B2/.27525510/,B3/.05176536/,
                   8  B4/2.72474500/,PISQ/1.128379167/
0004                S=X*X-Y*Y
0005                T=2.*X*Y
0006                IF(Y.GE.5..OR.X.GE.5.) GO TO 111
0007                IF(Y.GE.1.8 .OR. X.GE.3.0) GO TO 112
0008                XSER=Y
0009                YSER=-X
0010                XN=Y
0011                YN=-X
0012                X2=-S
0013                Y2=-T
0014                N=6.842*X+8.0
0015                IF(N.GT.29) N=29
0016                IF(X.EQ.0.0) N=15
0017                DO 10 I10=1,N
0018                XNEW=XN*X2-YN*Y2
0019                YNEW=Y2*XN+YN*X2
0020                XSER=XSER+XNEW*AN(I10+1)
0021                YSER=YSER+YNEW*AN(I10+1)
0022                XN=XNEW
0023                YN=YNEW
0024             10 CONTINUE
0025                ZVOIGT=DEXP(-S)*(DCOS(-T)*(1.-PISQ*XSER)+PISQ*DSIN(-T)*YSER)
0026                RETURN
0027             112 R=T*T
0028                T=T*X
0029                F=S-A6
0030                G=S-A4
0031                H=S-A2
0032                ZVOIGT=A1*((T-H*Y)/(H*H+R))+A3*((T-G*Y)/(G*G+R))+
                   1    A5*((T-F*Y)/(F*F+R))
0033                RETURN
0034             111 R=T*T
0035                T=T*X
0036                F=S-B2
0037                G=S-B4
0038                ZVOIGT=B1*((T-F*Y)/(F*F+R))+B3*((T-G*Y)/(G*G+R))
0039                RETURN
0040                END
```

APPENDIX D

DATSET SUBROUTINE

The data processing routine used by the transmittance program to transfer data from tape to computer memory or disk is listed on the next page. The parameters of the FORTRAN IV subroutine are explained in section 5.6. The following JCL must be included for program execution. It defines the seven files of the tape so that the routine can more quickly select that portion of the tape from which to read data.

```
//GO.FT11F001  DD UNIT=2400,DSN=F1L1,
// LABEL=(02,BLP,IN),DISP=OLD,VOL=SER=T00388,
// DCB=(RECFM=F,BLKSIZE=3900)
```

Seven of these cards must be used, the remaining six are exactly the same except as shown.

```
...GO.FT12F001...DSN=F1L12...LABEL=(05,BLP,IN)...
...GO.FT13F001...DSN=F1L13...LABEL=(08,BLP,IN)...
...GO.FT14F001...DSN=F1L14...LABEL=(11,BLP,IN)...
...GO.FT15F001...DSN=F1L15...LABEL=(14,BLP,IN)...
...GO.FT16F001...DSN=F1L16...LABEL=(17,BLP,IN)...
...GO.FT17F001...DSN=F1L17...LABEL=(20,BLP,IN)...
```

The routine can transfer 3000 lines of data to core. If disk is to be used the necessary JCL and DEFINE FILE statements must be included, and in the DATSET routine the comment card used and the

SPECS(...)=

and KIND (...)= Cards

removed.

```
FORTRAN IV G LEVEL  21                  DATSET              DATE = 77108          11/01/30

0001                  SUBROUTINE DATSET(WAVLO,WAVUP,ICNT,MAX,SPECS,KIND,LTOTAL)
0002                  DIMENSION IDATE(40),ISO(40),MOL(40),GBG(23),ICNT(7)
0003                  DIMENSION WAV(40),STRGH(40),WDTH(40),ENGY(40),ROTID(40,5),VIB(40)
0004                  DIMENSION SPECS(3000,4),KIND(3000)
0005                  LTOTAL=0
0006                  DO 40 I40=1,7
0007               40 ICNT(I40)=0
0008                  NFIL=11
0009                  IF(WAVLO.GT.500.0) NFIL=12
0010                  IF(WAVLO.GT.1000.0) NFIL=13
0011                  IF(WAVLO.GT.2000.0) NFIL=14
0012                  IF(WAVLO.GT.5000.0) NFIL=15
0013                  IF(WAVLO.GT.7500.0) NFIL=16
0014                  IF(WAVLO.GT.10000.0) NFIL=17
0015               07 READ(NFIL,01,END=99) NUM,FREQ
0016               01 FORMAT(I1),F10.3)
0017                  IF(FREQ.LT.WAVLO) GO TO 07
0018                  BACKSPACE NFIL
0019                  BACKSPACE NFIL
0020               23 READ(NFIL,11,END=98) NUM,(WAV(K),STRGH(K),WDTH(K),
                     1  ENGY(K),(ROTID(K,J),J=1,5),VIB(K),IDATE(K),ISO(K),
                     1  MOL(K),K=1,40),(GBG(M),M=1,23)
0021               11 FORMAT(I10,40(F10.3,E10.3,F5.3,F10.3,5A6,A5,I3,I4,I3),23A30)
0022                  DO 10 I10=1,NUM
0023                  KMOL=MOL(I10)
0024                  MOLE=10*KMOL
0025                  IF(WAV(I10).LT.WAVLO) GO TO 10
0026                  IF(WAV(I10).GT.WAVUP) GO TO 13
0027                  ICNT(KMOL)=ICNT(KMOL)+1
                   C  WRITE(MOLE+ICNT(KMOL)) WAV(I10),STRGH(I10),WDTH(I10),ENGY(I10)
0028                  LTOTAL=LTOTAL+1
0029                  IF(LTOTAL.GT.MAX) GO TO 97
0030                  SPECS(LTOTAL,1)=WAV(I10)
0031                  SPECS(LTOTAL,2)=STRGH(I10)
0032                  SPECS(LTOTAL,3)=WDTH(I10)
0033                  SPECS(LTOTAL,4)=ENGY(I10)
0034                  KIND(LTOTAL)=MOL(I10)
0035               10 CONTINUE
0036                  GO TO 23
0037               13 CONTINUE
0038                  REWIND NFIL
0039                  GO TO 999
0040               99 WRITE(6,21) NFIL
0041               21 FORMAT(1X,35HLOWER WAVE NUMBER NOT FOUND ON TAPE,/,
                     1  1X,15HFILE NUMBER IS:,I10,/,1X,18HPROGRAM TERMINATED,//)
0042                  STOP
0043               98 WRITE(6,31) NFIL,WAV(40),WAVUP
0044               31 FORMAT(//,2X,31HEND OF FILE ENCOUNTERED ON FILE,I3,/,2X,
                     1  34HBEFORE UPPER WAVE NUMBER WAS FOUND,/,2X,
                     2  20HLAST WAVE NUMBER IS:,F10.3,3X,
                     3  25HUPPER LIMIT SPECIFIED WAS,5X,F10.3,//2X,
                     4  18HPROGRAM CONTINUING,///)
0045                  REWIND NFIL
0046                   NFIL=NFIL+1
0047                  IF(NFIL.GE.17) NFIL=17
0048                  GO TO 23
0049               97 WRITE(6,41) (ICNT(M),M=1,7),WAV(40)
0050               41 FORMAT(//,1X,31HEXPECTED RECORD NUMBER EXCEEDED,/,1X,
```

```
                      1  34HNUMBER OF RECORDS OF EACH TYPE IS:,/,2X,7(I6,2X),/,
                      2  20HLAST WAVE NUMBER IS:,2X,F10.3,/,2X,18HPROGRAM CONTINUING,///)
0051                   ICNT(KMOL)=ICNT(KMOL)-1
0052                   REWIND NFIL
0053                999 RETURN
0054                   END
```

APPENDIX E

TRANSMITTANCE PROGRAM

The transmittance program written as a result of this work follows. The important variables of the routine are defined in Appendix F. The logic and a flow chart for the program is contained in Chapter six.

```
0001                IMPLICIT REAL*8(A-H,O-Z)
0002                REAL WAVLO,WAVUP,FREQ,HIGH,SIZE,EGY,BOUND
                C
0003                REAL*4 TEMP(033),PRESS(033),CJ(7)/1.5,1.0,1.5,2*1.0,1.5,1.0/,
                   1  WTMOL(7)/18.,44.,48.,44.,28.,16.,32./,H2OMIX(033),O3MIX(033),
                   1  SPECS(3000,4)
0004                INTEGER*4 KIND(3000),MAX/3000/
0005                DIMENSION QV(33,7),ABSK(33,7),ICNT(7),TRANS(33),X1(33),X2(33),
                   1          X3(33)
0006                DATA P0/1013.1/122500/,T0/296.00000000/,HCKT0/4.860728216E-03/
0007                DATA ALG2/0.8325546112/,SQRPIV/0.5641895835/
0008                READ(5,01) NCHNL,LEVS,BOUND,INTVLS
0009              01  FORMAT(1X,I3,1X,I3,1X,F10.3,1X,I4)
0010                DO 10 I10=1,LEVS
0011              10  READ(5,11) PRESS(I10),TEMP(I10),H2OMIX(I10),O3MIX(I10)
0012              11  FORMAT(6X,F9.3,F5.1,1X,E9.3,1X,E9.3)
                C
                C                    CNE TIME CALCULATIONS
                C
0013                DO 160 I160=1,LEVS
0014                T2=TEMP(I160)*TEMP(I160)
0015                QV(I160,1)=.99504424+.44933103D-04*TEMP(I160)-.98896039D-07*T2
0016                QV(I160,2)=1.0707513+.51691420D-03*TEMP(I160)-.25483461D-05*T2
0017                QV(I160,3)=.98969448+.67787503D-03*TEMP(I160)-.21673751D-05*T2
0018                QV(I160,4)=1.1201483+.42823000D-03*TEMP(I160)-.28101372D-05*T2
0019                QV(I160,5)=1.00000000
0020                QV(I160,6)=.98548537+.22766513D-03*TEMP(I160)-.60069938D-06*T2
0021                QV(I160,7)=.99504424+.44933103D-04*TEMP(I160)-.98896039D-07*T2
0022                X1(I160)=T0/TEMP(I160)
0023                X2(I160)=(PRESS(I160)/P0)*DSQRT(X1(I160))
0024                X3(I160)=HCKT0*(1.-X1(I160))
0025              160  CONTINUE
                C
                C                         CHANNEL LOOP
                C
0026                DO 20 I20=1,NCHNL
0027                READ(5,21) WAVLO,WAVUP
0028              21  FORMAT(2(1X,F10.3))
0029                WAVLO=WAVLO-BOUND
0030                WAVUP=WAVUP+BOUND
0031                SEARCH=BOUND
0032                IF(BOUND.EQ.0.0) SEARCH=(WAVUP-WAVLO)/2.0
0033                CALL DATSET(WAVLO,WAVUP,ICNT,MAX,SPECS,KIND,LEND)
0034                INCR=INTVLS+1
0035                IF(INTVLS.NE.0) SPACE=(WAVUP-WAVLO-2.*BOUND)/INTVLS
0036                DO 40 I40=1,LEVS
0037                TRANS(I40)=0.0
0038              40  CONTINUE
                C
                C                    INCREMENT LOOP
                C
0039                IFIRST=1
0040                CNTR=WAVLO+BOUND
0041                IF(INTVLS.EQ.0) CNTR=(WAVLO+WAVUP)/2.0
0042                DO 60 I60=1,INCR
0043                UP=CNTR+SEARCH
0044                DOWN=CNTR-SEARCH
0045                DO 70 I70=IFIRST,LEND
```

```
0046                CHECK=SPECS(I70,1)
0047                IF(CHECK.GE.DOWN) GO TO 13
0048             70 CONTINUE
0049                IFIRST=1
0050                GO TO 23
0051             13 IFIRST=I70
0052             23 CONTINUE
0053                DO 80 I80=IFIRST,LEND
0054                CHECK=SPECS(I80,1)
0055                IF(CHECK.GE.UP) GO TO 33
0056             80 CONTINUE
0057                ILAST=LEND
0058                GO TO 43
0059             33 ILAST=I80
0060             43 CONTINUE
                 C
                 C                  LEVEL LOOP
                 C
0061                DO 30 I30=1,LEVS
0062                DO 50 I50=1,7
0063                ABSK(I30,I50)=0.0
0064             50 CONTINUE
                 C
                 C                    LINE LOOP
                 C
0065                DO 90 I90=IFIRST,ILAST
0066                ITYPE=KIND(I90)
0067                AD=3.580-07*SQRT(TEMP(I30)/WTMOL(ITYPE))
0068                X4=X1(I30)**CJ(ITYPE)*QV(I30,ITYPE)
0069                ALFAD=AD*SPECS(I90,1)
0070                ALFAL=X2(I30)*SPECS(I90,3)
0071                YFAC=ALG2/ALFAD
0072                U=ALFAL*YFAC
0073                RKO=(DEXP(X3(I30)*SPECS(I90,4)))*SPECS(I90,2)*X4)*YFAC
0074                Y=DABS(CNTR-SPECS(I90,1))*YFAC
0075                SHAPE=ZVOIGT(Y,U)
0076                ABSK(I30,ITYPE)=ABSK(I30,ITYPE)+RKO*SHAPE
0077             90 CONTINUE
0078             30 CONTINUE
                 C
                 C            ABSORPTION COEFFICEINT * MIXING RATIO
                 C
0079                DO 130 I130=1,LEVS
0080                ABSK(I130,1)=(ABSK(I130,1)*2.743475499D16*H2OMIX(I130)+
                   1  ABSK(I13),2)*6.954682447D15+ABSK(I130,3)*1.279623310D19*
                   2  03MIX(I130)+ABSK(I130,4)*5.897035858D12+
                   3    ABSK(I130,5)*1.589430793D12+ABSK(I130,6)*3.381698754D13+
                   4  ABSK(I130,7)*4.443139014D18)*(SQRPIV)
0081            130 CONTINUE
                 C
                 C                      TRANSMITTANCE
                 C
0082                LSTOP=LEVS-1
0083                TAU=1.
0084                DO 150 I150=1,LSTOP
0085                INUM=1
0086                HSTEP=(PRESS(I150+1)-PRESS(I150))/1000.
0087                TPRED=TAU-HSTEP*ABSK(I150,1)*TAU
```

```
FORTRAN IV G LEVEL  21                MAIN                DATE = 77108          11/01/30

0088          63  TAUNEW=TAU-(HSTEP/2.)*(ABSK(I150,1)*TAU+ABSK(I150+1,1 )*TPRED)
0089              IF(DABS(TPRED-TAUNEW).LE.0.0001.OR.INUM.GE.10) GO TO 53
0090              TPRED=TAUNEW
0091              INUM=INUM+1
0092              GO TO 63
0093          53  TAU=TAUNEW
0094              K=I150+1
0095              TRANS(K)=TRANS(K)+TAU
0096         150  CONTINUE
0097              CNTR=CNTR+SPACE
0098          60  CONTINUE
0099              TRANS(1)=INCR
0100              WAVLO=WAVLO+BOUND
0101              WAVUP=WAVUP-BOUND
0102              WRITE(6,31) I20,WAVLO,WAVUP
0103          31  FORMAT(1HI,51X,14HCHANNEL NUMBER,1X,I2,/,25X,
                 1  23HBEGINNING WAVENUMBER OF,1X,F10.3,1X,3HAND,1X,
                 2 20HENDING WAVENUMBER OF,1X,F10.3,/,25X,70(1H*),/,25X,70(1H*),/)
0104              WRITE(6,101)
0105              LEVEL=LEVS
0106              DO 140 I140=1,LEVS
0107              TRANS(I140)=TRANS(I140)/INCR
0108              WRITE(6,91) LEVEL,PRESS(I140),TEMP(I140),TRANS(I140)
0109              LEVEL=LEVS-I140
0110         101  FORMAT(/,19X,5HLEVEL,11X,8HPRESSURE,15X,11HTEMPERATURE,9X,
                1  22HAVERAGED TRANSMITTANCE,/,16X,85(1H=))
0111          91  FORMAT(20X,I3,11X,D10.4,17X,F5.1,14X,D17.10)
0112         140  CONTINUE
0113          20  CONTINUE
0114              STOP
0115              END
```

APPENDIX F

DEFINITION OF VARIABLES USED IN THE TRANSMITTANCE PROGRAM

The following is a list of the important variables and their definition, used in the transmittance program.

ABSK(33,7)	Array of absorption coefficients
ALFAL	α_L
ALFAD	α_D
A1G2	$(1n2)^{1/2}$
BOUND	Amount by which channel limits are changed.
CJ(7)	Array of rotational partition function exponents.
CNTR	Frequency at which transmittance is calculated.
DOWN	Lower limit of the range of lines included in transmittance calculations.
EGY	Energy of a line (E) = SPECS(I,4).
FREQ	Line wavenumber (ν_0) = SPECS(I,1).
HIGH	Line strength (S) = SPECS(I,2).
HSTEP	dP in bars.
H2OMIX(33)	Array of water vapor concentrations.
IFIRST	Subscript of the lower limit line used in transmittance calculations.
ILAST	Subscript of the upper limit line used in transmittance calculations.

INTVLS	Number of intervals in a channel.
KIND(3000)	Array of molecular types.
LEVS	Number of layers of the atmosphere.
NCHNL	Number of channels.
03MIX(33)	Array of ozone concentrations.
PO	Reference pressure = 1013.17mb.
PRESS(33)	Array of layer pressures.
QV(33,7)	Array of vibration partition functions.
SEARCH	Range from CNTR within which effects of lines are added together.
SHAPE	Voigt profile value.
SIZE	Line width (α_0) = SPECS(I,3).
SPACE	Distance between points where transmittance is computed.
TAU	Iterative transmittance.
TAUNEW	Corrected iterative transmittance.
TEMP(33)	Array of layer temperatures.
TO	Reference temperature = 296.
TPRED	Predicted transmittance.
TRANS(33)	Transmittances of each layer.
U	$\frac{\alpha_L}{\alpha_D} (\ln 2)^{1/2}$
UP	Upper limit of the range of lines included in transmittance calculations.
WAVLO	Channel lower limit.
WAVUP	Channel upper limit.
WTMOL(7)	Molecular weights of atmospheric gases.

Y $\frac{\nu-\nu_0}{\alpha_D} (\ln 2)^{1/2}$

APPENDIX G

MONOCHROMATIC TRANSMITTANCES

The results of monochromatic transmittance calculations for the seven channels of the HIRS are listed. The frequency at which the transmittance was computed was the channel center-frequency. Only lines between the channel limits were used.

CHANNEL NUMBER 1

BEGINNING WAVENUMBER OF 665.200 AND ENDING WAVENUMBER OF 670.800

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.10000000000D 01
32	0.6710E-01	218.0	0.99999932D 00
31	0.9510E 00	276.0	0.99998918835D 00
30	0.1760E 01	270.0	0.99997533333D 00
29	0.3330E 01	258.0	0.99994430430D 00
28	0.6520E 01	245.0	0.99987048950D 00
27	0.1320E 02	234.0	0.99970339910D 00
26	0.2770E 02	224.0	0.99938433670D 00
25	0.3220E 02	223.0	0.99930258840D 00
24	0.3760E 02	222.0	0.99921257620D 00
23	0.4370E 02	220.0	0.99911961300D 00
22	0.5100E 02	219.0	0.99901778600D 00
21	0.5950E 02	218.0	0.99890878590D 00
20	0.6950E 02	217.0	0.99879009500D 00
19	0.8120E 02	216.0	0.99866044700D 00
18	0.9500E 02	216.0	0.99851623980D 00
17	0.1110E 03	216.0	0.99835706470D 00
16	0.1300E 03	216.0	0.99817582630D 00
15	0.1530E 03	216.0	0.99796458620D 00
14	0.1790E 03	216.0	0.99773405050D 00
13	0.2090E 03	222.0	0.99747757100D 00
12	0.2430E 03	229.0	0.99719837260D 00
11	0.2810E 03	235.0	0.99689389680D 00
10	0.3240E 03	242.0	0.99657360798D 00
9	0.3720E 03	248.0	0.99622502110D 00
8	0.4260E 03	255.0	0.99584771810D 00
7	0.4870E 03	261.0	0.99543699850D 00
6	0.5540E 03	267.0	0.99500102640D 00
5	0.6280E 03	273.0	0.99453442030D 00
4	0.7100E 03	279.0	0.99403218440D 00
3	0.8020E 03	285.0	0.99348372730D 00
2	0.9020E 03	290.0	0.99290212630D 00
1	0.1013E 04	294.0	0.99227078150D 00

CHANNEL NUMBER 2

BEGINNING WAVENUMBER OF 665.300 AND ENDING WAVENUMBER OF 692.700

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.10000000000D 01
32	0.6710E-01	218.0	0.10000000000D 01
31	0.9510E 00	276.0	0.99999999950D 00
30	0.1760E 01	270.0	0.99999999830D 00
29	0.3330E 01	258.0	0.99999999370D 00
28	0.6520E 01	245.0	0.99999997520D 00
27	0.1320E 02	234.0	0.99999989440D 00
26	0.2770E 02	224.0	0.99999951950D 00
25	0.3220E 02	223.0	0.99999934730D 00
24	0.3760E 02	222.0	0.99999910580D 00
23	0.4370E 02	220.0	0.99999878640D 00
22	0.5100E 02	219.0	0.99999833920D 00
21	0.5950E 02	218.0	0.99999772990D 00
20	0.6950E 02	217.0	0.99999689090D 00
19	0.8120E 02	216.0	0.99999574100D 00
18	0.9500E 02	216.0	0.99999415450D 00
17	0.1110E 03	216.0	0.99999200650D 00
16	0.1300E 03	216.0	0.99998902660D 00
15	0.1530E 03	216.0	0.99998479750D 00
14	0.1790E 03	216.0	0.99997920050D 00
13	0.2090E 03	222.0	0.99997176490D 00
12	0.2430E 03	229.0	0.99996221840D 00
11	0.2810E 03	235.0	0.99995019360D 00
10	0.3240E 03	242.0	0.99993492040D 00
9	0.3720E 03	248.0	0.99991587560D 00
8	0.4260E 03	255.0	0.99989204760D 00
7	0.4870E 03	261.0	0.99986221750D 00
6	0.5540E 03	267.0	0.99982604000D 00
5	0.6280E 03	273.0	0.99978220100D 00
4	0.7100E 03	279.0	0.99972921000D 00
3	0.8020E 03	285.0	0.99966468720D 00
2	0.9020E 03	290.0	0.99958893910D 00
1	0.1013E 04	294.0	0.99949849900D 00

CHANNEL NUMBER 3

BEGINNING WAVENUMBER OF 677.400 AND ENDING WAVENUMBER OF 702.600

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.1000000000D 01
32	0.6710E-01	218.0	0.1000000000D 01
31	0.9510E 00	276.0	0.9999999999D 00
30	0.1760E 01	270.0	0.9999999997D 00
29	0.3360E 01	258.0	0.9999999991D 00
28	0.6520E 01	245.0	0.9999999967D 00
27	0.1320E 02	234.0	0.9999999867D 00
26	0.2770E 02	224.0	0.9999999431D 00
25	0.3220E 02	223.0	0.9999999235D 00
24	0.3760E 02	222.0	0.9999998962D 00
23	0.4370E 02	220.0	0.9999998605D 00
22	0.5100E 02	219.0	0.9999998109D 00
21	0.5950E 02	218.0	0.9999997437D 00
20	0.6950E 02	217.0	0.9999996517D 00
19	0.8120E 02	216.0	0.9999995265D 00
18	0.9500E 02	216.0	0.9999993541D 00
17	0.1110E 03	216.0	0.9999991205D 00
16	0.1300E 03	216.0	0.9999987961D 00
15	0.1530E 03	216.0	0.9999983352D 00
14	0.1790E 03	216.0	0.9999977244D 00
13	0.2090E 03	222.0	0.9999968936D 00
12	0.2430E 03	229.0	0.9999957783D 00
11	0.2810E 03	235.0	0.9999943110D 00
10	0.3240E 03	242.0	0.9999923668D 00
9	0.3720E 03	248.0	0.9999898332D 00
8	0.4260E 03	255.0	0.9999865384D 00
7	0.4870E 03	261.0	0.9999822295D 00
6	0.5540E 03	267.0	0.9999767394D 00
5	0.6280E 03	273.0	0.9999699206D 00
4	0.7100E 03	279.0	0.9999612582D 00
3	0.8020E 03	285.0	0.9999502341D 00
2	0.9020E 03	290.0	0.9999367155D 00
1	0.1013E 04	294.0	0.9999198948D 00

CHANNEL NUMBER 4

BEGINNING WAVENUMBER OF 686.100 AND ENDING WAVENUMBER OF 717.900

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.10000000000D 01
32	0.6710E-01	218.0	0.10000000000D 01
31	0.9510E 00	276.0	0.99999999980 00
30	0.1760E 01	270.0	0.99999999940 00
29	0.3330E 01	258.0	0.99999999770 00
29	0.6520E 01	245.0	0.99999999100 00
27	0.1320E 02	234.0	0.99999996600 00
26	0.2770E 02	224.0	0.99999990110 00
25	0.3220E 02	223.0	0.99999988200 00
24	0.3760E 02	222.0	0.99999985870 00
23	0.4370E 02	220.0	0.99999983210 00
22	0.5100E 02	219.0	0.99999980000 00
21	0.5950E 02	218.0	0.99999976200 00
20	0.6950E 02	217.0	0.99999971610 00
19	0.8120E 02	216.0	0.99999966050 00
18	0.9500E 02	216.0	0.99999959140 00
17	0.1110E 03	216.0	0.99999950540 00
16	0.1300E 03	216.0	0.99999939570 00
15	0.1530E 03	216.0	0.99999925310 00
14	0.1790E 03	216.0	0.99999908060 00
13	0.2090E 03	222.0	0.99999885010 00
12	0.2430E 03	229.0	0.99999852350 00
11	0.2810E 03	235.0	0.99999807490 00
10	0.3240E 03	242.0	0.99999745810 00
9	0.3720E 03	248.0	0.99999663170 00
8	0.4260E 03	255.0	0.99999552470 00
7	0.4870E 03	261.0	0.99999404810 00
6	0.5540E 03	267.0	0.99999216050 00
5	0.6280E 03	273.0	0.99998974680 00
4	0.7100E 03	279.0	0.99998666430 00
3	0.8020E 03	285.0	0.99998269350 00
2	0.9020E 03	290.0	0.99997778920 00
1	0.1013E 04	294.0	0.99997168830 00

CHANNEL NUMBER 5

BEGINNING WAVENUMBER OF 698.500 AND ENDING WAVENUMBER OF 733.500

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.1000000000D 01
32	0.6710E-01	218.0	0.1000000000D 01
31	0.9510E 00	276.0	0.1000000000D 01
30	0.1760E 01	270.0	0.1000000000D 01
29	0.3330E 01	258.0	0.9999999999D 00
28	0.6520E 01	245.0	0.9999999994D 00
27	0.1320E 02	234.0	0.9999999974D 00
26	0.2770E 02	224.0	0.9999999912D 00
25	0.3220E 02	223.0	0.9999999892D 00
24	0.3760E 02	222.0	0.9999999866D 00
23	0.4370E 02	220.0	0.9999999835D 00
22	0.5100E 02	219.0	0.9999999797D 00
21	0.5950E 02	218.0	0.9999999753D 00
20	0.6950E 02	217.0	0.9999999703D 00
19	0.8120E 02	216.0	0.9999999649D 00
18	0.9500E 02	216.0	0.9999999588D 00
17	0.1110E 03	216.0	0.9999999521D 00
16	0.1300E 03	216.0	0.9999999441D 00
15	0.1530E 03	216.0	0.9999999341D 00
14	0.1790E 03	216.0	0.9999999222D 00
13	0.2090E 03	222.0	0.9999999069D 00
12	0.2430E 03	229.0	0.9999998860D 00
11	0.2810E 03	235.0	0.9999998576D 00
10	0.3240E 03	242.0	0.9999998181D 00
9	0.3720E 03	248.0	0.9999997641D 00
8	0.4260E 03	255.0	0.9999996898D 00
7	0.4870E 03	261.0	0.9999995877D 00
6	0.5540E 03	267.0	0.9999994530D 00
5	0.6280E 03	273.0	0.9999992753D 00
4	0.7100E 03	279.0	0.9999990412D 00
3	0.8020E 03	285.0	0.9999987302D 00
2	0.9020E 03	290.0	0.9999983342D 00
1	0.1013E 04	294.0	0.9999978275D 00

CHANNEL NUMBER 6

BEGINNING WAVENUMBER OF 715.400 AND ENDING WAVENUMBER OF 750.600

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.10000000000D 01
32	0.6710E-01	210.0	0.10000000000D 01
31	0.9510E 00	276.0	0.10000000000D 01
30	0.1760E 01	270.0	0.10000000000D 01
29	0.3330E 01	258.0	0.99999999990D 00
28	0.6520E 01	245.0	0.99999999970D 00
27	0.1320E 02	234.0	0.99999999900D 00
26	0.2770E 02	224.0	0.99999999610D 00
25	0.3220E 02	223.0	0.99999999490D 00
24	0.3760E 02	222.0	0.99999999320D 00
23	0.4370E 02	220.0	0.99999999110D 00
22	0.5100E 02	219.0	0.99999998820D 00
21	0.5950E 02	218.0	0.99999998440D 00
20	0.6950E 02	217.0	0.99999997920D 00
19	0.8120E 02	216.0	0.99999997240D 00
18	0.9500E 02	216.0	0.99999996300D 00
17	0.1110E 03	216.0	0.99999995040D 00
16	0.1300E 03	216.0	0.99999993290D 00
15	0.1530E 03	216.0	0.99999990810D 00
14	0.1790E 03	216.0	0.99999987540D 00
13	0.2090E 03	222.0	0.99999982890D 00
12	0.2430E 03	229.0	0.99999976130D 00
11	0.2810E 03	235.0	0.99999966530D 00
10	0.3240E 03	242.0	0.99999952880D 00
9	0.3720E 03	248.0	0.99999933950D 00
8	0.4260E 03	255.0	0.99999907720D 00
7	0.4870E 03	261.0	0.99999871580D 00
6	0.5540E 03	267.0	0.99999823380D 00
5	0.6290E 03	273.0	0.99999761220D 00
4	0.7100E 03	279.0	0.99999679400D 00
3	0.8020E 03	285.0	0.99999572140D 00
2	0.9020E 03	290.0	0.99999437800D 00
1	0.1013E 04	294.0	0.99999269020D 00

CHANNEL NUMBER 7

BEGINNING WAVENUMBER OF 730.600 AND ENDING WAVENUMBER O. 767.400

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3300E-03	210.0	0.1000000000D 01
32	0.6710E-01	218.0	0.1000000000D 01
31	0.9510E 00	276.0	0.1000000000D 01
30	0.1760E 01	270.0	0.1000000000D 01
29	0.3330E 01	258.0	0.1000000000D 01
28	0.6520E 01	245.0	0.9999999999D 00
27	0.1320E 02	234.0	0.9999999994D 00
26	0.2770E 02	224.0	0.9999999983D 00
25	0.3220E 02	223.0	0.9999999979D 00
24	0.3760E 02	222.0	0.9999999975D 00
23	0.4370E 02	220.0	0.9999999970D 00
22	0.5100E 02	219.0	0.9999999965D 00
21	0.5950E 02	218.0	0.9999999959D 00
20	0.6950E 02	217.0	0.9999999952D 00
19	0.8120E 02	216.0	0.9999999946D 00
18	0.9500E 02	216.0	0.9999999939D 00
17	0.1110E 03	216.0	0.9999999932D 00
16	0.1300E 03	216.0	0.9999999925D 00
15	0.1530E 03	216.0	0.9999999916D 00
14	0.1790E 03	216.0	0.9999999905D 00
13	0.2090E 03	222.0	0.9999999892D 00
12	0.2430E 03	229.0	0.9999999872D 00
11	0.2810E 03	235.0	0.9999999843D 00
10	0.3240E 03	242.0	0.9999999800D 00
9	0.3720E 03	248.0	0.9999999737D 00
8	0.4260E 03	255.0	0.9999999645D 00
7	0.4870E 03	261.0	0.9999999511D 00
6	0.5540E 03	267.0	0.9999999323D 00
5	0.6280E 03	273.0	0.9999999062D 00
4	0.7100E 03	279.0	0.9999998701D 00
3	0.8020E 03	285.0	0.9999998197D 00
2	0.9020E 03	290.0	0.9999997528D 00
1	0.1013E 04	294.0	0.9999996640D 00

APPENDIX H

AVERAGED TRANSMITTANCE

The result of the averaged transmittance for the first HIRS channel is listed. Ten monochromatic transmittances were averaged over the band. Each separate transmission calculation included only lines that were within a distance of 5 wavenumbers of the transmission frequency.

CHANNEL NUMBER 1

BEGINNING WAVENUMBER OF 665.200 AND ENDING WAVENUMBER OF 670.800

LEVEL	PRESSURE	TEMPERATURE	AVERAGED TRANSMITTANCE
33	0.3000E-03	210.0	0.1000000000D 01
32	0.6710E-01	218.0	0.9999066290D 00
31	0.9510E 00	276.0	0.9998104601D 00
30	0.1760E 01	270.0	0.9995925830D 00
29	0.3330E 01	259.0	0.9991349821D 00
28	0.6520E 01	245.0	0.9981519939D 00
27	0.1320E 02	234.0	0.9960567790D 00
26	0.2770 02	224.0	0.9924551851D 00
25	0.3220E 02	223.0	0.9916018443D 00
24	0.3760E 02	222.0	0.9906909679D 00
23	0.4370E 02	220.0	0.9897847863D 00
22	0.5100E 02	219.0	0.9888350224D 00
21	0.5950E 02	218.0	0.9878738255D 00
20	0.6950E 02	217.0	0.9868923173D 00
19	0.8120E 02	216.0	0.9858998059D 00
18	0.9500E 02	216.0	0.9848380995D 00
17	0.1110E 03	216.0	0.9838723632D 00
16	0.1300E 03	216.0	0.9823274423D 00
15	0.1530E 03	216.0	0.9817300016D 00
14	0.1790E 03	216.0	0.9806588348D 00
13	0.2090E 03	222.0	0.9795605491D 00
12	0.2430E 03	229.0	0.9784326343D 00
11	0.2910E 03	235.0	0.9772799180D 00
10	0.3240E 03	242.0	0.9760785790D 00
9	0.3720E 03	248.0	0.9748323430D 00
8	0.4260E 03	255.0	0.9735181849D 00
7	0.4870E 03	261.0	0.9721146528D 00
6	0.5540E 03	267.0	0.9706458051D 00
5	0.6280E 03	273.0	0.9690860738D 00
4	0.7100E 03	279.0	0.9674117597D 00
3	0.8020E 03	285.0	0.9655307443D 00
2	0.9020E 03	290.0	0.9636315701D 00
1	0.1013E 04	294.0	0.9615054266D 00

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