

NOTE TO USERS

PREVIEW

This reproduction is the best copy available.

UMI[®]

PREVIEW

ACCURACY COMPARISON IN CALCULATIONS
OF ATMOSPHERIC TRANSMITTANCE
BY THREE NUMERICAL METHODS

by

Gregory A. Stolt

THESIS

Presented to the Faculty of the Graduate School of
The University of Texas at El Paso
in Partial Fulfillment
of the Requirements
for the Degree of
MASTER OF SCIENCE

THE UNIVERSITY OF TEXAS AT EL PASO

December 1978

UMI Number: EP01482

PREVIEW

UMI[®]

UMI Microform EP01482

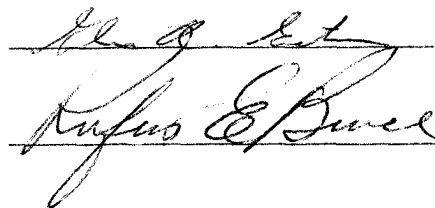
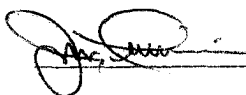
Copyright 2003 by ProQuest Information and Learning Company.

All rights reserved. This microform edition is protected against
unauthorized copying under Title 17, United States Code.

ProQuest Information and Learning Company
300 North Zeeb Road
P.O. Box 1346
Ann Arbor, MI 48106-1346

ACCURACY COMPARISON IN CALCULATIONS
OF ATMOSPHERIC TRANSMITTANCE
BY THREE NUMERICAL METHODS

APPROVED:



Dean of the Graduate School

DEDICATED TO MOM AND DAD
AND
TO MY WIFE, JEY

PREVIEW

ACKNOWLEDGEMENTS

I would like to take this opportunity to express my thanks to those people who have helped me complete this project.

To Dr. Joseph H. Pierluissi who sponsored my work, I thank you. I would also like to extend a thank you to Dr. Glenn A. Gibson whose guidance in the area of computer modelling was very helpful. Additionally, for his assistance in setting up data files and modifying the computer program, I express my appreciation to Jim Brown.

To Paul Demshur, my friend and fellow student, I express my thanks for his encouragement and help along the way.

For the assistance he provided in assuring my computer programs were executed in a timely manner, I would like to express a special thanks to Mr. Leonard Chochrek and his staff at the University's Computer Center.

Finally, to Louise Rahman, Kathy Murphy, and Lucy Rodriguez who spent many hours in careful typing of this work, I express my thanks. And to Mrs. Beatrice G. Hollander for her advice and help in the publishing of this report, I express a special thank you.

To all these people I am most indebted. Thank you all.

ABSTRACT

The monochromatic transmittance profile for paths along inhomogeneous atmospheres is calculated using three well known numerical methods. The first method employs a fourth order Runge-Kutta technique to solve the first order differential equation form of Beer's Law. The second method utilizes the area of rectangles to approximate the integral over altitude in the Beer's Law exponent. The transmittance is calculated by summing the rectangular areas for a horizontally-stratified atmosphere of homogeneous layers which was assumed. The third method also assumes a stratified atmosphere of constant temperatures and absorber concentrations. The method transforms the Beer's Law exponent to a function of pressure and integrates analytically.

The three methods are compared for accuracy at ten different frequencies and two atmospheric models. Errors as large as 4% were found in the comparison of the Runge-Kutta method with the rectangular area method. The pressure integration method was found to introduce errors as large as 20% when compared to the other two techniques. Finally, the Runge-Kutta method was found to be unstable for certain computations where the transmittance was close to zero.

TABLE OF CONTENTS

	Page
ACKNOWLEDGEMENTS	iii
ABSTRACT	iv
TABLE OF CONTENTS	v
LIST OF FIGURES.	vii
I. INTRODUCTION	1
II. GENERAL THEORY OF SLANT PATH ATMOSPHERIC ABSORPTION	3
2.1 PREFACE	3
2.2 LAMBERT-BEER LAW.	4
2.3 LORENTZ BROADENING.	7
2.4 THE EARTH'S ATMOSPHERE.	13
2.4.1 General Atmospheric Constituents	14
2.4.2 Other Model Atmospheres.	17
2.5 PREVIOUS WORK	18
2.5.1 Layered Atmosphere Method.	18
2.5.2 Runge-Kutta.	21
2.5.3 Pressure Integration	23
III. SOLVING THE TRANSMITTANCE PROBLEM: HOW THE METHODS WERE TESTED.	26
3.1 RUNGE-KUTTA ITERATION OF THE DIFFERENTIAL EQUATION	26
3.2 SOLVING THE INTEGRAL USING THE RECTANGULAR APPROXIMATION	29
3.3 SOLVING THE INTEGRAL USING PRESSURE INTEGRATION.	33
3.4 CALCULATION OF GAS AMOUNTS, ABSORPTION COEFFICIENTS, AND A DISCUSSION OF UNITS	35
3.4.1 Picking the Points for Runge-Kutta	35
3.4.2 Picking the Points for Rectangular Integration.	40
3.4.3 Picking the Points for Pressure Integration...	43

Table of Contents (Continued)	Page
3.5 THE PROGRAM TO COMPARE METHODS	45
IV. DISCUSSION OF DATA AND PROGRAM RESULTS	55
4.1 WHICH FREQUENCIES WERE CHOSEN FOR	55
THE COMPARISON	
4.2 DETERMINING A STANDARD	57
4.3 RESULTS OF THE COMPARISON	59
4.3.1 The Basic Group Frequencies	59
4.3.2 The Strong Absorption Frequencies	63
4.3.3 The Frequency 2086.325 cm^{-1} ,	67
CO Laser	
V. CONCLUDING REMARKS	69
5.1 SUMMARY	69
5.2 CONCLUSIONS	70
REFERENCES	77
APPENDIX A: QUANTITIES USED TO COMPUTE	79
ATMOSPHERIC TRANSMITTANCE	
APPENDIX B: FORTRAN PROGRAM USED TO PERFORM	83
TRANSMITTANCE CALCULATIONS	
APPENDIX C: TRANSMITTANCE DATA USED FOR	102
ERROR ANALYSIS	

LIST OF FIGURES

Figure		Page
2.2-1	Zenith Angle	6
2.3-1	Lorentz Contour	11
2.4-1	Composition of the Earth's Atmosphere . .	14
2.4-2	Trace Gas Infrared Absorbers	15
3.1-1	Graphical Representation of Rectangular Integration	30
3.4-1	Definition of Divided Differences for Newton's method	36
3.5-1	Program Flow Chart	47
4.1-1	Frequencies Selected for Comparison . . .	56
4.3-1	Maximum Runge Kutta Error for Strong Absorption Frequencies	65
5.2-1	Summary of Error	71
5.2-2	High Percentage Errors for Rectangular Integration Method	73
5.2-3	Maximum Error Comparison: Rectangular . . vs. Pressure Integration	74
5.2-4	High Percentage Errors for Pressure Integration Method	75
5.2-5	High Percentage Errors of Pressure Integration as Compared to Rectangular Method	75

CHAPTER I

INTRODUCTION

The mathematical modeling of energy transmission through the atmosphere at frequencies in the infrared spectrum has been the subject of numerous research efforts in recent years. Reports by Anding^[1], McClatchey^[2] et. al., Drayson^[3], and Pierluissi^[4] et. al., have described various computational methods employed in determining the transmittance at a monochromatic frequency to given points in a vertical or slant path in the atmosphere. Some researchers have claimed levels of accuracy ranging from .001 to .0001 in the transmittance computation. Others have claimed no specific level of accuracy for their calculations. A Master of Science Thesis by Potter^[5] presented an accuracy comparison between two methods of computing the absorption coefficient. The thesis reported that the methods of Pierluissi and Gibson^[4] compared favorably with the line-by-line method of McClatchey^[2] which has historically been used in mathematical models. However, the report by Potter only partially answers the question of model accuracy. The real question which must be answered is "How accurate can different numerical methods compute transmittance along a slant path?" This report will attempt to answer this question for three well known methods. Since the accuracy of computing the absorption coefficient has already been determined^[5], the line-by-line method of

McClatchey^[2] will be employed in all three models.

The first of the three models is a fourth order Runge-Kutta method for solving the differential equation form of the Lambert Beer law. The method was employed by Pierluissi and Gibson^[4] at the University of Texas at El Paso. The second model is that employed by the reader of the McClatchey^[2] reports from the Air Force Geophysics Laboratory. Basically it employs the area of rectangles to perform numerical integration of the transmittance function. The third method is that of Drayson^[4]; it utilizes an analytic solution to the integration over pressure. All three methods will be completely developed in subsequent chapters of this report.

The report will outline a computer program to calculate transmittance by the three numerical methods discussed and compare the results. The work is organized into five chapters as follows. Chapter two discusses the atmospheric attenuation problem in more detail and outlines the method used to calculate the transmittance coefficients. Chapter three presents the comparison of the Runge-Kutta method, the rectangular integration method, and the pressure integration method. The results of the comparison are presented in chapter four while Chapter Five is used for analysis and concluding remarks. Where necessary the basic data is supported by more complete data in appendices.

CHAPTER II

GENERAL THEORY OF SLANT-PATH ATMOSPHERIC ABSORPTION

2.1 Preface:

This chapter provides background material necessary in the development of a program to compute atmospheric transmittance of energy in the infrared frequency spectrum. Numerous mechanisms are available to compute transmittance and many researchers have taken approaches different from those described here. However, the theory described and the methods used lead directly to the comparison in question and hence they are covered in detail. The following two sections review the mathematical modeling of infrared transmittance to include a discussion of the Lambert-Beer law for molecular absorption and the theory governing the line shape of discrete frequency lines which absorb infrared radiation in the atmosphere. A study of the atmosphere, presented in section 2.4, reviews the basic atmospheric constituents which contribute to absorption of infrared radiation and presents basic quantities and atmospheric models which were assumed to exist for the slant path calculations. Finally, previous work in the area performed by Dr. Joseph H. Pierluissi^[4] and Dr. Glenn A. Gibson at the University of Texas at El Paso, work performed under the direction of R. A. McClatchey^[2,6,7] at the Air Force Geophysics Laboratory, Hanscom Air Force Base,

Massachusetts, and work done by S. R. Drayson^[3] at the University of Michigan is presented with emphasis placed on the different computational methods for computing transmittance. In the work of Pierluissi^[2] et. al., the vertical path transmittance profile is computed using a fourth order Runge-Kutta numerical technique to solve the differential equation form of the Lambert Beer Transmittance Law. The research of McClatchey et. al, concentrates on calculation of the absorption coefficient in the Lambert Beer Law. The work employs a layered atmosphere and approximates the integral in the Beer's Law exponent by a summation of rectangular areas. The third research method [Drayson]^[3] employs a similar layered atmosphere approach, but transforms the exponent to a function of pressure and upon assuming an isothermal atmospheric layer integrates the resulting function analytically. The transmittance profile is realized by summing the areas resulting from the pressure integration. The three research efforts will be further discussed in section 2.5.

2.2 Lambert-Beer Law

In general, the attenuation of radiation along a slant path in the atmosphere can be largely attributed to molecular absorption of energy at discrete wavelengths. The general equation which quantitatively specifies the amount of molecular absorption along a path can be derived from the Lambert-Beer Law^[1]. The Law states that the

differential decrease in spectral intensity dI which is caused by absorption in a differential section of path dz is proportional to the length of the path dz , the incident radiation I , and to the concentration of the absorber ρ .

Mathematically stated:

$$dI = K[I\rho dz] \quad 2.2-1$$

where K is the constant of proportionality known as the absorption coefficient. Integration of equation 2.2-1 over a vertical path from a height z_1 to z_2 gives the monochromatic transmittance τ , where transmittance is defined as the ratio of incoming to outgoing intensities of radiation

$$\tau = \exp\left[-\int_{z_1}^{z_2} K\rho dz\right] \quad 2.2-2$$

The transmittance equation is sometimes expressed as the exponentiation of the integral of the absorption coefficient K times the differential gas amount dU where $dU = \rho dz$. A closer look at the quantities defined in equation 2.2-2 indicates that the concentration of absorbing gases in the atmosphere is a function of altitude and, as will be shown later the absorption coefficient K , is a function of frequency, temperature and pressure. Since temperature and pressure can be expressed uniquely as a function of altitude the absorption coefficient can be expressed as a function of frequency and altitude. Additionally, if slant paths are to be considered the differential absorber amount (dU) is modified by the secant of an angle known as the zenith

angle. Consider the path lengths travelled by two identical rays of radiation I_1 and I_2 , through differing paths in an identical, homogeneous atmosphere from altitude z_1 to z_2 as shown in Figure 2.2-1. If ray I_1 is incident vertically on the absorber and gas amount U_1 is known then the gas amount U_2 can be calculated by $U_2 = \sec \theta U_1$.

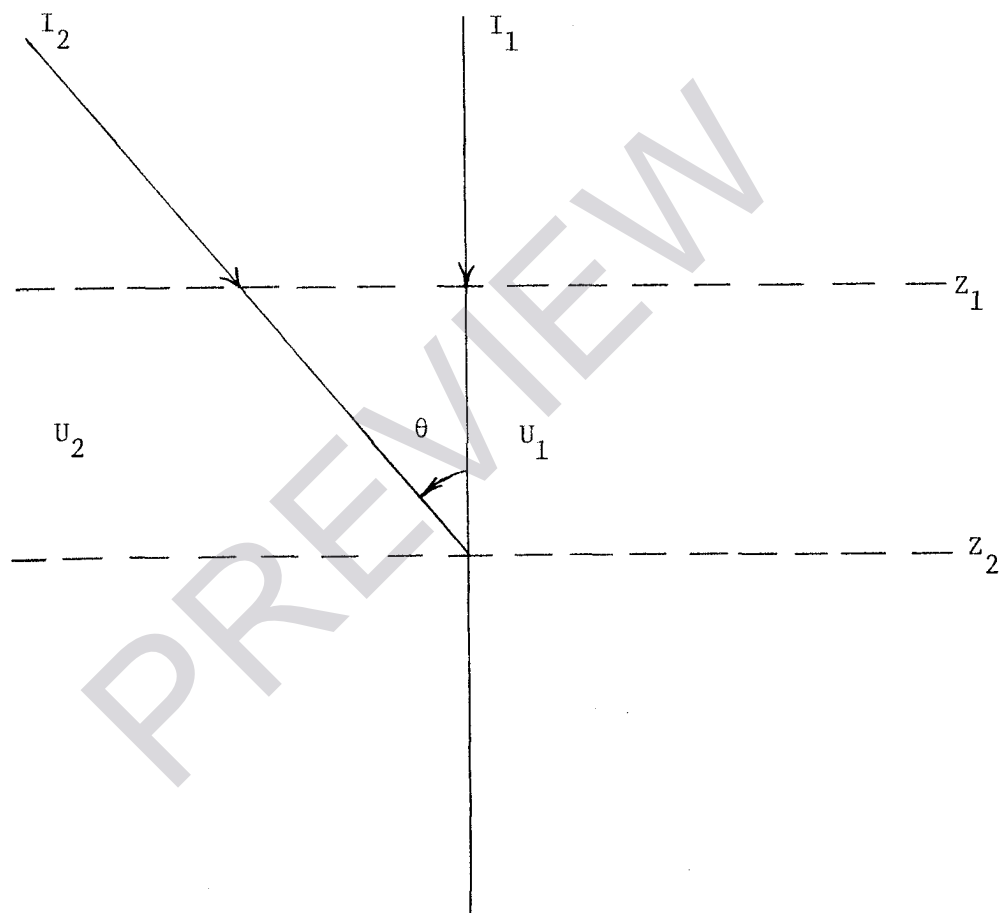


Figure 2.2-1

Zenith Angle

Hence, equation 2.2-2 can be rewritten more completely as:

$$\tau(\nu, z) = \exp[-\sec \theta \int_{z_1}^{z_2} K(\nu, z) \rho(z) dz] \quad 2.2-3$$

As an alternative to the numerical evaluation of 2.2-3 the numerical evaluation of the differential equation

$$d\tau(\nu, z) = -\sec \theta [K(\nu, z) \rho(z) \tau(\nu, z)] dz \quad 2.2-4$$

may be considered, which subject to the boundary conditions $\tau(\nu, z_1) = 1.0$, yields 2.2-3 as a solution^[4].

Transmittance is a measure of how much energy passes through a given amount of absorber. Conversely a measure of the amount of radiation which is attenuated is called absorptance, A, and is defined by

$$A = 1 - \tau. \quad 2.2-5$$

In research literature care must be taken to insure which quantity the author is using. In this report the quantity transmittance will be used, unless otherwise specified.

2.3 Lorentz Broadening

In the previous section it was shown that transmittance of infrared radiation can be described using the knowledge of absorber amount and a constant of proportionality known as the absorption coefficient. To understand the absorption coefficient a cursory review of molecular energy and spectra is necessary.

In molecular, as well as atomic particles, transitions

in energy levels may occur due to either absorption or emission of energy at a given frequency. When an energy transition occurs the frequency at which it occurs is governed by Plank's relation.^(9,10) Mathematically

$$\nu = \frac{\Delta E}{h} \quad 2.3-1$$

where ΔE is the change in energy and h is Plank's constant. The total energy of a single molecule is a function of translational motion, energy of the electrons (electronic energy), vibrational and rotational energies of the molecule, and combinations or interactions of two or more of the energy types. For the purposes of molecular absorption this report considers only the latter three types of energy and their combinations. In that the energy types differ in order of magnitude the spectra of energy absorptions (emissions) vary; the electronic spectra occupy the ultraviolet and visible, the vibrational spectra are in the near infrared, and the rotational spectra are in the far infrared. [Zuev]⁽⁹⁾ Therefore modeling transmittance in the infrared region is most sensitive to absorption of energy due to vibrational and rotational energies of molecules along the radiative path.

The problem of molecular absorption, however, deals with very large numbers of molecules intermixed in the atmosphere. Therefore, while it may be possible in principle to mathematically describe the motion of each molecule in practice the problem is beyond solution. Therefore scien-

tists have turned to statistical methods known as statistical mechanics^[10] to describe the effects of large numbers of particles in an absorbing gas. In fact, what is of interest is the average behavior of the interacting microscopic particles rather than the behavior of each particle.

In describing the effect of energy emissions or absorptions caused by transitions in discrete energy levels of a molecule, the assumption was made that these processes are characterized by well-defined monochromatic frequencies. In reality, due to many reasons including the interaction of molecules within the absorbing gas, this assumption of monochromatic frequency absorption (emission) is not true. The actual absorption spectra have fully defined contours whose shapes depend upon the conditions of the absorber that is its density, pressure, temperature, etc. For the earth's atmosphere the line shapes are determined predominantly by 1) radiative damping, 2) the Doppler effect and 3) effects of molecular collisions, (Zuev)^[9]. While the effects of radiative damping and the Doppler effect are important it is significant that their effects on transmittance are mainly recorded at higher levels in the atmosphere, levels where pressure drops below 10 millibars. For this report only the atmosphere where pressures ranged above 10 millibars was considered and hence only the effects of molecular collision known as pressure broadening were taken into account.

The interaction or collisions of neighboring molecules in a gas results in a deformation of energy levels and an absorption or emission of light. The interaction of molecules clearly depends on the observed pressure and temperature of the gas. According to Zuev^[9] "No exact solution of the problem of the influence of molecular collisions on spectral line broadening has yet been obtained....." Early theories of molecular-collision spectral line broadening took only strong collisions into effect. The best known of these theories was developed in 1906 by H.A. Lorentz^[9] and is widely used today to describe the contour of spectral lines which absorb light in a gaseous absorber. The mathematical representation for the line shape of the absorption coefficient given by the Lorentz theory is:

$$K(\nu) = \frac{S}{\pi} \frac{\alpha_L}{(\nu - \nu_0)^2 + \alpha_L^2} \quad 2.3-2$$

where S represents the intensity of the line at the line center ν_0 and α is the half width of the line. A contour of the Lorentz line shape for a single absorbing line is given in figure 2.3-1. The half width for the Lorentz contour is, as expected, pressure and temperature dependent. It is defined by the formula

$$\alpha_L = \alpha_0 \frac{P}{P_0} \sqrt{\frac{T_0}{T}} \quad 2.3-3$$

where α_0 is the half width under standard conditions. Standard

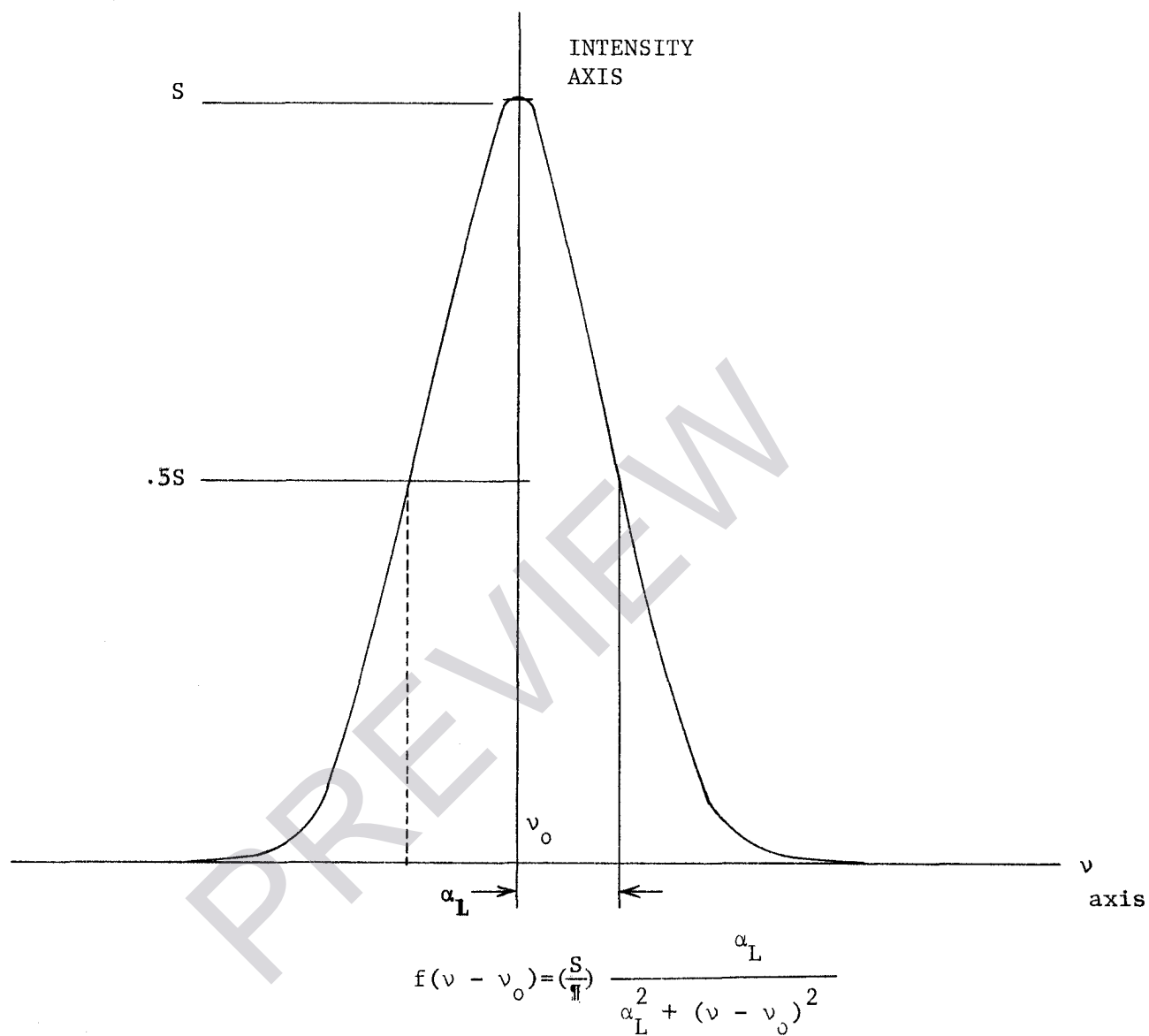


Figure 2.3-1

Lorentz Line Shape

conditions defined as $P_o = 1013$ millibars and $T_o = 296$ °K were adopted to conform with those outlined in "AFCRL Atmospheric Absorption Line Parameters Compilation"[7].

The line intensity S is also a function of temperature and for the Lorentz theory is given by:

$$S = S_o \left(\frac{T_o}{T} \right)^b Q_v \exp \left[\frac{-E_v}{kT_o} \left(\frac{T_o}{T} - 1 \right) \right] \quad 2.3-4$$

S_o is the line intensity at reference temperature and pressure as given above. Q_v is the vibration-partition function ratio for a given isotope of an absorbing gas; partition functions for the most abundant isotopes of the absorbing gas are given in table 1, Appendix A. The term

$\left(\frac{T_o}{T} \right)^b$ gives the temperature dependence for the rotational partition function⁽⁷⁾. The constant b equals one for linear molecules such as carbon dioxide, nitrous oxide, carbon monoxide, and oxygen; but has the value 1.5 for water vapor, ozone, and methane. The factor E_v in the exponential is the energy of the lower state of the molecular transition at a given frequency; k is Boltzman's constant.

A review of equations 2.2-3, 2.3-2, and 2.3-3 indicates the varied quantities needed to define transmittance through an absorbing medium. Assuming that the temperature, pressure, density, and path length for which the transmittance is desired are known; the quantities S_o = reference intensity,

E_v = base energy state, α_o = reference line half width, and v_o = line center position must be defined in order to perform the calculation. Fortunately, a compilation such as described above exists, and is available on magnetic tape adaptable to many computers. The compilation by R. A. McClatchey et. al., is discussed in "AFCRL Atmospheric Absorption Line Parameters Compilation" dated 26 January 1973. Recently, the magnetic tape has been superseded by a 1976 version which contains more up-to-date absorption line data^[11]. The calculation of the absorption coefficient for all numerical methods discussed in this report is done utilizing line parameters retrieved from the 1976 atmospheric line parameter compilation from the Air Force Cambridge Research Laboratory.

2.4 The Earth's Atmosphere

In previous sections the assumption was made that certain atmospheric parameters, i. e., temperature, pressure, and absorber concentration, were known for a given altitude. Based on data gathered in numerous rocket and balloon sounder experiments and data collected at various ground-based research stations, the assumption is certainly valid. However, variations in collected atmospheric data exist, and a final determination as to a specific model to use in testing the calculations was not easy.