# Evaluation of LOWTRAN and MODTRAN for use over high zenith angle/long path length viewing 

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# EVALUATION OF LOWTRAN AND MODTRAN FOR USE OVER HIGH ZENITH ANGLE/ LONG PATH LENGTH VIEWING 

by<br>Jonathan C. Wright

# A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in the Center for Imaging Science in the College of Graphic Arts and Photography of the Rochester Institute of Technology 

May 1991

Signature of the Author Jonathan C. Wright


# COLLEGE OF GRAPHIC ARTS AND PHOTOGRAPHY ROCHESTER INSTITUTE OF PHOTOGRAPHY ROCHESTER, NEW YORK 

## CERTIFICATE OF APPROVAL

M. S. DEGREE THESIS

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The M.S. Degree Thesis of Jonathan C. Wright has been examined and approved
by the thesis committee as satisfactory for the thesis requirement for the Master of Science degree
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# EVALUATION OF LOWTRAN AND MODTRAN FOR USE OVER HIGH ZENITH ANGLE/ LONG PATH LENGTH VIEWING 

by<br>Jonathan C. Wright<br>Submitted to the Center for Imaging Science in partial fulfillment of the requirements<br>for the Master of Science Degree at the Rochester Institute of Technology

## ABSTRACT

LOWTRAN and MODTRAN were evaluated in the $2.0-5.5$ micron region against field collection data at high zenith angle/long path lengths to determine the degree of uncertainty associated with these models under these conditions. Matching data sets were developed using data from the Air Force Geophysics Laboratory Flying Infrared Signatures Technology Aircraft (FISTA) as the field reference. The Kolmogorov-Smirnov test was applied to determine the degree to which the outputs of LOWTRAN and MODTRAN follow the same distribution as the field data. The percent difference between the model and field data was also studied.

Agreement between the model and field data was found to be better than $97 \%$ for most cases. Median percent difference was within $10 \%$ for zenith angles less than 90 degrees.

It is said that no man is an island. This thesis is certainly a reflection of that concept. While it is only fair and fitting that any inaccuracies of fact, failing of intellect and insight, or butchery of standard written diction be laid at the feet of the author, the accomplishment of this thesis was by no means a solo feat. Thus, a few words of thanks to some of those who made this thesis possible.

Each of my advisors contributed in a unique way. Discussions with Stokes Fishburne were responsible for the concept. John Schott kept my feet to the fire and is in many ways responsible for the necessary rigor of the discussions and results. Carl Salvaggio provided invaluable assistance in keeping the focus on results rather than computer gymnastics.

Brian Sandford of the Air Force Geophysics Laboratory provided the data set, as well as advance copies of work in progress within the Laboratory updating the description of the sensor platform. His prompt response to a call out of the blue requesting data generated years earlier as well as detailed sensor information was and is extraordinary. I only hope I have the opportunity of fulfilling such an obviously irrational request in the future to somehow return the favor.

Jim Lisowski of Scitec provided sanity whenever it was needed. He, along with Stu Augustin, helped decipher the final calibration issues for which $I$ am eternally grateful. They also kept my feet to the fire and corrected me when $I$ strayed from the straight and narrow, something only friends would do. But that's another story.

## Dedication <br> To my wife Kathy and my daughter Caitlin.

They graciously allowed me to satisfy my academic curiosity. Why, I'll never know. Something about love I guess.

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1. INTRODUCTION

Proper interpretation of events viewed through the earth's atmosphere requires that the effects of atmospheric transmission and radiance be quantified when analysis of the remotely sensed data is performed. Computer models of the atmosphere have been developed to allow system designers and data analysts to perform this quantification. Two of the more commonly used models are LOWTRAN and MODTRAN, developed by the USAF Geophysics Laboratory. These models are computer codes which calculate atmospheric transmission and background radiance in the ultraviolet (UV) through infrared (IR) regions of the electromagnetic spectrum.

Traditionally, remote sensing has been performed within a viewing cone $\pm 45^{\circ}$ from earth normal, either uplooking or downlooking. This self-imposed limitation by remote sensing system designers and data analysts was due to concerns over optical system quality and atmospheric effects. The increased call for remote sensing to fill needs in both commercial (industrial and environmental) and military areas is resulting in systems which are required to make use of wider viewing. Examples of this are the desire to use data from
meteorological satellites for use in nonmeteorological applications (eg like LANDSAT images) and broader area coverage from environmental missions of high altitude aircraft such as the NASA U-2.

This thesis reviews the modeling by the LOWTRAN and MODTRAN codes and compares them statistically against actual field measurements in high zenith angle viewing (60-90 degrees) with long path distances ( $>50 \mathrm{~km}$ ). By testing the codes along these extreme viewing conditions it is hoped that the effectiveness of the modeling can be ascertained. Key to this focus on modeling errors is the use of high altitude measurements. By using high altitude measurements atmospheric variability is significantly reduced (the atmosphere is relatively stable and predictable at tropospheric and stratospheric altitudes). In a statistical sense this allows the effects of atmospheric uncertainty in any given measurement to be blocked out and only modeling errors should remain.

Determining the modeling errors is important for two general classes of problems. In many remote sensing applications either LOWTRAN or MODTRAN are used to determine the effect of the atmosphere on data collected in a measurement program. This effect is then used to back out the
losses to arrive at the original radiance of the object of interest. Modeling errors would thus lead directly to measurement errors in the processed data. These errors could lead to incorrect results in the analysis of that data. The codes are also useful in this problem's inverse. Sensors are usually designed against a minimum signal of interest. This signal is often defined as the signal of the target less the attenuation of the atmosphere. The attenuation is determined using codes such as either LOWTRAN or MODTRAN. Errors in the codes can thus lead to incorrect system design. Incorrect designs are either lacking in sensitivity or have excess sensitivity resulting from overdesign. Either is an inefficient use of resources. The intent of this thesis is to determine the level of error in these codes due to modeling. This characterization can be used to isolate errors in both sensor design and data analysis to allow for more efficient utilization of scarce remote sensing resources.

## 2. BACKGROUND

Performance of this thesis required an understanding of three major areas, (A) atmospheric transmission and radiance modeling programs or codes, (B) data used as reference against which the codes will be compared, and (C) the statistical tools and terminology used in comparing the code output with these reference data. This discussion outlines these three major areas, their underlying theory, and the procedures used in performing the work associated with each area.
2.1. Atmospheric Transmission

The propagation of energy is central to remote sensing. Remote sensing can be taken to imply any sensing and analysis of events while not in direct proximity to them. This thesis shall employ a convention that defines remote sensing in a macroscopic sense; viewing of large scale events over relatively large distances. This is best defined by using the common examples of airborne or satellite sensing, although ground based systems can also be included. In addition, this thesis focuses on remote sensing performed in the part of the electromagnetic spectrum that can be optically imaged. This spans the region from 0.2 to 25 microns (ultraviolet through
deep infrared). Energy sensed in this region is dominated by two sources, propagation of the energy from the sun into the earth's atmosphere (primarily in the visible region) and thermal emissions from either the target or the earth background (dominant in the long wave infrared region).

Energy passing through the atmosphere is affected primarily by atmospheric scattering and absorption (Lillesand and Kiefer, 1987) ${ }^{1}$. Scattering is largely dependent on the size of the atmospheric constituents(molecules, particles, and aerosols) compared to the wavelength of the energy. Particles with a much smaller diameter than the wavelength of the energy cause Rayleigh scatter. Rayleigh scatter is inversely proportional to the fourth power of the wavelength, so shorter wavelengths are scattered much more than longer wavelengths. This form of scattering manifests itself in the blue color of the sky. Particles with diameters approximately the same diameter as the wavelength result in Mie scattering. Mie scattering, primarily caused by dust and water vapor, effects longer wavelengths than Rayleigh scatter. While both Rayleigh and Mie scatter have fairly well defined scattering patterns, not all scattering is so well behaved. Nonselective scatter, which results when the particle diameter is larger than the wavelength of the energy, scatters all wavelengths in random
patterns.
Absorption is the other primary source of loss in energy transfer through the atmosphere. Absorption is caused by the interaction of energy with the constituent gases of the atmosphere; including water vapor, ozone, and carbon dioxide. The characteristic energy absorption pattern of each of these gases results in blocking bands (where energy is absorbed) and window bands (where energy passes through with minimal absorption effects). Absorption is an inherently wavelengthdependent phenomenon.

The effects of atmospheric transmission losses may be seen by examining Figure 1. The exoatmospheric source function, solar radiation reaching the earth's outer atmosphere, is the dotted line. The irradiance reaching the sensor is shown as the solid line. The difference between the two lines is caused by the transmission losses described in Figure 2. Major contributors to this transmission curve are shown in Figures 3-6.

Since the object of this thesis is to examine solely the effects of the atmosphere on energy propagation, care must be taken to ensure that other errors are not induced. Remote sensing often looks at the reflectance or emission of a target. This thesis avoids the uncertainties of that problem
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（yコIW－ટWコ／S11甘M z－0I）ヨコNHIO甘yyI

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(eg. specular vs lambertian reflection, wavelength dependent emission, effects of background) by looking directly at the sun. The sun may be approximated as an exoatmospheric blackbody with a temperature of $-6000^{\circ} \mathrm{K}$. Both LOWTRAN and MODTRAN have detailed solar source models which will make this assumption unnecessary. If this is taken as direct illumination of the focal plane, the only other sources of energy are path radiance due to the atmosphere having a finite thermal temperature and forward scatter of solar radiance.

The transmission through the atmosphere may be written using Beer's Law:

$$
\begin{equation*}
\tau_{\beta}=e^{-\beta z} \tag{1}
\end{equation*}
$$

where $\tau_{B}$ is the transmission through the path length $z$ and $B$ is the loss coefficient representing losses due to both scattering and absorption. This equation is solved for each homogeneous path of length $z$, and for each wavelength of interest, to find a point to point transmission for a given wavelength. A homogeneous path is defined as a path distance where the atmosphere has a constant temperature, pressure, and constituents.

Radiance at a sensor then may be approximately written including losses as (Schott, 1989) ${ }^{2}$ :

$$
\begin{equation*}
L=\left(E_{s}^{\prime} \cos \sigma e^{-\tau^{\prime} \sec \sigma}\right) / \pi+\sum L_{\mathrm{T}}(1-\tau) \tau^{\prime \prime}+\sum E_{s}^{\prime} \tau_{1} \beta(\theta) \tau^{\prime \prime} \tag{2}
\end{equation*}
$$

where $L$ is the radiance received at the sensor (assuming a standard flat focal plane). Angles are defined for a hemisphere (Figure 7).

This term may be more easily understood by viewing it as three input terms. The first term is direct solar radiance:

$$
\begin{equation*}
\left.L_{\text {solar rad }}-\left(E_{s}^{\prime} \cos \sigma e^{-\tau^{\prime} \operatorname{seco} \sigma}\right) / \pi\right) \tag{3}
\end{equation*}
$$

where $E_{s}{ }^{\prime}$ is the exoatmospheric solar irradiance outside the atmosphere on a plane perpendicular to the axis of propagation, $\sigma$ is the angle between the normal to the surface and the sun, and $\tau^{\prime}$ is the optical depth through the atmosphere normal to the earth at the target.

The second term is the path thermal radiance:

$$
\begin{equation*}
L_{\text {path thermal rad }}-\Sigma L_{T}(1-\tau) \tau^{\prime \prime} \tag{4}
\end{equation*}
$$

where $L_{\mathrm{T}}$ is the radiance associated with a blackbody at the temperature ( T ) of the atmospheric layer and (1- $\tau$ ) is the emissivity of the layer, and $\tau^{\prime \prime}$ is the transmissivity of the path from the layer to the sun. This term is summed over the homogeneous layers from the point of emission to the sensor.

Figure 7


Hemispheric Viewing Angle
for Equation 2

The third term is the forward scattered radiance:

$$
\begin{equation*}
L_{\text {forward scat rad }}-\Sigma E_{s}^{\prime} \tau_{1} \mathrm{~B}(\theta) \tau^{\prime \prime} \tag{5}
\end{equation*}
$$

$B(\theta)$ is the angle dependent loss coefficient for the scattered emission, and $\tau_{1}$ and $\tau^{\prime \prime}$ are the transmissivity of the portions of the path viewed prior to and after forward scatter. This term is summed over the homogeneous path distances traveled by the scattered radiation.

Thus, the energy received at the sensor is the energy emitted by the sun corrected for the angle by a cosine term, multiplied by the transmissivity of the atmosphere (corrected for the angle), and the thermal path radiance summed for each layer along the path (corrected for the emissivity of the path, its angle, and atmospheric transmission), and forward scattered energy of each layer along the path.

This equation, like equation 1 , must be solved over homogeneous paths, 2 , and for each wavelength of interest. This gives rise to two effects that must be corrected for in the codes. The first is that the atmosphere is not composed of homogeneous paths. An approximation must be made to generate an estimate of atmospheric transmission, either through forced establishment of homogeneous layers (LOWTRAN), development of an approximation of an equivalent homogenous layer path (LOWTRAN 5B and MODTRAN), or provision to allow for
solution of equations where local thermodynamic equilibrium does not exist (Fascode, a line by line transmission code also developed by the Air Force Geophysics Laboratory; (Smith, 1978 $)^{3}$ ). The second effect is known as curve of growth, an effect arising from the pressure broadening of absorption lines as a function of optical depth. This effect is not addressed in LOWTRAN (since it is a $20 \mathrm{~cm}^{-1}$ band model this effect is outside its effective resolution limits), but is addressed in LOWTRAN5B, MODTRAN and Fascode.

Neither LOWTRAN nor MODTRAN directly solve this radiative transfer equation. Instead, approximations are made to allow modeling to exist within the framework of available information and analytic tools.
2.2. LOWTRAN Model

The LOWTRAN model is a low resolution ( $20 \mathrm{~cm}^{-1}$ ) model originally developed by the Air Force Cambridge Research Laboratory (now the Air Force Geophysics Laboratory) in 1972 (Selby et al, 1972). Since then, considerable improvements have been made, expanding the code to include radiance in addition to transmission. It is useful to review the form and improvements to the code beginning with version 5 . LOWTRAN 5 (Kneizys et al, 1980) ${ }^{5}$, published in 1980, was a major software revision to the code and will be used as the baseline
reference for the rest of this discussion, as the extensions and improvements(Kneizys et al, 1983) (Kneizys et al, 1988)6,7 incorporated since then were built onto version 5's basic structure.

LOWTRAN 5 calculates atmospheric transmission based upon molecular band absorption and scattering (the $B$ term of Equation 1), aerosol extinction, and molecular continuum absorption. Absorption and scattering are not solved directly for the Beer's law formulation of equation 1. Instead, a single parameter (absorption coefficient, s/d) look-up table is employed for each of four components. These components are water vapor, ozone, nitric acid, and the uniformly mixed gasses $\left(\mathrm{CO}_{2}, \mathrm{~N}_{2} \mathrm{O}, \mathrm{CH}_{4}, \mathrm{CO}, \mathrm{O}_{2}, \mathrm{~N}_{2}\right)$. Each band is represented by a single parameter generation function using a look-up parameter based upon the atmospheric conditions given in the inputs.

Improvement of these parameters is one of the major changes incorporated in the most recent version, LOWTRAN 7. The need to upgrade the accuracy in the parameters chosen for the band model approach was outlined in Zachor (1981) ${ }^{8}$. This article examined the accuracy of $a$ band model approach to modeling the atmosphere. Zachor's primary conclusion was that the single parameter solution did not, and could not, contain
enough information to adequately describe the atmosphere. This was particularly true where multiple gasses were to be modeled in one curve. The move to independent curves for all of the major constituent gasses in LOWTRAN 7 addresses these concerns.

Using a method described by Pierluissi and Tsai (1987)9 the uniformly mixed gases are now treated individually rather than as a group. The overall formulation is similar to that of the earlier LOWTRAN versions in using a look-up table rather than a direct solution to Equation 1 . The effect of incorporating this change to the LOWTRAN 6 model was suggested and reviewed by cutten $(1986,1988)^{10,11}$. Similarly, the band models for $\mathrm{H}_{2} \mathrm{O}$ have also been upgraded (Pierluissi et al, 1989) ${ }^{12}$.

The continuum model for water vapor was upgraded in LOWTRAN $6^{5}$ to the form used in FASCODE 1B (Clough et al, 1981) ${ }^{13}$. This provided a major improvement in the 4.5-5.0 $\mu \mathrm{m}$ region. These authors note that there are still great uncertainties in the modeling at the atmospheric transmission windows in the $10 \mu \mathrm{~m}$ and $4 \mu \mathrm{~m}$ regions. Improved results were achieved in the $4.5-5.0 \mu \mathrm{~m}$ region.

The last major revision to the physics of the code has been in the treatment of scattering. In Version 5 all energy
scattered along the path was lost and no energy was scattered back in. As early as 1980 Ben-Shalom and others identified the effects that this would have over long path distances ${ }^{14}$. The lack of conservative scattering is estimated to cause errors as large as a factor of two under some viewing scenarios. LOWTRAN 6 introduced a single scattering model that allowed particles to scatter once before being lost. This still provided results significantly different from those shown using fully conservative scattering as suggested by BenShalom. This error was because single scattering treated scattering as a source of extinction but still not as a source of radiance. Fully conservative scattering had been implemented in Fascode $2^{15}$, but this proved to be inaccurate as well since now all energy was conserved, leading to an overestimate of radiance.

All of these shortcomings were well described in an article by Isaacs, et al (1987) ${ }^{16}$ in which they describe a multiple scattering modification to both LOWTRAN and FASCODE which greatly reduces errors (claimed to be less than $20 \%$ in all viewing geometries). Their approach is to model scattering using a finite stream approach. It is implemented in LOWTRAN 7. The actual results depend on the physical parameters of the single scattering albedo and the viewing
geometry (representing the scattering phase function).
Another modification that was performed to the LOWTRAN model was the inclusion of band models which gave true $5 \mathrm{~cm}-1$ accuracy. (Standard LOWTRAN output may be obtained at this resolution but it is interpolated from the $20 \mathrm{~cm}-1$ calculations.) This version, known as LOWTRAN 5B, developed by Robertson et al (1980) ${ }^{17}$, was more numerically accurate than the interpolation from the $20 \mathrm{~cm}^{-1}$ output of LOWTRAN since it calculated these points. It also predated LOWTRAN 7's treatment of the uniformly mixed gases as separate parameters. However, it still lacked individual band models for all of the gasses described in LOWTRAN 7 and lack of multiple scattering. Due to the significant differences in the development of the band model parameters it will be discussed in detail at the beginning of the MODTRAN section.

Both LOWTRAN and MODTRAN treat the atmosphere as layers above the earth surface, not unlike layers of an onion around its core. This modeling form defines both how energy is propagated through the atmosphere (path length) and how the different atmospheric models are developed with their characteristic components.

The LOWTRAN 5 manual states that in general earth curvature has a greater effect on path length than refraction,
except at angles approaching $90^{\circ}$. With zenith angles close to $90^{\circ}$ the increase in path length may be up to $30 \%$. The effect of increasing path distances is to increase optical depth. Optical depth refers to the "thickness" of the viewing atmosphere. If the observer is looking straight up the depth is one atmosphere as each layer is traversed once by the energy beam along the shortest (normal) path. As the viewing angle is changed to more oblique zenith angles each layer of the atmosphere has a longer effective depth and the atmosphere appears denser. At the 90 degrees zenith viewing optical depth is approximately 39.65 atmospheres (Bemporad 1907) ${ }^{18}$.

Refraction within the atmosphere is governed by standard optical principles, principally Snell's law for the transition of energy between layers. The angle of refraction from one layer to another is defined as:

$$
\begin{equation*}
\sin \theta=n_{0}\left(R_{0}+H_{1}\right) \sin \theta_{0} / n\left(R_{0}+z\right) \tag{6}
\end{equation*}
$$

Where $\theta$ is the zenith angle, $n$ is the index of refraction between layers, $R_{0}$ is the earth radius, $H_{1}$ is the height of the lower layer, and $z$ is the layer depth. The subscript 0 on the sine term indicates arrival. The term for effective path length between layers $z_{i}$ and $z_{i+1}$ is derived (Figure 8) where $B$ is the angle subtended at the center of the earth as:

$$
\begin{equation*}
D S_{i}-\left(R_{0}+z_{i+1}\right) \sin \beta_{i} / \sin \theta_{i} \tag{7}
\end{equation*}
$$

Version 7 was modified to account for surface heights of other than sea level. (Previous versions enforced a uniform earth radius with all surface points at sea level.) LOWTRAN now generates a modified version of the Beer's law formula; most significant at altitudes up to six kilometers. This modification was suggested by Novoseller (1987) ${ }^{19}$ and fully outlined by Shettle (1989) ${ }^{20}$. The effect of this modification is to compress the atmospheric layers so that areas where ground level is above sea level no longer suffer what amounted to truncation of the lower atmospheric layers. It should be noted that this does not change the molecular content at the upper altitudes, rather it effectively compresses the effects of lower altitudes into a single term so that the extinction is properly calculated.

Molecular content at an altitude is defined within the scope of the layer concept. Molecular quantities for important species are defined within the layers at predefined levels for the different aerosol models available in LOWTRAN and MODTRAN. The different models attempt to provide a reasonable approximation to conditions within a specified geographic area or type when measurements of atmospheric conditions are not available. Most changes in these

Figure 8


Geometry for Path Viewing
conditions are seen in the lower atmosphere. Above these lower levels (altitudes $>\sim 10 \mathrm{~km}$ ) the atmosphere is fairly uniform globally and seasonally, in the absence of volcanic activity.

In summary, the improvements to LOWTRAN focus on the addition of multiple scattering and separate band models for the most important atmospheric gasses. This is not to discount other major improvements such as the revised and highly upgraded extraterrestrial source function, aerosol models, and cirrus cloud models; it simply points out the major changes that justify a review of LOWTRAN capabilities now that more accurate results can be expected.

### 2.3. MODTRAN

MODTRAN can be viewed as an extension of the band model approach used in LOWTRAN 5B with the updated aerosol and scattering functions of LOWTRAN 7. Because of its close similarities to MODTRAN, LOWTRAN $5 B$ is included in this section and will be discussed first.

LOWTRAN 5B was the first of the moderate resolution codes. It retained the same aerosol models as LOWTRAN 5, but utilized a significantly different method of developing the band model parameters.

It included, besides the increased spectral resolution
discussed earlier, addition of temperature dependence of the molecular absorption coefficients, and use of a multi parameter, Doppler-Lorentz band model.

The basic forms of LOWTRAN have their band model coefficients defined for an absorption coefficient, s/d, defined for standard temperature and pressure (STP; 1 atm, 273 K ). LOWTRAN 5B calculations for the coefficients are based on multiple temperatures $(200,225,250,275$, and 300 K ) and line density, $l / d$, as well as the absorption coefficient $s / d$. Curve of growth effects are included through the combined Doppler-Lorentz band model. The Curtis-Godson approximation is used for multilayer transmittance calculations, replacing an inhomogeneous path with a homogeneous one by using average values for the various band model parameters. ${ }^{21}$
"MODTRAN ${ }^{22}$ is a moderate resolution model and computer code used to predict atmospheric transmittance and background radiance in the microwave, infrared, visible, and near ultraviolet spectral regions ( 0 to $50,000 \mathrm{~cm}^{-1}$ or 0.2 micron to infinity). The code maintains complete compatibility with LOWTRAN 7, specifically, MODTRAN retains all of the capabilities of the LOWTRAN 7 model. Both codes contain the same six built-in model atmospheres; spherical refractive geometry, aerosol models, clouds (water and ice), rain
attenuation and options to calculate single scattered solar/lunar radiance, solar/lunar irradiance and multiply scattered thermal and solar radiance.
"The MODTRAN code improves LOWTRAN's spectral resolution from 20 to $2 \mathrm{~cm}^{-1}$ full width/half maximum (fwhm) with an option to vary the resolution between 2 and $50 \mathrm{~cm}^{-1}$ (fwhm). The band model parameters were formulated from the HITRAN line atlas for twelve atmospheric gasses: $\mathrm{H}_{2} \mathrm{O}, \mathrm{CO}_{2}, \mathrm{O}_{3}, \mathrm{~N} \mathrm{O}, \mathrm{CO}, \mathrm{CH}_{4}, \mathrm{O}_{2}$, $\mathrm{NO}, \mathrm{SO}_{2}, \mathrm{NO}_{2}, \mathrm{NH}_{3}$, and $\mathrm{HNO}_{3}$. These parameters were calculated for $1 \mathrm{~cm}^{-1}$ bins from $0-17900 \mathrm{~cm}^{-1}$ at five temperatures from 200 to 300 K , all stored on an external data file which is accessed by the program (for the region from 17,900 to $50,000 \mathrm{~cm}^{-1}$ the program defaults to the LOWTRAN 7 band parameters.)
"The transmittance is calculated with an equivalent-width formulation which accounts for the finite spectral width of each interval and the number of lines contained within the one $\mathrm{cm}^{-1}$ bin. LOWTRAN 7 uses a one-parameter band model (absorption coefficient, $S / d$ ) plus molecular density scaling functions, while MODTRAN relies on three temperature dependent parameters, an absorption coefficient (S/d), a line density parameter (l/d), and an average line width. The absorption due to line centers, within the one $\mathrm{cm}^{-1}$ bin, is modeled separately from the absorption due to line tails (from regions
whose line centers are outside the specified fwhm interval). The absorption due to lines within each bin is calculated by integrating over a voigt line shape. The line tail parameters consist of line contributions within $\pm 25 \mathrm{~cm}^{-1}$ (of the center of the fwhm region). The line tail absorption coefficient band model parameters are determined by integrating the Lorentz line shape over this interval of $\pm 25 \mathrm{~cm}^{-1.123}$

The improvements to the band model parameters and supporting data structures (eg solar model, scattering model, and aerosol models) as well as the introduction of the true $2 \mathrm{~cm}^{-1}$ MODTRAN model suggests that computer models may now be expected to accurately model field data.

### 2.4 Field Data

Determining the transmission and radiance accuracy of the two codes requires some form of standard against which the output is judged. In this research the object is to isolate out most possible sources of error. The simplest means of doing this would be to obtain the reference measurements in a laboratory. However, laboratory measurements cannot fully duplicate the effects on transmission and radiance in the atmosphere over long path lengths.

However, field measurements are not without their own shortfalls. The accuracy of the reference measurements can be
thought of as a function of the accuracy of the meteorological assumptions of the code inputs, the accuracy of the reference source, and the accuracy of the instrument taking the measurement. Chief among these difficulties is obtaining meteorological data to fully describe the atmospheric path through which the measurement is taken.

Ideally, meteorological data would be available over the whole path of interest. This is unrealistic for long paths. In the absence of meteorological data throughout the path model inputs will be used instead.

An additional difficulty is obtaining a good reference signal. In this thesis the sun will be used as the reference signal. The exoatmospheric source function of LOWTRAN and MODTRAN has recently been upgraded in all wavebands using data from numerous sources ${ }^{24}$; it will be assumed to be accurate (maximum discontinuity error is reported as three percent in the midwave infrared), ignoring the day to day variations induced by sun flares and other disturbances.

The accuracy of the field measurements is defined by the accuracy of the instrument. The measurements used as reference in this thesis were taken by the Air Force Geophysics Laboratory Flying Infrared Signatures Technology Aircraft (FISTA). The particular mission reference is Mission

8202 flown on 18 November 1981. The FISTA program is a suite of instruments flown on a NKC-135 aircraft. The particular instrument used for this experiment was interferometer 105. Measurements were taken of the setting sun over the Pacific Ocean from altitudes of $39,000 \mathrm{ft}(11.89 \mathrm{~km})$ and $29,000 \mathrm{ft}$ (8.84 km); the majority of the measurements were obtained at the lower altitude. These heights are sufficient to allow use of the atmosphere models as inputs since most meteorological effects occur at lower altitudes. Additionally, the sky was observed to be cloud free, indicating a stable tropospheric viewing path.

Interferometer 105 is a Michelson type interferometer. Its output is a Fourier transform of the actual spectrum, which is inverse transformed to arrive at the spectral data. The theory of Fourier transform spectroscopy is covered in numerous articles and books (Huppi, et al, 1981 and Walker, 1979) ${ }^{2526}$ and will not be discussed in this thesis. The FISTA instrument follows conventional design and analysis practices for this type instrument (Draft AFGL document, 1990) ${ }^{27}$.

Of greater interest is the sensitivity and resolution of the instrument and the method of background calibration and removal. The parameters of concern for this instrument (are
stated below (Mills, 1989) ${ }^{28}$ :
Wavelength:
Field of View:
Spectral Resolution:
Detector:
Scan Time:
Sensitivity:
Solar signatures will be significantly (- factor of $10^{4}-10^{8}$ ) above the instrument sensitivity for the solar viewing cases, errors should be confined to removal of background effects. This sensitivity margin will not exist for the background signatures; this level of sensitivity may not be sufficient for viewing background radiation.

Target irradiance is provided as the calibrated data product from FISTA missions. The calibration involves correction for off-axis optics effects. This calibration is performed prior to release of the data. Each annular region is described by a weighing factor. The annular zones are then used to weight the contribution to target radiance using the form of the following equation:

$$
\begin{equation*}
T=\left(T_{0}-g B_{0}\right) /(1-g) \tag{8}
\end{equation*}
$$

$T=$ target signal
$T_{0}=$ center radiance
$B_{0}=$ outer radiance
$g=$ fractional value assigned to outer component (Figure 9). Since FISTA data has been extensively used and no problems have been noted with its calibration, it will be assumed that the FISTA data can be safely used as a standard against which to evaluate the codes.
2.5. Statistical Tools

Traditionally, differences between the codes and a standard have been defined as percent error over the waveband of interest. An excellent example of this type of review is available in a report by cundiff (1986) ${ }^{29}$. In many aspects this report is a direct precursor to my thesis, examining the earlier versions of these codes. The percent difference measure is adequate only over discrete wavebands or for broadband integrated radiance.

A more statistically rigorous method for determining accuracy of the code generated estimates is obtained by comparing the code output directly with the field data, point for point. This comparison allows use of both the chi-squared and Kolmogorov-Smirnov tests. The Kolmogorov-Smirnov test is more appropriate for testing two data sets and is conservative

Figure 9


Off-axis Integrated Total Response Zones for Interferometers 105
for count data (as opposed to cumulative percent data). It is a nonparametric test designed specifically to test if two independent samples come from identically distributed populations (Daniel, 1990) ${ }^{30}$. By using this test, as well as focusing on percent differences in specific wavebands, the results of this thesis give a statistically sound determination of the errors associated with the two codes.

The Kolmogorov-Smirnov test is particularly applicable since the statistical tools typically used (such as analysis of variance) require an assumption of normal distributions, an assumption which cannot be made in these data. General linear model techniques are inappropriate for the determination of significant error in the match between the codes and data since the object is to determine the degree of error between points, not the ability of a polynomial model (equation) to fit the data.
2.6. Previous Efforts

Characterization of the errors associated with atmospheric codes is not a new or unique topic. Examples include many of the references already provided as well as others of a more general nature (Royer, 1988) ${ }^{31}$. Interest in the midwave IR bands over long path lengths limits the number of published reports considerably. Examples of these are

Cutten's publications ${ }^{9,10}$.
Rather more indicative of the efforts performed in this area are internal memos and reports like Cundiff $\mathrm{f}^{28}$. This report used the same FISTA data as this thesis but earlier versions of the codes. Overall accuracy as well as band accuracy were examined as percent error figures. Extracts from this report are provided as Appendix 1. The percent differences showed maximum error in the bands where the models were the weakest, as well as when the zenith angle was increased. The charts representing these errors are presented in pages 15 and 17 of that report.

Summary results as presented from page 37 of that report are:

1. Errors increased as zenith angle increased,
2. Errors were largest in bands where the least modeling had been performed, eg the 2.1-2.4 micron $\mathrm{CH}_{4}$ band,
3. Percent error measures provide adequate diagnostics only for identifying gross trends,
4. Percent error is inadequate to determining overall quality of the codes. An example of this is shown in the 2.1-2.4 $\mu \mathrm{m}$ band at $91.7^{\circ}$ zenith. In this graph there are clearly large errors on the order of 100 percent, but the average error is shown as near 50 percent.

Note that both FASCODE and LOWTRAN show extreme errors at near $90^{\circ}$ zenith.

The errors near $90^{\circ}$ zenith may not be a failure in the physical modeling but rather in the implementation. Richter $(1985)^{32}$ demonstrates that the dip in radiance near this angle is an artifact of the single scattering model. It is thus reasonable to expect significantly improved performance from LOWTRAN 7 and MODTRAN near $90^{\circ}$. This is due to the change in modeling from single scatter to multiple scattering effects in LOWTRAN 7 and MODTRAN.

Examination of individual bands is shown in Cutten's work as well as in a follow on (Lisowski, 1988) ${ }^{33}$ to Cundiff's work also provided in Appendix 1. This work examined the $\mathrm{CO}_{2}$ band in an attempt to chose a band model for use in a data reduction process.

The discussion shows how the computer models have evolved and describes the field data and statistical tools chosen for evaluation of the computer models. The next section will describe the approach used for this evaluation.

## 3. APPROACH

The goal of this thesis, a statistical estimate of error
between a computer model (LOWTRAN or MODTRAN) and a baseline measurement (the AFGL data set), required generation of both a calibrated field data set and a model data set. It was then necessary to make any corrections necessary to ensure that the two data sets were equivalent before making the error analysis. This section is logically divided into a discussion of these three activities.
3.1. Field Data Generation

The data utilized in this thesis was obtained on 18 November 1982 by the FISTA platform. The aircraft flew an orbit off of the Pacific Coast; with March AFB, CA the takeoff and landing point. During the orbit the setting sun was observed. Matching observations of the background sky were obtained on each orbit. The data are thus in pairs with the background observations oriented 180 degrees from the sun (Figure 10). The physical parameters for each observation pair are provided in Table 1.

The AFGL data set arrived as a VAX backup tape. Unfortunately, the files on the tape were in a format unique to the AFGL file storage system. The most efficient means of reading the files was to dump the files in both word and decimal format. These files were then edited using a text

Figure 10



TABLE 1
Air Force Geophysics Laboratory (AFGL)
Flying Infrared Signatures Technology Aircraft (FISTA)
Mission 820218 November 1982
Interferometer 105 (1799.26-5199.15 wavenumbers)

| Run Pair | GMT | North Lat. | West Long. | Alt <br> (km) | Solar <br> Elevation <br> (Declination) | Solar <br> Azimuth <br> ( ${ }^{\circ}$ East <br> of <br> North) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1/2 | 21.980 | 34.67 | 121.63 | 11.887 | 61.96 | 214.29 |
| 3/4 | 22.195 | 34.96 | 121.86 | 11.887 | 63.63 | 216.94 |
| 5/6 | 22.428 | 35.21 | 121.96 | 8.839 | 65.55 | 219.85 |
| $7 / 8$ | 22.620 | 34.96 | 121.80 | 8.839 | 67.00 | 222.49 |
| 9/10 | 22.859 | 34.80 | 121.60 | 8.839 | 69.05 | 225.61 |
| 11/12 | 23.100 | 34.83 | 121.84 | 8.839 | 71.08 | 228.21 |
| 13/14 | 23.286 | 35.00 | 121.95 | 8.839 | 72.86 | 230.17 |
| 17/18 | 23.736 | 34.68 | 121.59 | 8.839 | 77.31 | 235.25 |
| 19/20 | 23.921 | 34.86 | 121.78 | 8.839 | 79.18 | 236.94 |
| 21/22 | 0.069 | 34.84 | 121.63 | 8.839 | 80.81 | 238.48 |
| 23/24 | 0.338 | 35.00 | 121.57 | 8.839 | 83.78 | 241.03 |
| 25/26 | 0.530 | 34.65 | 121.81 | 8.839 | 85.53 | 242.66 |
| 27/28 | 0.687 | 34.88 | 121.84 | 8.839 | 87.34 | 244.03 |
| 29/30 | 0.824 | 34.82 | 121.74 | 8.839 | 88.92 | 245.29 |
| 31/32 | 0.976 | 34.66 | 121.84 | 8.839 | 90.48 | 246.54 |
| 33/34 | 1.096 | 34.68 | 121.67 | 8.839 | 91.98 | 247.65 |
| 35/36 | 1.205 | 34.82 | 121.68 | 8.839 | 93.26 | 248.55 |
| 37/36 | 1.296 | 34.76 | 121.67 | 8.839 | 94.30 | 249.31 |

Table 1 Notes:

1. 60 dB Neutral Density Filter used in all runs except 37. 2. Position Locations are for the midpoint of each data run.
2. Odd numbered runs are solar observations, even numbered runs are background observations.
3. Even numbered runs use position information generated during matching odd run.
editor to confirm the text information in the file header (already available in text format in the information provided by AFGL with the VAX backup tape, Appendix 2), and edit the data into a numeric format suitable for efficient processing on the computer. A sample text output is shown below.

Table 2
Sample Output of AFGL Mission 8202 File Header Run 01


#### Abstract

Scale Factor: $0.95367 \mathrm{E}-06$


Frequency Spacing: 1.92847
Beginning Frequency: 1799.26
Data values in the array:1765
AFGL Mission Designator: MISSION 8202
Archival Tape Designator:FILE e:n00010 101.MIS202. NUU FROM R395-398/R491

Notes: SUN ND IN

The numeric files were processed using the Minitab statistical spread sheet program. The routine written using this software read in the decimal numeric file, corrected the order of the data (the files should read left to right but the numeric file was inverse order, right to left), stacked the data into a single file (the AFGL tape contained numeric data in two records which together formed a composite numeric data set), and then ordered the data in column format. The output
of this process was a file with the raw calibrated counts, irradiance in watts/cm2-cm, the wavenumber for the particular irradiance data point in inverse centimeters and the equivalent wavelength in microns.

Files from the first run are provided as an example. The decimal numeric file is Appendix 3. The resulting data file is Appendix 4. Due to its length (1768 data points, over 30 pages of output) only the first and last pages of the file are provided in Appendix 4.

The relative calibrated irradiance is found by multiplying the raw count number (eg. 2026 for the first point) by the scale factor (.95367E-06 for this file). The effects of the neutral density filter utilized in this mission for solar viewing are included in this scale factor. The wavenumber is obtained by finding the offset from the initial wavenumber. The initial wavenumber is defined as 1799.26 and the step interval between each data point is 1.92847 wavenumbers. The wavenumber for the second data point is thus $1799.26+1.92847=1801.19$ wavenumbers.

The next manipulation was to derive fully calibrated data. The irradiance values generated so far did not include any correction for sensor effects. This correction was applied by multiplying the data files point-by-point with
values from the smoothed correction curve (Figure 11). The smoothed response curve is derived from laboratory measurements taken in a Nitrogen atmosphere. The effect of this curve is shown in the plot of the corrected response curves with and without the neutral density filter (Figures 12 and 13). Only one correction curve was required. (The neutral density filter is a combination of a metal oxide filter and an adjustment to the instrument electronics and has a uniform linear effect across the spectrum of interest. ${ }^{34}$ ) This plot closely matches other laboratory reference curves for this and other AFGL interferometers. ${ }^{35}$ The notch visible in both response curves is a result of adding a correction factor to compensate for $\mathrm{CO}_{2}$ gas that will be present in the aircraft environment.

It was necessary to determine the irradiance in units of watts/cm ${ }^{2}$ - micron. A simple linear interpolation was used to convert data from a reference to inverse centimeters to a reference of microns: $x$ * delta wavelength/delta wavenumber / a unit correction factor $=y$, where $x$ is irradiance (wavenumbers) and $y$ is irradiance (microns). As example, for the second point, $1.06 \mathrm{E}-06 *(.0154 / 5) / 1 \mathrm{E}-04=3.44 \mathrm{E}-04$.

One final manipulation was required to place the data in the format desired for analysis. The AFGL data had a higher


słunos
45

spectral resolution than LOWTRAN could output. Data to correspond to the five inverse centimeter LOWTRAN output was generated by interpolating the $A F G L$ data to that resolution. This was accomplished using a shape conserving cubic spline interpolation routine available in the IMSL $^{36}$ software package. The resulting data file for use in the statistical comparisons is shown in Appendix 5. (All comparisons were referenced to wavelength values in microns.)
3.2. Computer Model Data Generation

Files were generated using both LOWTRAN 7 and MODTRAN for direct solar illumination and radiance with multiple scattering viewing conditions. The physical parameters used were those recorded by $A F G L$ during the field data collection (Table 1). The mission data sheet did not provide a separate set of conditions for background viewing. Thus, the same physical conditions were used as inputs to generate both direct solar irradiation files and the paired radiance with multiple scattering files.

An annotation on the flight record stated that no clouds were visible in the viewing path. Due to the extremely long path lengths (ex. 183 km for Run 01 and 982 km for Run 29) it was necessary to utilize the standard atmospheres and aerosol models built into the codes. The most applicable standard
atmosphere was the tropical atmosphere. All of the other LOWTRAN 7 and MODTRAN model atmospheres were tailored to conditions of more northerly latitudes. Table 2 shows that similar results were obtained using midlatitude summer conditions (the next closest match to tropical viewing conditions) as the atmospheric model.

Several different aerosol models were examined as inputs. The most logical choice was the Maritime 23 km visibility. The Navy Maritime model was not used since it required knowledge of surface conditions in the viewing area during the preceding 24 hours. This data was not available. Analysis of Table 3 indicates that the most critical factor regarding aerosols in the computer models is simply their inclusion in the model inputs. The particular choice of aerosol model is of lesser importance.

The data for the LOWTRAN files were generated using the IBM Personal Computer (PC) based version of LOWTRAN. Table 4 shows that similar results were obtained for both the PC and mainframe versions. The PC data was used for comparison as it provided the most rigorous test and had been subject to the least review at the time of my thesis.

All of the AFGL data was in units of irradiance at the sensor. The output from the direct solar illumination models

Table 3
Effects of Aerosol Models Choice on Radiance Values (Radiance values in Watts/cm²-ster-cm)

|  | Tropical Atmosphere |  |  | Midatitude <br> Summer |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| wave- <br> number | No <br> Aerosols | 23 km <br> Rural | 5 km <br> Rural | 23 km <br> Maritime | 23 km <br> Maritime |
| 1800 | $3.67 \mathrm{E}-09$ | $3.75 \mathrm{E}-09$ | $3.75 \mathrm{E}-09$ | $3.64 \mathrm{E}-09$ | $3.75 \mathrm{E}-09$ |
| 2050 | $7.77 \mathrm{E}-10$ | $8.46 \mathrm{E}-10$ | $8.46 \mathrm{E}-10$ | $1.02 \mathrm{E}-09$ | $8.46 \mathrm{E}-10$ |
| 2300 | $4.78 \mathrm{E}-09$ | $4.78 \mathrm{E}-09$ | $4.78 \mathrm{E}-09$ | $4.46 \mathrm{E}-09$ | $4.78 \mathrm{E}-09$ |
| 2550 | $2.80 \mathrm{E}-11$ | $1.53 \mathrm{E}-10$ | $1.53 \mathrm{E}-09$ | $1.57 \mathrm{E}-09$ | $1.53 \mathrm{E}-09$ |
| 2800 | $1.51 \mathrm{E}-11$ | $1.77 \mathrm{E}-10$ | $1.77 \mathrm{E}-10$ | $1.79 \mathrm{E}-10$ | $1.77 \mathrm{E}-10$ |
| 3050 | $1.33 \mathrm{E}-11$ | $2.14 \mathrm{E}-10$ | $2.14 \mathrm{E}-10$ | $2.14 \mathrm{E}-10$ | $2.14 \mathrm{E}-10$ |
| 3300 | $1.24 \mathrm{E}-11$ | $2.70 \mathrm{E}-10$ | $2.70 \mathrm{E}-10$ | $2.70 \mathrm{E}-10$ | $2.70 \mathrm{E}-10$ |
| 3550 | $1.39 \mathrm{E}-11$ | $2.57 \mathrm{E}-10$ | $2.57 \mathrm{E}-10$ | $2.57 \mathrm{E}-10$ | $2.57 \mathrm{E}-10$ |
| 3800 | $2.34 \mathrm{E}-11$ | $4.37 \mathrm{E}-10$ | $4.37 \mathrm{E}-10$ | $4.37 \mathrm{E}-10$ | $4.37 \mathrm{E}-10$ |
| 4050 | $4.06 \mathrm{E}-11$ | $7.11 \mathrm{E}-10$ | $7.11 \mathrm{E}-10$ | $7.11 \mathrm{E}-10$ | $7.11 \mathrm{E}-10$ |
| 4300 | $4.48 \mathrm{E}-11$ | $7.49 \mathrm{E}-10$ | $7.49 \mathrm{E}-10$ | $7.49 \mathrm{E}-10$ | $7.49 \mathrm{E}-10$ |
| 4550 | $7.03 \mathrm{E}-11$ | $1.12 \mathrm{E}-09$ | $1.13 \mathrm{E}-09$ | $1.13 \mathrm{E}-09$ | $1.13 \mathrm{E}-09$ |
| 4800 | $1.05 \mathrm{E}-10$ | $1.61 \mathrm{E}-09$ | $1.61 \mathrm{E}-09$ | $1.61 \mathrm{E}-09$ | $1.61 \mathrm{E}-09$ |
| 5050 | $1.49 \mathrm{E}-10$ | $2.17 \mathrm{E}-09$ | $2.18 \mathrm{E}-09$ | $2.18 \mathrm{E}-09$ | $2.18 \mathrm{E}-09$ |

Table 4
Comparison of LOWTRAN PC and Mainframe Results

|  | Irradiance (Watts/cm -cm ) |  |  |
| :---: | :---: | :---: | :---: |
| wavenumber | PC | Mainframe | \% Difference |
| 1800 | $7.34 \mathrm{E}-07$ | $7.14 \mathrm{E}-07$ | 2.88 |
| 2050 | $9.64 \mathrm{E}-07$ | $9.37 \mathrm{E}-07$ | 2.88 |
| 2300 | $5.33 \mathrm{E}-09$ | $5.18 \mathrm{E}-09$ | 2.89 |
| 2550 | $1.55 \mathrm{E}-06$ | $1.51 \mathrm{E}-06$ | 2.65 |
| 2800 | $1.74 \mathrm{E}-06$ | $1.69 \mathrm{E}-06$ | 2.96 |
| 3050 | $1.91 \mathrm{E}-06$ | $1.85 \mathrm{E}-06$ | 3.24 |
| 3300 | $2.23 \mathrm{E}-06$ | $2.17 \mathrm{E}-06$ | 2.76 |
| 3550 | $1.74 \mathrm{E}-06$ | $1.69 \mathrm{E}-06$ | 2.96 |
| 3800 | $2.44 \mathrm{E}-06$ | $2.38 \mathrm{E}-06$ | 2.52 |
| 4050 | $3.22 \mathrm{E}-06$ | $3.22 \mathrm{E}-06$ | 0.00 |
| 4300 | $2.88 \mathrm{E}-06$ | $2.79 \mathrm{E}-06$ | 3.23 |
| 4550 | $3.60 \mathrm{E}-06$ | $3.50 \mathrm{E}-06$ | 2.86 |
| 4800 | $4.36 \mathrm{E}-06$ | $4.24 \mathrm{E}-06$ | 2.83 |
| 5050 | $5.01 \mathrm{E}-06$ | $4.87 \mathrm{E}-06$ | 2.87 |

Mean Percent Difference $=2.68$
was in irradiance units but the output of the radiance with multiple scattering model is in radiance units. Since all of the AFGL data is in irradiance units it was necessary to convert the output of the radiance models to irradiance units. Using the formula outlined in slater (1980) ${ }^{37}$ the conversion from radiance to irradiance is defined by knowing the field of view of the sensor. The sensor has a nominal one degree field of view. The radiance values may be converted to irradiance values for this sensor by multiplying by $2.39 \mathrm{E}-04$ steradians. (It was learned after completion of the thesis that AFGL uses an empirically derived value of 2 .5E-04 value for converting values from this particular instrument.)

### 3.3. Data Set Equivalence

Even though both sets of data (field and computer generated) had now been established as calibrated sets with equivalent viewing conditions and units a final correction was found necessary. While attempting to compare the background files it was found that two sensor effects still existed that required correction.

The first effect was that the computer models were predicting results below the noise floor of the instrument. While not strictly a calibration issue, the effect was the same. Predictions below the noise floor have no meaning since
they cannot be obtained by the sensor. The correction for this issue was to set a noise floor for the computer values equal to the stated noise floor of the instrument. Any predicted values below this level were adjusted up by the value of the noise floor.

This adjustment allowed inclusion of points that otherwise would have had to have been discarded from the analysis. While it does not allow for full evaluation of the radiance portion of the models it does allow their evaluation within the bounds imposed by the instrument.

The second effect was apparent blackbody radiation affecting data in the longer ( 5.5 micron) end of the spectrum. This radiation is a result of any small temperature shift in the interferometer sensor system between the times of the cold calibration and the field collection. This effect is also believed to include emission from the telescope barrel and the instrument optics. This effect that is not removed using the smoothed correction curve ${ }^{38}$. (The smoothed correction curve is developed from the cold calibration data.) The effect was on the order of $7 \mathrm{E}-09$ Watts $/ \mathrm{cm}^{2}$-micron at its maximum (near the 5.5 micron region).

The correction was to add greybody radiation as if the optics had been a blackbody source. A series of curves was
plotted against the data. These curves utilized blackbody temperatures from 270 to 285 K and emissivities from . 1 to . 2 . A curve from a blackbody with emissivity of $15 \%$ and temperature of 285 degrees Kelvin was found to provide a good fit to the data (Figures 14-17). These values were felt to be reasonable since the optics material, $\mathrm{CaF}_{2}$, has a stated emissivity of $10 \%$ for pure material ${ }^{39}$ and the temperature is also a reasonable approximation for a transition between the outside and inside of the aircraft platform. Figures 18 and 19 provide a graphic reference for the similarities between the calibrated MODTRAN and LOWTRAN and the AFGL data.
4. RESULTS

Two sets of tests were made on the data sets. The results of the Kolmogorov-Smirnov test determine if the field data and computer data follow the same distribution. The results of the percent difference test provide details at specific wavelengths and insight into error trends.

Equivalent inputs were used in both sets of tests. For background viewing conditions (even numbered AFGL runs) the comparison took the form:


microns
irradiance (watts/cm2-micron)


microns

| $\cdots \cdots \cdots \cdots$ | MODTRAN |
| :--- | :--- |
| $\cdots \cdots$ | AFGL |



| $\begin{aligned} & \text { z } \\ & \text { 管苋 } \\ & 0 \end{aligned}$ |
| :---: |
|  |  |





$$
\begin{equation*}
E_{M}=E_{A F G L} \text { vS } E_{\text {RadiancewithmultipleScattering }}=E_{C} \tag{9}
\end{equation*}
$$

For solar viewing conditions (odd numbered AFGL runs) the comparison took the form:

$$
\begin{equation*}
E_{M}=E_{A F G L} \text { VS } E_{D i r ~ s o l a r ~ I r Y}+E_{\text {Rad with Mult scat }}=E_{C} \tag{10}
\end{equation*}
$$

(AFGL solar viewing captures at the instrument both direct solar irradiance and irradiance from the sky background with multiple scattering of both sky and solar radiance). Thus, for all comparisons, $E_{M}$ is the measured irradiance (field data) and $\mathrm{E}_{\mathrm{c}}$ is the equivalent calculated irradiance (computer data) at the instrument.
4.1. Kolmogorov-Smirnov Analysis

The Kolmogorov-Smirnov test is a hypothesis test that two sets of data have the same probability density function. The form of the hypothesis is as follows for the two sided case:

$$
\begin{gather*}
H_{0}(x): F_{1}(x)=F_{2}(x) \text { forall } x  \tag{11}\\
H_{1}: F_{1}(x) \neq F_{2}(x) \text { for at least one } x \tag{12}
\end{gather*}
$$

The test results (Table 5) are generated in terms of the two sided test statistic, $D$, and are shown in terms of the

Table 5
Results of Kolmogorov-Smirnov Test

| AFGL Run Number | Probability of Greater D, Two-Sided Test |  |
| :---: | :---: | :---: |
| (Solar Elevation) | LOWTRAN Comparison | MODTRAN Comparison |
| 1 (61.960) | 0.0001 | 0.0003 |
| $2\left(61.96^{\circ}\right)$ | 0.0000 | 0.0000 |
| $3\left(63.63^{\circ}\right)$ | 0.0003 | 0.0010 |
| $4\left(63.63^{\circ}\right)$ | 0.0000 | 0.0000 |
| $5\left(65.55^{\circ}\right)$ | 0.0073 | 0.0206 |
| $6\left(65.55^{\circ}\right)$ | 0.0000 | 0.0000 |
| $7\left(67.00^{\circ}\right)$ | 0.0005 | 0.0034 |
| $8\left(67.00^{\circ}\right)$ | 0.0000 | 0.0000 |
| $9\left(69.05^{\circ}\right)$ | 0.0007 | 0.0042 |
| $10\left(69.05^{\circ}\right)$ | 0.0000 | 0.0000 |
| 11 (71.08 ${ }^{\circ}$ ) | 0.0004 | 0.0034 |
| $12\left(71.08^{\circ}\right)$ | 0.0000 | 0.0000 |
| 13 ( $72.86^{\circ}$ ) | 0.0000 | 0.0000 |
| 14 (72.86 ${ }^{\circ}$ ) | 0.0000 | 0.0000 |
| $17\left(77.31^{\circ}\right)$ | 0.1735 | 0.1195 |
| $18\left(77.31^{\circ}\right)$ | 0.0000 | 0.0000 |
| 19 (79.18 ${ }^{\circ}$ ) | 0.0388 | 0.0284 |
| 20 (79.18 ${ }^{\circ}$ ) | 0.0000 | 0.0000 |
| $21\left(80.81^{\circ}\right)$ | 0.3368 | 0.1537 |
| $22\left(80.81^{\circ}\right)$ | 0.0000 | 0.0000 |
| $23\left(83.78^{\circ}\right)$ | 0.0332 | 0.0332 |
| $24\left(83.78^{\circ}\right)$ | 0.0000 | 0.0000 |
| 25 (85.53 ${ }^{\circ}$ ) | 0.0801 | 0.0451 |


| $26\left(85.53^{\circ}\right)$ | 0.0000 | 0.0000 |
| :--- | :--- | :--- |
| $27\left(87.34^{\circ}\right)$ | 0.0206 | 0.0061 |
| $28\left(87.34^{\circ}\right)$ | 0.0000 | 0.0000 |
| $29\left(88.92^{\circ}\right)$ | 0.0000 | 0.0000 |
| $30\left(88.92^{\circ}\right)$ | 0.0000 | 0.0000 |
| $31\left(90.48^{\circ}\right)$ | 0.0000 | 0.0000 |
| $32\left(90.48^{\circ}\right)$ | 0.0000 | 0.0000 |
| $33\left(91.98^{\circ}\right)$ | 0.0000 | 0.0000 |
| $34\left(91.98^{\circ}\right)$ | 0.0000 | 0.0000 |
| $35\left(93.26^{\circ}\right)$ | 0.0000 | 0.0000 |
| $36\left(93.26^{\circ}\right)$ | 0.0000 | 0.0000 |
| $37\left(94.30^{\circ}\right)$ | 0.0000 | 0.0000 |

Table 4 Notes:

1. Odd Runs are Solar Viewing, Even Runs Background Viewing.
2. Runs 1-4 are at 11.887 km , all others are at 8.839 km .
resulting probability. Probability is defined as 1-alpha where alpha is the risk of rejecting the null hypothesis when it is true. Table 4 shows that for most of the runs $H_{0}$ is true with a probability greater than $97 \%$. It is thus concluded that the two sets of data, field and computer, have the same probability distribution function. From this it can be inferred that they have statistically the same shape and that the computer models provide a good representation of the observed irradiances.
4.2. Percent Difference Analysis

The percent difference was defined as:

$$
\begin{equation*}
\Delta \%(\lambda)-\frac{E_{c}(\lambda)-E_{m}(\lambda)}{E_{m}(\lambda)} \tag{13}
\end{equation*}
$$

where $E_{c}$ (lambda) is the calculated value at a given wavelength and $E_{m}(l a m b d a)$ is the measured value at a given wavelength. A positive percent difference represents an under estimate of the irradiance by the models.

Singularly large differences at a given wavelength can be generated using equation 13 , especially in the blocking bands of $\mathrm{H}_{2} \mathrm{O}$ at 2.7 microns and $\mathrm{CO}_{2}$ at 4.3 microns. These large differences arise from small differences between the actual concentrations of these atmospheric gasses and the
concentrations predicted by the computer codes. In the blocking bands small; changes in concentration result in relatively large changes in transmissivity. These large changes in transmissivity of the atmosphere have large effects on the irradiance at the sensor. Thus, it is possible to arrive at large percent changes in irradiance from errors in the calculated data that result not from errors in the model itself, but from the atmospheric parameters input to the model.

Therefore, a limit was applied to the results of the percent difference calculations. This limit sets results from equation 13 that exceed a percent difference of $\pm 200 \%$ to $\pm 200 \%$. This was done so that singularly large differences at a given wavelength would not impede generation of useful plots or analysis at other wavelengths. The number of "limited" points can also be used as a diagnostic tool to evaluate the level of error in a given comparison; runs with larger numbers of "limited" points have greater overall error (Table 6). A tabular summary of the statistics is provided (Table 7). Plots of these values are provided as Figures 20-29.

The choice to "limit" the data was made over the alternative of declaring data in these regions invalid, as in Cundiff. Either approach has merit. Since the intent of this

Table 6
Summary Results from "limiting" Percent Difference Calculations

| AFGL Run \# | \# of LOWTRAN points "limited" | \% of LOWTRAN points "limited" | \# of MODTRAN points <br> "limited" | $\%$ of MODTRAN points "limited" |
| :---: | :---: | :---: | :---: | :---: |
| 1 | 16 | 2.35 | 14 | 2.06 |
| 2 | 106 | 15.63 | 105 | 15.49 |
| 3 | 17 | 2.51 | 16 | 2.35 |
| 4 | 116 | 17.11 | 116 | 17.11 |
| 5 | 22 | 3.24 | 30 | 4.43 |
| 6 | 78 | 11.50 | 80 | 11.80 |
| 7 | 22 | 3.24 | 27 | 3.98 |
| 8 | 74 | 10.91 | 73 | 10.76 |
| 9 | 23 | 3.39 | 32 | 4.72 |
| 10 | 76 | 11.21 | 74 | 10.91 |
| 11 | 27 | 3.98 | 37 | 5.46 |
| 12 | 57 | 8.41 | 59 | 8.70 |
| 13 | 27 | 3.98 | 36 | 5.31 |
| 14 | 51 | 7.52 | 53 | 7.82 |
| 17 | 41 | 6.05 | 43 | 6.34 |
| 18 | 174 | 25.66 | 172 | 25.37 |
| 19 | 39 | 5.75 | 44 | 6.49 |
| 20 | 31 | 4.57 | 30 | 4.42 |
| 21 | 42 | 6.19 | 55 | 8.11 |
| 22 | 27 | 3.98 | 30 | 4.42 |
| 23 | 54 | 7.96 | 62 | 9.14 |
| 24 | 12 | 1.77 | 134 | 19.76 |


| 25 | 70 | 10.32 | 57 | 11.06 |
| :---: | :---: | :---: | :---: | :---: |
| 26 | 12 | 1.77 | 127 | 18.73 |
| 27 | 87 | 12.83 | 92 | 13.57 |
| 28 | 6 | 0.09 | 123 | 18.14 |
| 29 | 112 | 16.52 | 116 | 17.11 |
| 30 | 9 | 1.33 | 59 | 8.7 |
| 31 | 162 | 23.89 | 185 | 27.29 |
| 32 | 772 | 69.62 | 57 | 8.41 |
| 33 | 13 | 1.92 | 509 | 75.07 |
| 34 | 25 | 39.71 | 676 | 7.22 |
| 35 | 4 | 0.59 | 71 | 99.71 |
| 36 |  |  | 26 | 10.47 |
| 37 |  |  |  | 3.83 |

Table 7
Statistics for "limited" Percent Difference Comparisons

|  | Statistics of "limited" LOWTRAN Comparisons |  |  | Statistics of "limited" MODTRAN Comparisons |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AFGL <br> Run \# | Mean | Median | Std Dev | Mean | Median | std Dev |
| 1 | 4.10 | 5.90 | 35.78 | 3.87 | 5.79 | 33.35 |
| 2 | -43.45 | -12.08 | 91.13 | -43.66 | -11.66 | 91.25 |
| 3 | 2.49 | 4.86 | 36.58 | 1.67 | 4.78 | 34.96 |
| 4 | -35.14 | 6.88 | 96.93 | -35.24 | 7.17 | 97.02 |
| 5 | -2.07 | 3.03 | 44.14 | -5.43 | 3.34 | 47.61 |
| 6 | -29.98 | -1.65 | 86.28 | -30.27 | -2.01 | 86.30 |
| 7 | -3.10 | 3.22 | 45.11 | 39.71 | 51.52 | 52.95 |
| 8 | -31.96 | -4.21 | 84.95 | -31.66 | -4.69 | 84.97 |
| 9 | -2.72 | 3.27 | 45.46 | -6.72 | 3.06 | 50.04 |
| 10 | -31.87 | -3.77 | 88.53 | -32.25 | -4.40 | 88.67 |
| 11 | -3.97 | 3.17 | 46.72 | -7.96 | 3.70 | 51.64 |
| 12 | -20.46 | 4.48 | 82.40 | -20.86 | 4.49 | 82.67 |
| 13 | 0.12 | 9.00 | 49.15 | -2.25 | 9.07 | 52.95 |
| 14 | -18.88 | -1.96 | 81.79 | -19.34 | -2.41 | 81.94 |
| 17 | -18.21 | -7.49 | 52.49 | -20.38 | -7.88 | 53.11 |
| 18 | -54.40 | -29.78 | 107.96 | -55.05 | -30.87 | 108.09 |
| 19 | -22.65 | -11.79 | 52.19 | -25.38 | -11.74 | 53.39 |
| 20 | -13.22 | -1.73 | 73.84 | -13.94 | -2.04 | 74.21 |
| 21 | -15.24 | -3.58 | 55.58 | -22.45 | $-5.13$ | 58.42 |
| 22 | -2.20 | 16.74 | 12.46 | -2.97 | 15.55 | 73.18 |
| 23 | -12.83 | 3.05 | 62.14 | -15.53 | 2.30 | 63.38 |
| 24 | 5.44 | 9.82 | 63.81 | -41.35 | -6.26 | 96.17 |


| 25 | -23.65 | -4.21 | 67.43 | -27.44 | -5.70 | 69.11 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 26 | 5.44 | 6.19 | 62.76 | -50.03 | -17.01 | 94.06 |
| 27 | -25.51 | 0.38 | 73.58 | -28.11 | -1.20 | 73.43 |
| 28 | 1.96 | 0.03 | 58.41 | -62.24 | -39.11 | 88.38 |
| 29 | -27.10 | 5.22 | 82.59 | -31.61 | 2.52 | 81.97 |
| 30 | 27.81 | 30.43 | 55.75 | -22.78 | 5.18 | 82.63 |
| 31 | -52.44 | -8.09 | 91.59 | -65.19 | -18.61 | 91.27 |
| 32 | 25.02 | 31.67 | 58.29 | -38.58 | 74.54 | 84.97 |
| 33 | -167.25 | -200.00 | 57.77 | -169.68 | -200.00 | 58.02 |
| 34 | 40.50 | 54.28 | 65.43 | 2.47 | 26.17 | 82.43 |
| 35 | -199.12 | -200.00 | 16.28 | -199.12 | -200.00 | 16.28 |
| 36 | 41.22 | 70.84 | 75.10 | 3.10 | 30.72 | 90.13 |
| 37 | 66.82 | 97.22 | 50.25 | 46.35 | 71.09 | 73.17 |


sju!od ..pep!u!!.. to səqunn
Figure 21
Number of $L O W T R A N$

słu!od ..pa!!m!l.. to səquinN
70

..pel!u!l.. slu!̣d to puassod

..pal!u!l.. siu!od 10 łuəつ」əd
72


$73$

asuada!! $\ddagger$ luaว


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thesis was to evaluate performance over the full 2.0-5.5 micron region, "limiting" the data provided better insight into the errors of the codes. In addition, it is difficult to decide on an single set of intervals that should be excluded as invalid due to curve of growth effects.

The optimum approach, which would have avoided the uncertainty in band exclusion intervals would have been to perform a signal to noise analysis. Data with a signal to noise ratio of less than three could be regarded as having insufficient strength to justify analysis. since the AFGL data was provided as a processed signal this analysis could not be performed using this data set.

Plots for every fourth run are provided as Figures 30-65 in Appendix 8. Analysis of these plots and Table 7 provided the following observations:
4.2.1. Median errors are relatively small in the lower zenith angles. Errors tend to stay below an average of $10 \%$ at zenith angles less than 90 degrees (Runs 1-30), as example Figure 30. Errors are well above $10 \%$ at zenith angles equal to or larger than 90 degrees (Runs 31-37) (Figure 37). The results from the direct solar viewing cases indicate that the models for transmission and solar irradiance are essentially correct (Figures 66 and 68), except for the regions noted in
paragraphs 4.2.5 and 4.2.6. The plots of median error for background viewing indicate a slightly larger error band at low zenith angles, but without the extreme excursions at high zenith angles (Figures 67 and 69). However, this result may be due to the large number of points affected by the correction for the sensor noise floor and greybody optics. 4.2.2. Errors occur largely in the regions of the primary atmospheric absorbers.

| Wavelength Region | Primary Atmospheric |
| :---: | :---: |
| (microns) | Absorber |
| 2.0 | $\mathrm{H}_{2} \mathrm{O}$ |
| 3.75 | $\mathrm{H}_{2} \mathrm{O}$ |
| 4.3 | $\mathrm{CH}_{4}$ |
| 4.8 | $\mathrm{CO}_{2}$ |
| 5.5 | $\mathrm{CO}_{2}, \mathrm{O}_{3}$ |
| 4.8 |  |

4.2.3. The large percent differences in the major blocking regions, 2.7 micron $\mathrm{H}_{2} \mathrm{O}$ and 4.3 micron $\mathrm{CO}_{2}$, are numerical artifacts. The low transmission of these regions (Figures 3 \& 4) mean that relatively small changes in transmission (irradiance at the sensor) result in disproportionately large




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percent difference measurements.
4.2.4. The increased viewing of higher density regions of the atmosphere results in broadened absorption lines. Curve of growth effects are clearly visible in the results of the 2.75 , 3.3, and 4.3 micron regions for both MODTRAN and LOWTRAN. This causes the bands of large percent difference in these regions to "grow" in width as the zenith angle increases. 4.2.5. The error trend in the 2.0-2.4 micron region of the solar viewing observations appears to have a consistent shape. This shape arrears independent of zenith angle and is the similar for both MODTRAN and LOWTRAN. The error indicates that the models are predicting more solar irradiance than is received by the sensor (Figures 18 and 19). Since this error does not change with angle it is not likely to be a result of error in transmission, which will change with view angle. The two other major sources of error are errors in the solar model or in the instrument calibration. Since the solar model was compiled based on multiple observations taken by many observers over time it is not as likely to contain the $-20 \%$ error indicated in the results. This suggests that the calibration curve for the AFGL instrument is in error in this wavelength region.
4.2.6. The error in the 5.2-5.5 micron region is angle
dependent. This indicates a possible failing in the transmission modeling. The primary constituent of this region is $\mathrm{H}_{2} \mathrm{O}$. As noted in the discussion (Section 2), the modeling of the continuum transmission of $\mathrm{H}_{2} \mathrm{O}$ continues to be an area of research. Errors in the transmission could come from the water content provided by the standard model and from the transmission curve for water vapor continuum. since errors exist in the primary water band at 2.7 microns as well as in this band it is suspected that the error in the 5.2-5.5 region is a result of both sources of error.
4.2.7. Standard deviation measurements (Figures $28 \& 29$ ) are a poor indicator of quality. Normally a smaller standard deviation is an indication of better data since it means there is less variance in the data. In the case of the percent difference measurements this is a false indication since the reduction of variation is a result of greater "limiting" of the results. The runs with lowest standard deviation are also the runs with the greatest number of "limited" points. These runs are at the highest zenith angles, already noted as the runs with the largest errors.
4.2.8. The difference in results in LOWTRAN and MODTRAN results in the low zenith angle runs where errors are essentially zero is an indication that the $2.68 \%$ upward bias
of the LOWTRAN PC generated values (shown in Table 4) is true bias and not just an artifact. This would indicate an upward bias of the PC based LOWTRAN results compared to field data. These results suggest that if accuracy is critical then a mainframe computer should be used to perform the calculations. (As part of the installation of MODTRAN a limited comparison was made between MODTRAN and LOWTRAN 7 results when both codes were run on the same mainframe. This limited comparison showed the two codes generating results that agreed much more closely than the results shown in Table 4. This suggests that the bias shown in Table 4 is due largely to the computer, not the model.)
4.2.9. Close examination of Table 7 shows the following discrepancies from the general trends noted above 4.2.9.a. There is a difference between the MODTRAN and LOWTRAN results for Runs 7, 26, 28, and 30. The difference for Run 7 lacks an explanation. The difference for runs 26,28 , and 30 (Figures 45 and 63 for Run 28) may be due to the increase in observed irradiance. For runs 26 and 28 LOWTRAN sees a lower value due to its coarser structure. It thus has a greater number of matches enforced by the fit to the sensor noise floor. By run 30 , MODTRAN has sufficient
irradiance to achieve a match while LOWTRAN is now seeing just sufficient irradiance to be above the noise floor but not enough to achieve a match.
4.2.9.b. Increasing errors for both MODTRAN and LOWTRAN are observed in both Runs 18 and 22. This is due to an insufficient match to the data by the greybody and sensor noise corrections.
4.2.9.c. Runs 33 and 35 exhibit extreme error for both LOWTRAN and MODTRAN.

## 5. CONCLUSIONS AND RECOMMENDATIONS

The results of my thesis strongly parallel the results reported by Cundiff ${ }^{28}$ in his analysis. As with Cundiff, errors increased as zenith angle increased. MODTRAN results closely mirror his results for LOWTRAN $5 B$, an expected result since the band models share a similar formulation. LOWTRAN 7 shows a significant improvement over LOWTRAN 6, as expected. both models show improved performance in the $4.3 \mu \mathrm{~m}$ region, compared to the results obtained by Cundiff.

Several overall conclusions can be drawn from the analysis and results.
5.1. LOWTRAN and MODTRAN give similar results. However, the
bias in the PC generated LOWTRAN data (most clearly indicated in the solar viewing cases at low zenith angles) indicates that the mainframe versions of the codes should be used whenever practical to obtain the most accurate results. In the region reviewed in this thesis no preference is indicated for either model. This conclusion may be due to the smoothing effect of the interpolation of the field data to $5 \mathrm{~cm}^{-1}$ resolution, the similar smoothing effect obtained in the interpolation of LOWTRAN $20 \mathrm{~cm}^{-1}$ resolution data to $5 \mathrm{~cm}^{-1}$ data, and limiting output resolution of the MODTRAN model to the $5 \mathrm{~cm}^{-1}$ resolution of LOWTRAN.
5.2. The computer models have error results within $10 \%$ for most viewing cases at zenith angles less than 90 degrees (Figures 67 and 68). This is especially true where transmission is the major factor.
5.3. Results for radiance with multiple scattering require further investigation. The adjustments for sensor noise floor and greybody radiation precluded full analysis of this part of the computer models. The large number of points affected by these corrections and the relative magnitude of the correction compared to the predicted values leaves doubt whether any observed differences are derived from the corrections imposed for analysis or a result of differences between the models and
real world conditions.
5.4. The inability to model the fine structure of the $\mathrm{CH}_{4}$ lines in the 3.3 micron region indicates a fundamental limitation of any band model code. If specific structural features are important in either data analysis or sensor design then a line-by-line code such as Fascode is required. 5.5. Improvements are required in the continuum modeling of $\mathrm{H}_{2} \mathrm{O}$ in the 2.1 and 5.5 micron regions. These improvements should correct the errors in the transmission curves in these regions. Since the errors in these regions could also be a result of errors in the atmospheric input parameters to the codes it is recommended that research into this area utilize data from a set of measurements where the atmospheric viewing path is closely defined both in geometry (little or no refraction) and in atmospheric constituents.

Further conclusions require acquisition of additional data to verify the radiance with multiple scattering models. The sensor used to obtain this data must have sufficient sensitivity to confirm radiance modeling results in the region 2.7-4.5 microns. It was this region that was limited by the FISTA instrument noise floor. Calibration should include matching of the response in the $\mathrm{H}_{2} \mathrm{O}$ regions and in the $\mathrm{CO}_{2}$ region at 4.3 microns to allow discrimination between sensor
calibration and computer model errors.
It is suggested that a separate set of measurements (similar to Cutten's ${ }^{10,11}$ ) be obtained at 90 degree zenith viewing. These measurements will require accurate site measurements of atmospheric data. The purpose of this experiment would be to separate errors due to the spherical refractive geometry and the transmission modeling at the high zenith angles, indicating which part of the computer model needs revision.

This experiment should be performed under controlled conditions where the atmosphere and path are well defined. Such a path could be achieved by setting up a path between two locations and fixing mirrors at each location. By arranging the viewing path such that it was bounced back and forth between the buildings a series of long paths could be obtained (by controlling the number of reflected paths). Atmospheric data could be collected for the path between the buildings, removing the other source of non-model error.

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Appendix 1
Cundiff and Lisowski Report Extracts

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CUNDIFF EXTRACT
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The derived atmospheric transmissions are presented in this chapter. The original solar spectral radiance data, collected by AFGL, is compiled in Appendix A.

The following table summarizes the major absorption regions and the absorbing molecule:

| Wavelength <br> Region ( ) | Primary <br> Atmospheric <br> Absorber |
| :---: | :---: |
| 2.0 | $\mathrm{H}_{2} \mathrm{O}$ |
| 2.75 | $\mathrm{H}_{2} \mathrm{O}$ |
| 3.3 | $\mathrm{CH}_{4}$ |
| 4.3 | $\mathrm{CO}_{2}$ |
| 4.8 | $\mathrm{CO}_{2}, \mathrm{O}_{3}$ |
| 5.5 | $\mathrm{H}_{2} \mathrm{O}$ |

Figures 4 through 8 are the atmospheric transmission at the remaining zenith angles. The same general features described above are evident in these. The overall transmission decreases as the zenith angle increases. At the largest zenith angle there is no transmission above 0.8 and most bands usually considered atmospheric windows show average transmissions of 0.5 or less.

### 2.2 Comparison of LOWTRAN6 to Data

The models were compared to the data by calculating the percent difference between the data and model. The percent difference is defined as:

$$
\Delta_{\mathscr{*}}(\lambda)=\frac{\tau_{c}(\lambda)-\tau_{m}(\lambda)}{\tau_{m}(\lambda)}
$$

where $\tau_{c}(\lambda)$ is the calculated transmission, and $\tau_{m}(\lambda)$ is the measured transmission. A positive percent difference represents an overestimate of
the atmospheric transmission by the model and a negative value an underestimate. If $\tau_{m}(\lambda)$ is less than $5 \%, \Delta_{q}(\lambda)$ is undefined as it is felt that there is insufficient intensity to make an accurate measurement of the transmission.

LOWTRAN6 accurately models the atmospheric transmission at the smaller zenith angles. Figure 9 is the percent difference between LOWTRAN6 and the data. At $61.9^{\circ}$ and $65.5^{\circ}$ zenith, the percent difference is close to zero at most wavelengths. In the $\mathrm{H}_{2} \mathrm{O}$ and $\mathrm{CO}_{2}$ absorption bands there is a significant deviation, but the transmission is very low in these regions, causing a small (5\%) difference in transmission to be a large percent difference. As the zenith angle increases, so does the uncertainty.

There are a few noticeable features in the percent difference at the larger zenith angles. A large uncertainty, with a distinct structure, exists in the 2.1-2.4 micron region. This absorption is due to $\mathrm{CH}_{4}$. This absorption band is entirely missing from the LOWTRAN6 data base (note that it is not apparent at the smaller zenith angles). We made a modification to the LOWTRAN6 data base to include this band; it is discussed in Section 5. On the edge of the 2.8 micron $\mathrm{H}_{2} \mathrm{O}$ and 4.3 micron $\mathrm{CO}_{2}$ absorption bands, there is a large difference. This is primarily due to low transmission as mentioned previously. A large difference also exists at 4.75 microns. Two molecules absorb in this region: $\mathrm{O}_{3}$ - 4.75-4.8 microns and $\mathrm{N}_{2} \mathrm{O}$ - 4.8-4.9 microns. If the $\mathrm{O}_{3}$ concentration is adjusted to obtain better agreement, the agreement in the 3.6 micron $\mathrm{O}_{3}$ absorption band is lost, $\mathrm{N}_{2} \mathrm{O}$ is part of the uniformly mixed gases, so its concentration cannot be adjusted individually. This example indicates a basic modeling problem in LOWTRAN6.

### 2.3 Comparison of LOWTRAN5B Model to Data

LOWTRAN5B is a mid resolution atmospheric transmission model. It uses a band model parameter formulation to calculate the atmospheric transmission. This approach more accurately takes into account the changes in the transmission due to different line shapes at different temperatures







Figure 9. Percent Difference Between LOWTRAN6 Calculations and AFGL Data.
and pressures. Consequently, it is a more accurate model. It also has a data with a resolution of $5 \mathrm{~cm}^{-1}$ as compared to the $20 \mathrm{~cm}^{-1}$ resolution of LOWTRAN6. Due to this increased resolution, the calculations of LOWTRAN5B more accurately represent the structure of the atmospheric transmission, much of this structure is not present in the LOWTRAN6 calculation. The transmission data display much finer structure than the LOWTRAN5B calculation (on the order of $0.01 \mathrm{~cm}^{-1}$ ) and $\operatorname{FASCODE}$ must be used if modeling of this fine structure is necessary. Note that there is more detail in the percent difference for LOWTRAN5B and FASCODE than for LOWTRAN6; this is because of the higher resolution of the claculations.

Figure 10 indicates the percent difference between LOWTRAN5B and the data. At the small zenith angles LOWTRAN5B does a fairly good job of modeling the atmosphere; essentially equal to LOWTRAN6. The percent difference at the $61.7^{\circ}$ zenith angle is approximately 0 at most of the wavelengths, again, excepting the areas of the $\mathrm{CO}_{2}$ and the $\mathrm{H}_{2} \mathrm{O}$ absorption bands where the atmospheric transmission drops quite low. It is quite good at the $65.5^{\circ}$ zenith angle with small spikes being observed in the region of the $\mathrm{CH}_{4}$ absorption at 3.3 microns and the beginnings of an inaccuracy in modeling the ozone at 4.75-4.8 microns. This apparent modeling deficiency is of the same nature as that mentioned for LOWTRAN6. Attempting to correct the ozone content to make it more accurately model the 4.75 micron region decreases the ability to accurately model the ozone absorption at 3.6 microns. At a zenith angle of $87.3^{\circ}$, the methane absorption at 3.3 microns is more evident as being an area of uncertainty. There is significant structure to the $\mathrm{CH}_{4}$ absorption in this band. LOWTRAN5B does a significantly better job of modeling this structure than LOWTRAN6 which is inherent in the designed resolution of the respective models. At 2.3 microns, the sharp positive spike is due to methane absorption which is completely unmodeled in the LOWTRAN5B data base. This was mentioned in LOWTRAN6 as being a problem and the problem increases with increasing zenith. At a $90.3^{\circ}$ zenith and at 4.8 microns the inaccuracy of modeling the $\mathrm{CO}_{2}$ absorption band is beginning to become evident as a positive percent difference.


Figure 10. Percent Difference Between LOWTRAN5B Calculations and AFGL Data.

The investigation was undertaken to determine the potential effects of uncertainties in actual $C 02$ concentration (relatively minor), the difference between the band model codes and the line-by-line codes (significant), and the effects of convolving the different code spectral transmissivity predictions with the spectral radiant intensity of the plume. The investigation has been performed for a number of scenarios and the complete results will be presented in a report which is currently being prepared. This effort has been exclusively devoted to the understanding of the atmospheric transmission effects in the 4.3-4.6 micron region.

Near the end of the computational phase of the effort we realized that the optical paths for each of the target altitudes were very similar to those encountered by AFGL during spectral radiant intensity measurements of the setting sun from an altitude of 29,000-39,000 ft. Therefore, we compared the code predictions with the AFGL measurements. The nomenclature and conditions are indicated in Table 1.

Table 1

| AFGL Run | Aircraft <br> Altitude | Zenith <br> Angle |
| :---: | :---: | :---: |
| 1 |  |  |
| 5 | $39,000 \mathrm{ft}$ | 61.9 |
| 27 | $29,000 \mathrm{ft}$ | 65.5 |
|  | $29,000 \mathrm{ft}$ | 87.3 |

Figure 2 indicates the comparison between the actual data and the predictions employing FASCOD2, LOWTRAN5B, and LOWTRAN6 for Run 1 (similar to a target at 30 km altitude in our computational scenario). Clearly, the LOWTRAN6 computations do not describe the spectral characteristics of the atmospheric transmission as well as either FASCOD2 or LOWTRAN5B. In fact, LOWTRAN5B gives slightly better agreement than FASCOD2.

Figures 3 and 4 indicate the results of the comparison between the predictions and data for Runs 5 and 27 . For both cases LOWTRAN6 does not provide an adequate spectral description. In Run 5, both FASCOD2 and LOWTRAN5B provide very similar results, both quite good. For Run 27, FASCOD2 provides much better agreement with data.

A further test was conducted by convolving the actual transmission and the computed transmissions with a plume spectrum and a sample sensor spectral filter. The results are provided in Figures 5, 6, and 7 for Runs 1,5 , and 27 , respectively. These results echo those stated in the previous paragraphs namely, LOWTRAN6 is not to be used, LOWTRAN5B does better at higher target altitudes, FASCOD2 does better at low target altitudes.


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Figure 4. Comparison of Atmospheric Transmission Predictions with AFGL Data Run 27 Zenith Angle of 87.3 Degrees.
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Appendix 2
AFGL File Format and VAX Backup Notes

Tape is $1 / 2$ inch, 800 bpi, 9 track and consista of files separated by EOF marks, with two EOF marks at the end of the data.

Each file consists of multiple recorda, the mumber depending on the type and amount of data in the file. Data will be of two typea: apectral and spatial. Their respective formats wll be discussed separately.

## Spectral

The first physical record in a spectral data file will be a 180 byte ASCII header record. The ASCII header is broken down aa follows:

1 to 11 bytes, 11 bytes - Amitiplicative scale factor for the binary integer data array in Ell. 5 format

12 to 19 bytes, 8 bytes - The time or frequency spacing of the data array in 78.5 format

20 to 27 bytes, 8 bytes - For frequency data, the starting frequency of the data array in F8. 2 format

28 to 32 bytes, 5 bytes - The mumber of data valuea in the data array in 15 format

33 to 47 bytes, 15 bytes - The AFGL mission designator in the ASCII format: "MISSION", 3A2

48 to 57 bytes,
10 bytes - The AFGL archival tape designator in the ASCII format:


11 bytes - The AFGL archival tape record number or Ostomer Service Number (CSN) in the ASCII format: "RECORD ", or" "CSN_" I3. If this file ia constructē from more than one archival record the record number will be zero and the source records description will be placed in the last 108 bytes.
$X 69$ to 72 bytes,
4 bytes - ASCII blanks
73 to $\frac{180}{113}$ bytes, 108 bytes (Tmincate. yo The AFGL archival record descriptor in 114-180 Llanks
The remaining records in the file are binary records 2880 bytea long. They consist of 144016 bit words in twos-compliment format. Each word represents one data point in the data array. If the record contains leas than 1440 data points, it is zero filled. The number of data records in the file can be determined by dividing the mumber of data values as determined from bytes 28-32 in the header record, by 1440 and rounding
to the next larger integer. The value of esch data point can be determined by multiplying the scale factor from header bytes l-ll, by the aigned integer value in the dsta record. For frequency data, the frequency of the first data point and the frequency increment per dats point are contalned in bytes $12-27$ of the header. For time domain data, the interferometer path increment is contained in bytes 12-19 of the hesder.

## Norelco SWIR Spatial

The first physical record is also a 180 byte ASCII header record. The header As broken down as follows:


Description
A multiplicative scale factor for the data array
The verticsl angular spacing of the data points within a scen in milliradians

| $17-21$ | F5.2 |  |
| :--- | :--- | :--- |
| $22-25$ | 14 | The horizontal angular spacing <br> between scens in milliradians |
| $26-29$ | 14 | data points/scan (vertical) |

30-33 I4
$\begin{array}{ll}34-41 & - \\ 42-47 & 3 A 2\end{array}$
48-53 - $\quad$ TAPE ' 6 ASCII charscters
54-57 2A2 The AFGL Archival Tspe ID (4 ASCII characters)

66-68 I3 Record on AFGL archival tape
69-72 - 4 ASCII Blanks (spaces)
73-144 36A2
73-73
79-90
81-92
93-96
97-98

58-65 - $\quad$ RECORD ' 8 ASCII characters.

- records/file
$\underbrace{\text { n }}$ FILE 8 ASCII characters
The AFGL file name in ASCII

Archival header info
'MMM/RR' mission/run
2 ASCII Blanks (spaces)
' $\mathrm{HH}: \mathrm{MM}: S S: C C$ ' Zulu Tlme and opace
'fFF'filter designator and space
'dB' $d B$ setting in ASCII








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| :---: | :---: | :---: |
|  |  |  |

$$
\therefore \because=\therefore=\because 2 \mathrm{O}=\therefore 1 \mathrm{~N} \quad 22: 51: 110 \text { (39) }
$$



$$
\therefore \because=4=40-101 \mathrm{~N} 23: 06: 320 \text { (35) }
$$





| ice |  |
| :---: | :---: |
|  |  |






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 EdF -oun fo: file $\quad 2 \mathrm{O}$

23：49：14：0（31）










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 Ei＝foun fer fals $\ddagger=7$



23: 49:14.0 (31)











EIT foridforfise $\ddagger$ Z


 Enf found for fite \# Ie




Et fand far file \＃ze

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& \text { :こ feund fer fi:e \# } \\
& \text { シeronc egF Faria }
\end{aligned}
$$



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## Appendix 3

Run 01 Numeric File


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| ここ14 | つこうこ | タこ？ | ちここら | ちこうこ | －292 | こごこ | －－ |
| ＊54 | ミミここ | 二4 | 542？ | 江こ | $\leq こ こ$ | くここ | ミここ |
| ここ？ | 5535 | $\because 257$ | $5 \leq 15$ | ぐ「ご | くここミ | ここち | 4.4 |
| コこ：？ | $こ こ!$ | ごいこ | くこここ | の－ | ごこ | －－－ | ミここ |
| $\therefore$ ¢ 1 | 5015 | Sore | $s=-1$ | －－${ }^{\text {－}}$ | $\therefore$ ミヲ | $21^{-1}$ |  |
| $\because 5: \vdots$ | 55.2 | 9．4こう | 554 | $\pm 5=$ | 654： | 2こち「 | こ？ |
| 」らここ | $\leq 5$ | 62.7 | 57－5 | $\bigcirc \rightarrow$ | 6721 | $\leq 7 \div 0$ | ＝7？ |
| ¢5ここ | 勺ご | ○きっこ | $\leq 7 \div 0$ | 5ここ 4 | 57？ | 5； | 吅ご |
| $\leq: 15$ | ！ | $\leq ミ け も$ | $6 \because 5$ | くこここ | －T4 | $\leq 75$ | $\bigcirc{ }^{\text {a }}$ |
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| ¢ \％＝ |  | にここ | $\leq こ こ$ | ？ここう | 71． | こここ |  |
|  | くアッシ | ア¢15 | $\pm 0$ こ | らくつ三 | ミヲプ | $=5=1$ | －117 |
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| こフこ | こご河 | ？こここ | ？1号 | ニTシ | ここご | こっこ | －こ！－ |
| ？ここ | ここのに | $\leq こ 67$ | くこう1 | วร $\leq \leq$ | でちここ | $\rightarrow$－－－ |  |
| $\pm 377$ | ちここ？ | 7ごう | いこうら | 5511 | くここう | $こ ゙ く$ | 1？ 3 |
| ？ 15 | 7695 | フミ07 | てこきこ | ファn6 | T－00 | こここう | 112 |
| 7315 | 5457 | くこ1う | 5 ¢จ§ | 701こ | 5S17 | $5 \pm 6 i$ | 65： |
| 277 | ？ 4 ここ | 7654 | 7357 | $6 \leq 21$ | 5540 | つこと？ | Tこん |
| フミこ7 | 7509 | ¢ 207 | Sヒこ： | 7こヒす | ？579 | ここここ | 6714 |
| 7257 | 6757 | フ0゙こ | TちJt | 7712 | 6965 | 5ここつ | 7147 |
| 7110 | ？ 566 | 75？ | 7532 | 5929 | 79 こ0 | 7560 | 7000 |
| 7250 | 8534 | 7743 | 733 \％ | 7659 | $70 こ 9$ | 7341 | 725 |
| こ256 | $\rightarrow$ 987 | 77こ9 | 7 ¢き6 | 3010 | 7377 | 7500 | $\rightarrow$ ここ |
| 2167 | き〕．2 | ミロダ | セここち | 3034 | ここ 15 | 吅 | こここう |
| こ356 | ジミ1 | E－5． | 7529 | 7922 | 7？ 0 | アタミこ | －150 |
| 7971 | 7959 | $738=$ | 8122 | 5213 | ¢1 53 | 8505 | 7c5 |
| 5005 | 799こ | 788 | 7927 | E127 | 8225 | E140 | E0： 1 |
| E067 | 3150 | 321 こ | 3177 | 314 三 | $8: 77$ | マここ5 | こここム |
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| と4ご | 3ここ4 | \％ 215 | 3こう5 | ここ47 | 3295 | ここっ1 | －215 |
| 3238 | E290 | 3363 | 347c | 3443 | 8333 | $2-1 t$ | 2518 |
| 8645 | 8639 | 8739 | 3853 | 8693 | 8445 | 3263 | 8175 |
| 3756 | 8564 | 8725 | 8691 | 8600 | 8597 | $265 ?$ | E640 |
| 8722 | 3827 | 8815 | 8789 | 8788 | 8763 | 3753 | を 791 |
| 2815 | 5802 | 8 こ01 | 2772 | －750 | 9777 | 2741 | 8663 |
| E 904 | 3501 | 2701 | 2752 | 8890 | 8915 | 3909 | E2tS |
| 9014 | 3034 | 9166 | 9206 | 0056 | 9991 | 3959 | 8944 |
| 9213 | 9130 | 9109 | 7016 | 8983 | 9016 | 8：86 | 9030 |
| 9034 | 9091 | 9091 | 9125 | 9204 | 9177 | 9131 | 9220 |
| 9110 | 9122 | 9150 | 9108 | 9005 | 8985 | 9045 | 9082 |
| 5625 | ¢ 850 | 9947 | 9121 | 2229 | 9349 | 0293 | 9170 |
| ミ64 | 2344 | －964 | 90.0 | 3005 | 9374 | 9018 | ¢ 711 |
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| ここここ | 2544 | 327こ | 3ご¢ | 5515 | 0443 | 3562 | こここの |
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| 1268 | 2052 | 2163 | 1210 | 404 | 233 | 216 | 65 |
| 530 | 473 | 485 | 435 | 292 | 434 | 597 | 792 |
| 5207 | 5 573 | 玉こ1t | 450E | $\because 755$ | 3こころ | 2こ1こ | 1こアこ |


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| 1ここós | 13974 | 109ア9 | 11122 | 11くら7 | 11117 | 11174 | 7 c |
| 1177\％ | $11 \pm 34$ | 1107 | 11350 | 11650 | 11712 | 11427 | 0. |
| 11567 | 11634 | 11763 | 11729 | 116？ | 11742 | 11794 | $6=$ |
| 12003 | 11ここ6 | 11752 | 11711 | 11 c50 | 11459 | 112 ？ | 11411 |
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| 1172 | 1172 | 1135 J | $115 \% 4$ | 11 E1三 | 11204 | 119 こム | 1196 ？ |
| 1167 | 115ご | 116 ？ | 117 ？ 0 | 11936 | 12 J 1 | 11 E太コ | 11735 |
| 1173 O | 11737 | 11945 | 12054 | 12074 | 12251 | 12ご玄 | 1 |
| 12340 | 121是 | 11710 | 117ヨ | 12169 | 12245 | 1 |  |
| 1こ277 | 12ミコを | 12974 | 12Eここ | 12422 | 12091 | 12 O72 |  |
| 12ごき | 11ヶ15 | 11 ¢ ${ }^{\text {－}}$ | 12441 | 1297t | 12508 | 11954 | 7 |
| 1こ144 | 11951 | $117 ミ 4$ | 11543 | 11917 | 12375 | 11 ¢2？ |  |
| 10こ1玉 | $11=47$ | 12261 | 127ミ3 | 12427 | 12210 | 1ここるs |  |
| 12601 | 12424 | 12547 | 12638 | 12398 | 12412 | 12307 | 337 |
| 12344 | 12424 | 12341 | 12239 | 12342 | 12869 | 13380 | 13060 |
| 12046 | 12125 | 12242 | 12136 | 12162 | 12157 | 12430 |  |
| 12013 | 12745 | 12551 | 12772 | 12745 | 12606 | 12591 | 12362 |
| 12764 | 12752 | 12 239 | 12712 | 13172 | 13249 | 12695 | 12665 |
| 12514 | 12734 | $1 \geq 154$ | $\uparrow 3057$ | 12938 | 12953 | 12795 | 12749 |
| 12976 | 12842 | $12 \varepsilon 74$ | 13061 | 12409 | 11350 | 12157 | 1 |
| 12792 | 12033 | 12285 | 12800 | 13186 | 12953 | 12630 | 12788 |
| 12323 | 13039 | 12056 | 12366 | 12138 | 12635 | 13109 | 13 |
| 1こ72\％ | 13147 | 12969 | $12 \leq 13$ | 12546 | 12523 | 12338 |  |
| 125？ | 1224： | 1202 |  | 13290 | 13072 | 12750 |  |
| 1こ7シ0 | $1 ? 6 ?$ | 12015 | $127 \leq 3$ | 12711 | 12650 | 124 |  |
| 12030 |  | 12379 | 12557 | 1250c | 1269 ？ | 1こ11过 |  |
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| 1－11 | 1？「こと | 1：ここ＝ | 1アテこ5 | 14こ1～ | 13 | 1 |  |
| － |  | 1 こ： | 1－5 |  |  |  |  |
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| 14271 | 14725 | 14370 | 13623 | 12261 | 1311 안 | 15309 |  |
| 13243 | 12ミこう | 13911 | 13777 | $1 ? 640$ | 125：1 | 13512 |  |
| $1: 5.5$ | 1こ175 | 12965 | $1305 ?$ | $123 ?$ | 1271＝ | $1 ? 7$ |  |


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| 0344 | 10377 |  |  |  |  |  |  |
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| 2632 | 12147 | 11516 | 120＜1 | 92く3 | －5シ2 | 9くミこ |  |
|  | 12041 | $1: 557$ | 1221i | 127－5 | 13114 |  |  |
|  | 1270 | 12655 |  |  | 1こう？ |  |  |
| 64 | 1こロう | 13152 | 1325．5 | 13 | 13634 |  |  |
| 1745 | 12027 | 12954 | 12720 | 124？7 | 13367 | 1ごイ12 | 12 E 17 |
|  | 12012 | 13004 |  | 13247 | 12014 | 1こ1＞1 |  |
| ここ25 | 11503 | $110 \equiv 4$ | 13947 | 13914 | 10647 | 11： |  |
| ここちき | 12ヶ5 | 121 ミ1 | 115 こ？ | 115 | 13455 | 137E |  |
|  | 12143 | 13108 | 13595 | 12770 | 11952 |  |  |
| 2733 | 13115 | 125 こ？ | 1411 S | 1455 | 13540 | 13－22 |  |
|  | 13757 | 14386 | 14421 | 13 こ60 | 14366 | 13359 |  |
| 4325 | 1435 1 | 14846 | 15458 | 14347 | 12703 | $1 \geq 512$ |  |
| 50 | 14181 | 13754 | 13775 | 12656 | 13509 | 13753 |  |
|  | 0 |  | － | 12422 | 14569 | $14 \pm 00$ |  |

## Appendix 4

## Run 01 Data File



| 1769 | 14421 | $う$ | ＝154． |  |
| :---: | :---: | :---: | :---: | :---: |
| 1741 | 14395 | 0.0137105 | 5150．？ 2 | 1 |
| 1742 | 15757 | 0．013115 | 515E．t $=$ | 3．00こ1きシこムつ |
| 1743 | 14524 | 0.2141457 | 5152． 5 ¢ | J． 09 |
| 174． | 155ご | こ．こ145うす7 | －1－2．51 |  |
| 17ヶ5 | 1251？ | －こ1こミ・枵 | 5164．44 |  |
| 174 C | 12703 | C． 1 12114 | 5160．こ7 | $2 \mathrm{C}=1$ |
| 1747 | 1424？ |  | 515¢．こ？ | O．rñ1 |
| 1745 | 1540\％ |  | 51アごくる | こ．こ0う1ロごイミ |
| 17：9 | 1 15 こち | 3． 2141 こここ | ミ172．15 | 2．こ0017マこく？ |
| 175こ | 1－3c | こ．こイアアここる | 「174．心爯 |  |
| 1751 | 14こここ | C． 1 1こ 5 ¢ | 5176．：1 | こ．こここ12ア1く2 |
| 1アミこ | 14157 | こ．21玉．519 | 5177.94 | 0.5 |
| 17 17 | 1ミア5き | D． 313115 E | 5170．97 | － |
| 1754 | $1 \geq 500$ | －． 1 －35こ1 | 519： 5 | －． $0001=2$ |
| 175 | 13655 | こ．－1302ミこ | 51？${ }^{\text {c．7 }}$ | 「．0う「イニ2 |
| 175 | 1ミア75 | こ．こ1？1295 | 5195． 5 | － |
| $17 ミ 7$ | 13アラ4 | C．013112 | 5187．5？ | こ．こうこイ |
| 17ジ | $1+1$ ¢1 | コ．ごミミごつ | 51 － 5 ． 1 | －．Cうこ1 |
| 175 | 14530 | 0.0139522 | 5101.44 | こ． $2=3102025$ |
| 1750 | 14376 | －C13T10J | 519 こ． 37 | 0．00こ1？？ |
| 1751 | 14500 | $0.014120 う$ | 5105.30 | 0．0こ01こ？ |
| 175こ | 14508 | 0.0135542 | 517 T .22 | 0． $0.30172+10$ |
| 1763 | 12402 | 0.0115274 | 5199.15 | 2．00017こうこ9 |
| 1754 | 0 | 0.0000000 | 52.21 .00 | $0.0001 \div 22 \leq 5$ |
| 1765 | 0 | 0.0000000 | 5203.01 | 0.000192190 |
| 1750 | 0 | C．0000000 | 5204.94 | 0.050192125 |
| 175 | 0 | 0.0000000 | 5206.87 | 0.000132054 |

## Appendix 5

$$
\text { Run } 01 \text { Calibrated Data File }
$$

1720．2ヶ
$1 \geq 31.1 \div$
1シうこ． 12
$1=55.0=$
1ミ52．07
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1こ1に．7
$1: 14.50$
$1: 16.65$

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1こ24．シき
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1ショシ．1く
1こここ．こん
1シここ・テ〉
1きこち．9
1まこ？．とこ
1ミミと．76
1こん1．67
1くらう． 61
$1 \hat{3} 45.54$
$1=47.47$
1849.40
1851.33

135 ． 26
1955．17
1ま57． 11
$1 \equiv 50.04$
1260.97
1862.90

1ことム．とう
1こちも．7も
1ミち8．6E
1870.61
1872.54
1874.47
1276.40

1878．33
1380.26
1832.18
1834.11
1226.04

1327．97
1859．90
1と51．ミ3
1このシ．7ム
1ショシ．もを
1こ07．01

1．4：
1ン」ミーム
1535．35
1907.25

1909．18
1911.11

1513．04













「．Sミ451こ5619テ5s6ミーつ0コ7 7．3930こ462200110ミ－0057
 6．5755太22この9ヲ41 ミミーつ007 ミ．9099きここう700227ミー00べ 5．78051127199615E－0007 $6.15716245400480 E-0007$ 6.3465 ç539699429ミ－0007勺． 3400155399 ล971ミ－0007 6．745シミ525ミ59620ミ－0007 0．441574312001E6E－0007 6．52952719052550E－0007 6．52119312499349E－0007 5．78จ99361499420ミ－0007 7．コ1E1632035テ507E－2007 7．13679717590613E－0007 E．33．3155405997？6ミ－0007 6．56222337099173E－0007 7.06027912799 こコ9ミー0007 $7.74184067999818 \mathrm{E}-0007$ 7．？ $2221101793967 \equiv-0007$ 7．93512590097927E－0007 7．©6？ $51255090334 E-0007$ 7．？9322175898919E－0007 8．02635500399411E－0007 3．06622517399505E－0007 8．1320425119ミ934ミ－0007 7．70778Е20599982E－0007 7．231こ5242359199ミ－00C7 2．184



 3．25930 ミこア7 $8.23141974399368 \mathrm{E}-0007$ 8． 30326494799540 E－0007 8．18602019499876E－0007 3.15294937098546 こ－0007

よ．ジアミ
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$5.4 \leq 00$
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5.3903
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5.3650
5.3624

5．3559
5.3514
5.3458
5.3403

5． 3348
5.3594
5.3239

5． 3154
5.3130
5.3075
5.3021
5.2967
5.2913
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5.2805

5．2751
「ころうき

5．こ4
5.2431
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 2．35605820967941E－0004 2．43546845071707E－0004 2．4927774444749三． $37245213304553 \mathrm{E}-0004$ 2.294400562827 ع1E－0004 2．47301072926550E－0004 2．72163069264905E－0004 2． 81125314642416 ミ－0004 2．79978286957583ミ－0004 $2.73171414607176 E-0004$ $2.81596069454881 \mathrm{E}-0004$ 2．86887226692123E－0504 2.86700084925260 E－0004 2.9034343892275 EE－0004 2．e4249266932515E－0004 2．80419061039373ミ－0034 2．930678281507505－cさ04 2．96903871357927ミー00う4

 3．00215204025315E－0204 2．97633263473429E－0004 3．02364172886094E－0004 2．9922394433955うミ－000＇ 2．980150050961 ミt

シ154．35 ミ156．7ミ $51 \equiv 3.65$ 51s0． 5 5102．51 5154．～に， ミ16．．こ． ミ168．ここ 5170．23 シ1？こ． 15 ミ17．． 05 こ17e．01 5177．こム E179．87 ミ1こ1．53 $51 \div 3.73$ こ105．0 シ1ミ7．シき こ129．51 5191.44 5192． 27 5195.35 5177．22 519 シ． 15

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## Appendix 6

Run 01 Interpolated Data File ( $\mathrm{cm}^{-1}$ units)

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| 1－1E．こコココロのこのことこの | $\because 1$ |
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| こ゚こここい？ |  |
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| 1ミマこ．ひこと？ここここのnこ： | ア．1ここ |
| 1ミミミ・コここうごさここさ？ | T．Eers |
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| ここここここっのこのご | 2．こつテここマイ |
| 1こ5う．こここうここここごご |  |
| 1 |  |
|  | こ．5くらここき |
| コロここのこのここ | 7．2こここここここーグ |
| －ここつつこここうごこここ | 二． |
| －こここことつここことに？ | ？－Eミ2 |
| ここここことここのま！ | ？ミ号号 |
| 1こここ．うここうくらこここにこの |  |
| 15：こ．らこつつにつこつここここ | 7．$=-1 \leq 5$－$=-7$ |
|  | シ．ミことここヒミミーラフ |
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|  | ミ．ここ゚ヒシこここー・， |
| 131こ．Cここうくここのここの） | こ．？¢¢っここここー？7 |
| 1715．0う0こう00うcron | －．3ムこつムイジーご |
|  | 7．E£911tここ－こ7 |
| 1925．090003000c00 | 2．1000464E－27 |
| 1530.000000000000 | ع．7257ミ365－57 |
| 193う．0000000コ0000 | 7．9999239E－37 |
| 1942．000000000000 | E．9世74813E－27 |
| 954 ．Cocococooros |  |
| 1 3 5C．00030300000 | と．£¢うことテ1ミーラ7 |
| 1055．000000020000 | ع． $85597645-27$ |
| 1950．こJこコ0コこ00000 | 8．9569くごちーご |
| 1955．000000000030 | 9．08406765－0？ |
| 197コ． 3 コ0コロコココこコロ？ |  |
| 19「シ．030002000002 |  |
| 1920.000000000000 | 9．10LE 2 27 |
| 1985.000000000000 | 9．37973145－07 |
| 1990.000000000000 | 9.1300069 －07 |
| 1995.000000000000 | 8．9944803E－97 |
| 2000．000500000002 | 9．2425373こ－07 |
| 2005.000300000003 | 9.4066612 E－07 |
| 2010．000300000000 | 9．4う¢1953 |
| 2015.000000000000 | 9．6141727E－07 |
| 2020.000003500000 | $9.3310496 \leq-07$ |
| 2025．000000000000 | 9．4712982 5 －07 |
| 2030.000000000000 | 9．5こここと215－3？ |
| 20こ5．0こ0000000000 | 9．6291501E－07 |
| 2043．0う0JcJコロ0coo | 9．41ミ5395こ－07 |
| 2045． 00000000000 | 9．369？755E－37 |
|  | c．ここC7095 |
| ここう5．こうこのコこうこことこの |  |
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| ミ．さここのこここここの | －とこここご，－「 |
|  | シーシミミミ15゙ー－ |
| ご75．030000020002 | £．ミタこちミイコこーブ |
| 2080.000000000000 | 6．3176437E－37 |
| 2055．000000000000 | 8．4590229E－07 |
| 2090．000000000000 | ع．37529？ |
| 2075.000000000000 | 8.15 こここ71E－07 |


|  | 5．こうつつへらすこのこここ |
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|  | こイフリ．こうこうこつこうことくこ |
|  | こイフ三．こここうくつのこうcc！ |
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|  | 155．こうつこちこうつちロこ2 |
|  | ミ19こ．とここつここここcさここ |
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## Appendix 7

$$
\text { Run } 01 \text { Interpolated Data File (micron units) }
$$

| 5.5556 | $2.73614746168160 \mathrm{E}-0004$ |
| :--- | :--- |
| 5.5402 | $3.44623184438841 \mathrm{E}-0004$ |
| 5.5249 | $2.64916325576792 \mathrm{E}-0004$ |
| 5.5096 | $2.45294805028884 \mathrm{E}-0004$ |
| 5.4945 | $2.92718332189246 \mathrm{E}-0004$ |
| 5.4795 | $2.37297160558203 \mathrm{E}-0004$ |
| 5.4645 | $2.37804637632566 \mathrm{E}-0004$ |
| 5.4496 | $2.53837491130948 \mathrm{E}-0004$ |
| 5.4346 | $2.48221218797973 \mathrm{E}-0004$ |
| 5.4201 | $2.0618633852961 \mathrm{E}-0004$ |
| 5.4054 | $2.13310328229577 \mathrm{E}-0004$ |
| 5.3908 | $2.17641420239945 \mathrm{E}-0004$ |
| 5.3763 | $2.26670505224735 \mathrm{E}-0004$ |
| 5.3619 | $2.44081523913753 \mathrm{E}-0004$ |
| 5.3476 | $2.29580397804297 \mathrm{E}-0004$ |
| 5.3333 | $2.75424762871346 \mathrm{E}-0004$ |
| 5.3191 | $2.77343834369503 \mathrm{E}-0004$ |
| 5.3050 | $2.86103607588295 \mathrm{E}-0004$ |
| 5.2910 | $2.83379016730922 \mathrm{E}-0004$ |
| 5.2770 | $2.97484850249496 \mathrm{E}-0004$ |
| 5.2632 | $3.03151975418636 \mathrm{E}-0004$ |
| 5.2493 | $3.00043975834718 \mathrm{E}-0004$ |
| 5.2356 | $3.00861904585226 \mathrm{E}-0004$ |
| 5.2219 | $3.05367736157969 \mathrm{E}-0004$ |
| 5.2083 | $2.90067046442299 \mathrm{E}-0004$ |
| 5.1948 | $3.02704114900187 \mathrm{E}-0004$ |
| 5.1813 | $3.26411967609186 \mathrm{E}-0004$ |
| 5.1680 | $2.98761158019190 \mathrm{E}-0004$ |
| 5.1546 | $3.36630280605821 \mathrm{E}-0004$ |
| 5.1414 | $3.19811225904854 \mathrm{E}-0004$ |
| 5.1282 | $3.37301739544493 \mathrm{E}-0004$ |
| 5.1151 | $3.37878817687987 \mathrm{E}-0004$ |
| 5.1020 | $3.43211582344960 \mathrm{E}-0004$ |
| 5.0891 | $3.49898442390195 \mathrm{E}-0004$ |
| 5.0761 | $3.4452770422219 \mathrm{E}-0004$ |
| 5.0633 | $3.64809621550943 \mathrm{E}-0004$ |
| 5.0505 | $3.59564714996985 \mathrm{E}-0004$ |
| 5.0378 | $3.6865158332982 \mathrm{E}-0004$ |
| 5.0251 | $3.60648967337784 \mathrm{E}-0004$ |
| 5.012 |  |


| 4.7619 | $3.63832675388309 \mathrm{E}-0004$ |
| :--- | :--- |
| 4.7506 | $3.71590832725754 \mathrm{E}-0004$ |
| 4.7393 | $3.56688142099326 \mathrm{E}-0004$ |
| 4.7281 | $4.14258633242959 \mathrm{E}-0004$ |
| 4.7170 | $3.5073009727414 \mathrm{E}-0004$ |
| 4.7059 | $3.40153165542004 \mathrm{E}-0004$ |
| 4.6948 | $3.73480422829697 \mathrm{E}-0004$ |
| 4.6838 | $4.46410314082879 \mathrm{E}-0004$ |
| 4.6729 | $4.77697684249989 \mathrm{E}-0004$ |
| 4.6620 | $4.91548832754596 \mathrm{E}-0004$ |
| 4.6512 | $4.77864923284610 \mathrm{E}-0004$ |
| 4.6404 | $4.76513082822816 \mathrm{E}-0004$ |
| 4.6296 | $4.76484878179306 \mathrm{E}-0004$ |
| 4.6189 | $4.73659883116095 \mathrm{E}-0004$ |
| 4.6083 | $4.74536077258225 \mathrm{E}-0004$ |
| 4.5977 | $4.75119391791345 \mathrm{E}-0004$ |
| 4.5872 | $4.60853292963304 \mathrm{E}-0004$ |
| 4.5767 | $4.51580107350580 \mathrm{E}-0004$ |
| 4.5662 | $4.19850472815675 \mathrm{E}-0004$ |
| 4.5558 | $4.03634201825209 \mathrm{E}-0004$ |
| 4.5455 | $3.81772197367347 \mathrm{E}-0004$ |
| 4.5351 | $3.50159053903010 \mathrm{E}-0004$ |
| 4.5249 | $3.29570843089488 \mathrm{E}-0004$ |
| 4.5147 | $3.03273511154778 \mathrm{E}-0004$ |
| 4.5045 | $3.07358216494968 \mathrm{E}-0004$ |
| 4.4944 | $3.95815170368241 \mathrm{E}-0004$ |
| 4.4843 | $3.27296886787121 \mathrm{E}-0004$ |
| 4.4743 | $2.5049969712491 \mathrm{E}-0004$ |
| 4.4643 | $2.12343106723800 \mathrm{E}-0004$ |
| 4.454 | $2.1807389881554 \mathrm{E}-0004$ |
| 4.4444 | $2.36823638584793 \mathrm{E}-0004$ |
| 4.4 .40 |  |


| 4.1667 | $7.53896068758309 \mathrm{E}-0004$ |
| :--- | :--- |
| 4.1580 | $7.60075199529808 \mathrm{E}-0004$ |
| 4.1494 | $7.50687935606287 \mathrm{E}-0004$ |
| 4.1408 | $7.37796610533081 \mathrm{E}-0004$ |
| 4.1322 | $7.42594525260820 \mathrm{E}-0004$ |
| 4.1237 | $7.49476580351072 \mathrm{E}-0004$ |
| 4.1152 | $7.67927269716751 \mathrm{E}-0004$ |
| 4.106 E | $7.73746061244474 \mathrm{E}-0004$ |
| 4.0984 | $7.76324118550775 \mathrm{E}-0004$ |
| 4.0900 | $7.98686151196826 \mathrm{E}-0004$ |
| 4.0816 | $7.94329194158117 \mathrm{E}-0004$ |
| 4.0733 | $8.10422241801945 \mathrm{E}-0004$ |
| 4.0650 | $8.12128707833537 \mathrm{E}-0004$ |
| 4.0568 | $8.16402564537633 \mathrm{E}-0004$ |
| 4.0486 | $7.92166262735705 \mathrm{E}-0004$ |
| 4.0404 | $8.31285970459561 \mathrm{E}-0004$ |
| 4.0323 | $8.50238460751385 \mathrm{E}-0004$ |
| 4.0241 | $8.66002264505283 \mathrm{E}-0004$ |
| 4.0161 | $8.67871992105584 \mathrm{E}-0004$ |
| 4.0080 | $8.69921010813179 \mathrm{E}-0004$ |
| 4.0000 | $8.84705855590973 \mathrm{E}-0004$ |
| 3.9920 | $8.83496966828545 \mathrm{E}-0004$ |
| 3.9841 | $8.86320273039587 \mathrm{E}-0004$ |
| 3.9761 | $9.02914931622867 \mathrm{E}-0004$ |
| 3.9683 | $9.16929644708020 \mathrm{E}-0004$ |
| 3.9604 | $9.25048421510866 \mathrm{E}-0004$ |
| 3.9526 | $9.24525938814647 \mathrm{E}-0004$ |
| 3.9448 | $9.32927168388886 \mathrm{E}-0004$ |
| 3.9370 | $9.27611049839072 \mathrm{E}-0004$ |
| 3.9293 | $9.18760874436764 \mathrm{E}-0004$ |
| 3.9216 | $9.23007419489252 \mathrm{E}-0004$ |
| 3.91 |  |

3.7037
3.6969
3.6900
3.6832
3.6765
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3.6630
3.6563
3.6496
3.6430
3.6364
3. 6298
3.6232
3.6166
3.6101
3.6036
3.5971
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| 2.1368 | 8. $29679073810041 \mathrm{E}-0003$ |
| 2.1345 | $7.63352866097478 \mathrm{E}-0003$ |
| 2.1322 | 7.55352557573730E-0003 |
| 2.1299 | 8.23197375015638E-0003 |
| 2.1277 | $8.25357882184742 \mathrm{E}-0003$ |
| 2.1254 | 7.95987019891697E-0003 |
| 2.1231 | 7.93043580688391E-0003 |
| 2.1209 | 7.66953628933464E-0003 |
| 2.1186 | $7.79256028284436 \mathrm{E}-0003$ |
| 2.1164 | $7.60021093051932 \mathrm{E}-0003$ |
| 2.1142 | $7.90565608048155 \mathrm{E}-0003$ |
| 2.1119 | $8.05862470835450 \mathrm{E}-0003$ |
| 2.1097 | 8.06947038392991E-0003 |
| 2.1075 | 8.07373997074023E-0003 |
| 2.1053 | $7.44014505334434 \mathrm{E}-0003$ |
| 2.1030 | $7.84597042243718 \mathrm{E}-0003$ |
| 2.1008 | 7.82007182908728E-0003 |
| 2.0986 | 8.32160356522138E-0003 |
| 2.0964 | 8.22793610126382E-0003 |
| 2.0942 | $8.05614968317059 \mathrm{E}-0003$ |
| 2.0921 | $7.82771660489345 \mathrm{E}-0003$ |
| 2.0899 | 8.48049372430637E-0003 |
| 2.0877 | 7.90820766304989E-0003 |
| 2.0855 | 8.09186863826028E-0003 |

2.0833
8.14194106982313E-0003
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2.0346
$2.0325 \quad 8.48706677133748 \mathrm{E}-0003$
$2.0305 \quad 9.20822923420417 \mathrm{E}-0003$
$2.0284 \quad 8.97163590437344 \mathrm{E}-0003$
$2.0263 \quad 8.67931977730052 \mathrm{E}-0003$
2.0243 7.99850450458450E-0003
2.0222 8.16961816332196E-0003
$2.0202 \quad 7.74314212848282 \mathrm{E}-0003$
$2.0182 \quad 6.86167551414485 \mathrm{E}-0003$
2.0161 6.68562420630536E-0003
2.0141 6.31084572711416E-0003
2.0121 6.30905156200612E-0003
2.0101 6.88906990927762E-0003
$2.0080 \quad 7.19839195352989 \mathrm{E}-0003$
$2.0060 \quad 6.50060137762409 \mathrm{E}-0003$
$2.0040 \quad 5.73388425233645 \mathrm{E}-0003$
$2.0020 \quad 6.14175466127875 \mathrm{E}-0003$
$2.0000 \quad 6.27875146358292 \mathrm{E}-0003$
$1.9980 \quad 7.95262542033015 \mathrm{E}-0003$
$1.9960 \quad 8.60370075525907 \mathrm{E}-0003$
$1.9940 \quad 8.37798855471306 \mathrm{E}-0003$
$1.9920 \quad 8.39449205881238 \mathrm{E}-0003$
$1.9900 \quad 9.24912381908882 \mathrm{E}-0003$
$1.9881 \quad 8.75290374968074 \mathrm{E}-0003$
$1.98618 .28182095445129 \mathrm{E}-0003$
$1.98418 .40984859802063 \mathrm{E}-0003$
$1.9822 \quad 8.85518998863688 \mathrm{E}-0003$
$1.98028 .93692503963450 \mathrm{E}-0003$
$1.9782 \quad 8.47596505848003 \mathrm{E}-0003$
$1.9763 \quad 8.31310506330851 \mathrm{E}-0003$
$1.9743 \quad 8.37897493104833 \mathrm{E}-0003$
$1.97248 .47482749369988 \mathrm{E}-0003$
$1.9704 \quad 8.75126636317702 \mathrm{E}-0003$
$1.96858 .74666109376676 \mathrm{E}-0003$
1.9666 $\quad 8.14208675387817 \mathrm{E}-0003$
$1.9646 \quad 7.14843876483684 \mathrm{E}-0003$
$1.9627 \quad 7.41898544578845 \mathrm{E}-0003$
1.9608 8.60221601162436E-0003
1.9589 8.88750327108312E-0003
$1.95698 .08256091956139 \mathrm{E}-0003$
$1.9550 \quad 8.45969611380326 \mathrm{E}-0003$
$1.95318 .07251584954827 \mathrm{E}-0003$
1.9512 9.18530439059850E-0003
1.9493 9.26816121842933E-0003
$1.9474 \quad 8.93776141629132 \mathrm{E}-0003$
$1.9455 \quad 9.21891788239293 \mathrm{E}-0003$
1.9436 8.77721833882106E-0003
1.9417 9.61099442051250E-0003
$1.9399 \quad 9.90863547512788 \mathrm{E}-0003$
$1.9380 \quad 9.85723073468137 \mathrm{E}-0003$
1.9361 8.97820529618798E-0003
$1.9342 \quad 1.05888191713319 E-0002$
$1.9324 \quad 9.86547132727367 \mathrm{E}-0003$
$1.9305 \quad 9.49855114660636 \mathrm{E}-0003$
$1.9286 \quad 9.48731497180688 \mathrm{E}-0003$
$1.9268 \quad 9.89364096572842 \mathrm{E}-0003$

## Appendix 8

Figures 30-65

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