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**GEOSTATIONARY ATMOSPHERIC SOUNDER (GAS):
SOUNDING RETRIEVAL PERFORMANCE STUDIES - YEAR 1**

Final Report to

AGS IR Sounder Program Office
Langley Research Center (LARC)
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By

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GEOSTATIONARY ATMOSPHERIC SOUNDER (GAS): SOUNDING RETRIEVAL PERFORMANCE STUDIES - YEAR 1

Abstract

The Geostationary Atmospheric Sounder (GAS) infrared sounder will offer a major advance in our capabilities for observing small spatial scale and short term temporal changes in the atmospheric state from space. It will provide quantitative measurements of variations in the distribution of water vapor, temperature and trace gases with high temporal resolution. The focus of this first year study was to conduct investigations of weather and chemistry sounding performance as a function of instrument design parameters. Specific tasks are classified: (1) to determine the optimal instrument configuration in terms of spectral resolution, spectral coverage, and signal to noise ratio for the sounding of thermodynamical and chemical gas concentration profiles; (2) to develop a fast radiative transfer model and implement a sounding retrieval algorithm to conduct performance analysis as described in (1); and (3) to define additional tasks for further detailed studies to determine incremental benefits of GAS observations from global, regional and mesoscale measurement conditions for both weather and chemistry applications.

1. Introduction

The primary mission of the NASA MTPE sponsored Advanced Geosynchronous Studies (AGS) program is to conduct intensive studies to demonstrate the use of advanced new technologies and instruments on geosynchronous satellites to improve our current capabilities of monitoring the global weather, climate, and chemistry. The Geostationary Atmospheric Sounder (GAS) mission, to be developed under AGS, is intended to demonstrate new space-based technology that is well suited for achieving the high temporal and spatial global coverage of cloud motion, water vapor transport, thermal and moisture vertical profiles, land and ocean surface temperature, and trace gas concentrations. The AGS technology demonstrations will show the capabilities of passive infrared observations from future NOAA geostationary operational sounders. These instruments will have much-improved spatial sampling and far more rapid coverage than the filter radiometer sounders. The proposed GAS characteristics are summarized in Table 1.

Table 1. Summary of Proposed GAS Characteristics and Approach

Spatial Footprints	Nominal 9 km square, composed of 3x3 array subpixels allowing higher resolution options
Spatial Coverage	Nominal 9 km contiguous sampling in 42x42 groups, with other options allowed by 128x128, 3 km pixel array
Spectral Resolution	1.0-0.1 cm^{-1} unapodized (0.5-5 cm Optical Path Difference)
Spectral Coverage (2 bands)	SW: 3.8-5.5 μm MW: 5.5-12 μm
Telescope Aperture	30.5 cm diameter (12 inches)
Interferometer	5-8 cm beam diameter, Dynamically Aligned Plane-Mirror Michelson (sized to keep angles small)
OPD Scan Drive Scan rate	TBD 0.05-0.1 cm/s (Maximize consistent with readout)
OPD Sampling Reference	Stabilized Diode Laser
Detector Arrays	128x128 elements with 60 μm pixel size InSb SW and PV HgCdTe LW bands With snapshot readout At rates of at least 500 frames/sec
Detector Cooler/temperature	Stirling Cooler/68-80 K
Noise Performance	< 0.2 K Brightness Temperature at 280 K, for the nominal configuration and 60 sec dwell time
Onboard Processing	Subpixel processing to Effectively Field Widen Plus Data Compression
Mass	<100 kg
Power	<300 Watts
Size	<0.25 m^3
Data Rate	TBD

The proposed GAS characteristics are used as the baseline instrument for the sounding retrieval performance study described in the next few sections.

2. Instrument Simulation

GAS measurements are simulated using the baseline instrument configuration with variable spectral resolution, spectral coverage, and signal to noise ratio for global scenes. Figure 1 shows two brightness temperature spectra computed from a fast radiative transfer model for tropical atmospheric conditions from a 5 cm and 1 cm optical path difference (OPD) interferometer. The baseline spectral coverage from 3.8 micron (2631 1/cm) to 12 micron (833 1/cm) show absorption characteristics from carbon dioxide, ozone, water vapor, carbon monoxide, methane and nitrous oxide. The significant spectral resolving power due to a 5 times difference in OPD is also clearly presented. The trade off between the spectral resolving power and the accuracy of the derived retrieval parameters such as temperature, water vapor, and trace gases are demonstrated using these kind of spectra.

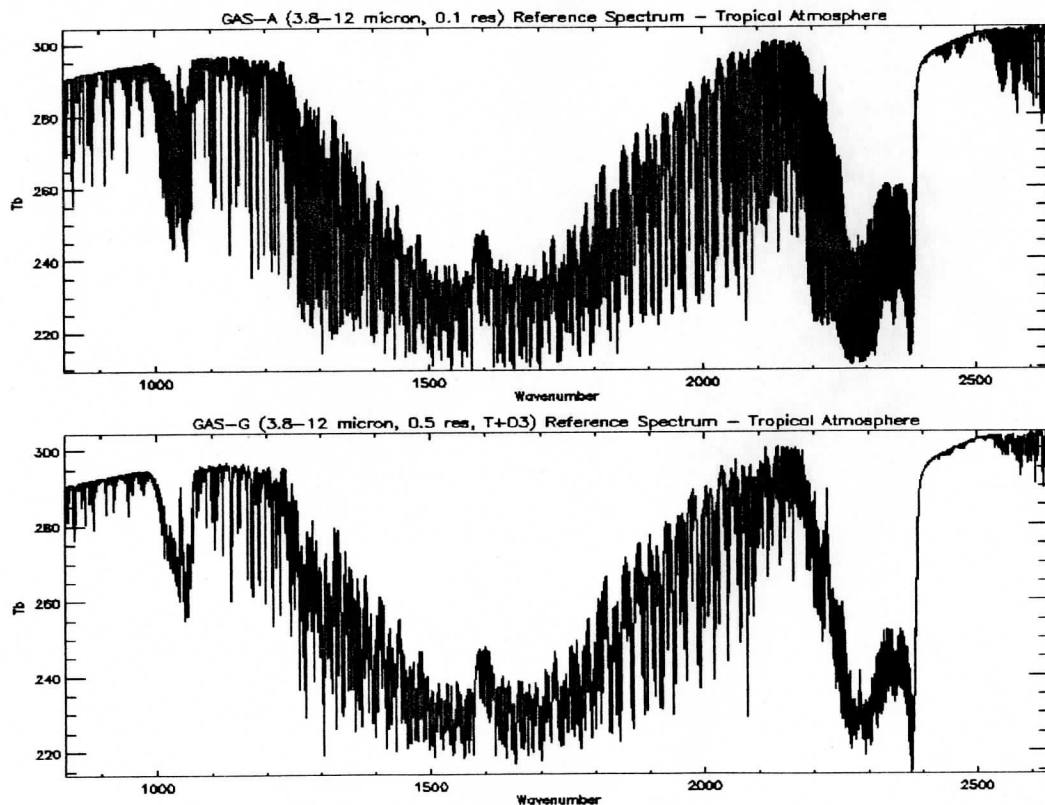


Figure 1. GAS brightness temperature spectra computed from tropical atmosphere for 5 and 1 cm OPD using GAS fast transfer model.

Chemistry applications will require that GAS spectral measurements have high sensitivity to trace gas constituents, such as ozone, methane, carbon monoxide, and nitrous oxide. Figure 2 shows 1976 U.S. standard atmosphere profiles used to analyze the measurement sensitivity for different spectral resolutions.

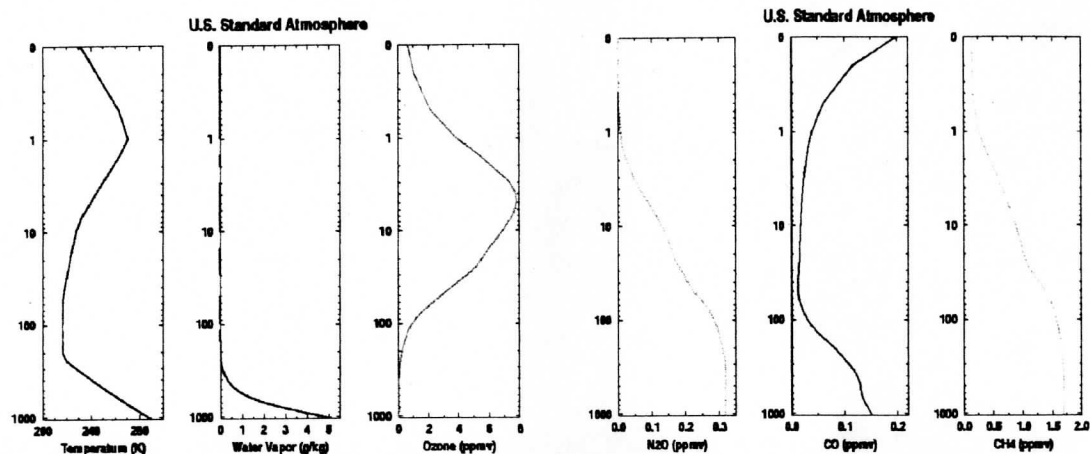


Figure 2. 1976 U.S. standard atmosphere temperature, water vapor and trace gas profiles.

Spectral differences are computed for different spectral resolutions (0.05, 0.1, and 0.2 1/cm) by using the U.S. standard atmosphere and increasing individual trace gas profiles by 20%. Figure 3 displays the measurement sensitivity with a 20% increase in the trace gas concentrations of ozone, methane, carbon monoxide and nitrous oxide at the three spectral resolutions.

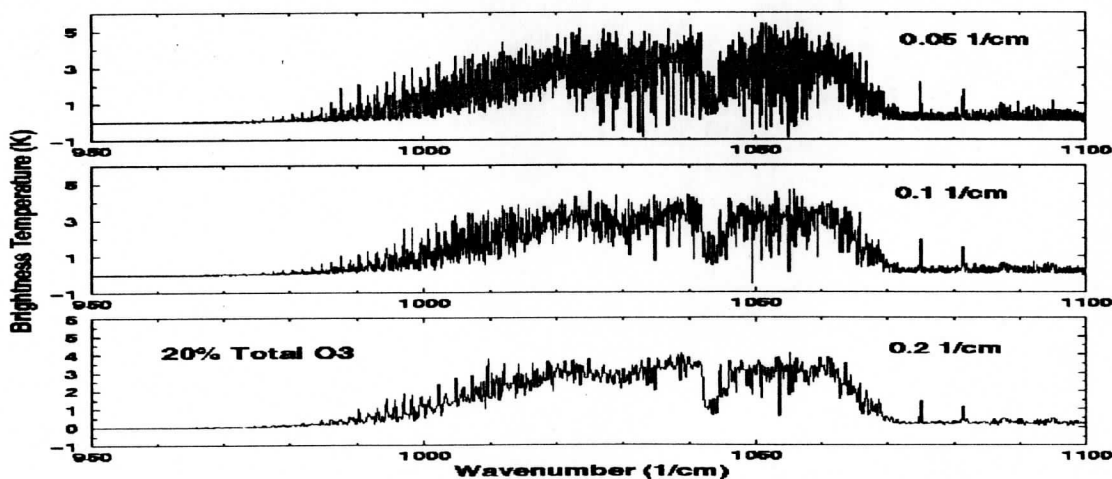


Figure 3a. GAS spectral measurement sensitivity with a 20% increase of ozone total concentration at spectral resolutions of 0.05, 0.1, and 0.2 1/cm.

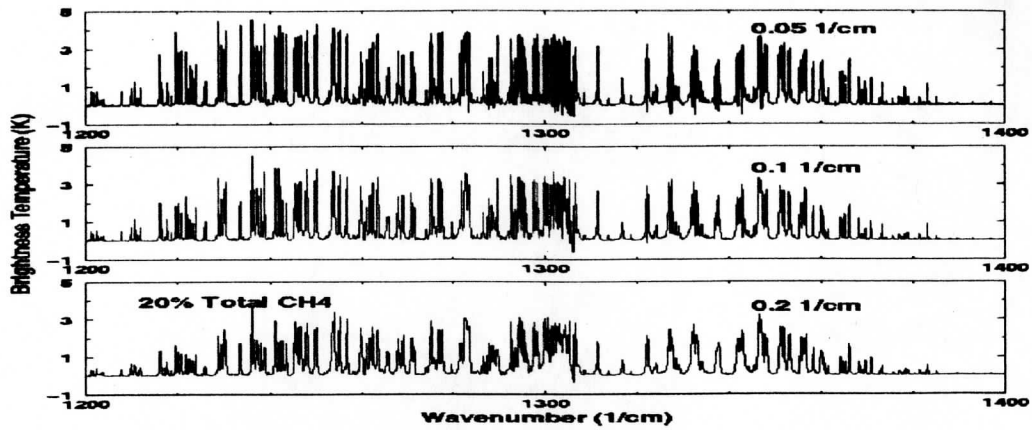


Figure 3b. GAS spectral measurement sensitivity with a 20% increase of methane total concentration at spectral resolutions of 0.05, 0.1, and 0.2 1/cm.

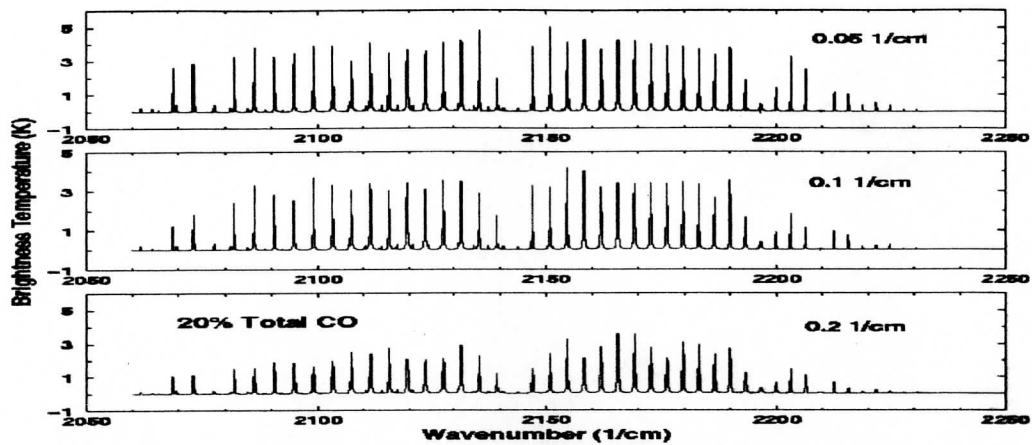


Figure 3c. GAS spectral measurement sensitivity with a 20% increase of carbon monoxide total concentration at spectral resolutions of 0.05, 0.1, and 0.2 1/cm.

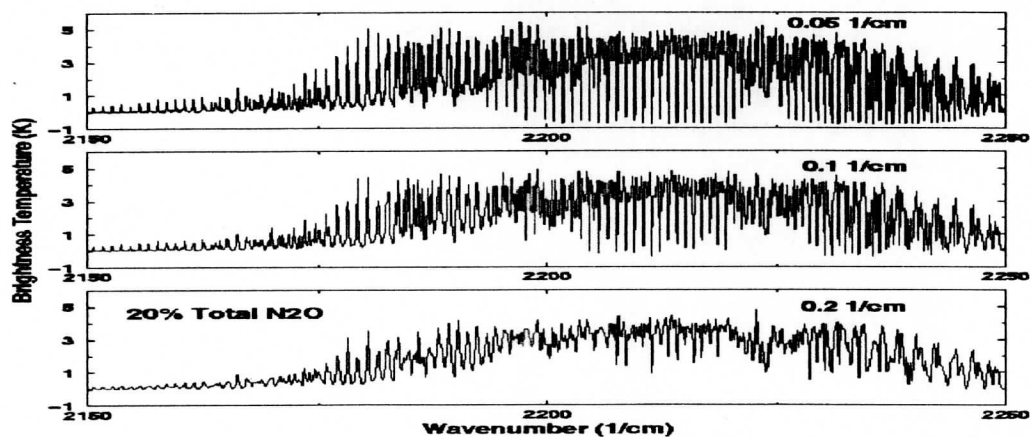
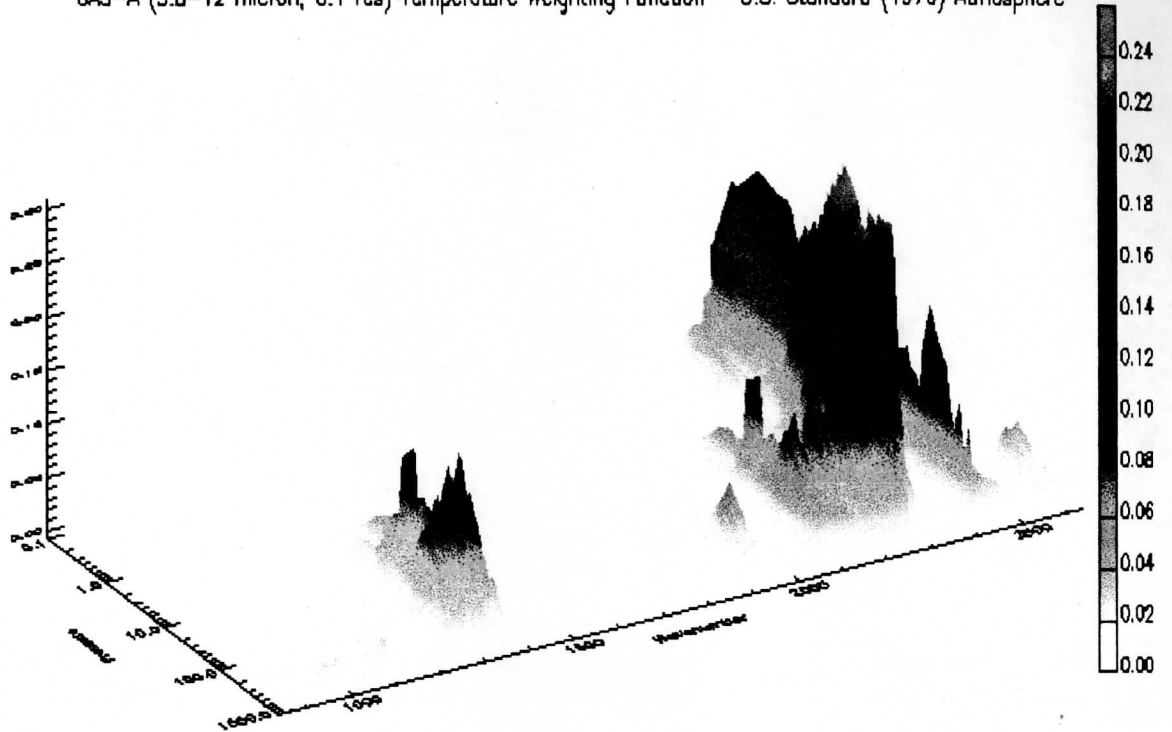


Figure 3d. GAS spectral measurement sensitivity with a 20% increase of nitrous oxide total concentration at spectral resolutions of 0.05, 0.1, and 0.2 1/cm.

Figure 3 shows that measurement sensitivity increases with higher spectral resolution. However, the signal to noise ratio does not necessarily favor higher spectral resolutions since at the same measurement dwell time, the higher spectral resolution will result in higher measurement noise. Figure 3 demonstrates that resolutions close to 0.2 1/cm might be enough to obtain useful and accurate retrieval information for the total concentration of ozone, methane, nitrous oxide and carbon monoxide. Further study is required to define the optimal spectral resolution for obtaining trace gas profiles and concentrations of boundary layer gases.

Figure 4 displays the weighting functions for temperature (upper panel) and water vapor (lower panel) at 0.1 1/cm spectral resolution. The temperature weighting function shows the sensitivity of carbon dioxide at the longwave and shortwave infrared measurement regions. The water vapor signal is mainly from the middle region of the spectral band. Figure 5 is similar to Figure 4 except that the spectral resolution is at 0.6 1/cm and the spectral coverage is extended to 15 micron. Figure 4 and 5 demonstrate that the temperature and water vapor signal of the interferometer's spectral measurements are very dependent on the spectral resolution and coverage. If GAS is designed to provide accurate weather (e.g. temperature and water vapor) and chemistry (e.g. ozone and carbon monoxide) information in an efficient and timely manner, one needs to perform a trade off study to determine the optimal relationship between the spectral measurements and the derived weather and chemistry parameters.

GAS-A (3.8–12 micron, 0.1 res) Temperature Weighting Function – U.S. Standard (1976) Atmosphere



GAS-A (3.8–12 micron, 0.1 res) Water Vapor Weighting Function – U.S. Standard (1976) Atmosphere

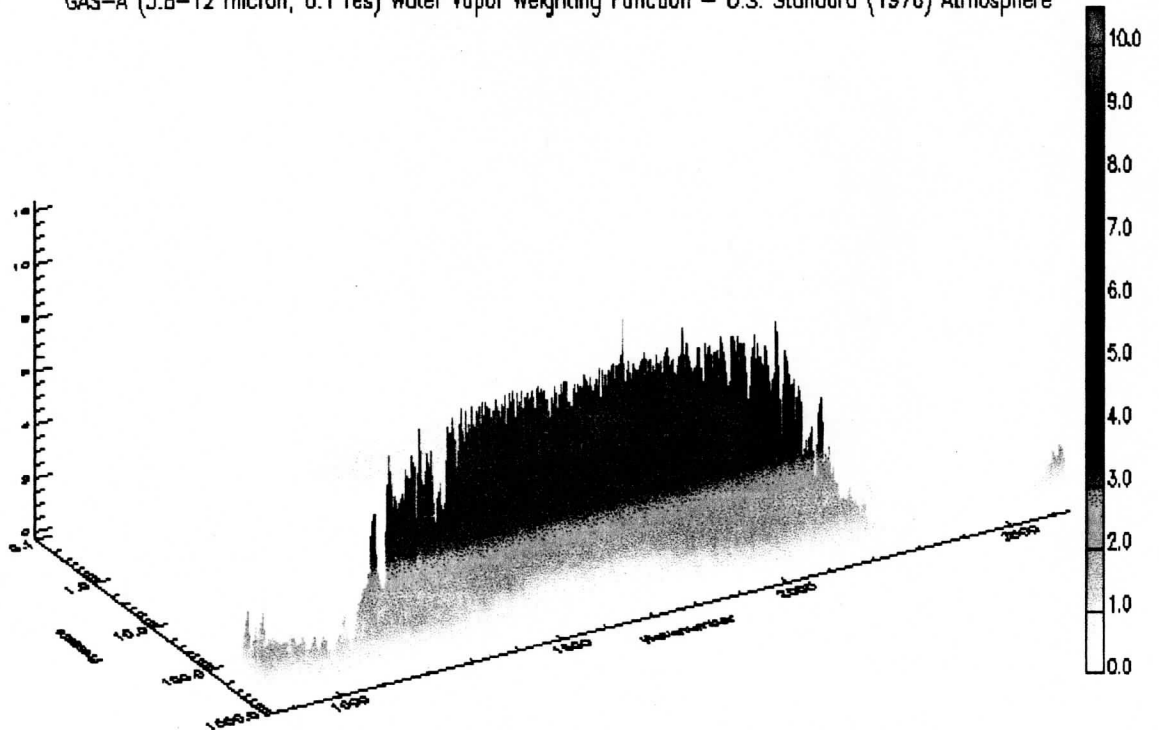
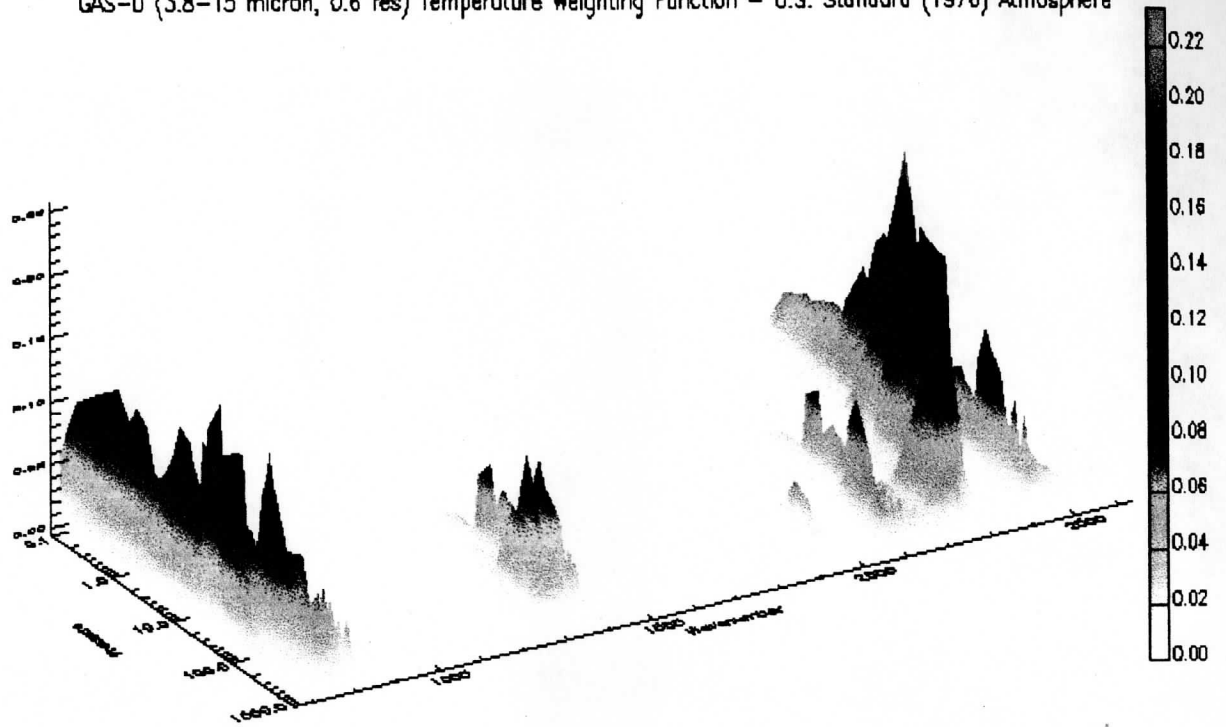


Figure 4. Temperature and water vapor weighting function 3-dimension spectra (5 cm OPD – 0.1 1/cm unapodized resolution) for the coverage of 3.8 to 15 micron.

GAS-D (3.8-15 micron, 0.6 res) Temperature Weighting Function - U.S. Standard (1976) Atmosphere



GAS-D (3.8-15 micron, 0.6 res) Water Vapor Weighting Function - U.S. Standard (1976) Atmosphere

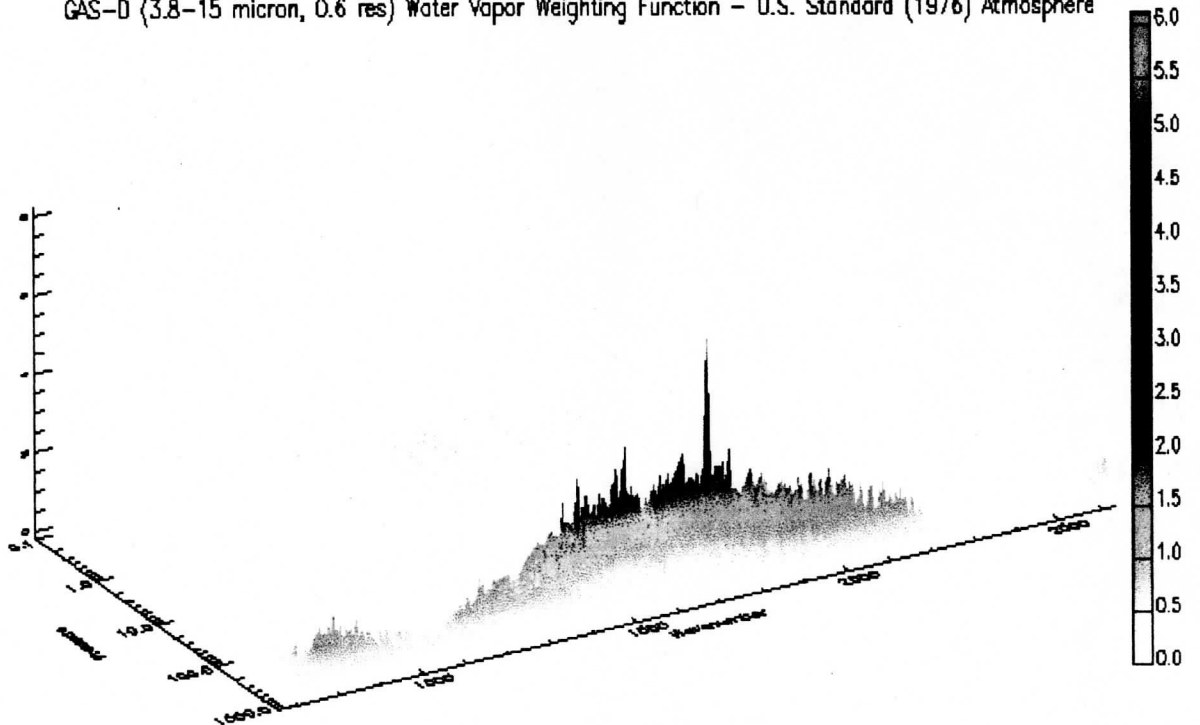


Figure 5. Temperature and water vapor weighting function 3-dimension spectra. (1 cm OPD - 0.5 1/cm unapodized resolution). Spectral coverage is different from figure 2 and extends to the 15 micron region.

Consider the carbon dioxide, ozone, and carbon monoxide detail absorption features in the center of each absorption band as shown in Figure 6. Carbon dioxide absorptions in the Q-branch region have regularly spaced spectral lines of about 1.6 wavenumber, the 0.1 wavenumber unapodized GAS radiances can resolve these features unambiguously. Since carbon dioxide is a well mixed species and its concentration is well known, one can use these spectral measurements to sound the temperature profile of the atmosphere (Huang, et. al., 1997). In addition, figure 6 shows the ozone absorption lines are irregularly spaced and the 0.1 wavenumber spectral radiances exhibit high frequency signals, and the spectral lines for carbon monoxide are regularly spaced within spectral band of 2100 to 2200 wavenumber.

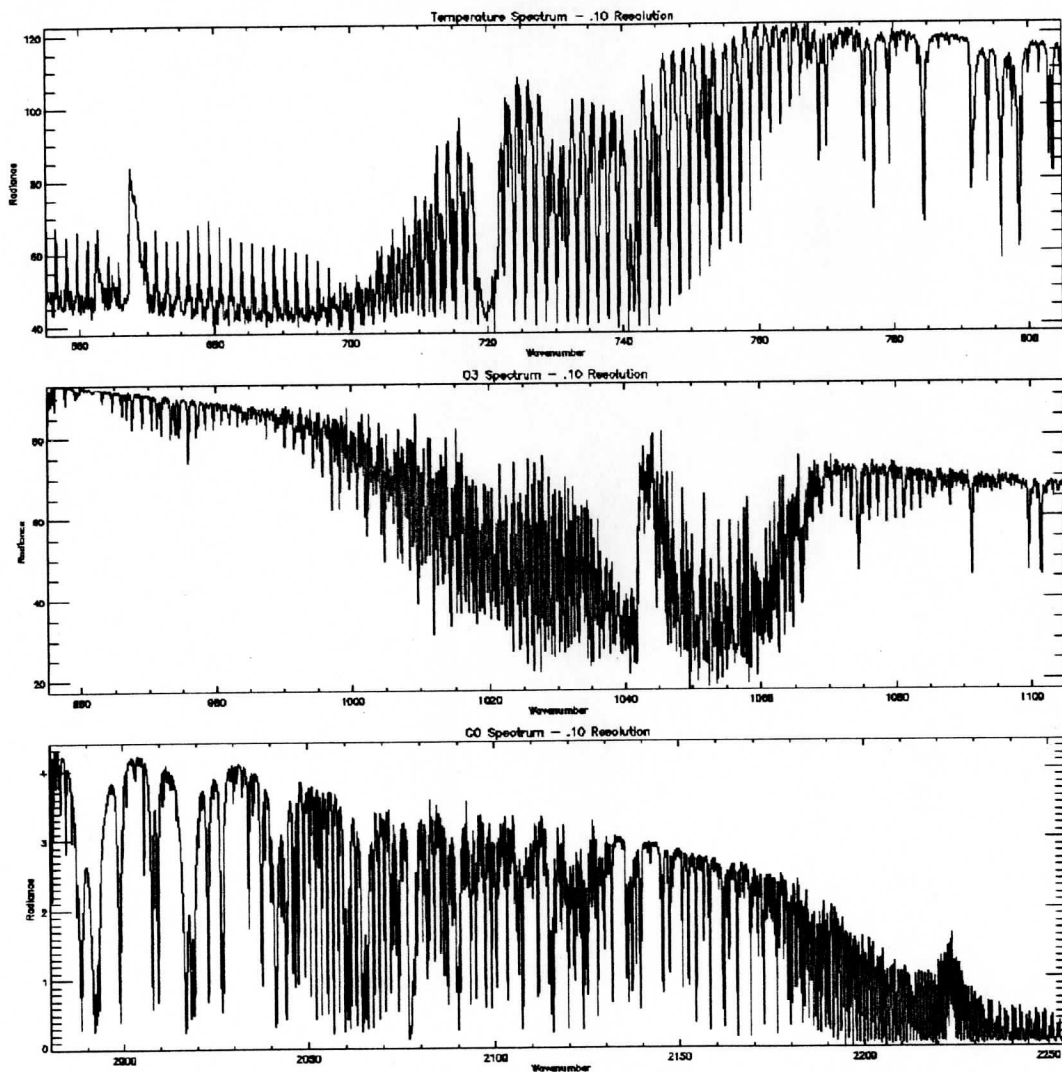


Figure 6. Major absorption bands of carbon dioxide (upper panel), ozone (middle panel) and carbon monoxide (lower panel) 0.1 1/cm unapodized brightness temperature spectra.

The spectral temperature information is shown using weighting function plots in Figure 7 (upper panel). The temperature information of GAS exists throughout the whole spectral coverage indicating that a highly accurate temperature profile is achievable.

The ozone and carbon monoxide spectral weighting functions are also displayed in figure 7. The ozone and carbon monoxide absorptions are concentrated in narrow spectral regions. Ozone is centered near 1040 wavenumber, while carbon monoxide is located near 2200 wavenumber. The ozone and carbon monoxide weighting function plots shown in Figure 7 demonstrate the possibility of obtaining profile information of both trace gases; however, this requires that GAS can measure these regions of interest with good signal to noise ratio and at the resolutions near 0.1 wavenumber.

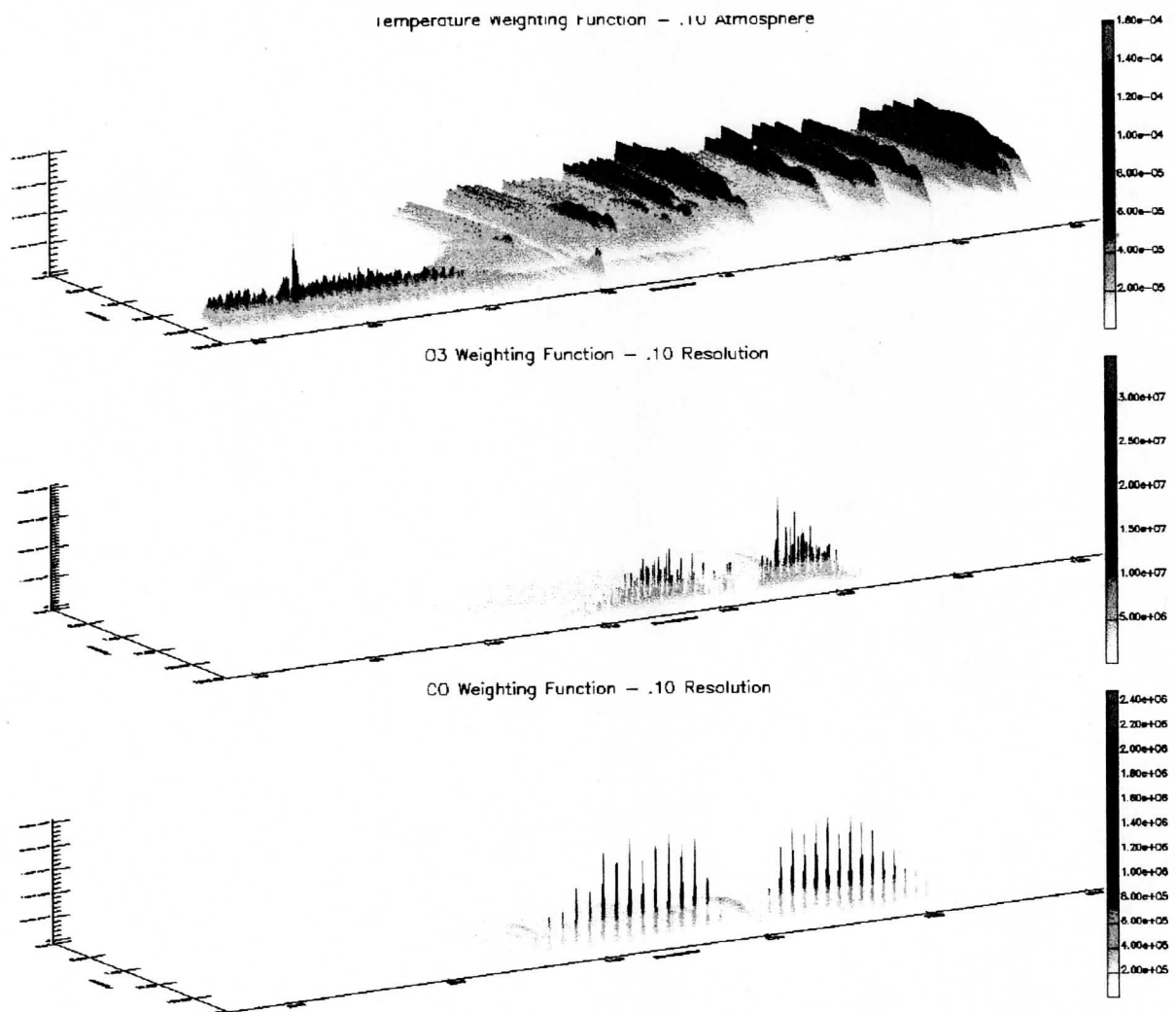


Figure 7. 3-dimension weighting function spectra of carbon dioxide (upper panel), ozone (middle panel) and carbon monoxide (lower panel) for 0.1 1/cm unapodized resolution of simulated GAS.

3. Instrument Performance Analysis

3-1. Linear Eigenvector Regression Retrieval Method

It has been found that the linear regression retrieval (Smith, W.L., and Woolf, H.M., 1976) can provide efficient and accurate initial estimates of temperature and trace gas profiles using simulated high spectral resolution infrared data (CIMSS/UW, 1996). A few hundred eigenvectors (empirical orthogonal functions or principal components) (Press, W.H. etc., 1990) of the brightness temperature covariance, calculated from a large global training data ensemble, can be used as basis functions to represent thousands of channels of infrared measurements with little loss of radiometric information. Two distinct advantages of this approach for analyzing the AGS instrument performance are the computational efficiency and maximization of the system's signal to noise ratio (i.e. measurement information of the system is fully utilized). The mathematical expression of the brightness temperature eigenvector regression retrieval is detailed in this section and is used as the fundamental approach for instrument performance analysis presented in this report.

Computed from the training ensemble of temperature, moisture and trace gases (ozone, carbon dioxide), the GAS brightness temperature spectra are used to conduct the eigenvector decomposition to obtain eigenvector spectra required for the regression retrieval analysis. The departure of the brightness temperature spectra from their ensemble mean, dT_b , for the entire training set has the dimension of NC (number of GAS channels) and NS (number of sample profiles). The covariance of the dT_b has the usual form,

$$\text{COV} = [dT_b * (dT_b)^T] / \text{NS}. \quad (1)$$

Where * denotes matrix multiplication and superscript T denotes matrix transpose. COV of dT_b is a square matrix with the dimensions NC by NC. The diagonal elements of COV represent the variance of the respective channel brightness temperatures, and the off diagonal elements represent the covariance between pairs of channels. The eigenvector decomposition of the COV matrix is,

$$\text{COV} = \text{VEC} * \text{VAL} * (\text{VEC})^T. \quad (2)$$

Where VEC is the [NC x NC] square matrix containing the eigenvectors of COV in its columns, and VAL is the [NC x NC] diagonal matrix of eigenvalues. The first diagonal element of VAL is the largest eigenvalue and last diagonal element is the smallest eigenvalue. The eigenvectors are also ordered such that the first eigenvector is associated with the largest eigenvalue and explains the most brightness temperature variance in the ensemble data set. The last few eigenvectors explain very little variance and do not appear to possess any significant radiometric information above the measurement radiometric noise level. Because of these subtle statistical properties, the use of truncated eigenvectors to represent thousands of channels of GAS measurements has the advantages of retaining most of the measurement information content while minimizing the effects of random measurement noise. The number of significant eigenvectors selected to be retained, NR, in general is much smaller than NC (NR << NC). The optimal choice of NR can be considered as the independent piece of information of GAS channel measurements; when NR eigenvectors are used in the retrieval analysis, it gives the optimal retrieval with the smallest root mean square temperature and trace gases profile errors. Many NR values have been used in the GAS regression retrieval and have been identified to be 200. Since the analysis so far uses 0.25 K at reference temperature 250 K as the GAS noise level, the NR of 200 is likely suboptimal when the improved radiometric noise model of GAS is used. The analysis results shown in the following sections will then need to be refined.

Using NR eigenvectors of GAS as the basis functions, the GAS brightness temperature measurements are transformed into expansion coefficients as,

$$\mathbf{COEF}_{ij} = \sum_{k=1}^{NC} \mathbf{VEC}_{i,k} * \mathbf{T}_{b,k,j}. \quad (3)$$

Where index i stands for number of 1 to NR, j is 1 to NS, and k is 1 to NC. Equation 3 represents the mapping of the whole spectrum information of NC channels into the eigen-space of NR coefficients, which significantly reduces the dimensionality of the matrix needed to be inverted later.

To achieve the linear regression relationship between expansion coefficients of GAS and temperature and trace gas profiles, one can use

$$\mathbf{RTV}_{ij} = \mathbf{REGC}_{i,i} * \mathbf{COEF}_{ij}. \quad (4)$$

Where l is the number of vertical levels representing the temperature and trace gas profile \mathbf{RTV} and i and j are the same as in eq. (2). \mathbf{REGC} becomes the regression retrieval coefficient matrix that needs to be derived from a very large training ensemble data set in order to perform regression retrieval analysis when other independent GAS measurements are simulated for a variety of instrument conditions. The least square solution for \mathbf{REGC} in eq. (4) can be written as,

$$\mathbf{REGC}_{i,i} = \mathbf{RTV}_{i,i} * (\mathbf{COEF}_{ij})^T * \{ \mathbf{COEF}_{ij} * (\mathbf{COEF}_{ij})^T \}^{-1}. \quad (5)$$

Where superscripts -1 and T stand for the matrix inverse and transpose. As can be seen, the matrix to be inverted has the size of NR by NR , which is around 200 by 200. In the case of using channel measurements directly in this regression analysis, the size of this matrix is significantly increased to NC by NC , where NC of the typical GAS spectrum is on the order of thousands.

Having successfully obtained the representative regression coefficient matrix \mathbf{REGC} from the ensemble training data set, it is easy to perform regression retrieval to the independent GAS simulated measurements with specific noise, spectral coverage and resolutions for temperature and other trace gases using eq. (6),

$$\mathbf{RTV}^{ind} = \mathbf{REGC} * \mathbf{COEF}^{ind}. \quad (6)$$

Where \mathbf{COEF}^{ind} is computed from eq. (3) using T_b simulated from independent GAS simulated conditions and \mathbf{REGC} is simply obtained from eq. (5) that is derived from the training data set described in the previous section. The regression results \mathbf{RTV}^{ind} are vectors of temperature and trace gases profiles that can be analyzed with the true profiles used to simulate the independent GAS T_b . The root mean square errors (RMSE) of many of these retrieval results for a variety of GAS measurement conditions and noises are shown in the subsequent two subsections 3-2 and 3-3.

3-2. Spectral Resolution and Noise Performance Analysis

Regression retrieval analysis is performed using GAS simulated spectral measurements computed from 834 independent global profiles of temperature, water vapor, and ozone. The

spectral resolutions of 0.1, 0.5 and 40 wavenumbers (unapodized) are assumed with channel random instrument noise of 0.2 K at a 250 K reference temperature, a 0.2 K forward model error is added to the spectra. Spectral coverage of 4 to 15 micron at three different resolutions of 0.1 (18344 channels), 0.5 (3666 channels) and 40 (46 channels) wavenumber GAS spectral data are simulated from the global profiles. The temperature RMSE for these three resolutions are shown in figure 8. It is obvious that the high spectral resolutions yield small RMSE. Figure 9 gives similar results for water vapor. The spectral resolution around 0.5 wavenumber unapodized resolution may be required for GAS measurements to be useful for weather applications.

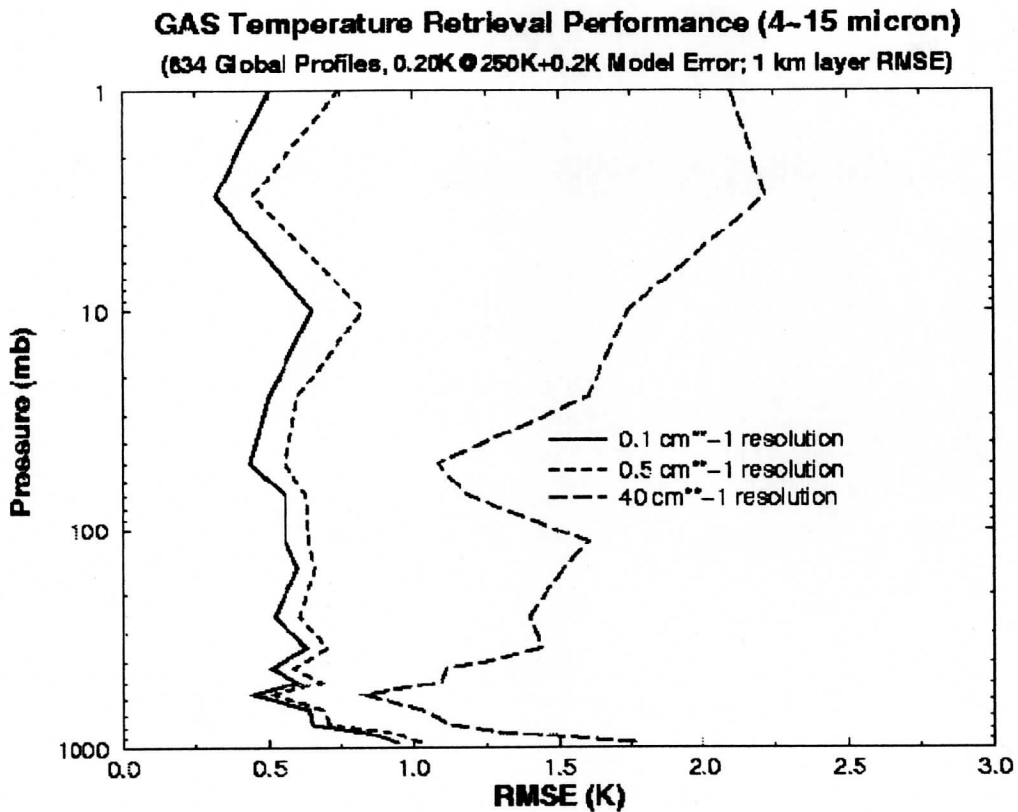


Figure 8. GAS temperature retrieval root mean square error derived from global profile simulation for three different spectral resolutions (0.1; 0.5 and 40 1/cm) simulated spectra.

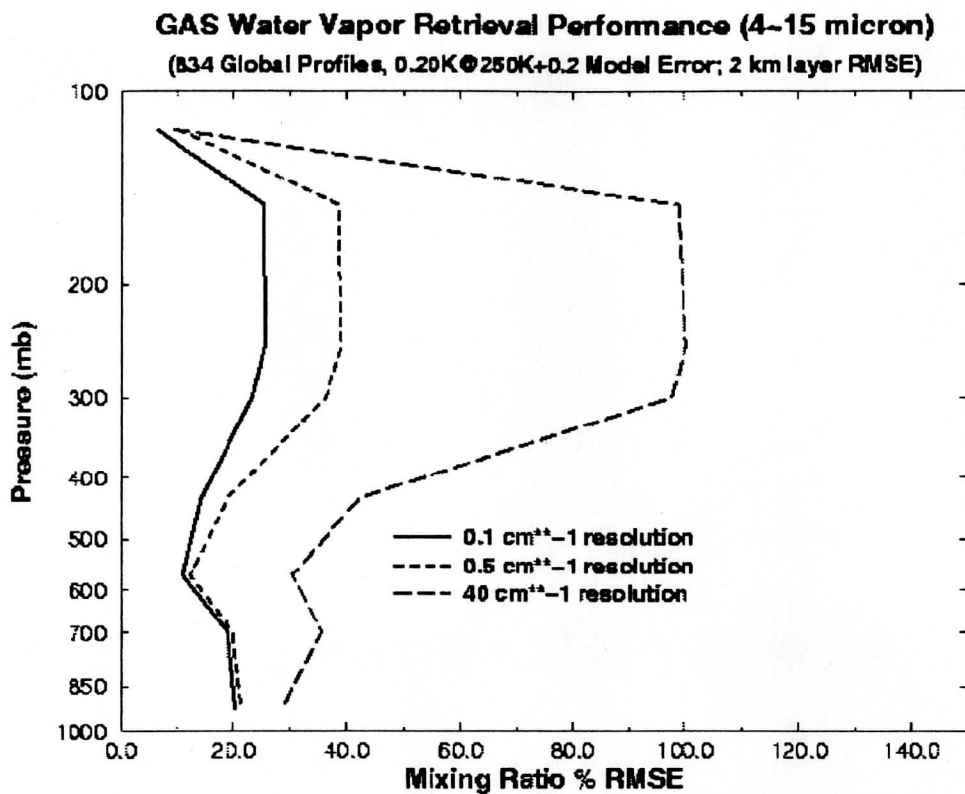


Figure 9. GAS water vapor retrieval root mean square error derived from global profile simulation for three different spectral resolutions (0.1; 0.5 and 40 1/cm) simulated spectra.

Carbon monoxide regression retrieval analysis was conducted to demonstrate the GAS trace gas sounding capabilities. Figure 10 shows thirty-eight independent GAS spectra retrieval RMSE for three different unapodized spectral resolutions of 0.05, 0.1 and 0.2 wavenumber with the same noise level as above (noise factor NF=1, 0.25 K at 250 K), and spectral coverage of 2025 to 2250 wavenumber (a major carbon monoxide absorption band). The result indicates that if the same noise level is maintained the increased spectral resolution greatly improved the carbon monoxide sounding accuracy. The highest spectral resolution of 0.05 might be needed to further improve the potential sounding of carbon monoxide to a higher accuracy.

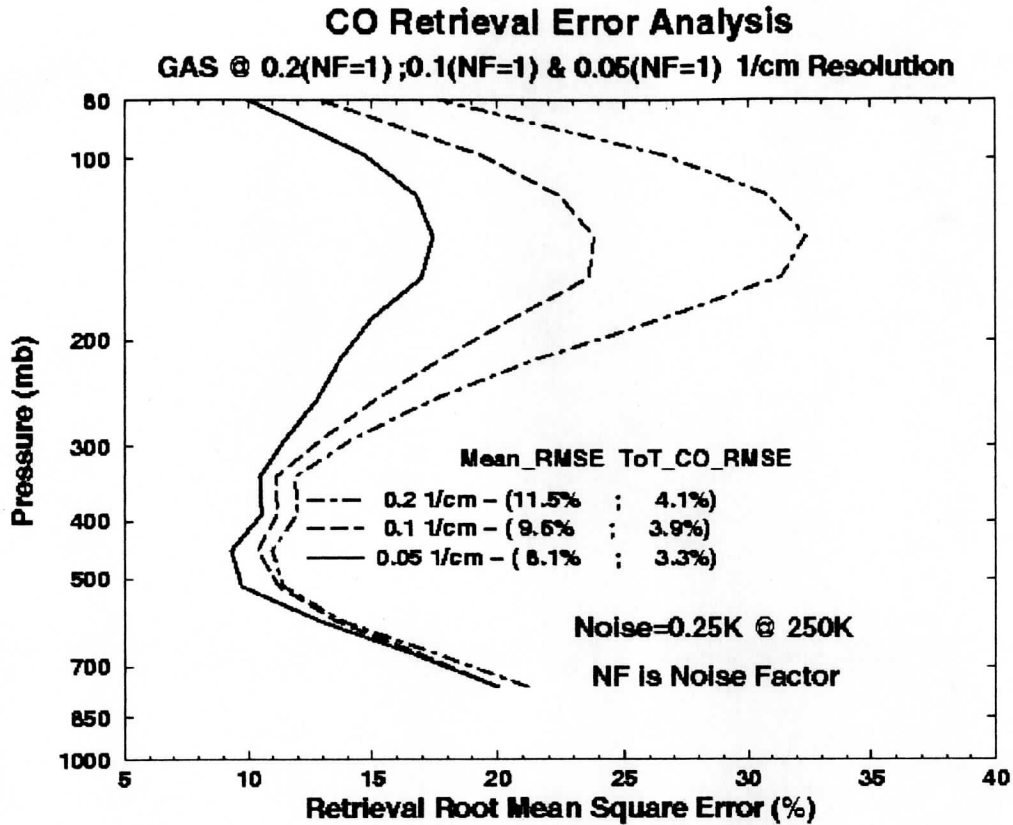


Figure 10. GAS carbon monoxide retrieval root mean square error profile derived from global profile simulation for three different spectral resolutions (0.05; 0.1 and 0.2 1/cm) simulated spectra with same noise value (0.25k).

Figure 11 gives the same analysis as figure 8 except that the dwell time of the GAS measurements at the three different spectral resolutions are the same. In other words, the noise level increases for the higher spectral resolution measurements; with these conditions the NF is 4 for 0.05, NF is 2 for 0.1 and NF is 1 for 0.2 resolution. The end results of this analysis show the carbon monoxide sounding performance is very sensitive to instrument noise. High spectral resolution with high level of noise underperforms the low spectral resolution with low level noise measurements. To achieve the benefits of high spectral resolution to accurately measure the carbon monoxide amount, GAS must be designed to meet the noise level required. This work indicates the required noise level is approximately 0.25 K (at 250 K reference temperature).

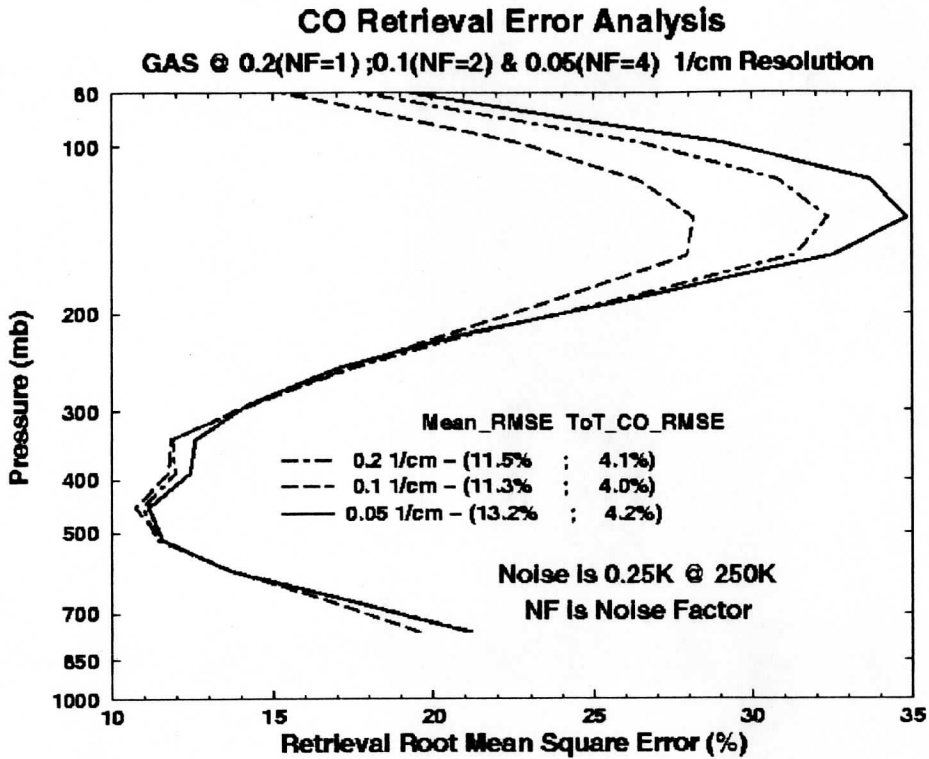


Figure 11. GAS carbon monoxide retrieval root mean square error profile derived from global profile simulation for three different spectral resolutions (0.05; 0.1 and 0.2 1/cm) simulated spectra with their respective noise value (0.25k; 0.5k and 1.0k).

3-3. Spectral Coverage Performance Analysis

Spectral coverage of the GAS measurements is of special concern given the limited detector materials offered by current technologies. It is important to look at the trade off from the different spectral cutoffs that might result in very different instrument designs.

Figures 12 and 13 look at the performance differences due to the spectral coverage with and without 10 to 15 microns at the same spectral resolution (0.5 wavenumber) and noise level (0.25 K). For temperature, there are significant differences above 300 mb due to the spectral coverage. It is not surprising to conclude that the major carbon dioxide absorption band present between 12 to 15 microns is crucial to the upper level temperature sounding accuracy. To have GAS only cover up to 10 microns and shorter will not meet the stringent requirements of the most weather applications that use upper level temperature profiles. Even for ozone, spectral coverage including the 15 micron band still outperforms the one without it.

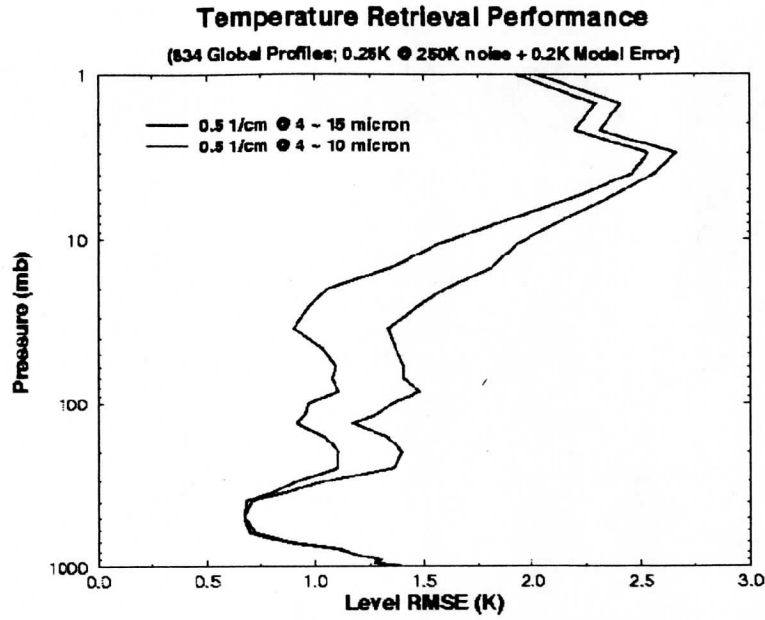


Figure 12. GAS temperature retrieval root mean square error profile derived from global profile for two different spectral coverage (4 to 15 micron and 4 to 10 micron) simulated spectra with 0.5 1/cm spectral resolution and 0.25 K noise value.

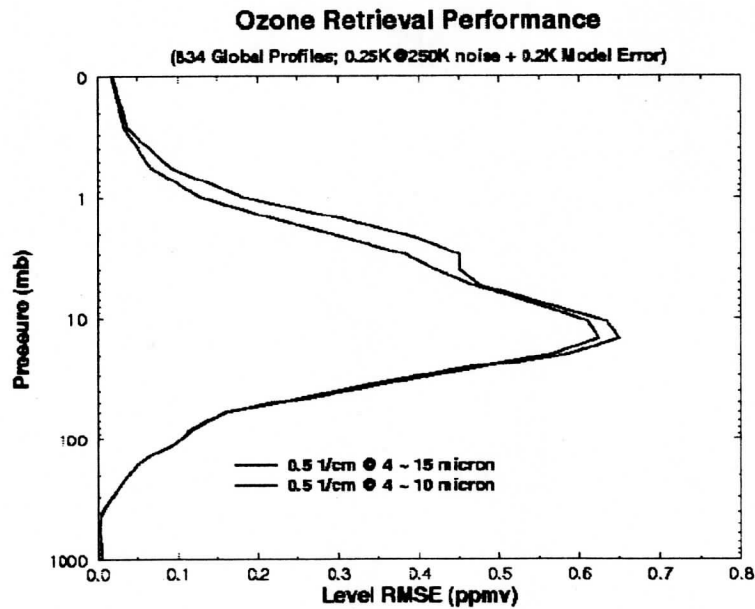


Figure 13. GAS ozone retrieval root mean square error profile derived from global profile for two different spectral coverage (4 to 15 micron and 4 to 10 micron) simulated spectra with 0.5 1/cm spectral resolution and 0.25 K noise value.

4. Summary

In this first year study, fundamental and necessary simulation tools have been built to allow some limited but useful analysis results to be achieved. Most of this groundwork required implementation of computer intensive tasks, especially for cases with spectral resolution of 0.1 wavenumber and higher. While we are continuing to develop more efficient techniques and use faster computers, we need to understand the fundamental instrumentation and resource limitations. In the second year we will focus on performing advanced trade off studies using much more elaborate schemes and using radiometric model specifications of arrays of the GAS design.

Based on this first year study and recognizing future tasks that must be investigated we conclude and recommend that

1. We need to develop a fast forward model for a few different spectral resolutions and the gas component transmittances have to be separated;
2. The GAS radiometric model has to be established to flowdown to the performance analysis study;
3. Trace gas ensemble data sets need to be collected and analyzed;
4. GAS has to extend spectral coverage beyond 12 microns, and the optimal cutoff needs to be analyzed;
5. Spectral resolutions of different sounding modes should be reanalyzed;
6. A nonlinear retrieval algorithm should be implemented;
7. Simulation of cloudy scenes should be considered; and
8. The development of cloud track and water vapor wind from GAS should be considered.

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