Improvement on sounding retrievals from GOES Sounder measurements


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Abstract

The Sounder instrument aboard the Geostationary Operational Environmental Satellite series (GOES-8, 9, 10, 11, and 12) currently provides information on changes in atmospheric state through a physically-based retrieval of vertical temperature and moisture profiles. The GOES Sounder typically samples the continental U.S. and surrounding oceanic regions on an hourly basis at a 10 km horizontal resolution. As a first step in the retrieval process, guess profiles of temperature and moisture are obtained, usually from short-term numerical model forecasts. Following this, the first guess profiles are then adjusted so that forward calculations match the Sounder measured radiances within some pre-determined noise level. This iterative process results in the final temperature/moisture retrieval. To date GOES moisture retrievals have provided a noticeable improvement over the first guess, while temperature retrievals have remained very similar to the first guess. The lack of temperature profile improvement in the physical retrieval process might be caused by insufficient use of the GOES Sounder radiance information, or the implementation of the radiative transfer calculation in the physical retrieval. This study demonstrates that both guess temperature and moisture profiles can be improved (by up to ~ 0.5 K for temperature and ~5% for Total Precipitable Water) when the GOES Sounder radiance measurements are used in a simple statistical retrieval approach that modifies the guess profiles prior to the physical retrieval. Another aspect of retrieval improvement involves taking into account both the time continuity of GOES Sounder radiance observations and the spatial stability of the upper atmosphere within the retrieval process. Lastly, a spatial and temporal filtering operator can be applied to reduce the random and striping noise in the GOES Sounder radiance measurements, while preserving the optimal information for subsequent sounding retrieval generation. The improvement of GOES Sounder products (sounding retrievals, total ozone, etc.) realized via noise reduction will be demonstrated. Together, these improvements are significant for better use of current GOES Sounder data, and are also important in preparation for the next generation of GOES Sounder – the Hyperspectral Environmental Suite (HES), scheduled for launch in 2013.

I. Introduction

The sounder instrument aboard the Geostationary Operational Environmental Satellite series (GOES-8, 9, 10, 11, and 12) currently provides information on the
changes in the atmospheric state using a physically-based retrieval of temperature and moisture profiles. The GOES Sounder typically samples the continental U.S. and surrounding oceanic regions on an hourly basis. As a first step in the retrieval process, guess profiles of temperature and moisture are generated, usually from short-term numerical model forecasts. Thereupon, the first guess profiles are adjusted so that forward calculations match the Sounder measured radiances; this iterative process results in the final retrievals. To date, GOES moisture retrievals have provided a noticeable improvement over the first guess, while temperature retrievals have remained very similar to the first guess. The lack of temperature profile improvement in the physical retrieval process might be caused by insufficient use of the GOES Sounder radiance information or the implementation of the radiative transfer calculation in the physical retrieval. This study demonstrates that both guess temperature and moisture profiles can be improved (by up to ~0.5 K for temperature and ~5% for Total Precipitable Water) when the GOES Sounder radiance measurements are used in a simple statistical retrieval approach.

2. Methodology

The GOES atmospheric temperature, moisture, and ozone retrieval algorithm in this paper is a statistical synthetic regression or regular regression with an option for a subsequent non-linear physical retrieval. The retrieval procedure involves linearization of the radiative transfer model and inversion of radiance measurements. To derive the statistical synthetic regression coefficients, GOES Sounder infrared band radiances are calculated from radiosonde observations of the atmospheric state, generating an ensemble of computed GOES Sounder radiances with associated observed atmospheric profiles. The radiative transfer calculation of the GOES Sounder spectral band radiances is performed using a transmittance model called Pressure layer Fast Algorithm for Atmospheric Transmittances (PFAAST) (Hannon et al. 1996); this model has 101 pressure level vertical coordinates from 0.05 to 1100 hPa. The fast transmittance model uses line-by-line radiative transfer model (LBLRTM) calculations and the high-resolution transmission molecular absorption spectroscopic database HITRAN 2000. The calculations take into account the satellite zenith angle, absorption by well-mixed gases (including nitrogen, oxygen, and carbon dioxide), water vapor (including the water vapor continuum), and ozone.

In the regression procedure, temperature and moisture are regressed together against radiances from CO₂, water vapor, and window bands. This method is often used to generate a first-guess for a physical retrieval algorithm, as is done in the International ATOVS Processing Package (IAPP) (Li et al. 2000) and the operational MODIS atmospheric profile product (Seemann et al. 2003). The statistical regression algorithm for atmospheric temperature is summarized below for cloud-free skies.

The general inverse solution of radiative transfer equation for the atmospheric profile can be written as (Smith 1970)

\[ X(i, k) = A(i, n)Y(n, k). \]  

(1)
Where \( i \) is the number of parameters to be retrieved, \( k \) is the number of profiles and surface data in the training sample, and \( n \) is the number of channels and other predictors used in the regression procedure. The statistical regression algorithm seeks a “best-fit” operator matrix \( A \) that is computed using least squares methods with a large sample of atmospheric temperature and moisture soundings and collocated radiance observations. Minimizing the difference between synthetic observations and the regression model

\[
\frac{\partial}{\partial A} |AY - X|^2 = 0, \tag{2}
\]

yields

\[
A(i,n) = X(i,k)Y^T(k,n)[Y(n,k)Y^T(k,n)]^{-1}, \tag{3}
\]

where \( (Y^TY) \) is the covariance of the radiance observations, and \( (Y^TX) \) is the covariance of the radiance observations with the atmospheric profile.

In the GOES Sounder regression procedure, the primary predictors (\( Y \) in Eq.1) are infrared spectral band brightness temperatures (BTs). The algorithm uses 15 infrared bands with wavelengths between 3.8 \( \mu \text{m} \) and 14.7 \( \mu \text{m} \). Quadratic terms of all BT predictors are also used as separate predictors to account for the non-linear relationship of moisture to the GOES Sounder BTs.

Ideally, the radiance predictors \( Y \) would be taken from actual GOES Sounder measurements and used with time- and space-collocated radiosonde profiles \( X \) to directly derive the regression coefficients \( A \). In such an approach (regular regression), the regression relationship would not involve any radiative transfer calculations. However, radiosondes are only routinely launched twice each day at 0000 UTC and 1200 UTC simultaneously around the earth; GOES Sounder has observation hourly each day. It is therefore possible to obtain many time- and space-collocated radiosondes and GOES Sounder radiances that are globally distributed at a wide range of locations. The advantage of regular regression is avoiding the bias and uncertainties related to the radiative transfer calculations, while the disadvantage is introducing the radiances and RAOB collocation error and lack of matchup samples over regions where RAOBs are not available.

In addition, the synthetic regression coefficients can be generated from GOES Sounder radiances calculated using a transmittance model with profile input from a global temperature and moisture radiosonde database. The advantage of this approach is that it does not need GOES Sounder radiances collocated in time and space with atmospheric profile data; it requires only historical profile observations. However, it involves the radiative transfer calculations and it requires an accurate forward model in order to obtain a reliable regression relationship. Any uncertainties (e.g., a bias of the forward model) in the radiative calculations will influence the retrieval. To address model uncertainties, radiance bias adjustments should be implemented in the retrieval algorithm (Seemann et al. 2003).
3. Training data

Synthetic regression retrievals of atmospheric properties from GOES Sounder require a hemispheric dataset of temperature, moisture, and ozone profiles in addition to estimates of skin temperature and emissivity to train the regression. A new data set consisting of more than 12,000 global profiles of temperature, moisture, and ozone has been created, drawing from NOAA-88, ECMWF, TIGR-3, ozonesondes, desert radiosondes. Radiance calculations for each training profile are made using the PFAAST 101 pressure layer transmittance model. These calculations require a skin T and emissivity value for each profile. In the past, skin temperature and emissivity were assigned relatively randomly to each profile in satellite regression retrieval algorithms, including MODIS atmospheric retrievals (Seemann et al., 2003), ATOVS retrievals (Li et al., 2000), NAST-I retrievals (Zhou et al. 2003). Emissivity was assigned using a mean of 0.84 and standard deviation of 0.15 at 4 μm, a mean of 0.95 at and standard deviation of 0.03 at 9 μm, and linear in between. Skin temperature/surface air temperature difference was given a mean of zero and standard deviation of 10K. Recently, work has been done to better characterize the skin temperature/surface air temperature difference and the global emissivity in order to assign these values to the training profiles using a more physical basis.

To characterize global skin temperature as a function of surface air temperature, and solar zenith and azimuth angles, the MODIS MOD11 land surface temperature product was used together with global radiosondes. For two years (2001-2002) of data, MOD11 and radiosondes were collocated within 3 hours and 0.1 degrees latitude and longitude. The resulting skin T/surface air T pairs were divided into ecosystem groups using the IGBP classification and further separated into 3 solar zenith angle and 7 solar azimuth angle bins.

Work toward preliminary high spectral surface emissivity estimates for use in the training data has also begun. Land surface emissivity is well characterized globally by the same MOD11 product used for land surface temperature, however it is only available at 6 discrete wavelengths: 3.7 μm, 3.9 μm, 4.0 μm, 8.5 μm, 11 μm, and 12 μm. For use with a training data set for high spectral resolution retrievals, the gaps between these wavelengths must be filled in. To address this, we took advantage of some laboratory measurements of emissivity from the MODIS emissivity library (UCSB, Dr. Zhengmin Wan) and the ASTER spectral library (JPL, JHU, and USGS). The drawback to the laboratory measurements is that the materials measured are not physically representative of global ecosystems. For example, the emissivity of a single leaf is not necessarily the same as the emissivity of a canopy of leaves in a forest as seen from a satellite. In order to combine the physically-relevant (though low spectral) MOD11 emissivity measurements and the high spectral laboratory measurements, the MODIS spectral response functions were used to reduce the spectral resolution of the high spectral laboratory measurements (a convolution of sorts). Then all lab spectra (> 200) were compared with the 6 MOD11 emissivity values for each 5km MOD11 point globally to
find the best match. Results were combined by ecosystem, and a histogram of all lab spectra matched with MOD11 points for each IGBP ecosystem was created.

This approach is a promising way to derive high spectral resolution emissivity for use with synthetic regression retrievals, however it would be better performed by matching MOD11 emissivities at 6 wavelengths to high spectral aircraft measurements of a range of real global ecosystems as opposed to laboratory measurements of basic minerals and pieces of vegetation.

In the GOES Sounder retrieval algorithm, the training data set described above is used to generate the regression coefficients. The emissivities at the MODIS spectral bands assigned to each profile are linearly interpolated into the GOES Sounder spectral bands. The radiative transfer calculation of the GOES Sounder spectral band radiances is performed with the PFAAST model for each profile from the training data set to produce a temperature-moisture-ozone profile/GOES Sounder radiance pair. The synthetic regression coefficients (see Eq.(3)) are generated using the calculated radiances and the matching atmospheric profile. 550 coefficients are generated for each training profile, corresponding to different local zenith angles from 10° to 65° with an increment of approximately 0.1°.

The estimated GOES Sounder instrument noise was added to the calculated spectral band radiances before creating the coefficients. The noise was randomly generated with a Gaussian distribution, a standard deviation equal to the NedT plus an estimated forward model error of 0.25K for each spectral band, and a mean of zero (white noise). The correlation in the noise between the spectral bands was not considered in the regression, and it is assumed that any impact of spectral noise correlation on the retrievals should be small. This impact will be further studied in future work.

The predictands, or the parameters to be retrieved by regression, include the temperature profile, the logarithm of the water vapor mixing ratio profile, the logarithm of the ozone mixing ratio, the surface skin temperature and the surface emissivities at 15 GOES Sounder spectral channels. To perform the retrieval, Eq. (5) is applied to the actual GOES Sounder measurements, where $Y$ is now the observed GOES Sounder radiances. Integration of the retrieved profiles yields the total precipitable water (TPW), total column ozone, and three layers of column water vapor (WV1, WV2, and Wv3). Other atmospheric parameters such as 40 levels of temperatures and moistures, as well as stability indices can also be derived from the predictands. The retrieved water vapor mixing ratio at each pressure level is checked for saturation and the mixing ratio at any level with relative humidity greater than 100% is set equal to the saturation mixing ratio at that level.

As a first step in the retrieval process, guess profiles of temperature and moisture are generated, usually from short-term numerical model forecasts. Thereupon, the first guess profiles are adjusted in a physical approach (Ma et al. 1999) so that forward calculations match the Sounder measured radiances; this iterative process results in the final retrievals. To date, GOES moisture retrievals have provided a noticeable
improvement over the first guess, while temperature retrievals have remained very similar to the first guess, at least over the CONUS. The lack of temperature profile improvement in the physical retrieval process might be caused by insufficient use of the GOES Sounder radiance information. In this study, the forecast profile is used together with GOES Sounder radiances to produce the first guess. In practice, the forecast temperature and moisture profiles are used as additional predictors in the regression Eq. (1) in both the regular regression or synthetic regression. Results for this study demonstrate that both guess temperature and moisture profiles can be improved (by up to \( \sim 0.5 \) K for temperature and \( \sim 5\% \) for Total Precipitable Water) when the GOES Sounder radiance measurements are used together with forecast temperature and moisture profiles in a simple statistical retrieval approach. This illustrates that the forecast profiles are used as reference or background in the regression retrieval, and the GOES Sounder radiances make adjustment to the forecast profiles for an improvement, thus the GOES Sounder radiance information are properly used to improve the first guess for the physical retrieval, or generate a simple statistical retrieval. The moisture first guess can be further improved by employing the physical approach (Ma et al. 1999) that accounts for the nonlinearity of moisture to the radiance measurements.

4. Preliminary results

Figure 1. The guess temperature (left panel) and water vapor mixing ratio (right panel) root mean square error (RMSE) (compare with RAOB) from the forecast alone (black line), the GOES Sounder radiances alone (red line), and the combination of the forecast and the GOES Sounder Radiances (green line).

GOES-12 Sounder radiances are used to test the algorithm. Figure 1 shows the guess temperature (left panel) and water vapor mixing ratio (right panel) root mean
square error (RMSE) (compare with RAOB) from the forecast alone (black line), the GOES Sounder radiances alone (red line), and the combination of the forecast and the GOES Sounder Radiances (green line). 368 independent profiles, mostly over the CONUS, are included in the statistics. Figure 2 shows TPW physical retrieval with model forecast as first guess (upper panel), and the TPW physical retrieval with regression (forecast + radiances) as first guess.
The combination of GOES sounder radiances and forecast temperature and moisture profiles provides a better first guess than either forecast alone or the regression retrieval from the GOES Sounder alone.

4. Noise filtering

Spatial filtering of the noise from IR radiance measurements has been tested using GOES-8 data (Plokhenko et al. 2003). The signal-to-noise ratio (SNR) of GOES Sounder radiances can be improved by filtering the spatial structure of the GOES Sounder measurement errors. For example, taking advantage of large spatial gradients in the upper atmosphere, a simple 5 by 5 field-of-view (FOV) radiance averaging would reduce
the noise of band 1 (a stratospheric channel), while still retaining the atmospheric structure in the retrievals. Subsequently, a 4 by 4 FOV radiance averaging can be applied to band 2 (sensitive to tropopause temperature), 3 by 3 radiance averaging to band 3 (sensitive to upper level temperature), and so on. The size of the box used for radiance averaging is based on the weighting function peak of each channel, and is smaller for lower-peaking channels. The surface-viewing channels (6, 7 and 8) will not have spatial smoothing applied, in order to retain the single FOV (10 km nominal spatial resolution) information. Figure 3 shows the GOES-12 Sounder band 1 (14.7 mm) and band 9 (9.7 mm) images before spatial filtering (left panels), after spatial filtering (middle panels), and difference images thereof (right panels). The random noise is filtered by this filtering operator, the impact of noise filtering on the ozone product is positive.

**Band 1: 14.7 µm**

**Band 9: 9.7 µm**

![Before filtering](image1)

![After filtering](image2)

![difference](image3)

Figure 3. The GOES-12 Sounder band 1 (14.7 mm) and band 9 (9.7 mm) images before spatial filtering (left panels), after spatial filtering (middle panels), and difference images thereof (right panels).

6. **GOES time continuity application**

The GOES Sounder provides hourly radiance measurements containing atmospheric sounding and cloud-top property information. Since atmospheric temperature and moisture evolution follows the dynamic rule, and the temperature profile typically doesn’t change dramatically within one hour, it is possible to take the time continuity of GOES observations into account in the sounding retrieval algorithm. For example, one can use the prior retrieval as the first guess, or use the averaged radiances from two time steps (previous and current) for the retrieval. Figure 4 shows the 850 hPa
water vapor mixing ratio from single time step (upper right) and two time steps (lower left). The retrievals are less noisy from two time steps than that from the single time step.

Figure 4. 850 hPa moisture retrieval image with GOES-12 Sounder radiances from current time (t2) (upper right), current time and previous time (t1) (lower left). The forecast (upper left) and retrieval from three times (lower right) data are also shown for comparison. Using time continuity is expected to be better than using a single time alone.

7. Conclusions

Both regular regression and synthetic regression can be used for improved first guess retrieval. The realistic assignment of surface skin temperature and emissivities for each profile in training data set is crucial for a synthetic regression procedure. When the GOES Sounder radiances are used together with the forecast temperature and moisture profiles as predictors in regression, the first guess can be better than either forecasts alone or the regression retrievals from the GOES Sounder radiances alone. Preliminary results demonstrate that the current GOES Sounder radiances can improve the forecast when their information is correctly used. The noise filtering and time continuity application are also studied. Noise filtering and application of time continuity are very important for improving the sounding retrieval.
References


