The Solar Spectrum 360 to 1050 nm from Rotating Shadowband Spectroradiometer (RSS) Measurements at the Southern Great Plains Site

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Abstract. Two years of Langley extrapolations made from the Southern Great Plains (SGP) site of the Atmospheric Radiation Measurement (ARM) Program using two very different RSS instruments and a NIST-derived irradiance scale show larger extraterrestrial solar irradiances in the 400 to 600 nm domain by as much as 4.5% compared to the Labs and Neckels (1968) data. Our results are more congruent with Thuiller et al. [1998] in this domain, but do not show larger irradiances than the Labs and Neckels data at wavelengths less than 400 nm. In addition to the question of the true extraterrestrial solar spectrum, the data we present here are directly useful for the interpretation of spectral measurements calibrated with current NIST irradiance standards, for which we believe this represents the most extensive determination of the solar irradiance.

Introduction. The Rotating Shadowband Spectroradiometer (RSS) is a field instrument developed for the ARM program which couples a CCD spectrograph spanning the wavelength range 360 to 1100 nm with a shadowbanded fore-optic. The RSS provides spectrally-resolved direct-normal, diffuse-horizontal, and total-horizontal irradiances. These three components are guaranteed to have the same passbands and responsivities; thus Langley calibrations can be used for the horizontal surface irradiances as well, producing self-consistent data for radiative transfer calculations.

RSS measurements at SGP have been taken with two versions of the instrument. In 1997 and 1998 the "first generation" RSS instrument was deployed, with a 512 pixel linear NMOS array. Most RSS data used to date for a variety of remote sensing and closure study efforts are from this 1st-generation RSS: Michalsky et al. [1999], Min and Harrison [2000], Mlawer et al. [2000] and Schmid et al. [1999]. In the summer of 1999 we deployed a substantially revised instrument. This "second generation" instrument uses a higher-performance 1024 x 256 CCD array; with this better detector a variety of other instrument design compromises could be revisited and performance substantially improved in resolution, out-of-band-rejection, and dynamic range. Other changes made on the basis of experience improved wavelength stability. Harrison et al. [1999] describe the RSS, compare data from the two instrument generations (which were operated side-by-side for a transition period at SGP), and show the first of the two Langley extrapolation data sets discussed in this paper. Here we show a more extensive Langley extrapolation data set taken with the 2nd-generation instrument, together with more extensive calibration, yielding results closely congruent with our earlier effort (Harrison et al. [1999]).

Langley Regression and Estimation of the Extraterrestrial Instrument Response, V_0

SGP is a low-altitude mid-continental site, with larger aerosol optical depths and associated variability than high-altitude sites commonly preferred for Langley extrapolation efforts. The ARM science mission for the RSS is continuous operation at the SGP facility; consequently calibration of the extraterrestrial instrument response needed for sun-photometry are derived from the routine data using an objective Langley algorithm developed by Harrison and Michalsky [1994]. This has proved practical only because the continuous operation yields sufficient events so that statistics can partially compensate for the higher event-to-event variance.

Here we analyze the "Langley events" observed by this 2nd-generation RSS at SGP from July 27, 1999 through May 23, 2000. This period spanned three irradiance calibrations of the instrument and contained the fall of 1999, which was unusually clear. In routine operation at SGP the RSS makes observations at 60 s intervals. The Langley regressions were done for two airmass ranges: 2 to 6 and 2 to 4.5, to aid statistical tests of aerosol-column impacts on the inferred extraterrestrial irradiances.

The 2-6 airmass range was used by Harrison et al. [1999] and will be shown first to permit closest comparison of the new observations with the earlier ones. Using its standard screening criteria the objective Langley algorithm returned 122 "Langley events" for the 2-6 airmass range analysis, and 115 for the 2-4.5 airmass range; of these 90 events match. The objective algorithm accepts events on the basis of the fraction and residual variance of observations within the airmass range which survive its tests to eliminate cloud passages. The majority of the events do have internal cloud-passage periods which survive the testing. It is not surprising that some events survive when tested over one airmass range, but not the other. The data reported in Harrison et al. [1999] were 27 events.

Each Langley regression is done on the raw instrument output data (instrument counts for each pixel), and yields an optical depth τ, an uncalibrated extraterrestrial instrument response V_0, and associated regression statistics for each pixel. A Langley optical depth spectrum taken by the 2nd-generation RSS from the morning of Nov. 2, 1999 at the SGP site is shown in figure 1. The optical depths are the slope of the Langley regression and do not depend on any instrument calibration. (The wavelength calibration of the instrument is done separately against low-pressure line-emission sources, and not discussed here. It controls the abscissa of the figure, but does not directly participate in the regression.) The top panel of figure 1 is a log-log plot showing the large range of optical depths observed, and the successive subtraction of the O_3 and NO_2 contributions inferred from the measurement. The 300 DU of O_3 inferred for this event is common, and negligibly different from the TOMS estimate of 297 DU for this location and time. However the 0.55 DU of NO_2 inferred for this event is a large column amount, an issue we will return to later. For the purposes of the Langley extrapolation of V_0 the partition of the extinction of these "weak absorptions" does not matter so long as their columns are invariant during the course of the time-series used for the Langley regression. Most of the remaining structure visible in the top panel is dominated by strong absorption bands of H_2O and O_2. Within these bands curve-of-growth causes Langley regression to fail; both τ and V_0, are undetermined. The underdrawn dotted line is the aerosol extinction inferred as an Angstrom distribution. This case is representative of the structure and signal-to-noise seen in the Langley regressions done over one airmass range, but not the other. The inferred aerosol optical depth (0.011 at 500 nm) and high column NO_2 inferred.

The lower panel of figure 1 shows the short-wavelength end of the optical depth spectrum in greater detail. Weak absorption features of O_2-O_2 are seen (Pfeilsticker et al. 1997, Michalsky et al., 1999) and the correlation of the optical depths with the superimposed NO_2 cross-sections is apparent to the eye in the range 400 to 440 nm, where other spectral features do not dominate. This high-NO_2 case was chosen in part so that these can be clearly seen. The K and H solar lines appear ubiquitously as negative residuals in these optical depth spectra, with nearly uniform magnitudes. In the simplest consideration they should not. We attribute these as consequences of both the "Ring Effect" (weak inelastic scattering by atmospheric gases) and less-than-perfect out-of-band rejection in the spectrometer. The inelastic scattering increases as the airmass increases, producing an apparent negative contribution to the local optical depth. Increasing airmass also attenuates the shorter wavelengths far more than longer ones, and very weak stray light contributions from longer wavelengths can manifest themselves similarly. We believe that the Ring Effect contribution is larger than the stray-light contribution for this second-generation RSS data, on the basis of both an estimate from our measured instrument stray-scattering functions (data from Harrison et al. 1999) and a comparison to data from the earlier instrument. For this reason the region below 400 nm is excluded from our V_0 retrieval, together with the weak O_2-O_2 bands. With the NO_2 removed the residual variance of the remaining optical depth is less than ~ 0.002 RMS; some of the remaining variability is due to inexact matching of NO_2 cross-section data to our instrument's observing function, and other weak trace-gas absorption not considered.

The Langley-extrapolated V_0 data from the 122 airmass-range 2-6 events are shown top-to-bottom in a false-color image in the lower panel of figure 2. These are the sequential events, with varying intervals between them. There are 23 days of events (~a third of the total events) which are the morning and afternoon of the same day. The longest interval between events is 12 days. Pixels are non-linearly short-wavelength to long, left to right. Each horizontal bar of pixels is a color-coded single V_0 spectrum with sequence black, brown, red ... gray, violet white. The thresholds were adjusted to maximize the perception of gradients.

A single raw V_0 spectrum is plotted conventionally for the comparison in the middle graph with the same pixel abcissa registration as the false-color presentation below it. This is the Nov. 2 event shown in figure 1; it is the 42nd spectrum in the image below. The undeviating vertical lines of the absorption features emphasize the long-term wavelength stability. No wavelength fitting has been necessary with these data. Horizontal "bars" are outlier Langley events, shown further below. Black spots are data where the regressions for individual pixels exceeded a variance criterion; these are not accumulated in further averaging. The lack of trend top to bottom is a general indicator of instrument throughput stability; the apparent exception seen around pixel 820 - 847 lies in the 820 - 847 nm H_2O band. Within strong absorption bands curve-of-growth causes Langley regression to fail; both τ and V_0 are underestimated. The seasonal trend in H_2O from July to December is then evident.

On closer examination trends in V_0 with time can be discerned in this rich Langley regression series. We compute the trends within the Langley series by applying linear and second-order least-squares polynomial fits. The ratio of the fitted V_0 are then computed for two date-pairs: July 7 199 and March 10, 2000, and then Feb. 8 2000 and March 10, 2000. On these three dates field irradiance calibrations were done on the instrument against our portable LiCor calibrator, which in turn had been calibrated against a pool of NIST FEL lamps (Kiedron et al. 1999) and concurrently as part of the ARESE II field calibration efforts (Kiedron, ??). These data show that the Langley estimates of the trend (a trend in instrument responsivity) closely match the ratios of responsivities seen against the portable calibrator. The close congruence of the linear and second--order fit predictions demonstrates that a linear trend explains the observations well. This conclusion is supported by the nearly identical values for the estimated 1-_fractional precision of the residuals from the regression for the two schemes; the second-order scheme does no better except in the H_2O bands, where it fits the seasonal artifact of the H_2O column discussed previously.

Figure 5 shows our extrapolated solar irradiances from the 1997 effort (Harrison et al., 1999, identified as "RSS-512," in blue) and the results of our 1999-2000 observations from the new instrument ("RSS-1024," in red) both presented as ratios to the "Old Kurucz" extraterrestrial spectrum from MODTRAN 3.4. This extraterrestrial spectrum has been superseded, but is used here for a common denominator for both as it was used for our earlier work.

The fidelity with which we reproduce the inferred ET spectrum in the two experiments is very encouraging. These two experiments are completely independent in the instrument used (the 2nd-generation RSS having 3 times the resolution, completely different detector and electronics), temporally, in angular fore optic calibrations), and the pool of observations. They share only the calibration to the ARM-NIST irradiance lamp pool, but that done two years apart. In the wavelength range 390 to 800 nm the largest apparent discrepancies which are not obvious curve-of-growth features are in the domain of the gamma band of O_2 (near 630 nm) and a weak H_2O feature at slightly longer wavelengths. (These can be seen in the top panel of figure 3.) Discounting these the smoothed discrepancy between our two sets of observations is congruent with the 0.1% - 0.2% (increasing to shorter wavelengths) 1-σ estimate of the precision of the V_0 values from the significantly smaller 1997 dataset.

Figure 1b: An Optical Depth (τ) Spectrum from a Langley Regression, Data at SGP Nov 2, 1999

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Figure 2: V_0 Spectra from Langley Regression 2-6 airmasses, 2nd generation RSS at SGP

Figure 3: Trends in V_0 (normalized to 1 AU), 2-6 airmass range, 2nd generation RSS at SGP

Estimation of systematic error due to aerosol optical depth interferences

The reproducibility demonstrated here is so good that the true error is almost certainly dominated by systematic issues not addressed simply by looking at the variances between the two independent efforts. Here we discuss potential systematic errors arising from the Langley extrapolations, and in a following section we further discuss potential systematic errors of our irradiance scale and transfer to the instrument.

Schmid et al. (1999) report an intercomparison of sunphotometers at the SGP in 1997 which included the first-generation RSS. While several of the participating sunphotometers used V_0 estimates obtained from high-altitude measurements conducted elsewhere, the RSS estimations of the aerosol optical depths were based solely on the V_0 results of the Langley pool discussed in Harrison et al. (1999) and repeated here in figure 5. The congruence of the aerosol optical depths obtained are thus an effective test for systematic discrepancies between either data quality or reduction methods between these very different instruments and sources of calibration. The first-generation RSS data produced aerosol optical depths which agreed with the AATS-6 instrument (taken to have the best calibration) to within the 1-σ error limit predicted from the variance of our Langley pool. This gives us confidence that we do not have a basic error in application of the Langley process.

Figure 6 shows a scattergram of the V_0 vs. total optical depth at 500 nm for the 2-6 airmass range cases, the data from figure 2. The abscissa value at the left limit of the plot is set to 0.1436, the Rayleigh optical depth for 500 nm from the Kasten approximation. The aerosol optical depths are thus approximately the total optical depth minus a further small decrement for Chappuis-band O_3; with the assumption of a climatological O_3 column of 339 DU the mean aerosol optical depth of the observations is 0.076 at 500 nm. The low correlation to the linear-fit is evident; the correlation coefficient is -0.0148. Thus there is no strong evidence for any systematic effect due to aerosol optical depth.

Nonetheless we were not completely relieved, because a modeling effort shows that aerosol optical depths can affect the extrapolated V_0 values when τ_{aer} is significant, and the aerosol is not distributed uniformly in altitude. The latter is of course almost a certainty. In this case if the airmass factor appropriate for a uniformly mixed species (e.g. Kasten's approximation) is assumed for simplicity as we have done for these data then the V_0 estimates exhibit a systematic error which grows approximately as m^2, where m is the limiting airmass factor used in the regression. In order to provide a direct assessment of the potential magnitude of such systematic effects on our data we re-ran the Langley regressions over the airmass range 2 - 4.5 and compared the ratios of V_0. We delay some further discussion to the conclusions.

Figure 6a: Ratios of V_0 determined from two airmass ranges.

Figure 6b: Scattergram of V_0 vs τ at 500 nm

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Figure 7: ARM's pool of NIST 1000 Watt FEL Lamps

The ARM/NIST Irradiance Scale

We maintain the ARM spectral irradiance scale, and transfer to the SGP site irradiance calibrator(s). The issue of ARM spectral irradiance scale is now particularly important as all ARESE II spectral calibrations have been done against this "ARM/NIST working standard." For the '97 IOP we established this as the mean of the three NIST FEL lamps F403 - F405, discarding F340 as an evident outlier. Measured spectral ratios of these lamps' outputs relative to their stated output are shown in figure 7, from Kiedron et al. (1999). The red and blue curves show the repeatability of these measurements 1 day apart. Repeatability over 6 months is not significantly worse.

NIST recalibrated our lamp F340 in July 1999. This recalibration demonstrates that the mean of the three ARM working lamps F403 through F405 is indeed very close to NIST's working irradiance source, and allows us to use this pool as representing the NIST standard despite the distressing variance among the individual lamps with their production calibrations by NIST seen here.

Figure 4: Precision of detrended V_0 estimates from Fig. 3

Figure 5: 1997 and 1999-2000 extrapolated Solar Irradiances, ratios vs "Old Kurucz"

References