Objective Algorithms for the Retrieval of Optical Depths from Ground-Based Measurements

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key words: radiometry, turbidity, optical depth, Langley regression, remote sensing

Abstract

Optical depth retrieval via Langley regression is complicated by cloud transits and other time-varying interferences. An algorithm is described that objectively selects data points from a continuous time series and performs the needed regression. The performance of this algorithm is compared by "double blind" test with analysis done subjectively. The limits to accuracy imposed by time-averaged data are discussed., and an additional iterative post-prrocessing algorithm is described that improves the accuracy of optical depth inferences made from data with time-averaging periods longer than 5 minutes. Such routine algorithms are needed to provide intercomparable retrievals of optical depths from widely varying historical data sets, and to support large networks of instruments such as the Multi-Filter Rotating Shadowband Radiometer (MFRSR).

Introduction

The analysis of direct beam extinction measurements by the technique of Langley regression[1] is the principal source of data for changes in atmospheric opacity due to changing aerosol burdens.[2,3,4,5,6] With current concerns over anthropogenic climate modification, and the effects of recent volcanic eruptions, a variety of research programs are placing increased emphasis on the routine measurement of atmospheric optical depths at a range of wavelengths, from a substantially increased number of sites. An objective and automated method of analysis is needed both to keep up with the substantially increased data flow, and to provide assurance that the results are not being biased (either by site, or over time) by change of analyst, or subtle changes of the analyst's preference.

Our particular motivation for this work has been the development of the Multi-Filter Rotating Shadowband Radiometer.[7] The MFRSR instruments provide spectrally resolved total-horizontal, diffuse-horizontal, and direct-normal irradiances at seven wavelengths through the use of an automated shadowband technique. The retrieval of the extra-terrestrial irradiance (E_0) via Langley regression is of particular utility for the MFRSR, because the automated shadowband technique guarantees that the calibration coefficient is identical for the three components, and so the observations of E_0 (suitably corrected for the astronomical distance) provide a long-term calibration for the instrument. However the algorithm described here is general to any measurement of direct-normal spectral irradiance at a passband that does not experience curve-of-growth deviation from the Bouguer law.[8]

Langley Regression

The basic Langley method is a straightforward application of the Bouguer law, and linear regression. In it's most familiar form the Bouguer law relates extinction through a path of a uniform medium

$$\frac{L(x)}{L(0)} = e^{-\tau x}$$

Here L is a measured spectral radiance, x is an arbitrary path length, and τ, the "optical depth," is a differential extinction per unit path length. The Langley method consists of using the progress of the sun's apparent motion that changes the observed path length through the atmosphere to compute an optical depth. The assumptions required are that the extinction of the atmosphere can be described as uniform horizontal lamina that do not vary during the course of the time-series used for the analysis, that the Bouguer law is applicable to the spectral passband in question, and that the effective path length through the atmosphere can be correctly calculated.

Several authors[9,10,11] discuss potential errors in this extrapolation due to violation of the principal assumptions of the regression; that the atmosphere can be described as stationary horizontal lamina. Curve-of-growth failure of the Bouguer law for finite passbands containing multiple absorption lines is explained by Goody.[8]

Standard techniques have been developed to estimate the path length by computing the apparent solar position from a known location and time, and applying corrections for the atmospheric refraction. The results are generally expressed in the unit of "airmass," where the value one represents the path at the zenith. In this work all calculations have been done using the solar ephemeris algorithm published by Michalsky[12], with refraction corrections applied using Kasten's approximation[13].

The Langley method then consists of transforming the Bouguer law into the form

$$l n E(A_n) - l n E(0) = - \tau A_n$$

where there are n observations (n >> 2) of the received direct-normal spectral irradiance E at calculated airmass values A_n. "Best-fit" values for the coefficients ln E(0) and τ in this over-determined linear system can then by found, most commonly by least-squares regression.

An Objective Langley Regression Algorithm

The simple-minded notion of using a least-squares regression on *all* the data only works under true clear-sky conditions. Cloud transits (even thin cirrus) produce "dips" that must be removed or the regression will produce nonsense results.

To date this has been done by subjective editing; a scientist examines the data graphically and chooses the points to be used for the regression. Aside from being quite labor intensive this process is subject to criticism on the basis that differing analysts may arrive at different results, and that descriptions of the criteria are difficult to use either for the training of analysts, or to standardize procedures.

An objective algorithm has been developed that operates on a time series of direct-normal irradiance observations. It can be described as a series of sequential filters that reject points:

* First the analysis intervals (either morning or afternoon) for each regression are selected by the airmass range from 2 to 6. Lower airmasses are not used (even if available in the data) because the rate-of-change of the airmass is small, creating a greater opportunity for changing atmospheric conditions to affect the regression. Higher airmasses are avoided due to greater uncertainty in airmass caused by refraction corrections that are increasingly sensitive to atmospheric temperature profiles.

* If needed by instruments such as the MFRSR, corrections to the direct-beam intensities (to correct non-ideal Lambertian diffuser performance) are made as described by Harrison et al.[7].

* A forward finite-difference derivative filter then identifies regions where the slope of dE/d(Airmass) is positive. These cannot be produced by any uniform airmass turbidity process, and are evidence of the "recovery" of the direct-normal irradiance from a cloud passage. The algorithm then computes a starting time for the interference by assuming an equal interval prior to the minimum. The entire region is then eliminated. If the data have been taken at rates higher than 1 per minute, then the derivative is calculated using a running "block average" over one minute samples -- this is done due to common experience that cloud transits generally last several minutes, and so that derivatives due to noise will not dominate this filtering process if very rapid sampling is done (where the real ΔE may then be small).

* A subsequent finite-difference derivative filter tests for regions of strong second derivatives. Regions are eliminated where the first derivative is negative, and more than twice the mean. This filter rejects points near the "edge" of intervals eliminated by the first filter if it was insufficiently aggressive, and

also eliminates any cloud passage that occurs at the end of the sampling interval where the data are truncated before a region of positive derivative can occur to trigger the first filter.

* *Two iterations* are then made to affect a robust linear regression as follows:

    A conventional least-squares regression is performed on the remaining points. The regression is done using the standard computational technique of LU Decomposition, with subsequent back-substitution.

    The standard deviation of the residuals of the remaining data points around the regression line are computed. A sweep is then made through the data points eliminating all points more than 1.5 standard deviations from the regression line.

* The points that remain are used for a final least-squares regression that yields the final analysis product. If time-averaged data are used a final correction step may be necessary as discussed in a following section.

Techniques such as singular-value decomposition are never needed for this simple system; only rarely does this system become close to singular, and in such cases visual examination of the data demonstrate that no retrieval of optical depths is conceivable.

In many cases the regression is non-singular, but not useful. This can occur simply because the entire interval was overcast. An important goal of this algorithm development has been to arrive at a method that is completely automated, and can simply be applied on a routine basis to the time-series data with no subjective preparation or subsequent selection. On the basis of the intercomparisons shown below two fixed error criteria select the Langley regressions that are to be kept for further use: a minimum of 1/3 of the initial data points must remain after the filtering; and these points must show a residual standard deviation the variance around the regression line $(\ln(E) -$

$(\ln(E_0)-\tau A))$ of no more than 0.006. This error estimator is a *ratio* of intensities, and hence is independent of both the optical depth being measured, and the absolute calibration of the detector.

Example Performance

The following example demonstrates the algorithm's behavior for a typical case where clouds are seen, but a Langley regression is still obviously possible. Figure 1a shows the time-series of the three irradiance components (direct-normal, diffuse horizontal, and total-horizontal) observed by the instrument. Only the direct-normal observations are used for the optical depth analysis. This example is taken from a multi-filter instrument operating at Rattlesnake Mountain Observatory (RMO, 46.40¡ N, 119.60¡ W, elevation 1088 m), rather than the data used for the intercomparisons shown later; the higher data rate taken at RMO makes the time-series of the irradiance components (figure 1a) much clearer to the reader.

Figure 1b shows the Langley regression for the morning interval identified by the objective algorithm, and the symbols illustrating the data points identify the filtering process: the points marked with a "+" contribute equally to the regression. Points marked with a small open box were discarded by the derivative filters. These remove the distinct cloud passage at ≈9:00 LMT.

The first iteration of the robustifying filters removes a weak cloud passage that is inconspicuous (but visible) in the time-series plot at ≈7:45 LMT. These points are marked with a box and cross. The second iteration removes two points marked with a solid black box. These would not materially affect the regression results if retained, but this second iteration is very important if the data are noisier.

The most convincing visual argument that the algorithm works well is to examine many cases, including those that clearly should not be used for optical depth analysis. We have done so, but cannot easily present them to the reader. Instead, statistical summaries are presented below. However these visual inspections demonstrate that the algorithm selects plausible subsets of the data that satisfy human observers in all but utterly hopeless cases. In total overcast, or conditions with a few very short (1-2 data point) intervals where the direct beam has perhaps been free of obstruction the algorithm may compute a clearly aphysical positive slope. However in all such cases the criteria used to determine whether the results of the regression should be kept are wildly exceeded.
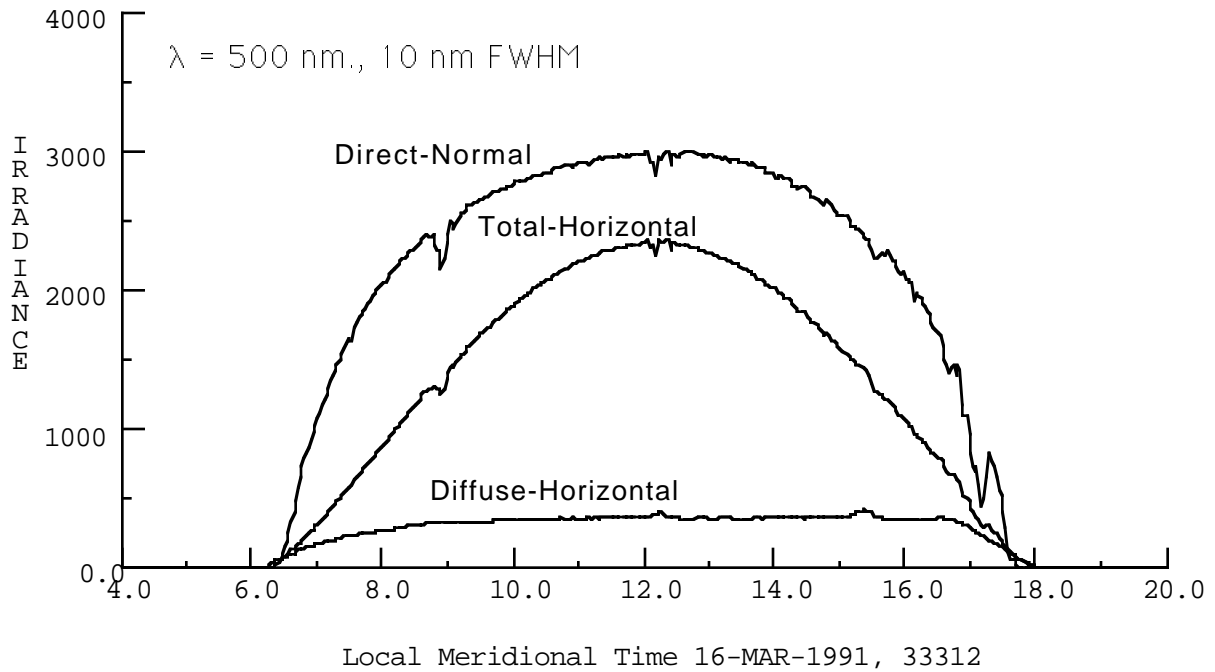
Figure 1a: Time-series of observed irradiance components for an example case
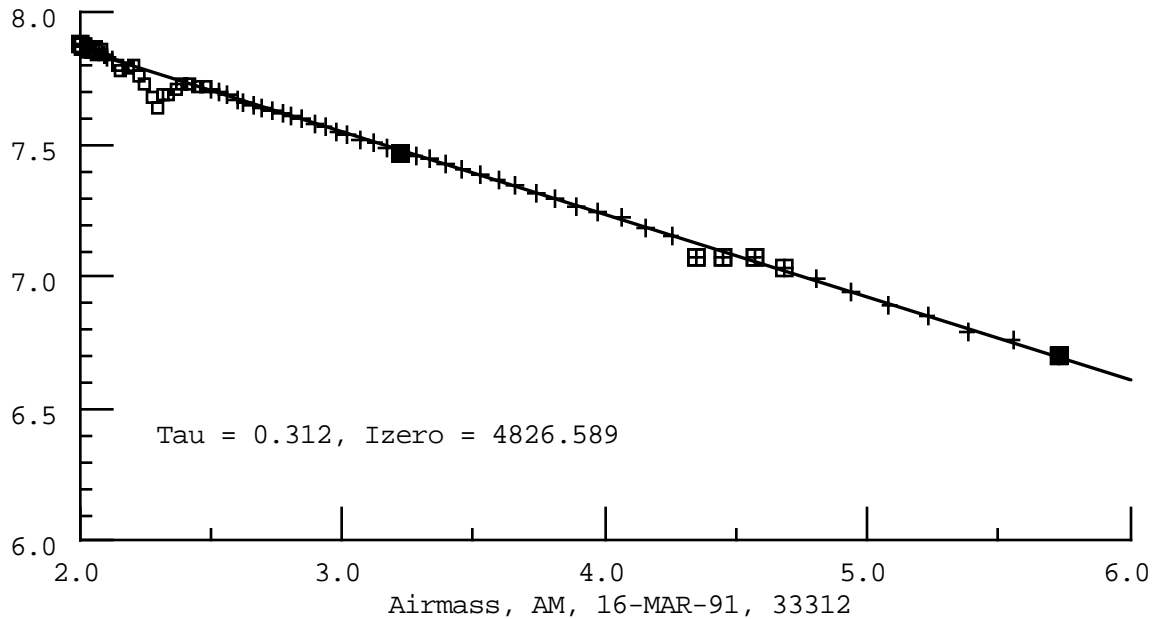(the irradiance scale is uncalibrated)

Figure 1b: Objective optical depth retrieval for the morning shown in **1a** [the ordinate
is ln(uncalibrated Direct-Normal irradiance)]

Algorithm Intercomparison Results

Tests of this algorithm were made using a data set taken at the NOAA Environmental Resources Laboratory in Boulder (40.0¡ N, 105.2¡W, 1634 m ASL) with a single-channel photopic passband Rotating Shadowband Radiometer. This instrument was one of our first to be deployed, and used a LI-COR 210SX detector (LI-COR Inc., Lincoln NB), rather than our more recent multiple-channel instruments.

These data are used for the algorithm testing because they were previously analyzed using conventional subjective analysis for the purpose of studying the Mt. Pinatubo eruption, and are a challenge for optical depth analysis. Boulder is known to be a difficult site due to circulation of the urban pollution in the Denver basin, and rapidly varying high-altitude cloud patterns associated with wave and advection phenomena caused by the Front Range to the west. Consequently NOAA maintains a separate facility at Niwot Ridge for photometer intercomparison rather than doing so at Boulder. Further, these data are *five-minute averages* of 15 second samples. This reduces the filtering efficiency of the derivative filters, and produces a very demanding test of the algorithm. We recommend that data used for Langley analysis be single observations; we present these data as evidence that the algorithm can work sensibly with data averaged up to such an interval. This is important for the application of this algorithm to historic data sets, as many of these were time-averaged during sampling.
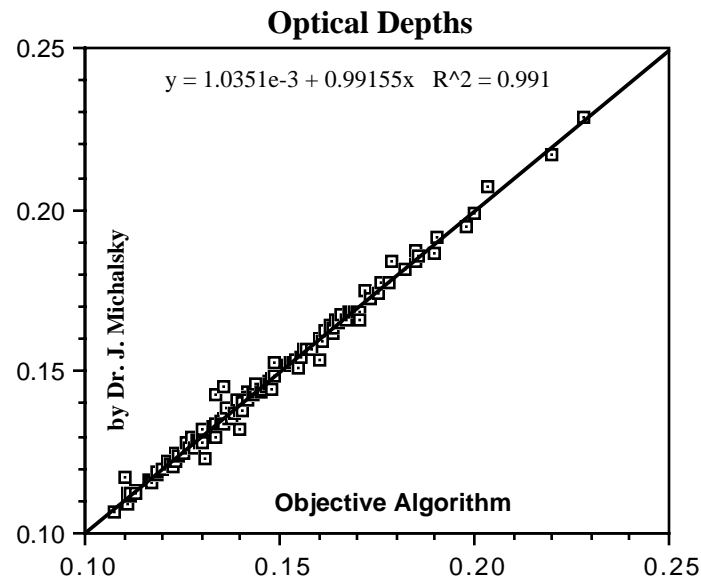
Optical Depths

$$y = 1.0351e\text{-}3 + 0.99155x \quad R^2 = 0.991$$

by Dr. J. Michalsky

Objective Algorithm

Figure 2: Comparison of total optical depths retrieved by the two analyses

Data files for the interval from May 23, 1990 to July 16, 1991 were selected for comparison; they contain 384 days of nearly uninterrupted operation of the instrument. The subjective analyst identified 151 Langley observations (either a morning or afternoon regression) during this period. When run using the selection criteria that require an minimum of 1/3 of the points to be retained, and standard deviation of ln(I) around the regression line less than 0.006, the objective algorithm identifies 143 observations. From these two lists 139 observations match. Figure 2 shows the correlation scattergram with a least-squares regression fit of the total optical depths recovered by the two analysis methods for these 139 matching events.

Readers familiar with data taken by hand-held sun photometers may be surprised by the large number of optical depths retrieved (≈ 0.36 events per day), particularly from an apparently difficult site. This is not a consequence of the retrieval methods, rather a demonstration of the advantage of automated observation. Even 5 minute averages produce many more points during the interval bounded by airmasses 2 and 6 than are typically taken by human operation. Further, people are rarely so dutiful morning and afternoon, day after day.

Figure 3 shows the correlation scattergram with a least-squares regression fit for the extrapolated extraterrestrial irradiance E_0 recovered by the two analysis methods. The units are the uncalibrated output of the detector, and this

irradiance has not been corrected for the variation in the astronomical distance, that accounts for approximately half of the range in these values.
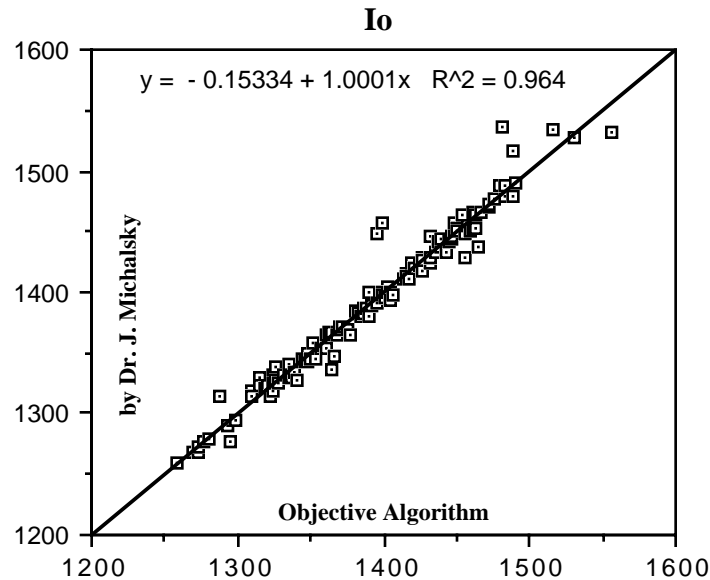

Figure 3: Comparison of the extrapolated zero-airmass irradiance retrieved by the two analyses (uncalibrated)

The E_0 value requires an extrapolation of at least one airmass (and as implemented by the objective algorithm at least two airmasses), and so small differences in the attributed optical depth may produce much larger changes in E_0. The remarkable agreement between the two algorithms as demonstrated by figures 2 and 3 (that show correlation coefficients of 0.995 and 0.982 for the retrieved optical depths and extraterrestrial irradiances respectively) enhances our confidence that the inferences are physically meaningful rather than a result of particular analyst or algorithm preference.

Study of the few cases rejected by one of the analysis methods but kept by the other demonstrate that the subjective analyst kept regressions based on a short contiguous interval (i.e. "one short hole in the clouds") that were rejected by the objective algorithm for an insufficient total number of points. Conversely the objective algorithm kept a few regressions that used points without nearby neighbors. This difference can be viewed as a preference, and in the absence of an external arbiter of truth the relative merit is difficult to assess. These few cases do not affect the aggregate statistics.

Using $E_0(\lambda)$ for In-Situ Calibration against the Solar Constant.

After adjustment for the variation in the astronomical distance the extraterrestrial irradiance should match the solar output. Through the visible and near infrared the solar output is stable to $\approx 0.3\%$ and is strongly correlated with sunspot number.[14] Our sun is a far better standard than light sources commonly used for irradiance calibration. Thus in principle the observations made by an instrument measuring the direct-normal irradiance over a passband for which the Bouguer law applies can be made self-calibrating against the solar constant through the mechanism of Langley regression.

Individual regressions do not constitute a suitable calibration unless made under remarkably good conditions (e.g. Mauna Loa). However these variations are not systematic, and so accuracy can be improved by averaging provided that the instrument's response remains stable for the averaging period. Figure 4 shows the distribution of E_0 values observed by the instrument using the detector calibration coefficient provided by the manufacturer, and normalizing all measurements to an earth-sun distance of 1 AU.
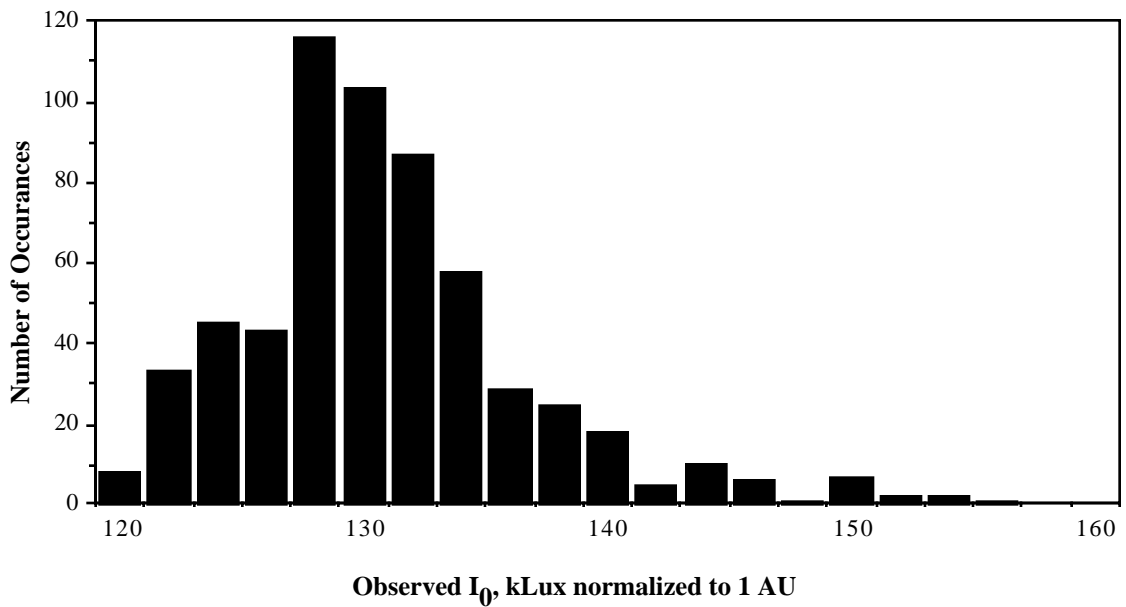
Figure 4: Histogram of retrieved I_0 using a laboratory calibration

Figure 4 contains almost four years of Langley observations, so that the distribution can be shown with a greater number of bins. The photometer was calibrated by the manufacturer using a standard lamp[15] with a spectral response traceable to the National Institute of Standards and Technology, at a 3σ uncertainty of 5%.

The mean of the distribution shown in figure 4 is 130.79 kLux, with a standard deviation of 5.94. It is a common practice to use the E_0 value as a quality control estimator for Langley regressions, and discard extreme events. If only the central $- 2\sigma$ range of this distribution around its mean is sampled then this subset contains 95% of the points, with a mean and standard deviation of 130.02 and 4.57 kLux respectively -- no substantial change. Another commonly used robust estimator is the median: 129.99 kLux with 95% confidence-interval limits of 129.61 and 130.37 kLux respectively.

The standard estimator of the uncertainty of the mean estimated from a finite sample of a random process is $c\sigma n^{-1/2}$, where $1 < c < 2$ depending on the distribution of the process. Thus roughly 40 Langley observations are needed *at this rather difficult site* to reduce the 1σ uncertainty in the inferred E_0 to less than one percent. At the Boulder site this can be typically obtained in less than three months of operation. Sub-intervals of the data show no statistically significant trend, thus demonstrating excellent stability.

A calibrated retrieval can be directly compared to published values. The CIE recommends[16] the value of 127.5 kLux (Lux = lumens/meter^2) for the direct normal illuminance at the mean solar distance. However the convolution of the CIE photopic response and the extraterrestrial spectral irradiance data from Neckel and Labs[17] produces 133.6 kLux for this photopic solar constant. Further there are additional uncertainties associated with the photopic response of the LI-COR photometer, that does not match the ideal photopic response exactly, and the subsequent impact on the laboratory calibration against the standard lamp.

The retrieval of the photopic solar constant done above has a smaller uncertainty in precision, and is centered within the range of the laboratory uncertainties. This is remarkable considering the difficult site. Thus the ongoing retrievals of E_0 are a better estimator of instrument stability than typical laboratory calibrations, and provide a mechanism whereby instrument calibrations can be retrospectively analysed, and data adjusted for improved understanding of the solar spectrum or instrument passband.

Laboratory uncertainties are reduced for narrower passbands. The correction of residual errors in Lambertian response (that is an important contributor to errors in retrieved E_0) is much better for our newer MFRSR instruments compared to the Li-COR detector. Consequently we expect the agreement between laboratory calibration and inferred solar constant to have lower uncertainties, but have not yet acquired sufficient data to demonstrate this.

The Consequences of Time-Averaging

Modern automated instruments operating at wavelengths from the UV-A through the near infrared have little need to average data over time spans sufficiently long to be of concern for Langley regression. However most of the historic data were time averaged, and new instruments with high spectral resolution working at more extreme wavelengths (e.g. UV-B spectroradiometers, and interferometric Fourier transform instruments in the infrared) have intrinsic integrating times that may limit the utility of Langley regression.

It has been common practice to assume for the purposes of Langley regression that a time-averaged irradiance measurement can be treated as a instantaneous measurement made at the airmass calculated for the center time of the measurement interval. This is only approximately correct; in general the mean irradiance measured over a range of airmass is not equal to the instantaneous irradiance measured at either the mean airmass *or* the mean time associated with the interval. We might wish to compute an effective airmass A^* associated with an averaging interval from t_1 to t_2 to be used for Langley regression:

$$\frac{1}{t_2 - t_1} \int_{t_1}^{t_2} e^{-\tau A(t)} dt = e^{-\tau A^*}$$

This formulation assumes that the extinction is described by the Bouguer law, and requires the optical depth τ. It is not analytically tractable because of the complexity of the function $A(t)$, the airmass as a function of time, but can be numerically evaluated for any particular interval.

It is illustrative to consider the somewhat impractical case of a uniform average *as a function of airmass,* for which the direct-normal irradiance measured at A^* is equal to that averaged over the airmass interval A_1 to A_2

$$\frac{1}{A_2 - A_1} \int_{A_1}^{A_2} e^{-\tau A} dA = e^{-\tau A^*}$$

that easily integrates to

$$\frac{1}{-\tau(A_2 - A_1)} (e^{-\tau A_2} - e^{-\tau A_1}) = e^{-\tau A^*}$$

Thus for the purpose of retrieving optical depths and associated extraterrestrial irradiances the A^* airmass associated with the measurement interval should be substituted. The effect of the negative exponential of A^* in the equation above is that A^* is always smaller than the midpoint airmass. Further, if *time* averaging over intervals sufficiently long that the uniform airmass averaging assumption implicit in this formulation is violated then the apparent diminution of A^* (compared to the mid-interval airmass) is magnified by the fact that dA/dt is smaller at lower airmasses.

For averages comprised of a finite number of samples at known times or known airmass the magnitude of the A^* adjustment, and it's resulting impact on inferred optical depths and extraterrestrial irradiances, can be assessed by numerical test. For averaging intervals of five minutes, total optical depths no greater than 0.3, and using data from airmass 2 to 6 for Langley regressions, exact calculations applied to a set of real events show that the use of the airmass at mid-interval time causes errors no larger than ≈ 0.004 optical depths, and 0.18% for the extraterrestrial

irradiances. We judge these to be negligible in comparison to other errors, and so the analyses done in this paper have used this approximation.

However these errors grow as a high order of the averaging time. Corrections should be considered for averaging intervals longer than five minutes or large optical depths. The objective algorithm implements an additional iterative correction step if the data are averaged for more than 5 minutes. For such data an initial trial for the objective regression is made using the airmass associated with the mid-interval time. This retrieves an estimate of the τ. A* values are then computed for each of the averaged observations kept by the objective algorithm, and the least-squares regression redone. It is not necessary to iterate this process more than once to drive residuals below 0.001 optical depths.

Conclusions

An objective analysis algorithm has been developed to perform the Langley regressions. This algorithm has been tested by intercomparison with subjective reduction, and comparison of the retrieved extraterrestrial irradiances against laboratory calibrations and the solar constant.

The objective algorithm retrieved 92% of the regressions retrieved by the subjective analysis. (This is a retrieval efficiency of "possible" events as defined by the subjective analysis, not fraction of all events.) It retrieved 2% of events rejected by the analyst.

The optical depths retrieved by the two methods intercompare with a geometric RMS deviation of 0.003 optical depth. This may be taken as the limit of accuracy for optical depth retrievals imposed *by the choice among reasonable methods of analysis* for time series that include the full range of clouds and other atmospheric phenomena.

The determinations of the extraterrestrial irradiance agree well with the known solar spectrum and laboratory calibrations. At a difficult site the standard deviation of single measurements is ≈5%. The deviations are not systematic, and repeated measurements can be used to reduce the uncertainty provided that the instrument has sufficient short-term stability. Thus these retrievals can provide a free long-term stability test for the instrument, and permit the instrument calibration to be tied to the solar output.

The algorithm operates well with single samples or time-averaged measurements. For instruments that can do so we recommend single samples at a data rate of at least 1 per minute. For averaging intervals of longer than 5 minutes a bootstrap technique is used to improve the accuracy of inferred properties. This is useful for the analysis of historic data or instruments that require such integrating times. However for averaging intervals substantially longer than 5 minutes the utility of Langley regression is reduced simply because the number of independent points can become marginally sufficient.

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