Objective algorithms for the retrieval of optical depths from ground-based measurements

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Optical depth retrieval by means of 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 required regression. The performance of this algorithm is compared by a double-blind test with an analysis done subjectively. The limits to accuracy imposed by time-averaged data are discussed, and an additional iterative postprocessing algorithm is described that improves the accuracy of optical depth inferences made from data with time-averaging periods longer than 5 min. Such routine algorithms are required to provide intercomparable retrievals of optical depths from widely varying historical data sets and to support large networks of instruments such as the multifilter rotating shadow-band radiometer.

Key words: Radiometry, turbidity, optical depth, Langley regression, remote sensing.

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 caused by changing aerosol burdens.[2–6] 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. Researchers need an objective and automated method of analysis 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 a change of analyst or by subtle changes of the analyst's preference.

Our particular motivation for this research was the development of the multifilter rotating shadow-band radiometer (MFRSR).[7] The MFRSR instruments provide spectrally resolved total-horizontal, diffuse-horizontal, and direct-normal irradiances at seven wavelengths through the use of an automated shadow-band technique. The retrieval of the extraterrestrial irradiance (E_0) by means of Langley regression is of particular utility for the MFRSR, because the automated shadow-band 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 its most familiar form the Bouguer law relates extinction through a path of a uniform medium,

$$\frac{L(x)}{L(0)} = \exp(-\tau x).$$

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 the use of the progress of the Sun's apparent motion that changes the observed path length through the atmosphere as a way 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

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spectral passband in question, and that the effective path length through the atmosphere can be correctly calculated.

Several authors[9–11] discuss potential errors in this extrapolation caused by a 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] Researchers have developed standard techniques to estimate the path length by computing the apparent solar position from a known location and time and by applying corrections for the atmospheric refraction. The results are generally expressed in units of air mass, in which the value one represents the path at the zenith. In this research we have made all calculations by using the solar ephemeris algorithm published by Michalsky,[12] with refraction corrections applied through the use of Kasten's approximation.[13]

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

$$\ln E(A_n) - \ln E(0) = -\tau A_n,$$

where there are n observations ($n \gg 2$) of the received direct-normal spectral irradiance E at calculated air-mass values A_n. Best-fit values for the coefficients $\ln E(0)$ and τ in this overdetermined linear system can then be found, most commonly by least-squares regression.

Objective Langley Regression Algorithm

The simple-minded notion of using a least-squares regression on *all* the data works only 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 different 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.

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

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

(3) A forward finite-difference derivative filter then identifies regions where the slope of $dE/d(\text{air mass})$ is positive. These cannot be produced by any uniform air-mass turbidity process, and they are evidence of the recovery of the direct-normal irradiance from a cloud passage. The algorithm can then be used to compute 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/min, then the derivative is calculated through the use of a running block average over 1-min samples. This is done because it is common knowledge that cloud transits generally last several minutes, and so that derivatives caused by noise will not dominate this filtering process if rapid sampling is done (where the real ΔE may then be small).

(4) We used a subsequent finite-difference derivative filter to test 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 it also eliminates any cloud passage that occurs at the end of the sampling interval where the data are truncated before a region of positive derivation can occur to trigger the first filter.

(5) 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 through the use of the standard computational technique of LU decomposition, with subsequent backsubstitution. 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 that are more than 1.5 standard deviations from the regression line.

(6) 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 demonstrates that no retrieval of optical depths is conceivable.

In many cases the regression is nonsingular but not useful. This can occur simply because the entire interval was overcast. An important goal of this algorithm development was 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 of 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 in which clouds are seen but a Langley regression is still obviously possible. Figure 1(a) 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 multifilter instrument operating at Rattlesnake Mountain Observatory; 46.40 °N, 119.60 °W, elevation 1088 m) rather than from the data used for the intercomparisons shown later; the higher data rate taken at Rattlesnake Mountain Observatory makes the time series of the irradiance components [Fig. 1(a)] much clearer to the reader.

Figure 1(b) 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 cross contribute equally to the regression. Points marked with an open square were discarded by the derivative filters. These remove the distinct cloud passage at ≈9:00 local meridional time. The first iteration of the filters removes a weak cloud passage that is inconspicuous (but visible) in the time-series plot at ≈7:45 local meridional time. These points are marked with crossed squares. The second iteration removes two points marked with a solid square. These would not materially affect the regression results if retained, but this second iteration is important if the data are noisier.

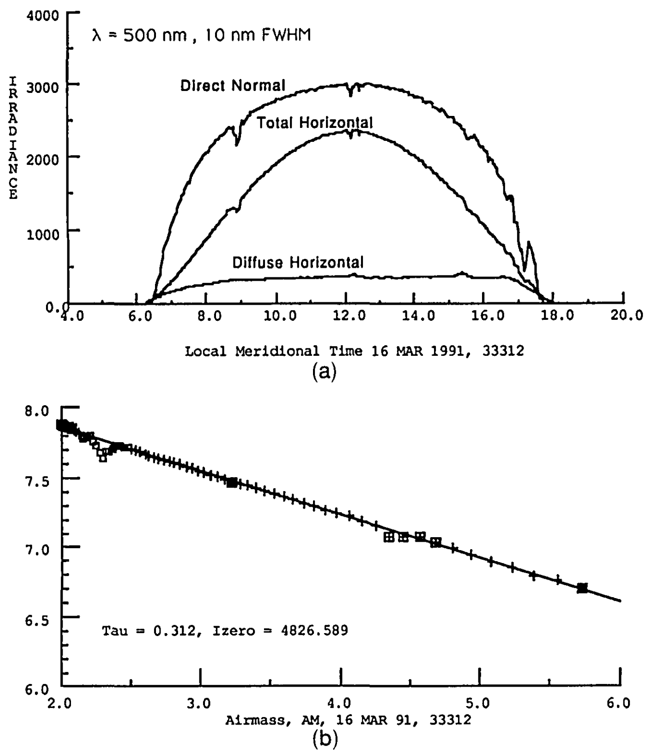

Fig. 1. (a) Time series of observed irradiance components for an example case (the irradiance scale is uncalibrated). (b) Objective optical depth retrieval for the morning shown in (a); the ordinate is ln(uncalibrated direct-normal irradiance).

The most convincing visual argument that the algorithm works well is for one to examine many cases, including those that clearly should not be used for optical depth analysis. We have done so but cannot easily present these cases 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 cases in which it is evident that no retrieval is possible. In total overcast, or in conditions with a few very short intervals (1–2 data points) in which 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.

Algorithm Intercomparison Results

We made tests of this algorithm by using a data set taken at the National Oceanic and Atmospheric Administration (NOAA) Environmental Resources Laboratory in Boulder, Colorado (40.0 °N, 105.2 °W, 1634-m elevation), with a single-channel photopic passband rotating shadow-band radiometer. This instrument was one of our first to be deployed, and it used a LiCor 210SX detector rather than our more recent multiple-channel instruments.

These data are used for algorithm testing because they were previously analyzed through a conventional subjective analysis for the purpose of studying the Mount Pinatubo eruption, and they are a challenge for optical depth analysis. Boulder is known to be a difficult site because of circulation of the urban pollution in the Denver basin, and because of 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. Further, these data are 5-min averages of 15-s samples. This reduces the filtering efficiency of the derivative filters and produces a 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 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.

Data files for the interval from 23 May 1990 to 16 July 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 with the selection criteria that require a minimum of 1/3 of the points be retained, and with a 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 it is a demonstration of the advantage of automated observation. Even 5-min averages produce many more points during the interval bounded by air masses 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 astronomical distance, which accounts for approximately half of the range in these values. The E_0 value requires an extrapolation of at least one air mass (and as implemented by the objective algorithm at least two air masses), 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 Figs. 2 and 3 (which show correlation coefficients of 0.995 and 0.982 for the retrieved optical depths and extraterrestrial irradiances, respectively) enhances our confidence that the interferences are physically meaningful rather than a result of a particular analyst or algorithm preference.

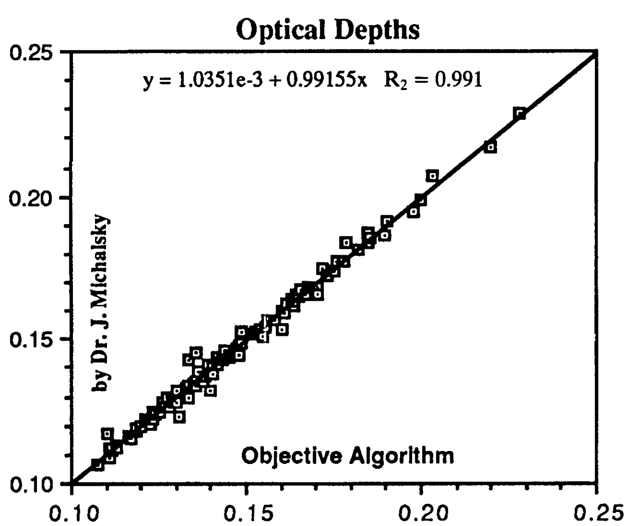

Fig. 2. Comparison of total optical depths retrieved by the two analyses.

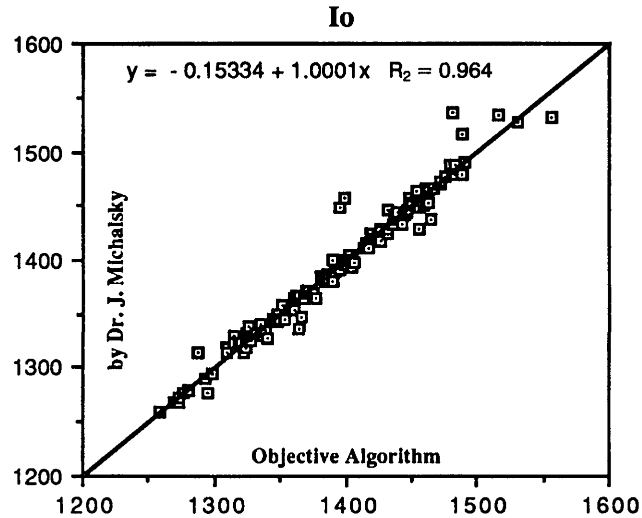

Fig. 3. Comparison of the extrapolated zero-air-mass irradiance retrieved by the two analyses (uncalibrated).

A study of the few cases rejected by one of the analysis methods but kept by the other demonstrates that the subjective analyst kept regressions based on a short contiguous interval (i.e., one short hole in the clouds), which 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 for one to assess. These few cases do not affect the aggregate statistics.

Use of $E_0(\lambda)$ for *In Situ* Calibration against the Solar Constant

After adjustment for the variation in 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 they are made under remarkably good conditions (e.g., at Mauna Loa). However, these variations are not systematic, so one can improve accuracy 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 when we use the detector calibration coefficient provided by the manufacturer, and when we normalize all measurements to an Earth–

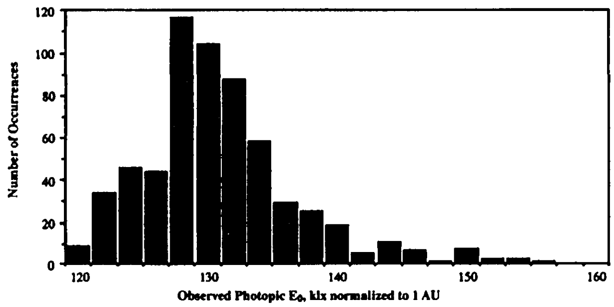

Fig. 4. Histogram of retrieved E_0 that uses a laboratory calibration for the irradiance scale.

Sun distance of 1 AU. Figure 4 contains almost 4 years of Langley observations so that the distribution can be shown with a greater number of bins. The photometer was calibrated by the manufacturer by 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 Fig. 4 is 130.79 klx, with a standard deviation of 5.94. It is common practice for one to use the E_0 value as a quality-control estimator for Langley regressions and to discard extreme events. If only the central $\pm 2\sigma$ 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 klx, respectively; this is no substantial change. Another commonly used robust estimator is the median: 129.99 klx with 95% confidence-interval limits of 129.61 and 130.37 klx, 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 difficult site for us to reduce the 1σ uncertainty in the inferred E_0 to less than 1%. At the Boulder site this can be typically obtained in less than 3 months of operation. Subintervals of the data show no statistically significant trend, thus demonstrating excellent stability.

A calibrated retrieval can be directly compared with published values. The Commission Internationale de l'Eclairage recommends[16] the value of 127.5 klx for the direct-normal illuminance at the mean solar distance. However, the convolution of this photopic response and the extraterrestrial spectral irradiance data from Neckel and Labs[17] produce 133.6 klx for this photopic solar constant. Further, there are additional uncertainties associated with the photopic response of the LiCor photometer, which 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 they provide a mechanism whereby instrument calibrations can be retrospectively analyzed 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 (which is an important contributor to errors in retrieved E_0) is much better for our newer MFRSR instruments than for the LiCor detector. Consequently, we expect the agreement between laboratory calibration and inferred solar constant to have lower uncertainties, but we have yet to acquire sufficient data to demonstrate this.

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

$$\frac{1}{t_2 - t_1}\int_{t_1}^{t_2} \exp[-\tau A(t)]\mathrm{d}t = \exp(-\tau A^*).$$

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 air mass as a function of time, but it can be numerically evaluated for any particular interval.

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

$$\frac{1}{A_2 - A_1}\int_{A_1}^{A_2} \exp(-\tau A)\mathrm{d}A = \exp(-\tau A^*),$$

which easily integrates to

$$\frac{1}{-\tau(A_2 - A_1)} [\exp(-\tau A_2) - \exp(-\tau A_1)] = \exp(-\tau A^*).$$

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

For averages comprising a finite number of samples at known times or known air mass, the magnitude of the A^* adjustment and its resulting effect on inferred optical depths and extraterrestrial irradiances can be assessed by numerical test. For averaging intervals of 5 min, total optical depths of no greater than 0.3, and through the use of data from air masses 2 to 6 for Langley regressions, exact calculations applied to a set of real events show that the use of the air mass at midinterval time causes errors no larger than ≈ 0.004 for optical depths and 0.18% for the extraterrestrial irradiances. We judge these to be negligible in comparison with other errors, and so our analyses reported in this paper use this approximation. However, these errors grow as a high order of the averaging time. Corrections should be considered for averaging intervals longer than 5 min or for large optical depths. The objective algorithm implements an additional interative correction step if the data are averaged for more than 5 min. For such data we make an initial trial for the objective regression by using the air mass associated with the midinterval time. This retrieves an estimate of the τ. We then compute A^* values for each of the averaged observations kept by the objective algorithm, and we redo the least-squares regression. It is not necessary for us to iterate this process more than once to drive residuals below 0.001 optical depths.

Conclusions

We have developed an objective analysis algorithm to perform the Langley regressions. This algorithm has been tested by intercomparison with subjective reduction and by 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 a 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 $\approx 5\%$. The deviations are not systematic and one can use repeated measurements 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 they 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/min. For averaging intervals of longer than 5 min, one should use a bootstrap technique 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 min, we find that the utility of Langley regression is reduced simply because the number of independent points can become marginally sufficient.

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