metrologia

New procedure for interpolating NIST FEL lamp irradiances

L. K. Huang, R. P. Cebula and E. Hilsenrath

Abstract. The Shuttle Solar Backscatter Ultraviolet (SSBUV) programme uses 1000 W, quartz-halogen, tungsten coiled filament (FEL) lamps as the primary radiometric calibration source in the 250 nm to 405 nm wavelength region. The National Institute for Standards and Technology (NIST) recommends using the product of a fifth-order polynomial and a Planck function as a fitting function for interpolating the NIST-calibrated FEL lamp irradiances to users' wavelengths. The NIST fitting procedure can result in more than a 1% overshoot in some data sets. This problem is related to the unconstrained properties of the fifth-order polynomial. Overshooting during lamp irradiance interpolation gives rise to corresponding errors in the SSBUV calibration and solar spectral irradiance measurements. Errors of this magnitude are unacceptably large for the SSBUV, and we have therefore developed a new interpolation scheme. A new fitting procedure has been developed to replace the NIST procedure in the SSBUV calibrations. Although it uses fewer fitting parameters, the new fitting function provides a better fit than the NIST fitting function does. The overshoot problems experienced with the NIST procedure do not exist in the newly interpolated lamp irradiances. We have also investigated the properties of the NIST FEL lamp interpolation scheme in the visible and near-infrared ranges, finding that the overshoot problem experienced in the ultraviolet extends into these regions, with potential errors of the order of 0.5% to 1%.

1. Introduction

The Shuttle Solar Backscatter Ultraviolet (SSBUV) spectrometer is a Space Shuttle-borne instrument [1, 2]. It flew eight times from 1989 to 1996. SSBUV measurements of both Earth radiance and solar irradiance in the spectral range from 200 nm to 406 nm are used to transfer NIST-traceable radiometric calibrations to satellite-based spectrometers [3, 4] that are part of the US and international programmes for monitoring ozone and solar activity [5]. Therefore, it is important to maintain the radiometric calibration accuracy of the SSBUV to approximately 1%. In the SSBUV calibrations, NIST-calibrated FEL lamps (the modified 1000 W, quartz-halogen, tungsten coiled filament lamps) were used as irradiance standards in the 250 nm to 406 nm wavelength range. This paper addresses one of the routine but critical aspects of the SSBUV calibration procedure: how to interpolate the NIST FEL lamp irradiances to users' wavelengths.

The NIST calibrated the spectral irradiances of the SSBUV FEL lamps at wavelength intervals equal to or larger than 10 nm, and recommends the following fitting function for the interpolation [6]:

$$B(\lambda) = \lambda^{-5} \exp(c_0 + c_1/\lambda) \times (a_0 + a_1\lambda^1 + a_2\lambda^2 + a_3\lambda^3 + a_4\lambda^4 + a_5\lambda^5), \quad (1)$$

where λ is the wavelength, and a_i and c_i are the fitting parameters. The term $P(\lambda) \equiv \lambda^{-5} \exp(c_0 + c_1/\lambda)$ is an approximation to a Planck function for $hc/\lambda \gg kT$, multiplied by a constant factor. The polynomial $K(\lambda) = (a_0 + a_1\lambda^1 + a_2\lambda^2 + a_3\lambda^3 + a_4\lambda^4 + a_5\lambda^5)$ is needed to account for differences between the FEL lamp irradiance and the black-body irradiance, which we call the lamp emissivity [differing from the conventional definition by the constant factor in $P(\lambda)$]. Details of the fitting procedure may be found in the NIST publication of 1987 [6], which is referred to as the NBS procedure in the following discussion (the National Bureau of Standards was renamed NIST in 1990). Before December 1994, all SSBUV FEL lamp source irradiances were interpolated using the NBS procedure.

Because of its flexible nature with the high-order polynomial, the NBS fitting function is not constrained by the physical characteristics of the lamp emission. As a result, the NBS procedure tends to overshoot the true irradiance between the input data points.

L. K. Huang and R. P. Cebula: Raytheon STX Corp., Lanham, MD 20706, USA.
E. Hilsenrath: NASA/Goddard Space Flight Center, Greenbelt, MD 20771, USA.

This problem becomes significant when the measured data are separated by 50 nm or more. Figure 1a presents an example of the overshooting with the NBS procedure for the 1992 calibration; the deviation is as great as 0.45% between 350 nm and 400 nm and –1.2% between 400 nm and 450 nm. When this lamp was recalibrated by the NIST in 1994, additional measurements were added at 360 nm, 370 nm, 380 nm, 390 nm and 410 nm. As shown in Figure 1b, the interpolated curve with these extra input points does not have the overshooting features of Figure 1a. However, if these extra input points are removed, the NBS procedure results in the same overshooting as seen in Figure 1a. Even though the NIST-calibrated lamp irradiance may be within the low quoted uncertainty ($2\,\sigma \approx 1\,\%$ at 400 nm), the interpolated lamp irradiance with the NBS procedure shows overshooting as great as about 1%. It is the latter value that the user must ultimately worry about. In many cases where the spectral profile is important, the overshooting can cause a 1.45% spectral bias at 435 nm relative to 375 nm (Figure 1). *Users of NIST data are encouraged to improve the fitting procedure in order to maintain as much absolute accuracy as possible in transferring the NIST calibration to their instruments.*

2. The SSBUV procedure

To overcome the overshooting problem associated with the NBS fitting procedure, a fitting function should be chosen to match the physical properties of the FEL lamp. The FEL lamp irradiance profile is the product of the black-body irradiance, the tungsten filament emissivity and the lamp envelope transmittance. The lamp emissivity is thus the product of the tungsten filament emissivity and the lamp envelope transmittance. The black-body radiation function is well known. The present task is to find the lamp emissivity function that accurately describes the difference between the FEL lamp and the black body. Laboratory measurements for both the tungsten ribbon emissivity [7] and the infrared-grade fused-silica envelope transmittance [8] have been reported. Both the emissivity and transmittance profiles decrease rapidly below 250 nm. The lamp envelope transmittance profile is approximately a straight line which increases slowly from 270 nm to 2.5 μm. For the tungsten ribbon emissivity profile, the second-order derivatives (thus, the curvature) are negative in the region below 300 nm and positive in the region above 450 nm (ignoring small spectral features around 1%, which were reported in [7] and are discussed below). In the region between 300 nm and 450 nm, the second-order derivatives are close to zero and the profile is close to a straight line. Therefore, the lamp emissivity function should be approximately linear from 300 nm to 450 nm. This agrees with the behaviour observed in the NIST calibrations in Figure 1.

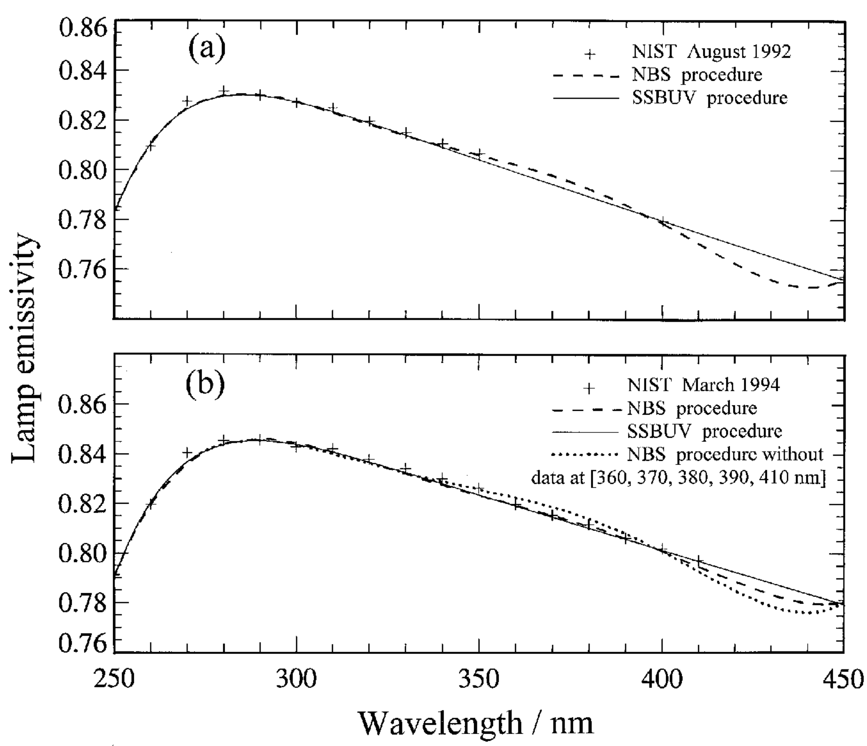

Figure 1. Interpolated FEL lamp UV emissivity for the SSBUV FEL lamp, serial number F216, (a) NIST August 1992 calibration (NIST Test No. 844/C-18-92-3) and (b) NIST March 1994 calibration (NIST Test No. 844/F-11-94-1). The + symbols are the NIST-calibrated irradiance divided by the fitted Planck function. The dashed curves are derived from the NBS interpolation procedure. The solid curves are obtained with the new SSBUV interpolation procedure.

The following function can be used to fit the FEL lamp irradiance profiles as described above:

$$F(\lambda) = \lambda^{-5} \exp[c_0 + c_1/\lambda] \times \exp\left[c_2 \lambda - c_3 \left| \frac{(\lambda - \lambda_0)}{500} \right|^{c_4}\right] \quad (\text{for } \lambda < \lambda_0), \tag{2}$$

and

$$F(\lambda) = \lambda^{-5} \exp[c_0 + c_1/\lambda] \times \exp\left[c_2 \lambda + c_5 \left| \frac{(\lambda - \lambda_0)}{500} \right|^{c_6}\right] \quad (\text{for } \lambda > \lambda_0), \tag{3}$$

where c_i are fitting parameters, c_3 and c_5 are positive, λ is the wavelength in nanometres and λ_0 = 450 nm. Two different fitting functions are needed to mimic the curvature of the lamp emissivity profile in the different wavelength regions. The function contains a factor of $\lambda^{-5} \exp(c_0 + c_1/\lambda)$ for the black-body emission, which is the same $P(\lambda)$ as in (1). However, the present function assumes the same black-body emission, thus the same c_0 and c_1 for the entire wavelength region. In contrast, the NBS fitting function $B(\lambda)$ defines two separate $P(\lambda)$ functions in the two wavelength regions, resulting in two lamp colour temperatures. This is physically less meaningful. The other factor in the new function, $E(\lambda) = \exp[c_2 \lambda - c_3 \,|(\lambda - \lambda_0)/500|^{c_4}]$, or, $E(\lambda) = \exp[c_2 \lambda + c_5 \,|(\lambda - \lambda_0)/500|^{c_6}]$, approximates the lamp emissivity to within a constant factor. The denominator in $(\lambda - \lambda_0)/500$ is separated from c_3 and c_5 in order to reduce the base value of the exponential function, $|(\lambda - \lambda_0)/500|^{c_4}$ and $|(\lambda - \lambda_0)/500|^{c_6}$, and thus to avoid overflow in numerical computation. The solid curve in Figure 2 shows an example of fitted $E(\lambda)$ functions in the wavelength range 250 nm to 1600 nm. For this lamp, c_2, c_3, c_4, c_5 and c_6 are about 0.000 29, 820, 9.8, 0.040 and 1.8, respectively. Thus, $\exp[-c_3|(\lambda - \lambda_0)/500|^{c_4}]$ is a modified Gaussian profile with a somewhat flattened top from 300 nm to 450 nm and a steep slope near 260 nm. The other factor, $\exp(c_2 \lambda) \approx (1 + c_2 \lambda)$, is approximately linear and is used to tilt the quasi-flat top as needed. On the long wavelength side, the lamp emissivity profile near λ_0 has the same value and slope as on the short wavelength side and $\exp[+c_5|(\lambda - \lambda_0)/500|^{c_6}]$ is tuned for the positive curvature.

In order to reduce the number of nonlinear fitting parameters, the fitting is performed in terms of $\log[\lambda^5 I(\lambda)]$. The lamp irradiance function, $F(\lambda)$, is transformed to

$$L(\lambda) = \log[\lambda^5 F(\lambda)] = c_0 + c_1/\lambda + c_2 \lambda - c_3 \left| \frac{(\lambda - \lambda_0)}{500} \right|^{c_4} \quad (\text{for } \lambda < \lambda_0), \tag{4}$$

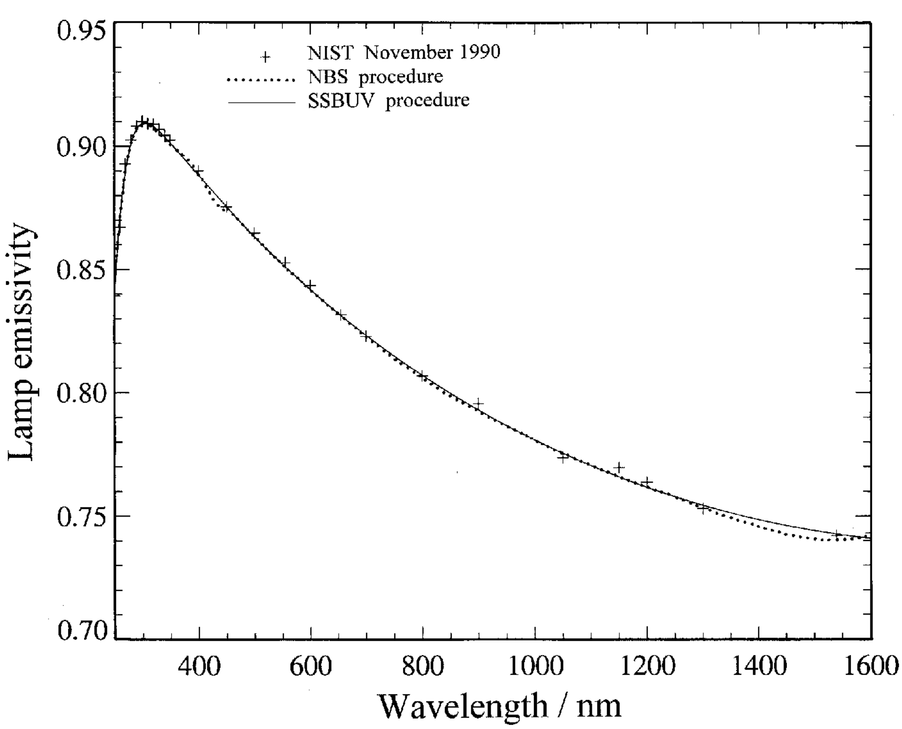

Figure 2. Interpolated FEL lamp emissivity from 250 nm to 1600 nm (lamp serial number FEL 316, NIST Test No. 534/C-12-91-1). The plot symbols are the same as in Figure 1.

or

$$L(\lambda) = \log[\lambda^5 F(\lambda)] = c_0 + c_1/\lambda + c_2\lambda + c_5 \left| \frac{(\lambda - \lambda_0)}{500} \right|^{c_6} \quad (\text{for } \lambda > \lambda_0). \tag{5}$$

When $L(\lambda)$ is used to fit $\log[\lambda^5 I(\lambda)]$, c_0, c_1, c_2, c_3 and c_5 become linear parameters. The nonlinear parameters are c_4 and c_6. In the SSBUV wavelength range (200 nm to 400 nm), c_4 is the only nonlinear parameter.

The constants in the new fitting function are determined by minimizing

$$\chi_1^2 = \Sigma_i \sigma_0^{-2} \{\log[\lambda_i^5 I(\lambda_i)] - L(\lambda_i)\}^2, \tag{6}$$

where σ_0 is the relative deviation in the calibrated irradiances, and the summation, Σ_i, is taken over λ_i for a set of the NIST-calibrated lamp irradiances $I(\lambda_i)$. The NIST-calibrated irradiances are assumed to have instrumental uncertainties, $\Delta I(\lambda_i) = \sigma_0 I(\lambda_i)$, with a constant relative uncertainty σ_0 [6]. This is the same assumption as is used in the NBS procedure. This uncertainty is weighted for the data in (6). Once the fitting parameters are determined, the NIST-calibrated lamp irradiances can be interpolated at a user's wavelengths. Fitting procedures for minimizing χ_1^2 which contains nonlinear parameters can be found elsewhere in commercial computer-software packages and in the statistical analysis literature [9].

3. Comparison of results

All NIST calibrations for the SSBUV FEL lamps were fitted using the newly developed SSBUV procedure. The relative deviations between the input and fitted data are plotted as functions of wavelength in Figures 3a, 3b and 3c according to calibration date: between 1992 and 1996, in 1990, and in the 1980s, respectively. Averages of the deviations are calculated at each of the calibrated data points and are connected with solid lines. A small number of fitting parameters makes it more difficult to minimize the differences between the fitted and the input data unless the fitting function has a well-established physical base. The SSBUV procedure has fewer fitting parameters than the NBS procedure. In each of the wavelength regions divided at 450 nm, $F(\lambda)$ of the SSBUV procedure has five fitting parameters and $B(\lambda)$ of the NBS procedure has eight fitting parameters. The NBS procedure is unable to cover the wavelength region 250 nm to 1600 nm in a single fit [6]. For the NBS procedure to cover the entire wavelength range, it is necessary to perform two fittings, which requires a total of sixteen fitting parameters. The SSBUV procedure can fit the full range of data with only seven fitting parameters. The relative standard deviations were calculated:

$$\sigma_v = [\![\Sigma_i \{[I(\lambda_i) - f(\lambda_i)]/I(\lambda_i)\}^2/(N - n - 1)]\!]^{1/2}, \tag{7}$$

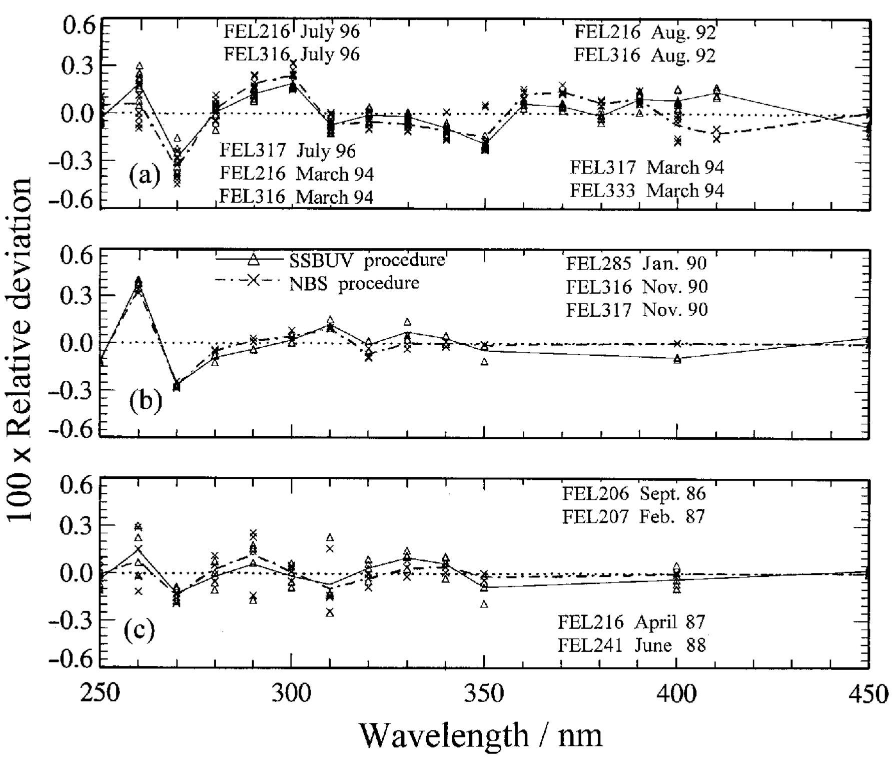

Figure 3. Relative deviations between the input and fitted data for the SSBUV FEL lamp irradiances. The NIST calibrations are listed with the lamp serial numbers and calibration date. Averages of the deviations are connected with solid lines for the SSBUV procedure, and with dashed lines for the NBS procedure.

where $n+1$ is the number of fitting parameters. *Even though it uses fewer fitting parameters, the SSBUV procedure has a smaller relative standard deviation than the NBS procedure in all cases.* For the SSBUV procedure, averages of the standard deviations over all SSBUV FEL lamps are 0.16% in the wavelength region 250 nm to 450 nm, and 0.22% in the region 450 nm to 1600 nm. For the NBS procedure, they are 0.20% and 0.23%. Note that σ_v^2 is proportional to the reduced chi-square χ_v^2 in the fitting test [9]. Therefore, the SSBUV procedure gives better fits than the NBS procedure.

Some observations are worth noting. First, in the wavelength region 280 nm to 410 nm, the average of the deviations is 0.25% (2 σ) and the NIST calibration uncertainty is 1.0% (2 σ). No clear pattern larger than 0.2% can be identified in this region. Therefore, these deviations are due to the measurement noise which is lower than the stated uncertainties. Second, the 1% spectral features in the referenced tungsten ribbon emissivity in the 300 nm to 400 nm wavelength region [7] do not exist in the FEL lamp emissivity. If these features existed in the FEL lamp spectrum, the deviations would be larger than they are. Third, in the 250 nm to 280 nm region, the average of the deviations is 0.49% (2 σ). The largest deviations are found at 260 nm and 270 nm. The deviations are correlated to the calibration date, as grouped in Figure 3. The deviations cannot be due to any fixed spectral features with each lamp since they are different for the same lamp in different calibration periods. If these deviations are due to some changing spectral features, these spectral features would correlate to the lamp production date, the lamp usage, the lamp storage, or the lamp transportation. In fact, the deviations for different lamps, brand new or aged, are about the same in each calibration period. Thus, we conclude that since the lamps in a given calibration period had very different histories, the deviations do not correspond to changing spectral features. The correlation between the deviations and the calibration dates suggests the existence of some systematic biases, within the NIST calibration uncertainty, in the NIST calibration standards at short wavelengths.

The overshooting problem with the NBS procedure in the wavelength range 350 nm to 450 nm does not exist with the new SSBUV procedure. The solid curves in Figures 1 and 2 give examples with the SSBUV procedure. In order to determine the minimum number of points that are required to interpolate the data with reasonable accuracy, two mini data sets were constructed from each complete data set (which contained lamp measurement data at 10 nm intervals from 250 nm to 350 nm and every 50 nm above 350 nm). The mini data sets are at wavelengths [250, 300, 350, 400, 450 nm] and [250, 280, 300, 350, 400, 450 nm], respectively. Each data set was fitted using the SSBUV procedure. All NIST calibrations for the SSBUV FEL lamps were tested. Since the SSBUV

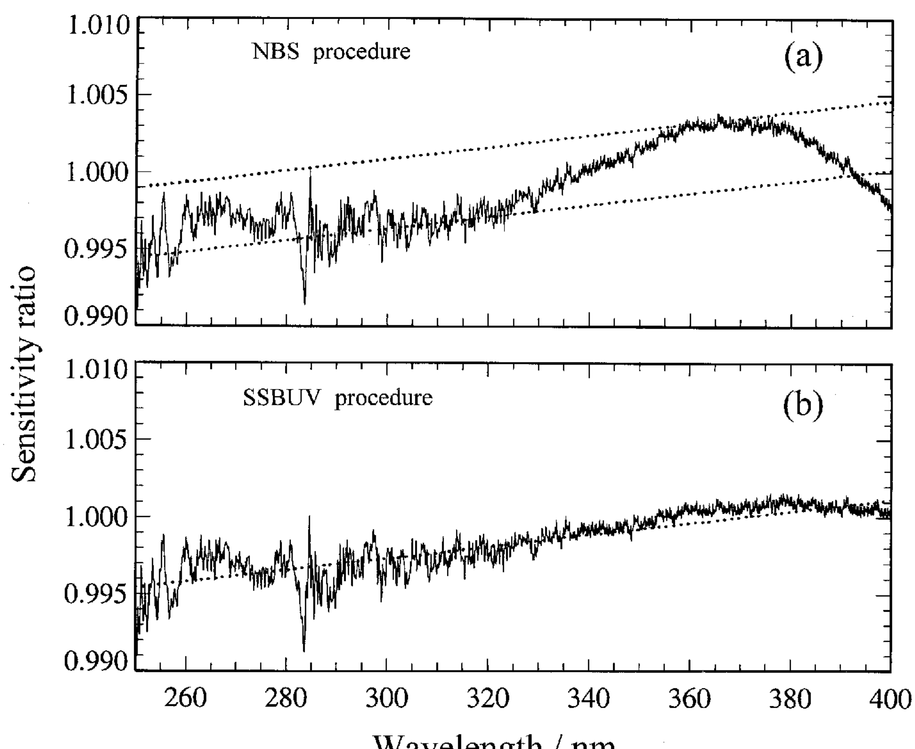

Figure 4. The SSBUV sensitivity ratios of different FEL lamps, (a) using the NBS procedure to interpolate the FEL lamp irradiance, (b) using the SSBUV procedure to interpolate the FEL lamp irradiance. The straight line in (b) is well fitted to the data. The straight lines in (a) are drawn parallel with the one in (b) to show the overshoot.

procedure works well with the complete data set, any significant discrepancies in the fitting results between the mini data sets and the complete data sets must be related to the problem of insufficient data points. Fits to the five-point data sets had overshooting less than 1.2% in the 250 nm to 300 nm region, and less than 0.3% in the 300 nm to 450 nm region. Adding one point at 280 nm to the mini data sets, the SSBUV procedure reduces the discrepancies to less than 0.3% in the 250 nm to 280 nm region, and to less than 0.12% in the 280 nm to 450 nm region. The SSBUV procedure can thus be of use to FEL lamp users for whom the lamps were calibrated at a minimal number of points.

The SSBUV irradiance sensitivities, which are equal to the instrument counts divided by the interpolated lamp irradiance, can be used to check the overshooting problems. Figure 4a shows ratios of the sensitivity based on lamp F216 to the sensitivity based on lamp F317 for the post SSBUV-5 calibration. Since the SSBUV instrument was calibrated against the two FEL lamps within a short period, the instrument sensitivity should be the same for the two calibrations. Ideally, the sensitivities derived from the two lamps should also be the same, thus the ratio of the two sensitivity data sets should be unity. Using the NBS procedure, the sensitivity ratio in Figure 4a shows a curved feature deviating from linearity by as much as 0.45% between 350 nm and 400 nm. This curved feature is related to the overshooting in the interpolated source irradiance for lamp F216 in Figure 1a. Figure 4b shows the ratio of SSBUV sensitivities based on the newly interpolated lamp source irradiances for two FEL lamps. The ratio of the two sensitivities is within 0.1% of unity at 400 nm, indicating good agreement between the sensitivities based on different FEL lamps. The ratio is within 0.5% of unity at 250 nm, which is within the NIST calibration uncertainty ($2\,\sigma_0 \approx 1.8\%$) at the shorter wavelengths. The sensitivity ratio in Figure 4b can be fitted with a straight line. The overshooting feature in Figure 4a is not seen in Figure 4b.

4. Conclusion

The newly developed SSBUV procedure for interpolating the NIST-calibrated FEL lamp spectral irradiances uses a fitting function that is constrained to a physical model for the FEL lamp emissivity. In the 250 nm to 450 nm wavelength region, both the NIST and SSBUV data confirm experimentally that the SSBUV procedure gives a better fit than the NBS procedure. The overshooting features of 0.45% to 1% that appeared in some fitting results with the NBS procedure can be eliminated with the SSBUV procedure. The SSBUV irradiance calibration data have been reprocessed using FEL lamp irradiances determined using the SSBUV procedure. Changes to the sensitivities before 1995 are less than 0.1% in the 250 nm to 350 nm region. In the 350 nm to 406 nm region, changes to the sensitivities due to reduction in overshooting are less than 0.25%, which is smaller than the overshooting observed with a single FEL lamp because multiple FEL lamps were used in the SSBUV calibrations.

In the 450 nm to 1600 nm wavelength region, the SSBUV procedure also gives better fitting results than the NBS procedure. However, we have no experimental data to check the overshooting problem in the long-wavelength region. Users of FEL lamps in the long-wavelength region may wish to follow the same methodology to interpolate their data.

Acknowledgements. Raytheon STX Corp. authors are supported by NASA contract NAS5-31755.

References

1. Frederick J. E., Niu X. F., Hilsenrath E., *J. Atmos. Ocean. Tech.,* 1990, **7**, 734-740.
2. Cebula R. P., Hilsenrath E., Guenther B., *Proc. SPIE,* 1989, **1109**, 205-218.
3. Hilsenrath E., Bhartia P. K., Cebula R. P., Wellemeyer C. G., *Adv. Space Res.,* 1997, **19**, 1345-1353.
4. Woods T. N. et. al., *J. Geophys. Res.*, 1996, **101**, 9541-9569.
5. National Plan for Stratospheric Monitoring and Early Detection of Change, 1988-1997, US Dept. of Commerce, NOAA, FCM-P17-1989, July 1989.
6. Walker et al., *Natl. Bur. Stand. Spec. Publ. 250-20*, 1987.
7. Elenbaas W., *Light Sources,* 1972, New York, Crame, Russat & Co., Inc., p. 23.
8. *ORIEL Catalog*, 1993, 250 Long Beach Blvd., Stratford, CT 06497, USA.
9. Bevington P. R., *Data Reduction and Error Analysis for the Physical Sciences*, New York, McGraw-Hill, 1969.