NMI TR 7
Source Distribution Temperature and its Uncertainty

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First edition — August 2005

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ABSTRACT

Methods are given for the calculation of the distribution temperature of a source and estimating its uncertainty from components of a typical measurement of spectral irradiance. Examples are given for common sources and typical measurement uncertainties of a spectral transfer from a reference lamp. Values and uncertainties are compared with those of correlated colour temperature for the same source. Shifts in distribution temperature due to the alternative of a direct fit of Planck’s distribution, and to including weights in the process, are compared to the estimated uncertainties.
1 INTRODUCTION

Distribution temperature of a source is defined [1] as the value of $T$ that minimises the integral

$$\int \left[ 1 - \frac{E(\lambda)}{aP(\lambda, T)} \right]^2 d\lambda$$

(1)

where $E(\lambda)$ is the spectral irradiance, and wavelengths $\lambda$ are taken in the range 400 to 750 nm. $P(\lambda, T)$ is Planck’s distribution for a temperature, $T$, and $a$ is a normalising constant. The spectral irradiance is only required in relative form – absolute scaling does not affect the fitted value of distribution temperature. If the spectral data are present at regular intervals, the integral can be written in sum form over the $N$ spectral points

$$\Delta\lambda \sum \left[ \frac{E_n}{aP_n(T)} - 1 \right]^2 = \Delta\lambda \sum f_n^2$$

(2)

where the $n$ subscript is used to denote wavelength.

Note: If the data are not present at regular intervals, the separation between points must be included in the summation – distribution temperature is not found by merely fitting a Planckian form to the values of the spectral energy distribution.

CIE in its definition [1] give the value of $c_2$ as $1.438 8 \times 10^{-2}$ m.K and do not clearly define whether air or vacuum wavelengths are used. The current value of $c_2$ is $1.438 775 2 \times 10^{-2}$ m.K, and we can take the refractive index of air as $n_a = 1.000 29$ to convert from the air-wavelengths at which measurements are made to the vacuum wavelengths needed for the calculation of photon energies assumed in the derivation of Planck’s law. However to be consistent with the CIE Illuminant values, we must use the value of $c_2$ as $1.438 8 \times 10^{-2}$ m.K and ignore the correction for the refractive index of air.

Distribution temperature only has meaning for sources close to the Planckian locus.

2 ESTIMATION OF DISTRIBUTION TEMPERATURE

Minimising with respect to the parameters $a$ and $T$ gives two equations

$$f_a = \sum \left[ \frac{E_n}{aP_n} - 1 \right] \frac{E_n}{P_n} = 0$$

(3)

and

$$f_T = \sum \left[ \frac{E_n}{aP_n} - 1 \right] \frac{E_n}{P_n^2} P_n' = 0$$

(4)

Distribution temperature can be determined iteratively by searching for a value of $T$, with a consistent value for $a$ found from Eq. (3).

Woeger [2] demonstrated a general method for least-squares fitting and uncertainty estimation, based on a generalised Newton-Raphson technique [3]. Determination of distribution temperature was used as an example. In that example, he considered a weighted fit, where the weighting used uncertainties of the spectral points, including correlations. The strict definition of distribution temperature requires an unweighted fit;
the method below follows Woeger, but removes the weighting and includes the constant 1 in the model definition.

The fitting equations are written in matrix form as

$$\mathbf{F} = \mathbf{M}_y^T \mathbf{M} = 0$$  \hspace{1cm} (5)

where

$$\mathbf{M}_y = \begin{pmatrix} \frac{\partial f_1}{\partial a} & \frac{\partial f_1}{\partial T} \\ \frac{\partial f_2}{\partial a} & \frac{\partial f_2}{\partial T} \\ \vdots & \vdots \\ \frac{\partial f_n}{\partial a} & \frac{\partial f_n}{\partial T} \end{pmatrix}$$  \hspace{1cm} (6)

is a $N \times 2$ matrix of the derivatives of the function with respect to the parameters being fitted and

$$\mathbf{M} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}$$  \hspace{1cm} (7)

is a $N \times 1$ matrix containing the model form being fitted. The derivatives are

$$\frac{\partial f_i}{\partial a} = \frac{E_n}{P_n}, \quad \frac{\partial f_i}{\partial T} = -\frac{E_n}{P_n^2} \frac{\partial P_n}{\partial T}$$  \hspace{1cm} (8)

where $P_n, \frac{\partial P_n}{\partial T}$ are, respectively

$$P_n = \frac{1}{\lambda_n^n (e^{\frac{c_2}{n \lambda_n^2}}) - 1}$$  \hspace{1cm} (9)

$$\frac{\partial P_n}{\partial T} = \frac{c_2 P_n}{n \lambda_n^2 T^2 (1 - e^{\frac{c_2}{n \lambda_n^2 T}})}$$  \hspace{1cm} (10)

The generalised Newton-Raphson technique is an iterative procedure to solve Eq. (5) by expanding the equations $\mathbf{F}$ in a Taylor series about the initial point, retaining only first-order derivatives, then setting the value at the new point (a better approximation to the solution) to zero; that is

$$\mathbf{F} (\mathbf{y} + \delta \mathbf{y}) = \mathbf{F} (\mathbf{y}_0) + \mathbf{J} \delta \mathbf{y} = 0$$  \hspace{1cm} (11)

Here $\mathbf{J}$ is the Jacobian matrix

$$\mathbf{J} = \begin{pmatrix} \frac{\partial F_i}{\partial y_j} \end{pmatrix}$$  \hspace{1cm} (12)

where $i = 1, 2$ for our two equation rows and $j = 1, 2$ for our two parameters. Hence

$$\mathbf{J} = \begin{pmatrix} \frac{\partial}{\partial y_j} \sum_n f_n \frac{\partial f_n}{\partial y_i} \\ \vdots \end{pmatrix} = \begin{pmatrix} \sum_n \frac{\partial f_n}{\partial y_j} \frac{\partial f_n}{\partial y_i} \end{pmatrix}$$  \hspace{1cm} (13)
where only first-order terms are retained, or
\[ J = M_y^T M_y \]  
(14)

It follows that, given the parameter matrix with some initial estimates \( y_0 = \begin{bmatrix} a \\ T \end{bmatrix} \), improved estimates are given by
\[
y = y_0 - (M_y^T M_y)^{-1} F(y_0) = y_0 - (M_y^T M_y)^{-1} M_y^T M
\]
(15)

This process is iterated until a required accuracy is reached. Convergence is rapid. For the typical spectra encountered in photometry and colorimetry, starting values \( T \) of 3000 K and a consistent value of \( a \) in the middle of the spectral range are used.

A practical consideration is that the differences generated in the matrix inversion process are subject to rounding errors. Even for the \( 2 \times 2 \) matrix \( J \), accuracy is improved if the scaling constant \( a \) is of order 1. This is achieved by scaling all the calculated Planck values and derivatives such that the starting value of \( a \) is 1, and applying this scaling throughout the solution.

Distribution temperature is calculated using spectral values only in the wavelength range 400 to 750 nm. For a given set of input spectral values and their correlations, only the subset in the required spectral range is used for this calculation.

3 UNCERTAINTY SENSITIVITY COEFFICIENTS FOR DISTRIBUTION TEMPERATURE

To calculate the uncertainties in the parameters \( a \) and \( T \) (input parameters \( y \)) from those in the spectral values \( E_n \) (input parameters \( x \)) we need the sensitivity coefficients \( \frac{\partial a}{\partial E_n} \) and \( \frac{\partial T}{\partial E_n} \). Given that \( \frac{\partial f_n}{\partial E_n} = \frac{\partial f_n}{\partial a} \frac{\partial a}{\partial E_n} + \frac{\partial f_n}{\partial T} \frac{\partial T}{\partial E_n} \), the sensitivity coefficients are carried in the matrix \( Q \) where \( M_x = M_y^T Q \) and

\[
M_x = \begin{pmatrix}
\frac{\partial f_1}{\partial E_1} & 0 & \ldots & 0 \\
0 & \frac{\partial f_2}{\partial E_2} & \ldots & 0 \\
0 & 0 & \ldots & \frac{\partial f_n}{\partial E_n}
\end{pmatrix}
\]
(16)

is a diagonal sensitivity matrix, with \( \frac{\partial f_n}{\partial E_n} = \frac{a}{P_n} \). Hence \( Q = -M_y^T M_x \) where \( M_y^{-1} \) is the generalised inverse of \( M_y \).
In Woeger’s method [2], the uncertainty matrix for the parameters \( y \) is given by

\[
U_y = QU_yQ^T \\
= M_y^{-1}M_yU_y(M_y^{-1}M_y)^T \\
= M_y^{-1}M_yU_yM_y^{-1}M_y^{-1} \\
= M_y^{-1}KM_y^{-1} 
\]  

(17)

The inverse is given by

\[
U_y^{-1} = (M_y^{-1}KM_y^{-1})^{-1} \\
= M_y^{-1}K^{-1}M_y 
\]  

(18)

where \( K \) is square and so we can calculate its inverse, form the product shown in the previous equation and take its inverse to get the covariance matrix between the fit parameters.

A problem here is that the uncertainties in spectral irradiance can be highly correlated. In fact, we wish to calculate uncertainties component by component. The systematic components are fully correlated and then matrix \( U_x \) has no inverse. The matrix \( K \) is ill-conditioned and the inverse calculation becomes unreliable. Hence we would like to calculate the sensitivity coefficients for \( T \) and use these to directly propagate uncertainties from spectral irradiance to temperature.

The generalised inverse of \( M_y \), and subsequently the sensitivity coefficients \( Q \), can be calculated as

\[
M_y^{-1} = (M_y^{-1}M_y)^{-1}M_y^{-1} 
\]  

(19)

The inverse required here is for a \( 2 \times 2 \) matrix. Again this calculation is subject to rounding errors, and the reliability of the inverse calculation should be checked. An immediate check on the values obtained is that the value of distribution temperature should not be affected by a constant relative error in the spectral irradiance values. The propagated uncertainty for this effect is proportional to the sum of the products of the sensitivity coefficients and the spectral irradiance values – this sum should be small (ideally zero).

As an alternative, the required sensitivity coefficients may be calculated directly. Each spectral irradiance value in turn is expanded, typically by 1.01, the temperature fitted and the sensitivity coefficient given as the change in temperature divided by the change in spectral irradiance. This direct numerical method was used to confirm the values of sensitivity coefficients calculated via the matrix method.

4 UNCERTAINTIES IN DISTRIBUTION TEMPERATURE

As detailed elsewhere [4, 5], the uncertainty in spectral irradiance for a given component effect described by a parameter \( p \) is given by

\[
u_s(E(\lambda)) = \frac{\partial E(\lambda)}{\partial p} u(p) 
\]  

(20)

The \( s \) subscript denotes a signed uncertainty – the sign is important in propagating uncertainties for effects that are systematic across wavelength. For effects that are random across wavelengths, the uncertainty in distribution temperature due to this component is
\[ u^2(T) = \sum (s_n u_{s,n})^2 \]  
where \( s_n \) is the sensitivity coefficient at the \( n \)th wavelength; for systematic effects

\[ u(T) = \sum s_n u_{s,n} \]  
The total uncertainty is then found by combining the independent components in quadrature.

5 \hspace{1em} TYPICAL UNCERTAINTY COMPONENTS

Measurements of spectral irradiance \( E_n \) at a given wavelength are generally made as a transfer against a reference standard, \( E_n^{\text{Ref}} \). The value at wavelength \( n \) is then given by

\[ E_n = t_n E_n^{\text{Ref}} \]  

Typical uncertainty components of a spectral measurement are given in the following sections.

5.1 \hspace{1em} Uncertainty in the Reference Value

For this component

\[ u(E_n) = t_n u(E_n^{\text{Ref}}) = \frac{E_n}{E_n^{\text{Ref}}} u(E_n^{\text{Ref}}) \]  

In general, reference spectral values are partly correlated due to the combination of systematic and random components in their derivation. Hence a complete propagation of uncertainty is required, including the covariance terms

\[ u(E_n, E_m) = \frac{E_n}{E_n^{\text{Ref}}} \frac{E_m}{E_m^{\text{Ref}}} u(E_n^{\text{Ref}}, E_m^{\text{Ref}}) \]  

However, reference values for spectral irradiance are often traced to the determination of a single temperature and all values are fully correlated; even after a transfer to working standards, random effects are small and values remain highly correlated and are able to be calculated from a single equivalent temperature uncertainty.

Reference spectra are usually provided at less wavelength points than required for a lamp measurement and then interpolated to the lamp wavelengths. The contribution of the reference uncertainty should be obtained by propagation over only the limited data set of the reference lamp, with the lamp data interpolated to the reference wavelengths for this calculation[]. This avoids the extra correlation introduced into the reference data by the interpolation process and properly calculates the averaging over random effects. For highly correlated reference data this difference is negligible.

5.2 \hspace{1em} Offsets in the Background

We treat background offsets as a fractions of the maximum measured signals, which in turn are taken as proportional to the reference and test spectral values themselves, ignoring variations in the efficiency of the measuring system. For measurements of the reference standard

\[ u(E_n) = u(t_n) E_n^{\text{Ref}} = t_n u(h^{\text{Ref}}) \]  

and for measurements on the test item

\[ u(E_n) = u(t_n) E_n^{\text{Ref}} = u(b) \]  

When propagating random offsets, the two uncertainty terms can be combined in quadrature and then propagated. The systematic offsets are propagated separately (as the linear sum of Eq. (22)) and then combined in quadrature, together with the random components.
5.3 Scaling of the Absolute Value

All components of this type can be propagated with the same expression

\[ u(E_n) = E_n^{\text{Ref}} \cdot u(t_n) = E_n u_{\text{rel}}(E_n) \]  

(28)

where \( u_{\text{rel}}(E_n) \) is constant. Random components of this type can be combined and then propagated. Systematic components must be propagated separately (again using the linear sum form) and then combined in quadrature, together with the random components.

5.4 Wavelength Errors

For wavelength errors in the reference measurement

\[ u(E_n) = u(t_n)E_n^{\text{Ref}} = -t_n \frac{\partial E_n^{\text{Ref}}}{\partial \lambda} \cdot u(\lambda) \]  

(29)

and for those in the test measurement

\[ u(E_n) = u(t_n)E_n^{\text{Ref}} = \frac{\partial E_n}{\partial \lambda} \cdot u(\lambda) \]  

(30)

(where again we have ignored spectral variations in the efficiency of the monochromator).

Random errors in wavelength depend on setting accuracy and the wavelength calibration. Combining random effects in wavelength setting now depends on the method used for recording the test spectrum. If the monochromator is stepped to a wavelength and the transfer at that wavelength is measured by switching between the test and reference sources (method 1), the wavelength uncertainty components are correlated at that wavelength. Hence the two terms, Eqs (29) and (30) are added and then propagated in quadrature between wavelengths. If the full spectrum is measured for the test lamp and then the reference lamp (method 2), the uncertainties at the one wavelength are uncorrelated and the components can be combined in quadrature and then propagated.

Systematic errors in wavelength depend on offsets between the illumination systems used for calibration and for measurement. High resolution is usually used for calibration to accurately define the scanning function, while lower resolution is used with broadband sources to improve signal levels. As for the random components, for method 1 scanning the two terms can be added linearly and the sum propagated linearly before combining in quadrature with the other uncertainty components; for method 2 scanning, the two terms are propagated linearly separately, then combined in quadrature with the other components.

6 EXAMPLE CALCULATIONS

Typical uncertainty components were chosen as in Table 1. Systematic offsets in the signals are generally estimated as average of the random background noise with a shutter closed and hence are smaller than the random noise at any one wavelength; the systematic values chosen in the table allow for a scattered background which may reach the detector with an open shutter. Systematic scaling of the spectral irradiance values does not contribute to the uncertainty in distribution temperature and hence only random scaling effects are included. Generally this is noise due to current fluctuations in the lamps. All calculations were made for data recorded at 5 nm intervals over the range 380 nm to 760 nm, selecting the subset from 400 nm to 750 nm for the actual calculation.
Table 1. Uncertainty components in a spectral irradiance measurement to be propagated through to uncertainty in distribution temperature (column 1 is an identifier for the plots shown below)

<table>
<thead>
<tr>
<th>Component</th>
<th>Identification</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>Reference standard (blackbody at 2800 K)</td>
<td>1 K</td>
</tr>
<tr>
<td>RO</td>
<td>Reference signal systematic offset</td>
<td>0.03% of the maximum</td>
</tr>
<tr>
<td>TRR</td>
<td>Transfer, random (relative signal noise)</td>
<td>0.1%</td>
</tr>
<tr>
<td>TRO</td>
<td>Transfer, random offsets (background noise)</td>
<td>0.03% of the signal maxima</td>
</tr>
<tr>
<td>SO</td>
<td>Spectrum signal systematic offset</td>
<td>0.03% of the maximum</td>
</tr>
<tr>
<td>WR</td>
<td>Wavelength, random (nm)</td>
<td>0.1 nm</td>
</tr>
<tr>
<td>WO</td>
<td>Wavelength, systematic offset (nm)</td>
<td>0.2 nm</td>
</tr>
<tr>
<td>Total</td>
<td>Sum of all components</td>
<td></td>
</tr>
</tbody>
</table>

Distribution temperatures and their uncertainties were calculated for actual data of lamps set near CIE Source A (Figure 1) and 3200 K (Figure 2), for a blackbody at 5500 K (Figure 3) and for CIE Illuminant D65 (Figure 4). The figures show the contributions of each component as well as their combined total. Figure 5 shows the relative spectral irradiance of these sources.

Figure 6 compares uncertainties in distribution temperature for the S20 source calculated from data at 50 nm intervals to that calculated at 5 nm intervals. Systematic components show little change, but random components are much smaller for the 5 nm data spacing; we would expect them to be of order √10 smaller, as seen in the figure, because more points of similar uncertainty are combined in quadrature. The fitted value of distribution temperature was 0.2 K higher for the 50 nm data spacing.

Another important parameter for a broad-band lamp is its correlated colour temperature. This parameter and its uncertainties [8], by component, are also shown in Figures 1 to 4. We see that the combined uncertainties for distribution temperature and for correlated colour temperature are similar, although the component contributions vary. Correlated colour temperature is calculated from chromaticity, in turn calculated from the 3 tristimulus values which are sums of the spectral irradiance data convolved with the colour-matching functions representing the colour response of the eye. Hence the sensitivity coefficients for the two temperatures at the different wavelengths are different. Sensitivity coefficients for the two temperatures for lamp S20 and a blackbody at 5500 K are shown in Figure 7; those for correlated colour temperature show structure related to the colour-matching functions.

CIE Source A is particularly important for calibration of colorimeters and photometers. It is defined as an incandescent source with a correlated colour temperature of 2856 K, which is the calculated value for the lamp shown in Figure 1. The fitted distribution temperature is ~ 5 K lower, outside the uncertainty placed on either value (but within the overlap – noting that the two values for the one source are highly correlated). Calculations on CIE Illuminant A as a true blackbody at 2856 K yield both distribution temperature and correlated colour temperature as 2856 K.
Figure 1. Uncertainty in distribution temperature, by component, for an incandescent lamp set near CIE Source A (see Table 1 for component identification).

Figure 2. Uncertainty in distribution temperature, by component, for a FEL incandescent lamp near 3200 K.
Figure 3. Uncertainty in distribution temperature, by component, for a 5500 K blackbody source

Figure 4. Uncertainty in distribution temperature, by component, for CIE Illuminant D65
Figure 5. Relative spectral irradiance for the sources whose uncertainties in distribution temperature are plotted in Figures 1 to 4.

Figure 6. Uncertainty components for the CIE Source A lamp S20, for data recorded at 5 nm intervals and 50 nm intervals.
Values for both distribution temperature and correlated colour temperature for all the above sources are shown in Table 2.

Table 2. Values of distribution temperature and correlated colour temperature for the sources whose uncertainty components are shown in Figures 1 to 4

<table>
<thead>
<tr>
<th>Source</th>
<th>Distribution temperature (K)</th>
<th>Correlated colour temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S20</td>
<td>2850.7</td>
<td>2856.0</td>
</tr>
<tr>
<td>FEL</td>
<td>3208.3</td>
<td>3208.1</td>
</tr>
<tr>
<td>BB 5500 K</td>
<td>5500.0</td>
<td>5500.0</td>
</tr>
<tr>
<td>CIE Illuminant D65</td>
<td>6240.2</td>
<td>6503.6</td>
</tr>
</tbody>
</table>

7 FITTING A DIRECT PLANCKIAN FORM

Instead of the expression in Eq. (2), we can directly fit a Planckian function by minimising

$$\Delta A \sum \left[ E_n - a P_\nu(T) \right]^2$$

This is equivalent to a shift in the weights given to different data, that is, a shift in the sensitivity coefficients at a given wavelength. In particular, wavelengths where the radiation is strongest have the strongest contribution to the sum being minimised. The same spectra fitted in Table 1 were fitted with this form, again using the generalised Newton-Raphson technique. Table 3 compares the results of the two methods.
Table 3. Comparison of a distribution temperature with that from a direct fit of Planck’s distribution

<table>
<thead>
<tr>
<th>Source</th>
<th>Distribution temperature (K)</th>
<th>Planckian (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S20</td>
<td>2850.7</td>
<td>2864.6</td>
</tr>
<tr>
<td>FEL</td>
<td>3208.3</td>
<td>3208.3</td>
</tr>
<tr>
<td>BB 5500 K</td>
<td>5500.0</td>
<td>5500.0</td>
</tr>
<tr>
<td>CIE Illuminant D65</td>
<td>6240.2</td>
<td>6180.1</td>
</tr>
</tbody>
</table>

8 WEIGHTING THE DATA

In principle, weighting the data by uncertainty, typically by the inverse of the variance at a given wavelength, takes into account more information of the measurement than the data value itself. Using the full variance-covariance matrix (Woeger’s method) would appear particularly advantageous. It requires the calculation of a inverse of the variance-covariance matrix of the input values, propagated through to the variance-covariance of the matrix \( F \) of Eq. (5). However, for highly correlated data, the variance-covariance matrix for spectral irradiance is ill-conditioned, as is its propagation to that of \( F \). In fact, if fully-correlated offsets in the data dominate, the variance-covariance matrix for spectral irradiance is of the form of a constant multiplied by a matrix with the value 1 in all positions, and this matrix has no inverse. Hence it is difficult to include systematic (i.e. correlated) effects into any weighting.

The form of Eq. (2) means that large and small values of spectral irradiance contribute equally to the fitting process. If relative uncertainties in the data dominate (source noise), then the weighting applied to the data can be taken as \( 1/E_i^2 \). Table 4 shows changes to the fitted values of distribution due to this weighting for the sources treated above. Shifts are significant for sources not exactly following a Planckian distribution, well beyond typical uncertainties in an unweighted fit.

Uncertainty due to offset is approximately constant across the spectrum, and hence weighting by this component leads to negligible change in the fitted value of distribution temperature. Hence for typical mixed uncertainties, weighting by uncertainty will lead to a shift somewhat lower than that shown in Table 4, but still significant for a practical source.

Table 4. Comparison of distribution temperature with that of a weighted fit where relative source noise dominates

<table>
<thead>
<tr>
<th>Source</th>
<th>Distribution temperature (K)</th>
<th>Weight by ( 1/E_i^2 ) (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S20</td>
<td>2850.7</td>
<td>2834.7</td>
</tr>
<tr>
<td>FEL</td>
<td>3208.3</td>
<td>3208.3</td>
</tr>
<tr>
<td>BB 5500 K</td>
<td>5500.0</td>
<td>5500.0</td>
</tr>
<tr>
<td>CIE Illuminant D65</td>
<td>6240.2</td>
<td>6160.8</td>
</tr>
</tbody>
</table>

Given the difficulty of properly estimating uncertainties, it is preferred to retain the unambiguous unweighted fit, of the form shown in Eq. (2), for the estimation of the value of distribution temperature and for the uncertainties to be propagated through to the uncertainty of that value.
REFERENCES


