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The treatment of uncertainties in SST measurements using radiation thermometers for the validation of satellite measurements.

E. Theocharous and N. P. Fox

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Engineering Measurement Division

ABSTRACT

A number of sea-borne radiation thermometers have been developed and are being used to validate sea surface temperature (SST) measurements made by satellite-borne instruments. Provided principles specified by Quality Assurance for Earth Observation (QA4EO) are followed, measurements carried out with these sea-borne radiation thermometers can be treated as Climate Data Records (CDRs). The purpose of this document is to summarise the minimum number of calibration steps that are required in order to ensure that SST measurements carried out with sea-borne radiation thermometers can be considered traceable to an SI standard. The treatment of uncertainties in SST measurements is summarised, and typical uncertainty budgets which satisfy each calibration step are presented in order to provide guidance to the preparation of uncertainty budgets and to ensure that SST measurements have an appropriate Quality Indicator (QI) associated with them. The uncertainty budgets presented in this document should only be considered as guidance, as the exact form of the uncertainty budgets will depend on the details of each calibration step.

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National Physical Laboratory
Hampton Road, Teddington, Middlesex, TW11 0LW

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Approved on behalf of NPLML by Teresa Goodman, Principal Research Assistant,
Engineering Measurement Division.

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1 INTRODUCTION

Radiometers are defined as instruments which are designed to measure one or more of the radiometric quantities or parameters used to quantify the characteristics of a source or beam or field of optical radiation (see Appendix 1 for the definition of the main radiometric quantities and units). A number of ship-borne instruments such as SISTER (Barton et al. 2004), ISAR (Donlon et al., 2008) and MAERI (Minnett et al. 2001) which are being referred to as “radiometers” have been developed to observe the Ocean as part of satellite calibration and validation activities. The aim of these instruments is to measure the sea surface temperature (SST) and thus validate measurements of the same parameter (SST) measured by satellite-based instruments such as ATSR+ series, MODIS etc. It should be noted that since the output of SISTER, MAERI and ISAR is in units of temperature ($^{\circ}\text{C}$ or K), they should really be called “thermometers”, or “radiation thermometers” in particular, as opposed to radiometers which would measure in terms of watts per unit area or solid angle and for a given spectral wavelength band.

Radiation thermometers vary in design and construction. Radiation thermometers measuring SST have to operate in the infrared (normally in the $8\text{ }\mu\text{m}$ to $12\text{ }\mu\text{m}$ wavelength range) where there is an atmospheric transmission window and, more importantly, the spectral radiance of blackbodies operating at near ambient temperatures has a maximum. SST measurements based on the $3\text{ }\mu\text{m}$ to $5\text{ }\mu\text{m}$ wavelength range are also possible but they are much more challenging and are best avoided for two main reasons:

- i. The spectral radiance of near ambient temperature blackbodies in the $3\text{ }\mu\text{m}$ to $5\text{ }\mu\text{m}$ wavelength range is much lower than in the $8\text{ }\mu\text{m}$ to $12\text{ }\mu\text{m}$ wavelength range, resulting in a lower signal and therefore measurements with poorer signal to noise ratio.
- ii. Solar radiation levels are much higher in the $3\text{ }\mu\text{m}$ to $5\text{ }\mu\text{m}$ wavelength range so measurements in this wavelength range are much more prone to solar radiation/sun reflection, resulting in their best performance being limited to night time observations.

Unfortunately the performance, in particular the stability, of photo-detectors responding in the infrared is far inferior to that of photo-detectors developed for the UV, visible and NIR spectral regions (Theocharous and Birch, 2002). For this reason, the minimum design of a SST-measuring radiation thermometer should include at least one internal reference blackbody to ensure that any drifts in the responsivity of the infrared photo-detectors utilised by the SST-measuring radiation thermometers can be accounted for. This means that in practice these instruments compare the spectral radiance of the observed sea surface with that of the internal reference blackbodies which are maintained at temperatures similar to the SST being measured. This provides a good method of minimising the effect of some of the problems associated with infrared radiometers such as drift in their responsivity (Theocharous, 2006), ageing, non-linear response (Theocharous, 2004), effect of the thermal background (Theocharous and Theocharous 2006), definition of “radiometric zero” (Theocharous et al., 1998), etc. However, the use of an internal reference blackbody still leaves a number of issues which have to be addressed if these radiation thermometers are to be used for the acquisition/validation of Climate Data Records (CDR)s. Amongst other things, the uncertainties associated with these reference blackbodies have to be quantified and used as a component uncertainty in the

uncertainty budget which is used to estimate the combined uncertainty of the final SST measurements acquired using these instruments.

The purpose of this document is:

- to summarise the minimum number of calibration steps which are required in order to ensure that SST measurements made with sea-borne radiation thermometers are traceable to an SI standard;
- to present methods for treating uncertainties in SST measurements;
- to provide guidance on the preparation of uncertainty budgets which satisfy each calibration step.

This document makes reference to the recently established, CEOS endorsed, Quality Assurance Framework for Earth Observation (QA4EO) <http://www.QA4EO.org>. This framework and its supporting guidelines, are based upon best practice and often are summaries or interpretations of existing standards (e.g. ISO, 2012) and documents developed for other communities. It should thus be noted that the QA4EO guidelines can be considered a convenient common reference point for more specific documents and not intended as a replacement for them.

2 UNCERTAINTIES AND THEIR TREATMENT

The acquisition of a CDR requires traceability to SI units, which requires documentary evidence of a correct treatment of measurement uncertainties. The definitions and meaning are clearly defined in QA4EO which is itself derived from the formal ISO guide to vocabulary in metrology recently revised in 2012 - Traceability is the **property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty** (ISO, 2012) (Ehrlich and Rasberry, 1997). Bell (2001) provides a basic introduction to measurement uncertainty, while a more detailed exposition is given by UKAS M3003 (2007). Each calibration step has to have its own, appropriate, uncertainty budget. Unfortunately the concept of traceability by some instrument manufacturers and users who declare the calibration of their instruments as being traceable to National Standards Laboratories is not always as rigorous as it should be, and can lead to misunderstandings and inappropriate interpretations by customers/users.

It also not uncommon for there to be confusion and misuse of the terms ‘measurement uncertainty’ and ‘measurement error’. The two terms are very different since measurement uncertainty refers to the limits within which the value of the parameter being measured may be reasonably presumed to lie, while measurement error refers to the difference between the value obtained from a measurement and the corresponding (presumed) true value. Since the true value is rarely if ever known, the value measured by a designated reference laboratory, typically one or more National Measurement Institutes (NMI)s, is usually considered to be representative of the true or SI value.

The calculation of the uncertainty of a measurement is very important because it allows the meaningful comparison of measurements made by different people or different institutions. Measurements made by two different people/institutions may differ, but if the difference is smaller than the combined uncertainty of their measurements, then the two results can be said to agree.

A brief and simplified overview of the steps required to calculate the overall uncertainty of a measurement is presented below. The reader is encouraged to consult Bell (2001), UKAS M3003 (2007), QA4EO and ISO (2012) and the references therein for more thorough discussion and detail.

The key steps to estimating the overall uncertainty of a measurement are as follows:

1. Determine what quantities are used as inputs to obtaining the measurement result;
2. Estimate the uncertainty of each input quantity, and express all uncertainties in similar terms. Input quantities that do not significantly affect the result can be ignored;
3. Calculate the combined standard uncertainty of the measurement. If the input quantities are not independent of each other, extra calculations may be required to take account of correlations;
4. Express the uncertainty in terms of a coverage factor, and state a level of confidence.

1. The treatment of uncertainties is straightforward, if the measurement procedure can be described by an analytical equation:

$$y = f\{x_{i;i=1:n}\} \quad (1)$$

where y is the result of the measurement and each x_i is one of n input quantities. For a measurement that results from many (m) separate measurements, equation (1) can be generalised to:

$$Y = f\{y_{k;k=1:m}\} \quad (2)$$

where Y is the overall result. However, for many measurements it is difficult to establish a complete analytical equation. In this case, a list of parameters/external influences which can contribute to the output of the measurement has to be assembled.

2. Uncertainty contributions can be one of two types:

- (i) **A Type A uncertainty contribution** is derived by a statistical calculation from a series of repeated measurements. The standard deviation of the mean of these measurements (also known as the standard error of the mean) is referred to as the Type A standard uncertainty (QA4EO guideline 6). For example, where n repeated measurements are carried out, and s is the calculated standard deviation of these measurements, the standard uncertainty is given by

$$u = \frac{s}{\sqrt{n}} \quad (3)$$

- (ii) **A Type B uncertainty contribution** is derived from non-statistical calculations. These include uncertainties taken from calibration certificates or derived from the characterisation of the performance of the instruments being used. They also include uncertainties taken from manufacturers' specifications. However, where this is not possible, it is acceptable for an estimate to be made based on

experience and/or ‘other knowledge’, provided the basis for this is made clear and is documented.

The standard uncertainty is defined as one standard deviation (ISO, 2012). The standard uncertainty of a particular parameter contributing to a measurement is derived from the uncertainty value (the spread parameter) of that parameter divided by a number associated with the assumed probability distribution of that parameter (UKAS M3003, 2007). The divisors for the probability distributions most likely to be encountered are 1 for normal distributions, $\sqrt{3}$ for rectangular distributions, $\sqrt{6}$ for triangular distributions and, $\sqrt{2}$ for U-shaped distributions (ISO, 2012).

- (iii) All uncertainty components must be expressed in similar units, usually the units of the measurement result. In cases where the input parameter to a measurement is different from the output, it is necessary to introduce a “sensitivity coefficient” so that the measurement result can be directly related to that particular input parameter. For example, when considering the effect of ambient humidity on SST measurements, the input parameter is humidity whereas the output parameter is temperature. The sensitivity coefficient is effectively a conversion factor from one unit into another (UKAS M3003, 2007).

3. Once all Type A and Type B standard uncertainty contributions have been estimated, they should be combined (QA4EO guideline 6) to produce the so called **combined standard uncertainty** of the measurement. The combined standard uncertainty $u_c(y)$ of y is the positive square root of the estimated variance, given by

$$u_c^2(y) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \left(\frac{\partial f}{\partial x_i} \right) \left(\frac{\partial f}{\partial x_j} \right) u(x_i, x_j) \quad (4)$$

The partial derivatives $\partial f / \partial x_i$ are the sensitivity coefficients, $u(x_i)$ is the standard uncertainty associated with x_i , and $u(x_i, x_j)$ is the covariance associated with x_i and x_j . For simplicity, we will assume that there are no correlations between x_i and x_j , i.e. the second term in the right-hand side of Eq. (4) is zero. In the situation where a measurement equation cannot be established, Eq. (4) can still be applied, using the standard uncertainties associated with the quantities/external influences which are known to contribute to the output of the measurement.

4. The combined standard uncertainty is usually converted to the **expanded uncertainty** by multiplying the combined standard uncertainty by the “**coverage factor**”, k (QA4EO guideline 6). The expanded uncertainty provides a larger range of values than the combined standard uncertainty so that the probability that the value of a measurement lies within that expanded range is higher.

3. UNCERTAINTY AND TRACEABILITY OF SST MEASUREMENTS

There are two different approaches which can potentially be used to enable a SST-measuring radiation thermometer to provide SI-traceable measurements.

3.1 The traceable calibration of the radiance temperature of the internal blackbodies contained within the SST-measuring radiation thermometer

The first approach involves the traceable calibration of the radiance temperature of the internal blackbodies contained within the SST-measuring radiation thermometer. This requires that the thermometers used to measure the temperature of the internal blackbodies of the SST-measuring radiation thermometer are traceably calibrated to SI units. It is important to note that this condition on its own is not sufficient. The internal blackbodies must also be fully characterised with respect to parameters that may affect their use in the particular application. Parameters such as their cavity emissivity and any temperature difference between the reading of the thermometers and the true temperature of the emitting surface of the blackbody cavity must also be known. The former requires that of the emissivity of the blackbody cavity coating over the range of wavelengths over which the radiation thermometer responds be known, along with the corresponding uncertainty. It also requires the emissivity of the blackbody to be calculated, ideally using a Monte Carlo based method. For this calculation, the exact geometry of the blackbody cavity, along with the size of the blackbody aperture must also be known. Any temperature differences must also be determined and these will be governed by the position and means of attachment of the thermometers relative to the blackbody cavity, the cavity geometry, the material out of which the cavity is made, the cooling or heating of the cavity surface due to radiative and convective cooling/heating, temperature uniformity over the surface of the cavity etc.

The internal blackbodies are restricted in size and therefore in the size of their exit apertures, so a Size of Source (SoS) correction (Pusnik et al., 2006) will also be required, along with the associated uncertainty contribution. Full evaluation of all these parameters can be difficult but SI traceability will require that the magnitudes of all these effects to be estimated and any appropriate corrections and uncertainties applied.

3.2 The use of an external traceably-calibrated blackbody.

The second approach requires the traceable calibration of the radiance temperature of an external blackbody which can subsequently be used to calibrate the SST-measuring radiation thermometer. This is considered a much better approach because it involves the calibration of a blackbody whose physical size is not restricted by the external dimensions of the radiation thermometer housing and portability. This means that the external blackbody can be physically larger and can therefore be designed to have a higher emissivity than the internal blackbodies. Moreover, the performance of the external blackbody can be re-calibrated/checked far more frequently than that of the internal blackbodies.

The radiance temperature of the external blackbody can be calibrated in two ways. The first involves the calibration of the external blackbody against a reference standard blackbody, which may either be one used by NMIs, or one with formal traceability to an NMI blackbody. The external blackbody then becomes a transfer standard blackbody, and a certificate will be issued when it is calibrated against the reference standard blackbody stating its radiance temperature at various temperature settings. The certificate will also include the combined uncertainty values associated with the radiance temperature of the transfer standard blackbody at the various temperature settings. The combined uncertainty values shown on the calibration certificate are calculated by the institute which would carry out the calibration of the transfer

standard blackbody (usually an NMI or accredited organisation), so can be considered sufficient evidence of traceability.

The second method of calibrating the radiance temperature of the external blackbody would be similar to that used for the calibration of the radiance temperature of the internal blackbodies (see section 3.1), i.e. it would require:

- α. The traceable calibration of the thermometers used to measure the temperature of the external blackbody.
- β. The calculation of the temperature difference between the reading of the thermometers and the true temperature of the surface of the blackbody cavity. This is governed by the position of the thermometers relative to the inside of the blackbody cavity, the blackbody cavity geometry, the material out of which the blackbody cavity is made of, the cooling/heating of the cavity surface due to radiative and convective cooling/heating, how uniform is the temperature over the surface of the cavity etc.
- γ. Knowledge of the emissivity of the blackbody cavity coating over the range of wavelengths over which the radiation thermometer responds so that the cavity emissivity can be calculated (using Monte Carlo methods).

3.3 *SST measurement recommendations*

For the purposes of the traceable measurement of SST using radiation thermometers such as SISTER (Barton et al. 2004), ISAR (Donlon et al., 2008) or MAERI (Minnett et al. 2001), the authors recommend that the traceability chain is via an external transfer standard blackbody which is itself calibrated by an NMI against a reference standard blackbody or of course directly against the NMI reference standard. This calibration chain would require the following minimum calibration steps:

- i. Calibration of the radiance temperature (related to spectral radiance via Planck's equation) of an external transfer standard blackbody against SI units (an NMI owned reference standard blackbody). The calibrated transfer standard blackbody will then be used to calibrate the SST-measuring radiation thermometer (see next step);
- ii. Calibration of the SST-measuring radiation thermometer against the calibrated transfer standard blackbody (which was calibrated under step (i));
- iii. Measurement of the SST of the ocean using the calibrated radiation thermometer (calibrated under step (ii));
- iv. Comparison with one or more independently calibrated radiation thermometers whilst viewing a common water body.

Step (iv) is not strictly a requirement as a calibration step in a minimal traceability chain to make a single point measurement of SST. However, it is highly valuable and recommended to establish the evidence needed to be demonstrated that the user of the instrumentation follows an appropriate and consistent procedure when taking measurements. This step is considered fundamental by NMIs as it is the only true way to evaluate that an uncertainty budget is complete and reliable. Consistency (within their combined uncertainties) between two independent measurements of the same parameter can be considered clear evidence and

justification for a declared uncertainty, whereas deviations are an indication that there is something wrong with one or both measurements.

QA4EO recommends that an uncertainty budget should be developed for each of the steps in the traceability chain. Note that if the calibration chain incorporated more steps, then each of these additional steps must also have its own uncertainty budget. Furthermore the combined uncertainty derived from the uncertainty budget for step (i) will be a component uncertainty in the uncertainty budget for step (ii). Finally, the combined uncertainty derived from the uncertainty budget for step (ii) will be a component uncertainty in the uncertainty budget for step (iii) and this will then be in the combined uncertainty of the comparison. Note that the uncertainty budget for each of the calibration steps may be better broken down into smaller steps (and consequent uncertainty budgets) depending on how the actual measurements are conducted.

The next sections provide some guidance on how to prepare an uncertainty budget for each of the calibration steps highlighted above.

4. EXAMPLES OF UNCERTAINTY BUDGETS FOR SST MEASUREMENTS

The radiance temperature of a test blackbody is defined as the temperature at which the cavity of a perfect blackbody (i.e. a blackbody with a cavity emissivity equal to 1.000) would have to be maintained so that its spectral radiance would be equal to the spectral radiance of the test blackbody. Since the emissivity of the test blackbody is a function of wavelength, the radiance temperature of the test blackbody will also be a function of wavelength so the operating wavelength must be quoted when specifying the radiance temperature of the test blackbody.

The most common SI reference standard for the calibration of the radiance temperature of a transfer standard blackbody is a reference blackbody. The reference blackbody should ideally be the radiance temperature standard of a National Measurement Institute (NMI) such as NPL or NIST but can be that of an organisation which can demonstrate robust traceability to an NMI. The radiance temperature of the reference blackbody is calculated by measuring its cavity temperature as well as the emissivity of its cavity at the operating wavelengths. International equivalence and thus validation of NMI primary SI scales such as radiance temperature are confirmed by regular formal comparisons with other NMIs (Gutschwager et al., 2012) as part of the Mutual Recognition Arrangement (BIPM MRA 1995). Traceability of the radiance temperature of the reference blackbody to SI units requires that the emitting surface temperature of the blackbody cavity be known as well as the emissivity of the of the same blackbody cavity at the wavelength of interest. Two methods are currently used to determine the cavity temperature of the reference blackbody in SI units:

- i. The reference blackbody cavity temperature is determined by immersing the blackbody cavity into a phase transition cell such as a gallium fixed-point blackbody. The melting point of gallium is a fixed point on the ITS-90 temperature scale so the cavity temperature will be traceable to SI via the Kelvin. Moreover, because the gallium melting point is a fixed point on the ITS-90 scale, there is no uncertainty associated with it (however, the radiance temperature of the gallium blackbody still has an uncertainty associated with it, as shown in Table 1).

- ii. The reference blackbody cavity temperature is determined by using a calibrated thermometer which is in good thermal contact with the blackbody cavity. In this case the blackbody radiance temperature will also be traceable to SI via the Kelvin. Note that it is the emitting surface temperature of the blackbody cavity which determines the blackbody radiance temperature so any temperature difference between the thermometer reading and the temperature of the emitting surface of the blackbody cavity should be known and used to correct measurements, and also used to calculate a corresponding uncertainty contribution.

It is worth mentioning that the temperature of reference blackbodies operating at high temperatures (over 1000 K) can also be calibrated using “Absolute Radiation Thermometers” (ARTs) (Fox et al., 1991). In this case the traceability to SI units is derived from radiometric units traceable to the cryogenic radiometer (Fox et al., 1995/1996). However, the performance of infrared detectors operating in the 8 μm to 12 μm wavelength range is not currently good enough for the reasons highlighted in Section 1, to enable this approach to have a sufficiently small uncertainty, so the traceability of the radiance temperature of all ambient temperature reference blackbodies is provided by either a fixed point blackbody or by a blackbody whose cavity temperature is measured using a calibrated contact thermometer. Measuring the temperature of the cavity alone is not sufficient to establish traceability to SI units. The cavity emissivity must also be known. The emissivity of the reference blackbody can be measured by direct cavity absorbance measurements, but is more frequently calculated using Monte-Carlo simulations. The latter approach requires that the emissivity of the material which forms the blackbody cavity be known over the range of wavelengths to which the radiation thermometer responds.

Note that the development of an uncertainty budget is also required in order to estimate the uncertainty with which the radiance temperature of the reference blackbody is known. This uncertainty budget will include a number of uncertainty contributions including:

- α) the uncertainty in the calibration of the thermometer which is used to measure the temperature of the cavity of the reference blackbody (this is zero in the case of fixed-point blackbodies such as the gallium fixed-point blackbody);
- β) the uncertainty in the knowledge of the emissivity of the cavity of the reference blackbody;
- γ) the uncertainty due to the temperature drop between the position where the thermometer is located and the inside surface of the blackbody cavity. In blackbodies which operate above ambient temperature, the cavity temperature is always lower than the temperature indicated by the thermometer due to radiative and convective cooling of the cavity. Conversely, in blackbodies which operate below ambient temperature, the cavity temperature is always higher than the temperature indicated by the thermometer due to radiative and convective heating of the cavity;
- δ) an uncertainty contribution to account for any ageing/drifts in the reference blackbody radiance temperature.

It is the responsibility of the primary calibration laboratory, ideally an NMI, to quantify these uncertainty contributions and collate them to produce an appropriate uncertainty budget to assign an overall combined uncertainty to the radiance temperature of the reference blackbody. Table 1 gives the uncertainty budget developed by NPL in order to calculate the combined uncertainty of the radiance temperature of a gallium fixed point blackbody which is used as a

reference blackbody in radiance temperature calibrations in the -40 °C to +80 °C temperature range.

Table 1: Standard uncertainty budget of the radiance temperature of an NPL Ga fixed-point blackbody

Contribution	Standard Uncertainty / mK	Comment
Uncertainty due to the Ga blackbody emissivity	29	Difference of cavity emissivity (0.9993) from unity is taken to be the uncertainty contribution (with rectangular distribution). The standard uncertainty is provided in mK.
Uncertainty due to Ga blackbody temperature “drop”	13	Estimated from the temperature drop between the Ga metal and the inside surface of the Ga blackbody cavity.
Stability of the Ga blackbody radiance temperature (as indicated by a high resolution radiometer such as AMBER).	4	Standard deviation of measurements over the measurement period e.g. 5 minutes.
Uncertainty due to radiation heat loss to the environment	2	Small since the Ga blackbody is operating just above ambient.
Uncertainty due to convective heat loss to the environment	2	Small since the Ga blackbody is operating just above ambient.
Uncertainty due to (spatial) temperature variation inside the cavity	3	
Uncertainty due to ambient temperature fluctuations	2	
Uncertainty due to the purity of the Ga metal	1	The Ga metal used to fill the blackbody cavity was 99.9999% pure.
Combined uncertainty ($k=1$)	32 mK	

The calibration of the radiance temperature of the transfer standard blackbody against an SI reference blackbody requires the use of a well characterised radiometer or radiation thermometer. This calibration step will usually be done by an NMI. The radiation thermometer will transfer the calibration from the reference blackbody to the transfer standard (customer) blackbody. This calibration should be done at a number of temperatures spanning the range of radiance temperatures over which the transfer standard blackbody will be used. This calibration will also require its own uncertainty budget which will include the uncertainty contribution of the reference blackbody as well as the appropriate uncertainty contributions introduced by the radiation thermometer which is used to provide the transfer to the test blackbody. By using dedicated, well characterised radiometers such as AMBER (Theocharous et al., 1998) or TXR

(Rice and Johnson, 1998), the uncertainties introduced by this calibration step can be minimised. However, it should be the responsibility of the calibration laboratory, usually the NMI which will be completing this calibration step, to prepare the appropriate uncertainty budget. The uncertainty budget must include all relevant uncertainty contributions for the calibration of the uncertainty of the radiance temperature of the transfer standard blackbody.

Table 2 gives the uncertainty budget developed by NPL in order to calculate the combined uncertainty of the radiance temperature of a suitable transfer standard blackbody calibrated by comparing its radiance temperature to that of a gallium fixed-point blackbody reference source using the AMBER radiometer (Theocharous et al., 1998). This uncertainty budget includes the uncertainty in the radiance temperature of the gallium blackbody (derived in Table 1) as a component uncertainty. It also includes uncertainty contributions to account for the non-linear response of the lock-in amplifier used by AMBER, fluctuations in ambient temperature over the duration of the calibration and drifts in the responsivity of AMBER over the duration of the calibration.

This calibration step results in a transfer standard (customer) blackbody whose radiance temperature is traceably calibrated to SI units (ITS-90) and with an appropriate uncertainty assigned to its radiance temperature.

The calibration of the SST measuring radiation thermometer against the calibrated transfer standard blackbody is the responsibility of the owner/user of the radiation thermometer and will require the development of an appropriate uncertainty budget. The following section provides some guidance on the development of this uncertainty budget e.g. the identification and estimation of the magnitude of the various uncertainty contributions which contribute to the combined uncertainty of this measurement.

5. UNCERTAINTY COMPONENTS WHICH HAVE TO BE CONSIDERED IN THE DEVELOPMENT OF THE UNCERTAINTY BUDGET ASSOCIATED WITH THE MEASUREMENT OF SST USING CALIBRATED RADIATION THERMOMETERS.

It is a well-established principle that a measurement has little if any meaning without an associated uncertainty budget. To ensure that SST measurements acquired with the radiation thermometer satisfy CDR conditions, every effort should be made to ensure that the radiation thermometers being used in SST measurements are fully characterised so that an appropriate uncertainty budget can be established.

All of the parameters/external influences which could potentially contribute to the output of the radiation thermometer being used, from the point of its calibration against a transfer standard blackbody to the point when it is used to measure the SST at a particular location of the sea should be identified. The first uncertainty contribution arises from the uncertainty in the calibration of the transfer standard blackbody against which the radiation thermometer is calibrated. The transfer standard blackbody which will be used to calibrate the radiation thermometer should be accompanied with a calibration certificate or some other evidence/record of the traceable calibration of its radiance temperature. The calibration certificate of the transfer standard blackbody should include the uncertainty with which the radiance temperature of the transfer standard blackbody is known at all temperatures of interest. The uncertainty value of the blackbody at a particular temperature will be included as a

component uncertainty in the uncertainty budget which will provide the uncertainty with which the radiation thermometer is calibrated at that temperature. When the calibrated radiation thermometer is used to measure SST, another uncertainty budget is required which will allow the combined uncertainty of that particular SST measurement (completed with that radiation thermometer, under specific conditions) to be estimated. That uncertainty budget will include the uncertainty of the radiation thermometer as a component uncertainty.

Table 2: Systematic standard uncertainties when AMBER is used to measure the radiance temperature of a test blackbody in the 10 °C to 50 °C (283K to 323 K) temperature range by comparison to a gallium fixed-point blackbody.

Contribution	Standard Uncertainty / mK	Comment
Uncertainty in the Ga blackbody radiance temperature	32	Taken from Ga blackbody uncertainty budget (see Table 1)
Uncertainty due to the lock-in amplifier non-linearity (Theocharous, 2008)	36	0.1% non-linearity in the lock-in amplifier. Depends on the difference between the Ga melting point temperature and the temperature of the target being measured.
Uncertainty in the relative spectral responsivity calibration of 10.1 μm filter radiometer	6	From the calibration of the relative spectral responsivity of the 10.1 μm filter radiometer
Uncertainty due to the definition of the "radiometric zero"	4	From monitoring the AMBER output when the 77 K blackbody is being viewed
Uncertainty in the measurement of the ZnSe AMBER window transmission	1	Common to all blackbody measurements, hence the uncertainty due to this window is small.
Uncertainty in the measurement of the ZnSe AMBER lens transmission	1	Common to all blackbody measurements, hence the uncertainty due to this window is small.
AMBER stability/drift over the period of a measurement	18	based on 0.05% drift over a measurement period i.e. 5 minutes
Uncertainty due to ambient temperature fluctuations	12	See reference (Theocharous and Theocharous, 2006)
Uncertainty due to chopper frequency fluctuations	2	Based on a 0.2 Hz drift in the chopper frequency during a measurement cycle.
Combined uncertainty ($k=1$)	53 mK	

A list of the parameters which are likely to influence the measurement of SST using a radiation thermometer is given below. This may not be a comprehensive list as this document is written without direct experience of any specific SST instrument or its use on the ocean. Furthermore, there are a large number of radiation thermometers currently being used for SST measurements, each of bespoke design (Theocharous et al., 2010). Each radiation thermometer may be affected differently by external influences and, therefore, may require a different approach in the development of the corresponding uncertainty budget.

All parameters, which determine (or can contribute to) the performance of a radiation thermometer must be fully characterised. This is essential in order to quantify the magnitude of their effect on the radiation thermometer output and to allow the uncertainty budget associated with measurements involving that radiation thermometer to be prepared. The uncertainty contribution due to external influences is most easily determined by changing the magnitude of the external influence by a known amount (while leaving all other parameters the same) and measuring the resulting change in the radiation thermometer output. The most important parameters which determine the performance of radiation thermometers are summarised below:

5.1 *Responsivity*

Responsivity is the main parameter measured during the calibration of the SST-measuring radiation thermometer against the transfer standard blackbody. The calibration should include an uncertainty budget which will provide the combined uncertainty of that calibration. That will in turn be used as a component uncertainty in the measurement of the SST when the calibrated radiation thermometer is used in SST measurements. The uncertainty budget will have a similar format to that shown in Table 2. If the transfer standard blackbody has a small aperture, then another uncertainty component will have to be included to account for the size-of-source (SOS) effect.

5.2 *Out-of-band response*

The characterisation of the radiation thermometer should include a consideration for its out-of-band response. This can arise due to the imperfect blocking by the band-pass filter which is used to define the spectral response profile of the radiation thermometer. Although the out-of-band response of visible radiometers can normally be suppressed to below 0.001% of the peak response relatively easily using good quality interference filters and absorbing glasses, things are considerably harder in the infrared. Furthermore, the out-of-band rejection of visible radiometers can be aided by the selection of an appropriate photodetector (for example, silicon detectors do not respond to wavelengths much longer than 1.1 μm , while InGaAs detectors do not respond to wavelengths much longer than 1.7 μm). However, a large fraction of infrared radiation thermometers employ thermal detectors (e.g. thermopiles and pyroelectric detectors) which have a flat, spectrally broad response. This means that if the wavelength selective filter has any out-of-band transmission, at any wavelength, this unwanted radiation passing through the filter will be detected by the radiation thermometer; the total effect of this out-of-band radiation can be large, even if the proportion at each individual wavelength is small. Characterisation of the out-of-band response can conveniently be done by adding a long-pass filter whose transmission starts just above the wavelength range of the radiation thermometer. If any signal is present then there are likely to be issues with out-of-band rejection at longer wavelengths. Similarly, the out-of band response at shorter wavelengths can be evaluated by inserting a low-pass filter in front of the radiation thermometer. The filter transmission is

chosen to stop wavelengths just below the wavelength band of the radiation thermometer. If any signal is present then there may be issues with out-of-band rejection of the radiation thermometer at short wavelengths.

5.3 *Linearity of response*

The linearity of response of a radiation thermometer is the property whereby the output reading of the instrument is directly proportional to the temperature of the target being measured. The linearity characteristics of radiation thermometers of the type being used to measure SST benefit greatly by the fact that one or more internal blackbodies are used within the instrument, as reference sources. However, the linearity characteristics of the test instrument should be investigated by measuring the radiance temperature of a test blackbody at different temperatures and comparing these values with the true blackbody temperatures, as indicated by the blackbody itself. The plot of the temperature read by the radiation thermometer versus the “true” blackbody temperature can provide the instrument non-linearity which can be used to correct subsequent measurements carried out by that radiation thermometer. It can also be used to estimate an uncertainty component due to the instrument non-linearity which can be added as a component uncertainty to the uncertainty budget associated with measurements carried out by that radiation thermometer.

5.4 *Temperature Coefficient of Response*

The temperature coefficient of response of a radiation thermometer quantifies the effect of the ambient temperature on the responsivity of the instrument. It is usually given by the percentage change in the responsivity of the instrument, resulting from an increase of the ambient temperature of 1 °C. It is calculated by measuring the output of the radiation thermometer while it is sequentially maintained at a number of temperatures around ambient. Figure 1 shows the output of a radiometer located in an enclosure, as the temperature of the enclosure was increased every 20 minutes in steps of 2 °C, from 20 °C to 30 °C. It is clear that the responsivity of this particular radiometer increases with increasing ambient temperature. From Figure 1, another plot can be generated of the radiometer output at different ambient/enclosure temperatures. From the slope of that plot, the temperature coefficient of response of that particular radiometer was estimated to be +0.29% °C⁻¹.

It so happens that the temperature coefficient of response of that radiometer arose due to the band-pass filter used to define its spectral response. If this cannot be resolved through better technology or some temperature stabilisation process then the effect on the measurement has to be evaluated, corrected and an appropriate uncertainty assigned. This requires:

- i. the ambient temperature to be recorded during the entire period during which measurements are acquired using this radiometer;
- ii. the maximum deviation of the ambient temperature during that period to be calculated (say ± 2 °C);
- iii. the maximum per cent fluctuation on the radiometer output during the monitoring period (± 2 °C at 0.29% per °C means a maximum deviation of $\pm 0.58\%$) to be estimated. This is now treated as an uncertainty contribution with a rectangular profile (QA4EO Guideline 6) which is equivalent to a standard uncertainty contribution equal to 0.58% divided by $\sqrt{3}$;

- iv. This uncertainty contribution should be added to the other uncertainty components to arrive at the combined uncertainty of the measurement completed with that radiometer.

One way of reducing the uncertainty contribution due to the temperature coefficient of response of the radiation thermometer is to actively stabilise the temperature around the instrument. However, this may not be practically feasible due to the extra power requirements which will be necessary. A second method would be to reduce the period of data acquisition to ensure that the drift in the ambient temperature during that period is minimised.

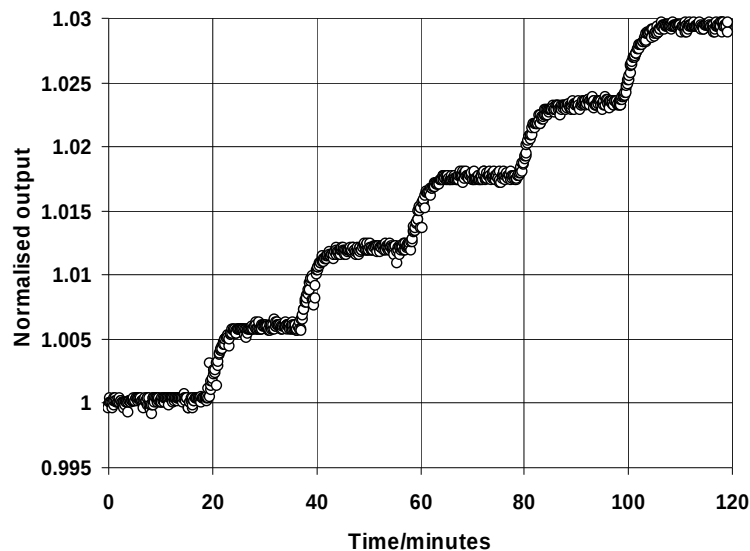


Figure 1: Normalised output of a radiometer as the ambient temperature was increased every 20 minutes in steps of 2 °C, from 20 °C to 30 °C.

5.5 *Ambient humidity fluctuations*

The effect of humidity fluctuations can be treated in the same way as the effect of ambient temperature fluctuation highlighted above. Water is known to absorb strongly in the infrared. Even though infrared radiation thermometers operate in one of the infrared atmospheric windows, it would not be surprising to find that the responsivity of a radiation thermometer is affected by the humidity of the environment in which it is operating. Again, dedicated experiments consisting of placing the radiation thermometer in an environmental chamber and measuring its responsivity to a constant input while the humidity in the chamber is changed allows a plot of the instrument output versus ambient humidity to be generated. The slope of this plot (humidity coefficient of response) can be treated in exactly the same way as the temperature coefficient of response (see section 5.4) to estimate the uncertainty contribution due to fluctuations in humidity during the period of the acquisition of the data. Note that, for this to be done, it will be necessary to record the ambient humidity during the period of data acquisition with the radiation thermometer.

5.6 *Polarisation*

The absolute spectral responsivity of radiation thermometers generally exhibits some dependence on the state of polarisation of the radiation being measured. This is not an issue when blackbody sources are being viewed because their output is completely unpolarised.

However, the output of many other sources, including skylight, are partially polarised. The dependence of the responsivity of the radiation thermometer on the state of polarisation of the incident radiation must be fully characterised. Each component of a radiation thermometer is expected to introduce some degree of polarisation (CIE, 1984). The polarisation contribution from each radiometer component should be analysed separately. This is because it can provide a better understanding of the polarisation characteristics of the instrument and can aid in the reduction of the polarisation effects through improvements in instrument design (CIE, 1984). Alternatively, at least the linear polarisation characteristics of the complete radiometer should be quantified. This can be done by measuring the instrument responsivity while the plane of polarisation of the incident radiation is rotated (CIE 1982) or vice versa. The appropriate uncertainty contribution should be introduced, to be representative of the polarisation characteristics of the source being viewed.

5.7 *Temporal response*

The response time of a radiometric sensor defines how quickly the output of the sensor can follow a rapidly changing incident signal. Mathematically it specifies how quickly the output of the sensor rises in response to a step change in the incident signal. The temporal response of the radiation thermometers used for SST is very long (well in excess of 10 minutes in some cases) because each measurement involves three separate measurements (the sea surface, the sky and the internal blackbody). During the period of such a measurement, the SST may change. An uncertainty component should be included in the uncertainty budget to account for any changes in the SST during the period of the measurement of the sea, the sky and the internal blackbodies.

5.8 *Repeatability, Type A (random) uncertainty*

Every uncertainty budget must include a repeatability or Type A uncertainty contribution. This is estimated by repeating the same measurement a number of times, without realignment and estimating the standard deviation of these measurements.

5.9 *Reproducibility*

The uncertainty budget should contain an uncertainty component related to how well the measurement system can reproduce the measurement. This should be estimated by making a repeat measurement of an observable e.g. blackbody output or sea surface temperature after re-aligning the measurement system. This can be difficult to evaluate if the observable is not stable and in such cases it is likely that this component will be small compared to that due to the observable under test.

5.10 *Radiation thermometer stability and ageing*

The responsivity of all measuring instruments can change slowly with time and this is known as ageing. Ageing is accelerated when the instruments are operated in harsh environments such as on the exposed decks of ships. Instruments using interference filters sometimes exhibit large, sudden changes in their responsivity of 1% or more. These changes are believed to originate from the relaxation of the dielectric constituent layers of the interference filter. The effect of ageing is minimised by frequent calibration. SST measuring radiation thermometers benefit greatly from possessing an internal calibration blackbody which serves to provide a first order

frequent calibration and thus minimises the effects of ageing. Another source of ageing which was identified in the responsivity of radiation thermometers utilising cryogenically cooled detectors arises due to the deposition of a thin film of ice on the cooled detectors (Theocharous, 2005) and cooled wavelength selecting filters (Theocharous et al., 2005). These ageing effects are reversible because they can be temporarily eliminated by evacuating the detector Dewars while they are baked at about 50 °C. The drifts are stronger in regions where ice has absorption bands such as the 2.9 μm to 3.3 μm and 9 μm to 12 μm wavelength bands (Theocharous, 2006). An uncertainty contribution due to instrument ageing should be estimated from the previous history of the instrument. This is likely to have a rectangular profile so it must be converted to a standard uncertainty and added as a component in the uncertainty budget.

5.11 “Background” or “dark” measurements

When radiometers are used to acquire measurements, it is important to include “background” or “dark” readings. The aim of the “dark” measurements is to eliminate the effects of clutter and stray light as well as any biasing due to the photodetector dark signal and the electrical amplification circuitry. The positioning of the optical shutter is critical in the acquisition of “dark” measurement. Infrared measurements are further hindered by the fact that bodies whose absolute temperature is above absolute zero emit infrared radiation so the presence of bodies at ambient temperature in the FOV of a radiation radiometer can affect the instrument reading. SST measuring radiation thermometers benefit greatly by using an internal blackbody to compare the spectral radiance of the sea surface with that of the internal blackbody. This reduces the need to acquire proper “dark” measurements. However, the contribution of the internal blackbody only eliminates errors due to the definition of “zero” when the SST is the same as the temperature of the internal blackbody. When there is a difference between the two, the advantages of the “null reading” are reduced. An uncertainty contribution should be included in the uncertainty budget to account for the inadequate definition of “zero”. This uncertainty component will depend on the temperature difference between the SST being measured and the temperature at which the internal blackbody is set. This uncertainty component is expected to be less in SST-measuring radiation thermometers which include two internal reference blackbodies.

5.12 Uncertainty contribution due to out-of-field stray light

The response of a radiation thermometer to optical radiation incident from different directions should be the same irrespective of the angle of incidence, provided the radiation comes within the instrument’s field of view. On the other hand, the response of the radiation thermometer to radiation which is outside its field of view should be zero. This is accomplished by placing a number of apertures/baffles at appropriate positions within the body of the radiation thermometer. In this case, radiation thermometer are characterised for their ability to reject the output from sources, which are not in their FOV. If the out-of-field stray light rejection of a radiation thermometer is poor then the appropriate uncertainty contribution should be added when the instrument is viewing a scene, with the sun or other radiation source being close to the field of view of the radiation thermometer.

5.13 Uncertainty contribution due to the water emissivity.

The sea water emissivity at particular angles is known from tables. These values should have uncertainty values associated with them. The uncertainty in the emissivity of sea water under

the conditions of the measurement should be used as an uncertainty contribution in the calculation of the combined uncertainty.

5.14 *Uncertainty contribution due to the viewing angle*

Water emissivity is a function of the “angle of incidence”. The observation angle of the radiation thermometer will depend on the tilting of the ship. The level of tilting of the ship should be recorded and the corresponding change in the observation angle should be estimated. The corresponding change in the water emissivity (due to changes in the observation angle) should then be calculated. The maximum and minimum emissivity values (corresponding to the smallest and largest angle of incidence to the sea surface) can be used to calculate the range of values, which will represent the uncertainty with rectangular distribution. This range should be divided by $\sqrt{3}$ to calculate the standard uncertainty due to changes in the viewing angle.

5.15 *Other uncertainty contributions*

In addition to the above the following sources of uncertainty should also be considered:

- i. Uncertainty contribution due to the “state of the sea surface” i.e. the presence of waves and the “speed of the wind”.
- ii. Uncertainty contribution due to the measurement of the sky radiance.
- iii. Uncertainty contribution due to relative spectral responsivity of the radiation thermometer response (partly covered by out of band response).

6. COMPARISON EVIDENCE TO SUPPORT UNCERTAINTY EVALUATIONS.

This final section emphasises the importance of regular independent comparison with peers to ensure that the uncertainty budgets developed above are internationally consistent with those of others. In principle, a comparison can be treated in exactly the same way as a calibration except that in this case there is no *a priori* true value to which one instrument is being referenced as in the case of an NMI reference black body. In this case each participant in a comparison can be considered equal (or at least to a level commensurate with their uncertainties) and results or consistency is usually determined with respect to a mean value from all the results of the comparison (ideally weighted by uncertainties if they can be considered reliable).

The uncertainty of the comparison and the level at which evidence of equivalence can be demonstrated is based on the combined uncertainties of the participants, which will be calculated from the recommendations in the treatment of uncertainties provided in sections 4 and 5. If the radiation thermometers being compared exhibit differences in their readings when observing the common parameter, in this case SST, then an additional uncertainty to account for these differences should be added the combined uncertainty of the comparison. If there are more than two participants in the comparison, as would be preferred, the comparison reference value will have an uncertainty determined by the combined uncertainties of all the participants but reduced by dividing by the square root of the number of participants. Guideline 4 of QA4EO provides details of how best to organise and analyse a comparison.

The level of agreement between any two participants in the comparison can be used as evidence to support the uncertainty they have estimated, however it cannot be used to reduce any estimated uncertainty.

7. SUMMARY

A number of sea-borne radiation thermometers have been developed and are being used to validate sea surface temperature (SST) measurements made by satellite-borne instruments. Provided the principles specified by QA4EO are followed, measurements completed with these sea-borne radiation thermometers can be treated as Climate Data Records (CDRs). This document summarises the minimum number of calibration steps which are required in order to ensure that SST measurements made with sea-borne radiation thermometers are traceable to an SI standard. The treatment of uncertainties in SST measurements was summarised and typical uncertainty budgets which satisfy each calibration step were presented in order to provide guidance on the preparation of uncertainty budgets and to ensure that SST measurements can have a Quality Indicator (QI) associated with them. The uncertainty budgets presented in this document are only intended as a guide, as the exact form of the uncertainty budgets will depend on the details of each calibration step.

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Appendix 1

Definition of the Main Radiometric Quantities and Units

Radiant power, sometimes referred to as radiant flux, is defined as the time derivative of radiant energy and represents the rate of flow of radiant energy. It is denoted by the symbol Φ and has units of watts (W). Radiant power is used, for example, to quantify the power of a laser beam. The total radiant power or flux is frequently encountered in radiometry and it is the total radiant power emitted by a source in all directions. Note that radiant energy or “exposure” can be calculated by integrating the radiant power over a period of time. Radiant intensity¹ is the radiant power radiated from a source into a unit solid angle² in a defined direction and is expressed in units of W sr^{-1} . Radiant intensity is denoted by the symbol I and is associated with point, isotropic³ sources and sources whose dimensions are small compared to the distance between the source being characterised and the observer. Irradiance is the radiant power incident on a surface per unit surface area from a hemisphere. It is denoted by the symbol E and has units of W m^{-2} . Radiant exitance refers to the radiant power radiated into a hemisphere from a surface of unit area. It is denoted by the symbol M and has units of W m^{-2} . Finally radiance, denoted by the symbol L , is defined as the radiant power per unit solid angle per unit projected area (Nicodemus, F. E., 1963, Radiance, *American Journal of Physics*, **31**, 368-377) and is expressed in units of $\text{W m}^{-2} \text{sr}^{-1}$.

¹ The term intensity has different meanings when it is used in different fields. In radiometry it is defined as radiant power per unit solid angle and has units of W sr^{-1} . The same term is (wrongly) used to mean irradiance or radiant power and it is even used to denote radiance in atmospheric physics (Palmer, J. M., 1993, “Getting intense on intensity”, *Metrologia*, **30**, 371-372).

² Solid angle is the three-dimensional equivalent of the plane angle. The solid angle of a cone is defined as the ratio of the area cut out on a spherical surface with its centre at the apex of that cone divided by the square of the radius of the sphere. It has units of steradians (sr). A hemisphere has a solid angle of 2π sr.

³ An isotropic source is a spherical source which radiates uniformly in all directions i.e. its radiant intensity is the same in all directions.