

1 **A review of uncertainty in in situ measurements and data sets of sea-surface**
2 **temperature**

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24 **Abstract**

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26 Archives of in situ sea-surface temperature (SST) measurements extend back more than
27 160 years. Quality of the measurements is variable and the area of the oceans they sample
28 is limited, especially early in the record and during the two World Wars. Measurements
29 of SST and the gridded data sets that are based on them are used in many applications so
30 understanding and estimating the uncertainties are vital. The aim of this review is to give
31 an overview of the various components that contribute to the overall uncertainty of SST
32 measurements made in situ and of the data sets that are derived from them. In doing so, it
33 also aims to identify current gaps in understanding. Uncertainties arise at the level of
34 individual measurements with both systematic and random effects and, although these
35 have been extensively studied, refinement of the error models continues. Recent
36 improvements have been made in the understanding of the pervasive systematic errors
37 that affect the assessment of long-term trends and variability. However, the adjustments
38 applied to minimize these systematic errors are uncertain and these uncertainties are
39 higher before the 1970s and particularly large in the period surrounding the Second
40 World War owing to a lack of reliable metadata. The uncertainties associated with the
41 choice of statistical methods used to create globally complete SST data sets have been
42 explored using different analysis techniques but they do not incorporate the latest
43 understanding of measurement errors and they want for a fair benchmark against which
44 their skill can be objectively assessed. These problems can be addressed by the creation
45 of new end-to-end SST analyses and by the recovery and digitization of data and
46 metadata from ship log books and other contemporary literature.

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48 **1. Introduction**

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50 Measurements of the temperature of the sea surface have been made for more than 200

51 years for a wide variety of purposes. The earliest measurements of sea-surface

52 temperature (SST) in the eighteenth century were taken out of pure scientific interest.

53 Later, after the connection between SST and ocean currents was made, large numbers of

54 measurements were made for the construction of navigational charts. In the twentieth

55 century, the needs of weather forecasting and, to an extent, the need to produce marine

56 climate summaries determined the quantity and quality of observations. Most historical

57 SST measurements were not made by dedicated scientific vessels, but by voluntary

58 observing ships (VOS) on the basis that they would contribute to the safety of life at sea.

59 This is reflected in the geographical distribution of observations, which are largely

60 confined to major shipping lanes.

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62 Nowadays, in situ measurements of SST – those made at the surface as opposed to those

63 made remotely by satellites or aircraft – are used in diverse applications. They are used

64 directly in calibration and validation of satellite retrievals and they are assimilated into

65 ocean analyses [*Roberts-Jones et al.*, 2012]. They are also used to construct data sets of

66 summaries of SST on regular grids and globally-complete SST fields are created using

67 statistical techniques to impute SSTs in regions where there are no observations. The SST

68 data sets and statistical SST ‘reconstructions’ or ‘analyses’ are widely used, for example

69 as an index of global climate change [*Morice et al.*, 2012], as a boundary condition for

70 climate simulations [*Folland, 2005*] and reanalyses [*Simmons et al., 2010*], as initial
71 conditions for decadal forecasts [*Smith et al., 2007*], in studies of hurricane formation
72 [*Saunders and Harris, 1997*] and in studies of the impact of climate change on marine
73 ecosystems [*Sheppard and Rayner, 2002*].

74

75 As the demands for SST measurements have changed, so have the instruments used to
76 make them, and so have the ships and other vessels from which the measurements were
77 made. The first systematic observations were made using buckets to collect a water
78 sample. Buckets made of wood, canvas, tin, leather, brass, rubber and plastic – of designs
79 as various as the materials employed in their construction – have all been used to measure
80 the temperature of the surface layers of the ocean. There are two problems with this
81 approach. The first is that during the collection and hauling, the temperature of the water
82 sample can be modified by the combined actions of latent and sensible heat transfer and
83 the warmth of the Sun. Even in the best conditions, an accurate measurement requires
84 diligence on the part of the sailor; that is the second problem. Improvements to minimize
85 the physical effects were made to bucket designs during the 1950s, but as ships became
86 larger and faster, the making of the measurements became not just thankless, but
87 dangerous.

88

89 After the advent of steam ships in the late nineteenth century, it was routine to measure
90 the temperature of the sea water that was circulated through the steam condenser.

91 Condenser inlet measurements and later, engine room inlet (ERI) measurements, were
92 often recorded in ship logbooks, but they were not entered into meteorological logs until

93 the 1930s. The convenience of using measurements that were made as a matter of routine,
94 and the attendant reduction in the risk of losing a bucket or sailor overboard, meant that
95 ERI measurements became the preferred method for measuring SST on board ships
96 during the latter half of the twentieth century. That is not to say that the method was
97 without its difficulties. Modification of the temperature of the water between inlet and
98 thermometer was still a problem and it was now compounded by the varying depth of the
99 measurements.

100

101 Since the 1970s, a growing number of ships have been fitted with dedicated sensors either
102 outside or inside the hull. These have been joined by a growing array of moored and
103 drifting buoys which make automated measurements that are relayed by satellite. At
104 present, around 90% of all SST observations come from buoys. In calm conditions
105 drifting buoys measure at a nominal depth of between 10 and 20 cm depending on their
106 size. However, wave motion means that in some conditions the buoy will be submerged
107 for part of the time and report temperatures that are representative of something like the
108 upper 2 m.

109

110 Moored buoys are fixed platforms, akin, in some ways, to meteorological stations on
111 land. They come in a variety of shapes and sizes. Most are a few meters in height and
112 width, but the largest in regular use are the 12 m Discus buoys designed to weather the
113 wilder climates of the northern oceans. There are two loose groupings of moored buoys:
114 the Global Tropical Moored Buoy Array (GT MBA) and a more diverse group of coastal
115 moorings mostly around the US. The GT MBA has regular arrays of moorings in the

116 tropical Pacific, Atlantic and Indian Oceans. The majority of moored buoys measure SST
117 at a nominal depth of 1 m. Some measure slightly deeper and some moorings make
118 measurements at a range of depths.

119

120 SST measurements from ships and buoys together with near-surface measurements made
121 by oceanographic cruises have been gathered in digital archives. The largest and most
122 comprehensive of these is the International Comprehensive Ocean-Atmosphere Data Set
123 (ICOADS, *Woodruff et al.* [2011]). The latest release of ICOADS, release 2.5, contains
124 individual marine reports from 1662 to 2007, but air and sea temperature measurements
125 only start to appear in the 19th Century. Metadata giving information about some of the
126 measurements and the ships that make them is also provided and is now complemented
127 by information from regular bulletins such as WMO publication 47
128 (<http://www.wmo.int/pages/prog/www/ois/pub47/pub47-home.htm>).

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130 Other digital archives exist. Research vessel (RV
131 <http://coaps.fsu.edu/RVSMDC/index.shtml>) data are gathered at the Research Vessel
132 Surface Meteorology Data Center at Florida State University. Woods Hole
133 Oceanographic Institute (<http://www.whoi.edu/>) maintains an archive of research
134 mooring data and the OceanSites website (<http://www.oceansites.org/data/index.html>)
135 provides links to other mooring data. The Pacific Marine Environmental Laboratory
136 maintains an archive of water temperature measurements from the GTMBA at a range of
137 depths and time resolutions that are not available in ICOADS
138 (<http://www.pmel.noaa.gov/tao/global/global.html>). Near-surface measurements from

139 other sub-surface sources such as the Argo array of autonomous profiling floats also
140 exist.

141

142 Despite being comprehensive, ICOADS is incomplete. Large archives of paper records
143 exist around the world and many of these have yet to be digitized. It is not possible yet to
144 know exactly how many undigitized records remain because there is no definitive
145 catalogue of global archives. What is known is that many archives that have been
146 identified are far from being exhausted. The potential for reducing the uncertainty in SST
147 analyses as well as in reconstructions of other marine variables is clear, but funding,
148 particularly sustained funding for the efforts to identify, image and key the data has
149 proved difficult to find. Nonetheless, there have been some successes such as a project to
150 crowd source the keying of Royal Navy logbooks from the First World War. Volunteers
151 on the OldWeather.org project keyed pages from the logbooks online. In the three years
152 since the project started more than 1.6 million weather observations have been digitized,
153 by around 16,400 volunteers.

154

155 The observing network was not created with a single purpose in mind. It was certainly
156 not intended to meet the stringent criteria demanded for monitoring long-term
157 environmental change. Nonetheless, historical SST measurements have been widely used
158 in such studies. In a 2010 paper, *Jones and Wigley* [2010] identified uncertainties
159 associated with pervasive systematic errors in SST data sets as an important uncertainty
160 in the estimation of global temperature trends. The obvious gulf between the ideal and the
161 reality leads naturally to questions about the reliability of the SST record. Often this

162 question is couched as a yes/no dichotomy: “are SST records reliable?” A more useful
163 question is "How reliable are they?" Although historical measurements were not made for
164 climate research, or any single purpose, it does not mean that it is impossible to derive
165 from them a record that is useful to a particular end. However, it does mean that special
166 care must be taken in identifying and, as best as possible, quantifying uncertainties.

167

168 In using SST observations and the analyses that are based on them, it is important to
169 understand the uncertainties inherent in them and the assumptions and statistical methods
170 that have gone into their creation. In this review I aim to give an overview of the various
171 components that contribute to the overall uncertainty of SST measurements made in situ
172 and of the data sets that are derived from them. In doing so, I also aim to identify current
173 gaps in understanding.

174

175 Section 2 provides a classification of uncertainties. The classifications are not definitive,
176 nor are they completely distinct. They do, however, reflect the way in which uncertainties
177 have been approached in the literature and provide a useful framework for thinking about
178 the uncertainties in SST data sets. The uncertainties have been tackled in ascending order
179 of abstraction from the random errors associated with individual observations to the
180 generic problem of unknown unknowns. In this review quoted uncertainties represent one
181 standard deviation of the relevant distribution unless otherwise stated. Section 3 applies
182 this framework to analyze progress and understanding under each of the headings. Some
183 shortcomings of the presentation of uncertainties are discussed in section 4 along with
184 possible solutions. Section 5 reviews how some analyses have used knowledge of likely

185 errors in SST data sets to minimize their exposure to uncertainty. Section 6 briefly
186 discusses SST retrievals from satellites and how these have been used to understand the
187 in situ record. The review concludes with a summary of possible future directions.

188

189 **2. General Classification of Uncertainties**

190

191 Throughout this review the distinction will be made between an *error* and an *uncertainty*.
192 The distinction between the two loosely follows the usage in the Guide to the Expression
193 of Uncertainty in Measurement (GUM) [BIPM, 2008]. The *error* in a measurement is the
194 difference between some idealized “true value” and the measured value and is
195 unknowable. The GUM defines the uncertainty of a measurement as the “parameter,
196 associated with the result of a measurement, that characterizes the dispersion of the
197 values that could reasonably be attributed to the measurand”. This is the sense in which
198 uncertainty is generally meant in the following discussion. This is not necessarily the
199 same usage as is found in the cited papers. It is common to see the word error used as a
200 synonym for uncertainty such as in the commonly used phrases standard error and
201 analysis error.

202

203 Broadly speaking, errors in individual SST observations have been split into two
204 groupings: random observational errors and systematic observational errors. Although
205 this is a convenient way to deal with the uncertainties, errors in SST measurements will
206 generally share a little of the characteristics of each.

207

208 *Random observational errors* occur for many reasons: misreading of the thermometer,
209 rounding errors, the difficulty of reading the thermometer to a precision higher than the
210 smallest marked gradation, incorrectly recorded values, errors in transcription from
211 written to digital sources and sensor noise among others. Although they might confound a
212 single measurement, the independence of the individual errors means they tend to cancel
213 out when large numbers are averaged together. Therefore, the contribution of random
214 independent errors to the uncertainty on the global average SST is much smaller than the
215 contribution of random error to the uncertainty on a single observation even in the most
216 sparsely observed years. Nonetheless, where observations are few, random observational
217 errors can be an important component of the total uncertainty.

218

219 *Systematic observational errors* are much more problematic because their effects become
220 relatively more pronounced as greater numbers of observations are aggregated.
221 Systematic errors might occur because a particular thermometer is mis-calibrated, or
222 poorly sited. No amount of averaging of observations from a thermometer that is mis-
223 calibrated such that it reads 1 K too high will reduce the error in the aggregate below this
224 level save by chance. However, in many cases the systematic error will depend on the
225 particular environment of the thermometer and will therefore be independent from ship to
226 ship. In this case, averaging together observations from many different ships or buoys
227 will tend to reduce the contribution of systematic observational errors to the uncertainty
228 of the average.

229

230 In the 19th and early 20th century, the majority of observations were made using buckets
231 to haul a sample of water up to the deck for measurement. Although buckets were not
232 always of a standard shape or size, they had a general tendency under typical
233 environmental conditions to lose heat *via* evaporation or directly to the air when the air-
234 sea temperature difference was large. *Folland and Parker* [1995] provide a more
235 comprehensive survey of the problem which was already well known in the early 20th
236 Century (see, for example, the introduction to *Brooks* [1926]). *Pervasive systematic*
237 *observational errors* like the cold bucket bias are particularly pertinent for climate studies
238 because the errors affect the whole observational system and change over time as
239 observing technologies and practices change. The change can be gradual as old methods
240 are slowly phased out, but they can also be abrupt, reflecting significant geopolitical
241 events such as the Second World War [*Thompson et al.*, 2008]. Rapid changes also arise
242 because the digital archives of marine meteorological reports (*ICOADS Woodruff et al.*
243 [2011]) are themselves discontinuous.

244

245 Generally, systematic errors are dealt with by making adjustments based on knowledge of
246 the systematic effects. The adjustments are uncertain because the variables that determine
247 the size of the systematic error are imperfectly known. The atmospheric conditions at the
248 point where the measurement was made, the method used to make the measurement –
249 ERI or bucket – the material used in the construction of the bucket if one was used, as
250 well as the general diligence of the sailors making the observations have not in many
251 cases been reliably recorded. Part of the uncertainty can be estimated by allowing
252 uncertain parameters and inputs to the adjustment algorithms to be varied within their

253 plausible ranges thus generating a range of adjustments (e.g., *Kennedy et al.* [2011c]).
254 This *parametric uncertainty* gives an idea of the uncertainties associated with poorly
255 determined parameters within a particular approach, but it does not address the more
256 general uncertainty arising from the underlying assumptions. This uncertainty will be
257 dealt with later as *structural uncertainty*.

258

259 First, however, there are a number of other uncertainties associated with the creation of
260 the gridded data sets and SST analyses that are commonly used as a convenient
261 alternative to dealing with individual marine observations. The uncertainties are closely
262 related because they arise in the estimation of area-averages from a finite number of
263 noisy and often sparsely-distributed observations.

264

265 In *Kennedy et al.*, [2011b] two forms of this uncertainty were considered: *grid-box*
266 *sampling uncertainty* and *large-scale sampling uncertainty* (which they referred to as
267 coverage uncertainty). Grid-box sampling uncertainty refers to the uncertainty accruing
268 from the estimation of an area-average SST anomaly within a grid box from a finite, and
269 often small, number of observations. Large-scale sampling uncertainty refers to the
270 uncertainty arising from estimating an area-average for a larger area that encompasses
271 many grid boxes that do not contain observations. Although these two uncertainties are
272 closely related, it is often easier to estimate the grid-box sampling uncertainty, where one
273 is dealing with variability within a grid box, than the large-scale sampling uncertainty,
274 where one must take into consideration the rich spectrum of variability at a global scale.

275

276 Although some gridded SST data sets contain many grid boxes which are not assigned an
277 SST value because they contain no measurements, other SST data sets – oftentimes
278 referred to as SST analyses – use a variety of techniques to fill the gaps. They use
279 information gleaned from data-rich periods to estimate the parameters of statistical
280 models that are then used to estimate SSTs in the data voids, often by interpolation or
281 pattern fitting. There are many ways to tackle this problem and all are necessarily
282 approximations to the truth. The correctness of the *analysis uncertainty* estimates derived
283 from these statistical methods are conditional upon the correctness of the methods, inputs
284 and assumptions used to derive them. No method is correct therefore analytic
285 uncertainties based on a particular method will not give a definitive estimate of the true
286 uncertainty. To gain an appreciation of the full uncertainty it is necessary to factor in the
287 lack of knowledge about the correct methods to use, which brings the discussion back to
288 structural uncertainty.

289

290 There are many scientifically defensible ways to produce a data set. For example, one
291 might choose to fill gaps in the data by projecting a set of Empirical Orthogonal
292 Functions (EOFs) onto the available data. Alternatively, one might opt to fill the data
293 using simple optimal interpolation. Both are defensible approaches to the problem, but
294 each will give different results. In the process of creating any data set, many such choices
295 are made. *Structural uncertainty* [Thorne *et al.*, 2005] is the term used to understand the
296 spread that arises from the many choices and foundational assumptions that can be (and
297 have to be) made during data set creation. The character of structural uncertainty is
298 somewhat different to the other uncertainties considered so far. The uncertainty

299 associated with a measurement error, for example, assumes that there is some underlying
300 distribution that characterizes the dispersion of the measured values. In contrast, there is
301 generally no underlying “distribution of methods” that can be used to quantify the
302 structural uncertainty. Furthermore, the diverse approaches taken by different teams
303 might reflect genuine scientific differences about the nature of the problems to be tackled.
304 Consequently, structural uncertainty is one of the more difficult uncertainties to quantify
305 or explore efficiently. It requires multiple, independent attempts to resolve the same
306 difficulties, it is an ongoing commitment, and it does not guarantee that the true value
307 will be encompassed by those independent estimates. Nevertheless, the role that the
308 creation of multiple independent estimates and their comparison has played in
309 uncovering, resolving, and quantifying some of the more mystifying uncertainties in
310 climate analyses is unquestionable. The most obvious – one might say, notorious –
311 examples are those of tropospheric temperature records made using satellites and
312 radiosondes [Thorne *et al.*, 2011] and sub-surface ocean temperature analyses [Lyman *et*
313 *al.*, 2010; Abraham *et al.*, 2013].

314

315 Which leads finally to *unknown unknowns*. On February 12th 2002, at a news briefing at
316 the US Department of Defense, Donald Rumsfeld memorably divided the world of
317 knowledge into three quarters:

318

319 “*There are known knowns. These are things we know we know. We also know there*
320 *are known unknowns. That is to say, we know there are some things we do not know. But*
321 *there are also unknown unknowns, the ones we don't know we don't know.*”

322

323 In the context of SST uncertainty, unknown unknowns are those things that have been
324 overlooked. By their nature, unknown unknowns are unquantifiable; they represent the
325 deeper uncertainties that beset all scientific endeavors. By deep, I do not mean to imply
326 that they are necessarily large. In this review I hope to show that the scope for revolutions
327 in our understanding is limited. Nevertheless, refinement through the continual evolution
328 of our understanding can only come if we accept that our understanding is incomplete.
329 Unknown unknowns will only come to light with continued, diligent and sometimes
330 imaginative investigation of the data and metadata.

331

332 **3. The Current State of Uncertainty in in situ SST Analyses**

333

334 The classification of uncertainties outlined in section 2 will now be used as a framework
335 to assess uncertainties in the global data sets based on in situ measurements. Preliminary
336 to this it will be helpful to define what exactly is meant by sea-surface temperature.

337

338 **3.1 Defining Sea-surface Temperature**

339

340 Traditionally, in situ SST analyses have been considered representative of the upper ten
341 or so meters of the ocean. However, the near-surface temperature structure of the ocean
342 can be rather complex. Under conditions of low wind speed and high insolation, a stable
343 stratified layer of warm water can form near the surface. For a recent review see *Kawai*
344 *and Wada* [2007]. The diurnal temperature range of the sea-surface can, under certain

345 conditions, exceed 5 K and, somewhat attenuated, penetrate to many tens of meters
346 [*Prytherch et al.*, 2013]. This can lead to strong temperature gradients in the upper few
347 meters of the ocean and consequently measurements made at the same time and location
348 but at different depths can record quite different temperatures. Temperatures measured at
349 the same depth but at different times of day can also differ markedly.

350

351 *Donlon et al.* [2007] proposed that the depth of the measurement be recorded along with
352 the temperature as a first step to reconciling measurements made at different depths and
353 different times of day. *Donlon et al.* [2007] also introduced the concept of an SST
354 foundation (SST_{fnd}) temperature. The current definition ([https://www.ghrsst.org/ghrsst-](https://www.ghrsst.org/ghrsst-science/sst-definitions/)
355 [science/sst-definitions/](https://www.ghrsst.org/ghrsst-science/sst-definitions/)) of “ SST_{fnd} , is the temperature free of diurnal temperature
356 variability, i.e., SST_{fnd} is defined as the temperature at the first time of the day when the
357 heat gain from the solar radiation absorption exceeds the heat loss at the sea surface.” It is
358 generally assumed that the upper few meters of the ocean are of approximately constant
359 temperature at this point. SST_{fnd} has proved a practical reference point for comparing and
360 combining satellite observations [*Roberts-Jones et al.*, 2012] and was intended to provide
361 “a more precise, well-defined quantity than the previous loosely-defined bulk SST”

362 *Donlon et al.* [2007].

363

364 Unfortunately, such niceties of definition are not readily applicable to historical SST
365 measurements and the effect of the interaction between measurement depth and water
366 temperature on SST measurements in in situ archives is not clear. For many ships that
367 measure the temperature of water drawn in below the surface, the depth of the

368 measurements is not known and is likely to have changed depending on how heavily the
369 ship was loaded. Nor is it clear to what extent any warm surface layer is mixed with
370 cooler subsurface water by the passage of the ship or by the interaction of wind, water,
371 Sun and hull [*Amot*, 1954; *Stevenson*, 1964]. Similar interactions have been noted closer
372 to the surface with moored buoys [*Kawai and Kawamura*, 2000]. *James and Fox* [1972]
373 found that ERI measurements from ships became progressively warmer relative to
374 simultaneous bucket observations as the depth of the ERI measurement increased, a
375 similar pattern to that seen by *Kent et al.* [1993]. *Reynolds et al.* [2010] found that
376 measurements made by ships, which were largely ERI measurements in their study
377 period, were on average warmer than nearby drifting buoy observations made nearer to
378 the surface.

379

380 Nonetheless, the concept of the foundation SST can be used to get an idea of how
381 changing measurement depth might have affected SST trends in the absence of other
382 considerations. Figure 1 shows an upper estimate of the potential size of the effect of
383 changing measurement depth on global average SST over time (for calculation details see
384 Appendix A). The assumption is that buckets and buoys measure in the upper 30 cm and
385 engine room measurements are measuring SST_{ind} . The estimated global average bias
386 (relative to the 1961-1990 average) is less than 0.1 K at all times and from 1945 onwards
387 is less than 0.05 K. The bias is largest in the early record when all measurements were
388 made using buckets which sample in the upper meter of the water column. In the more
389 recent period, the blend of buckets, ERI measurements and buoys leads to a smaller,

390 time-varying bias. Although the size of the effect is modest at a global level, locally the
391 average diurnal warming can exceed 0.5K, which would imply a larger effect.

392

393 A related problem is that changing times of observation could potentially interact with the
394 diurnal cycle of temperature leading to spurious trends in the data. *Kent et al.* [2010] note
395 "*The implicit assumption is that the sampling of conditions is regular enough that no*
396 *regional or time-varying bias is introduced into the datasets by neglecting such effects.*"

397 Ships currently make SST observations at regular intervals throughout the day, typically
398 every four or six hours, which is sufficient to minimize the aliasing of diurnal cycles,
399 particularly if the measurements are made at depth. During earlier periods when buckets
400 were widely used, there were systematic changes in the time of observation that might
401 have a more pronounced effect on average SSTs but this has not been quantified.

402

403 Even when the measurement depth is known, there are potential problems. Metadata in
404 WMO Publication 47 show that ships measure water temperatures through a wide range
405 of depths from the near surface down to around 25 m [*Kent et al.*, 2007]. Although the
406 average depth was typically less than 10 m, the deepest measurements could be sampling
407 water that is colder than the SST_{fnd} . How large this effect might be is not yet well
408 understood.

409

410 *Chiodi and Harrison* [2006] identified large-scale warm surface features using SST
411 retrievals from microwave satellite instruments that persisted for several days. The warm
412 layer was observed at night suggesting that the effect was independent from diurnal

413 warming and they hypothesized that the multi-day warming might have been confined to
414 a relatively shallow layer between 1 and 5 m thick. The implication is that the depth of
415 the SST foundation temperature can vary rapidly and that it can be much shallower than
416 the deepest in situ SST measurements. During a two week cruise, *Matthews and*
417 *Matthews* [2013] found persistent temperature difference between the surface and 3 m
418 depth in the tropical Pacific. Similar warm layers can be seen in data from moored buoys.
419 Figure 2 shows time series from several moorings showing multi-day near-surface warm
420 layers that do not penetrate down to 10 m and in some cases do not reach 5 m.
421 Climatologies of mixed layer depth (MLD, see for example *de Boyer Montégut* [2004])
422 indicate large areas – in regions of upwelling and in the summer hemisphere – where the
423 average MLD is shallower than 30 m, implying measurable temperature gradients within
424 the depth range of ship SST measurements. *Grodsky et al.* [2008] also found differences
425 between SST and temperatures in the mixed layer, which were largest in areas of
426 persistent upwelling – most notably the eastern Pacific – but they did not consider the
427 possible confounding effects of systematic errors in SST or other measurements.
428
429 To isolate the specific effect of multi-day or persistent temperature stratification of the
430 near-surface waters would require regular measurements of near-surface waters at a range
431 of depths. Such an analysis is now possible thanks to the network of Argo floats [*Castro*
432 *et al.*, 2013]. In what follows, it should be noted that variations in depth will contribute to
433 the variance of measurements and will therefore be partly, or wholly, counted in
434 estimates of random and systematic measurement errors.
435

436 **3.2 Individual Observational Errors**

437

438 The general quality of raw SST measurements recorded in digital archives is mixed.

439 Consequently, all SST analyses perform a stage of pre-screening, or quality control (QC)

440 in order to remove observations of low quality and minimize the number of egregious

441 errors. The size of the uncertainties of individual measurements will depend to a certain

442 extent on the QC that is applied but the effects of differences in QC have not been

443 assessed systematically.

444

445 **3.2.1 Random Measurement Errors**

446

447 Many estimates of random observational error uncertainty have been made. Although

448 thermometers issued to ships by many port meteorological officers are calibrated, such

449 calibration information is not routinely published, nor is there any guarantee that the

450 temperature of a water sample measured by a well calibrated thermometer is equal to the

451 actual SST when the sample has spent time in a bucket, or passed through the pipe work

452 of a ship. Consequently, estimates of measurement uncertainty from the literature are

453 empirical estimates derived from considerations of the variance of the data: for example,

454 spatial [*Lindau*, 2003; *Kent and Challenor*, 2006; *Emery et al.*, 2001] and temporal

455 [*Stubbs*, 1965] semivariograms, by comparing collocated observations [*O'Carroll et al.*,

456 2008], by resampling [*Shen et al.*, 2007], by using the variation of the variance with the

457 number of observations [*Rayner et al.*, 2006], or by comparison with a background field

458 [*Kent and Berry*, 2008; *Xu and Ignatov*, 2010; *Ingleby*, 2010; *Kennedy et al.*, 2011a;

459 *Atkinson et al.*, 2013]. Some of the analyses did not distinguish between random
460 observational errors and systematic observational errors, tending to combine them into
461 one estimate. In addition it is not always easy to separate the effects of spatial sampling
462 from measurement errors particularly in regions of high SST variability [*Castro et al.*,
463 2012].

464

465 A single SST measurement from a ship has a typical combined random and systematic
466 error uncertainty of around 1 K to 1.5 K. Results from individual analyses are
467 summarized in Table 1. The studies are mostly based on data from 1970 onwards.

468

469 Measurements are not all of identical quality. *Kent and Challenor* [2006] showed that in
470 the period 1970-1997 the uncertainties of measurements from ships varied with location,
471 time, measurement method and the country that recruited the ship. Uncertainties were
472 estimated to be larger in the mid-1970s probably due to data being incorrectly transmitted
473 in real time in the early days of the Global Telecommunication System. Their estimated
474 uncertainty for engine room measurements was larger than for bucket measurements.

475 *Tabata* [1978a] noted that bucket measurements *could* be accurate to 0.15 K, but that ERI
476 measurements were nearly an order of magnitude worse (1.16 K). *Ingleby* [2010]
477 estimated uncertainties for different subsets of the data and noted that manual VOSclim
478 (a high-quality subset of the VOS fleet) measurements and automated measurements
479 were of slightly higher quality than manual ship measurements in general. *Beggs et al.*
480 [2012] showed that Australia Integrated Marine Observing System ships had
481 uncertainties comparable to those from data buoys. Analyses that have looked at statistics

482 for individual ships and buoys have found that some ships and buoys take much higher
483 quality measurements than others [*Kent and Berry, 2008; Brasnett, 2008; Kennedy et al.,*
484 *2011a; Atkinson et al., 2013*]. The subset of ships (around 40-50% of ship observations)
485 that passed the more stringent quality control procedures of *Atkinson et al. [2013]* had
486 significantly lower measurement uncertainties assessed using the method of *Kennedy et*
487 *al. [2011a]* than did the full fleet of ships. Early results on hull sensors reported by *Emery*
488 *et al. [1997]* indicated the potential for these sensors to make accurate measurements.
489 Indeed, *Kent et al. [1993]* found that hull sensors installed on ships in the Voluntary
490 Observing Ships Special Observing Project for the North Atlantic (VSOP-NA) gave
491 consistent measurements during the two year observing period.

492

493 Drifting buoy measurements are generally more accurate and consistent than ship
494 measurements, but there is a greater relative spread between the estimates which are
495 summarized in Table 2. In part these differences are likely to arise from the level of pre-
496 screening that is applied to the observations. Where quality control is more stringent,
497 estimated uncertainties are likely to be lower and, where the error variance of the
498 observations is low already, the effects of quality control and processing choices are
499 likely to be more pronounced [*Xu and Ignatov, 2012*]. *Castro et al. [2012]* considered
500 differences between drifting buoys and two different satellite products and found that
501 there was little difference between buoys produced by different manufacturers. There is
502 some evidence that the quality of drifting buoy observations has improved slightly over
503 time [*Merchant et al., 2012*], but this has not been conclusively demonstrated. As a

504 comparison, temperature measurements from Argo have been reckoned to have an
505 uncertainty of around 0.002K [*Abraham et al.*, 2013].
506
507 Moored buoys have received less attention. Estimates of the measurement uncertainties
508 are summarized in Table 3. The two studies [*Kennedy et al.*, 2011a; *Xu and Ignatov*,
509 2010] that examined moorings from the GTMBA separately from other moorings found
510 that they had lower measurement error uncertainties. *Castro et al.* [2012] found that the
511 standard deviations of differences between moorings and satellite data were lower for
512 tropical moorings than for coastal moorings. They noted that in coastal waters there can
513 be large local variations in temperature, which satellites cannot resolve. Some moorings
514 along coastlines are located in estuaries and river mouths and are therefore less likely to
515 be representative of open ocean areas. This is perhaps one reason why *Wilkerson and*
516 *Earl* [1990], who studied US coastal buoys, found such large standard deviations between
517 ships and moorings (Table 1). *Merchant et al.* [2012] found that few coastal moorings
518 met their required stability criteria.

519

520 As noted in section 2, random observational errors are of relatively minor importance in
521 large-scale averages (see Figure 8 and section 3.5), particularly in the modern period
522 when observations are numerous. For an uncertainty of 1.0 K for a single observation due
523 to random observational error, the resulting uncertainty of a global annual average based
524 on 10000 observations would be of order 0.01 K.

525

526 **3.2.2 Random and Systematic Measurement Errors**

527

528 *Kent and Berry* [2008] and *Kennedy et al.* [2011a, 2011b] decomposed the observational
529 errors into random and systematic components. *Brasnett* [2008] and *Xu and Ignatov*
530 [2010] implicitly used the same error model – their analyses output the same statistics
531 produced by *Kent and Berry* [2008] – and the results are indeed very similar (Figure 3).
532 Estimates are summarized in Table 4. The possibility of correlated measurement errors is
533 also implicitly allowed for by *Ishii et al.* [2003] and *Hirahara et al.* [2013] who merge
534 observations from a single ship into a super observation before calculating uncertainties.
535 Adding the uncertainties in quadrature gives a combined observational uncertainty of
536 between 1 and 1.5 K, consistent with earlier estimates (Table 1) that did not differentiate
537 between the two.

538

539 In the studies listed in Table 4, the systematic component of the error was assumed to be
540 different for each ship, but this does not on its own capture the effects of pervasive
541 systematic errors. The data from *Kent and Berry* [2008], *Brasnett* [2008] and *Xu and*
542 *Ignatov* [2010] also show that the systematic observational error component for some
543 ships varies from month to month suggesting that the partitioning of systematic and
544 random effects is also a function of the time period considered.

545

546 The addition of a systematic component has a pronounced effect on the uncertainty of
547 large-scale averages comprising many observations. *Kennedy et al.* [2011b] estimated
548 that the effect of the correlations between errors was to increase the uncertainty of the
549 global annual average SST anomaly due to measurement error from 0.01 K (uncorrelated

550 case) to more than 0.05 K in the 19th Century and to more than 0.01 K even in the well-
551 observed modern period when millions of observations contribute to the annual global
552 average (see Figure 8). Systematic errors could also have a pronounced effect on
553 reconstructions when they project onto large-scale modes of variability, or on the
554 estimation of EOFs. However, because of the assumed independence of the errors
555 between ships, the correlated component of the uncertainty remains relatively
556 unimportant for the analysis of long-term trends of large-scale averages. Pervasive
557 systematic errors, which are correlated across a large proportion of the global fleet,
558 (section 3.2) are far more important from that point of view.

559

560 One of the difficulties with estimating the uncertainties associated with systematic errors
561 from individual ships is that not all observations in ICOADS can be associated with an
562 individual ship. Some of the reports have no more information than a location, time and
563 SST measurement. *Kennedy et al.* [2011b] had to make estimates of how the uncertainty
564 arising from systematic errors behaved as the number of observations increased by
565 considering the behavior at times when the majority of reports contained a ship name or
566 call-sign. They assumed that observations without call signs behaved in the same way.
567 *Kent and Berry* [2008] suggested that only ship reports with extant metadata be used in
568 climate analyses of the modern period to minimize such ambiguities. For earlier periods,
569 the gains in improved quantification of uncertainty would need to be balanced against the
570 increased uncertainty arising from reduced coverage.

571

572 Many gridded SST data sets and analyses, as well as the studies that depend on them,
573 assume that the observational errors are normally distributed, but this is not necessarily
574 the case for individual observations. *Kennedy et al.* [2011a] investigated the properties of
575 observations that had been quality controlled using the procedures described in *Rayner et*
576 *al.* [2006]. They found that in comparisons with satellite observations the distributions of
577 errors were 'fat-tailed' with the distribution of errors having a positive kurtosis. In the
578 creation of gridded data sets from SST observations, the effects of outliers can be
579 minimized somewhat by the use of resistant or robust statistics such as Winsorised, or
580 trimmed means (see e.g., *Rayner et al.* [2006]). The effect of outliers is further reduced in
581 large scale averages and the distribution of errors in large scale averages tends towards a
582 normal distribution as the number of observations increases [*Kennedy et al.*, 2011a].

583

584 **3.2.3 Summary of Individual Observational Errors**

585

586 Many estimates of uncertainties of ship and buoy SST measurements have been made. A
587 typical SST measurement made by a ship has an uncertainty of around 1-1.5K and a
588 drifting buoy observation a typical uncertainty of around 0.1-0.7K. More recent studies
589 split these uncertainties into random and systematic components, which better describe
590 the error characteristics of these platforms. However, a lack of metadata, most
591 particularly ship call signs, hampers the application of such an error model and it does not
592 capture behavior seen in SST measurements such as non-Normal distributions or
593 systematic errors that vary on time scales from months to years.

594

595 **3.3 Pervasive Systematic Errors and Biases**

596

597 *Kent et al.* [2010] conducted a review of literature on pervasive systematic errors (often
598 termed ‘biases’) in in situ SST measurements. Many studies have looked at the
599 differences in pervasive systematic errors between measurement methods, but fewer have
600 attempted to adjust SST records to minimize the effects of changes in instrumentation.

601

602 **3.3.1 Bias Adjustments 1850 to 1941**

603

604 The need for adjustments to minimize the cold bias associated with bucket measurements
605 in the period from 1850 to 1941 is well established. *Folland and Parker* [1995] calculated
606 adjustments using a simplified physical model of the buckets used to make SST
607 measurements combined with fields of climatological air-temperature, SST, humidity,
608 wind and solar radiation. Some parameters in their model were taken from literature and
609 others were estimated from the data. The length of time between the water sample leaving
610 the sea surface and the measurement was estimated by integrating their model until a
611 seasonal cycle in the SST was minimized. The fractional contributions of canvas and
612 wooden buckets were estimated by assuming a linear change over time from a mix of
613 wooden and canvas buckets to predominantly canvas buckets by 1920. The rate of this
614 change was estimated by minimizing the air-sea temperature difference in the tropics.
615 The same method was also used in *Rayner et al.* [2006] and *Kennedy et al.* [2011c].

616

617 *Smith and Reynolds* [2002] took an alternative approach. They adjusted SSTs based on
618 statistical relationships between Night Marine Air Temperature (NMAT) and SST. The
619 resulting adjustments were different to those produced by *Folland and Parker* [1995]
620 although the magnitude of the global average adjustment was similar. Both *Folland and*
621 *Parker* [1995] and *Smith and Reynolds* [2002] found a long term increase in the
622 magnitude of the adjustments – that is, an increasing cold bias – from the 1850s to 1941.

623

624 The methods employed by *Folland and Parker* [1995] and *Smith and Reynolds* [2002] are
625 not independent as they both rely on NMAT, which have their own particular pervasive
626 systematic errors [*Bottomley et al.*, 1990; *Rayner et al.*, 2003; *Kent et al.*, 2013]. The use
627 of NMAT to adjust SST data is, to an extent, unavoidable as the heat loss from a bucket
628 does depend on the air-sea temperature difference.

629

630 In data sets based on a ICOADS release 2.0 and later, the earlier bucket adjustments were
631 found to over-adjust SST in the period 1939-1941. *Rayner et al.* [2006] and *Smith et al.*
632 [2008] ramped the adjustments down to zero over this period. *Kennedy et al.* [2011c]
633 showed that the ramp-down corresponded to new data in that release of ICOADS that
634 included a large fraction of ERI measurements.

635

636 **3.3.2 Bias Adjustments 1941 to Present**

637

638 In the post-1941 period, *Folland and Parker* [1995], *Smith and Reynolds* [2003], *Smith*
639 *and Reynolds* [2005] and *Rayner et al.* [2006] opted not to adjust the data because they

640 found no clear evidence of the need for adjustments. However, *Rayner et al.* [2006] did
641 identify biases in Japanese and Dutch data after the Second World War. *Thompson et al.*
642 [2008] identified a discontinuity in global-average SST associated with a change in the
643 composition of ICOADS release 2.1 in late 1945. *Reynolds et al.* [2010] quantified a
644 relative bias between ship and drifting buoy measurements that they thought could lead to
645 an artificial cooling of the global average SST. *Kent et al.* [1999] applied adjustments to
646 ERI measurements, but removed the adjustment from later versions of their data set.

647

648 *Kennedy et al.* [2011c] and *Hirahara et al.* [2013] developed bias adjustments for the
649 period 1941 onwards. *Kennedy et al.* [2011c] used metadata from ICOADS, WMO
650 Publication 47, observer instructions, technical reports and scientific papers to estimate
651 biases for individual measurement types and to assign a measurement method to as many
652 observations as possible. *Hirahara et al.* [2013] used a narrower range of metadata. By
653 comparing subsamples of the data for which the metadata were known, they could
654 estimate appropriate metadata assignments for the remainder.

655

656 To estimate the bias adjustments for long-term analyses, an understanding is needed of
657 how biases varied for individual components of the observing system. Several studies
658 have examined ERI and bucket biases in ship data [*Brooks*, 1926; *Brooks*, 1928; *Lumby*,
659 1927; *Collins et al.*, 1975; *Wahl*, 1948; *Roll*, 1951; *Kirk and Gordon*, 1952; *Amot*, 1954;
660 *Perlroth*, 1962; *Saur*, 1963; *Walden*, 1966; *Knudsen*, 1966; *Tauber*, 1969; *James and*
661 *Fox*, 1972; *Tabata*, 1978a, 1978b; *Folland et al.*, 1993; *Kent et al.*, 1993] but only *Kent*
662 *and Kaplan* [2006] provide information that is time-resolved and traceable back to

663 ICOADS. There is a single study of pervasive systematic errors in hull sensor
664 measurements [*Kent et al.*, 1993], which analyzed data from a small number of ships over
665 a two year period and found that hull sensors were relatively unbiased and showed no
666 systematic change of bias with depth.

667

668 Few studies have looked at the long-term stability and calibration drifts of drifting buoys.
669 *Reverdin et al.* [2010] installed 16 drifters with high quality temperature sensors in
670 addition to their usual temperature sensors and found that the temperatures measured by
671 the drifters showed inaccuracies that were larger than the 0.1 °C target accuracy and that
672 they exhibited significant calibration drifts. This is consistent with the behavior seen by
673 *Atkinson et al.* [2013].

674

675 **3.3.3 Estimating Uncertainty in Bias Adjustments**

676

677 *Folland and Parker* [1995] did not explicitly estimate the uncertainties in their
678 adjustments. *Rayner et al.* [2006] explored the parametric uncertainty in the *Folland and*
679 *Parker* [1995] adjustments using a Monte-Carlo method. In *Smith and Reynolds* [2004]
680 the uncertainty in the bias adjustments was estimated by taking the mean-squared
681 difference between the *Smith and Reynolds* [2002] adjustments and the *Folland and*
682 *Parker* [1995] adjustments, a first-order estimate of the structural uncertainty.

683

684 *Kennedy et al.* [2011c] used a Monte-Carlo method to explore the parametric uncertainty
685 within their particular approach to bias adjustment. *Hirahara et al.* [2013] also provide

686 uncertainties on their adjustments that are a combination of analysis uncertainties and
687 regression uncertainty.

688

689 An important component of the uncertainty of adjustments for the effects of persistent
690 systematic errors arises from a lack of knowledge concerning how the measurements
691 were made. Metadata are often missing, incomplete or ambiguous and sometimes
692 different sources give conflicting information. *Kent et al.* [2007] assessed metadata from
693 ICOADS and WMO Publication 47. They found disagreement in around 20-40% of cases
694 where metadata were available from both sources. *Kennedy et al.* [2011c] allowed for up
695 to 50% uncertainty in metadata assignments based on the discrepancy between observer
696 instructions and measurement methods recorded in WMO Publication 47. *Hirahara et al.*
697 [2013] used differences between subsets of data to infer the fraction of observations made
698 using different methods.

699

700 Figure 6 compares estimated biases and metadata assignments from *Kennedy et al.*
701 [2011c] and *Hirahara et al.* [2013]. It shows that from 1945, the estimated biases agree
702 within their parametric uncertainty ranges (Figure 6a) and that the fractions of
703 measurement methods estimated by *Kennedy et al.* [2011c] from literature and other
704 metadata are consistent with the fractions inferred from the data by *Hirahara et al.* [2013]
705 (Figure 6b). However, there are two key differences that highlight the importance of
706 structural uncertainty for understanding the bias adjustments. The first difference is that
707 the phasing out of uninsulated buckets in *Hirahara et al.* [2013] happens earlier and
708 faster than allowed for in the parametric uncertainty analysis of *Kennedy et al.* [2011c]

709 (Figure 6c). In *Hirahara et al.* [2013] the changeover starts in the 1940s and is especially
710 rapidly in the early 1960s, being nearly complete by around 1962. The second difference
711 is that the estimated bias during the Second World War is higher in the analysis of
712 *Hirahara et al.* [2013] than in *Kennedy et al.* [2011c]. Further work is needed to
713 understand these differences and more complete, more reliable metadata would help
714 reduce uncertainty in SST records.

715

716 In the post-1941 period, *Smith and Reynolds* [2003] and *Smith and Reynolds* [2005]
717 estimated the uncertainty due to pervasive systematic errors by considering the difference
718 in estimated bias between measurements made in the engine rooms of the ships and
719 measurements from all ships between 1994 and 1997. They estimated a minimum 1-
720 sigma standard error in the global average of around 0.015 K. The range is similar to,
721 albeit slightly narrower than, that estimated by *Kennedy et al.* [2011c]. The difficulty
722 with the approach taken by *Smith and Reynolds* [2003], *Smith and Reynolds* [2005] and
723 *Smith et al.* [2008] is that the quoted uncertainty range is considered to be symmetric
724 whereas *Kennedy et al.* [2011c] and *Hirahara et al.* [2013] suggest that the true global
725 mean is consistently higher than *Smith et al.* [2008] in the period 1945-1960 (Figure 9).
726 It also suggests that the estimate of *Smith et al.* [2008] in the post World War 2 period
727 (1945-1950s) was slightly too conservative because it compared ERI measurements with
728 a mixture of ERI and insulated bucket measurements, whereas large numbers of
729 observations were made using buckets [*Kennedy et al.*, 2011c; *Hirahara et al.*, 2013].

730

731 **3.3.4 Refinements to Estimates of Pervasive Systematic Errors**

732 There are some factors that have not been explicitly considered in estimates of biases.
733 Refinements to the models of pervasive systematic errors will address with factors that
734 are implicitly included in random and systematic measurement uncertainties. If it is
735 possible to estimate the bias on a ship-by-ship, or observation-by-observation basis,
736 taking account of the conditions peculiar to that observation, then it might be expected
737 that uncertainties associated with random and systematic observational error will
738 decrease.

739

740 Both *Kennedy et al.* [2011c] and *Hirahara et al.* [2013] make simplifying assumptions
741 about the systematic errors associated with modern insulated buckets. Various bucket
742 designs have been used since the end of the Second World War, which are likely to have
743 different bias characteristics. Physical models could be developed for each type of bucket
744 similar to those used by *Folland and Parker* [1995], or statistical methods could be used
745 to estimate the biases as was done in *Kent and Kaplan* [2006].

746

747 Other simplifying assumptions used in all analyses include such things as assuming that
748 changes in the observing system happened linearly. Evidence suggests that changes in
749 measurement method were not always monotonic and sometimes happened abruptly (see
750 Figure 6). Improved metadata or more sophisticated statistical techniques could help
751 assess these uncertainties.

752

753 An uncertainty associated with pervasive systematic biases, which is not explicitly
754 resolved by current analyses, arises when the conditions at the time of the measurement

755 deviate from the climatological values assumed by the bias correction scheme. If, for
756 instance, the air sea temperature difference is larger than that assumed by the *Folland and*
757 *Parker* [1995] scheme, then there will be an additional systematic uncertainty that is
758 correlated strongly across synoptic spatial and temporal scales with a potential long-term
759 component where differences persist for months or years. Likewise conditions vary
760 during the day. Such discrepancies could be assessed by evaluating the systematic error
761 using local conditions. Such information could be taken from reanalyses, or an
762 appropriate bucket model could be explicitly included when SST observations are
763 assimilated into ocean-only and coupled reanalyses.

764

765 **3.3.5 Assessing the Efficacy of Bias Adjustments**

766

767 The efficacy of the bias adjustments and their uncertainties are difficult to assess. *Folland*
768 *and Parker* [1995] presented wind tunnel and ship board tests and also used their
769 adjustments to estimate the differences between bucket and ERI measurements in broad
770 latitude bands. These limited comparisons showed that their model could predict
771 experimental results to better than 0.2 K. *Folland and Salinger* [1995] presented direct
772 comparisons between air temperatures measured in New Zealand and SST measurements
773 made nearby. *Smith and Reynolds* [2002] used oceanographic observations to assess their
774 adjustments and those of *Folland and Parker* [1995]. In regions with sufficient
775 observations they found that the magnitude of the *Smith and Reynolds* [2002] adjustments
776 better explained the differences between SSTs and oceanographic observations, but the
777 phase of the annual cycle was better captured by *Folland and Parker* [1995]. *Hanawa et*

778 *al.* [2000] showed that the *Folland and Parker* [1995] adjustments improved the
779 agreement between Japanese ship data and independent SST data from Japanese coastal
780 stations in two periods: before and after the Second World War. However, the collection
781 of ship data (COADS and Kobe collections) used in *Hanawa et al.* [2000] might not have
782 had the same bias characteristics as assumed by *Folland and Parker* [1995] (based on the
783 Met Office Marine Data Bank) in developing their adjustments. Other long term coastal
784 records of water temperature exist. Some of these [*Hanna et al.*, 2006; *MacKenzie and*
785 *Schiedek*, 2007; *Cannaby and Hüsrevoğlu*, 2009] have been compared to open ocean SST
786 analyses (though not with the express intention of assessing bias adjustments), others
787 have not [*Maul et al.*, 2001; *Nixon et al.*, 2004; *Breaker et al.* 2005].

788

789 More recently, *Matthews* [2013] and *Matthews and Matthews* [2013] reported field
790 measurements of SST made using different buckets and simultaneous thermo-salinograph
791 measurements. They found negligible biases between different buckets, but their
792 experimental design involved larger buckets and shorter measurement times than were
793 used in *Folland and Parker* [1995]. Nevertheless, this highlights the potential for well-
794 designed field experiments to improve understanding of historical biases.

795

796 An analysis by *Gouretski et al.* [2012] compared SST observations with near-surface
797 measurements (0-20 m depth) taken from oceanographic profiles. It shows that the
798 overall shape of the global average is consistent between the two independent analyses,
799 but that there are differences of around 0.1 K between 1950 and 1970. These are most
800 likely attributable to residual biases, although, as noted above, actual physical differences

801 between the sea surface and the 0-20 m layer cannot be ruled out. Similar differences are
802 seen when comparing SST with the average over the 0-20 m layer of the analysis of
803 *Palmer et al.* [2007] (not shown).

804

805 Since the late 1940s, global and hemispheric average SST anomalies calculated
806 separately from adjusted bucket measurements and adjusted ERI measurements showed
807 consistent long-term and short-term changes [*Kennedy et al.*, 2011c]. From the 1990s,
808 there are also plentiful observations from drifting and moored buoys.

809

810 In contrast to the modern period, the period before 1950 is characterized by a much less
811 diverse observing fleet. During the Second World War, the majority of measurements
812 were ERI measurements. Before the war, buckets were the primary means by which SST
813 observations were made. This makes it very difficult to compare simultaneous
814 independent subsets of the data. In periods with fewer independent measurement types, it
815 might be possible to use changes in environmental conditions such as day-night
816 differences or air-sea temperature differences to diagnose systematic errors in the data.

817

818 Qualitative agreement between the long-term behavior of different global temperature
819 measures – including NMAT, SST and land temperatures – gives a generally consistent
820 picture of historical global temperature change (Figure 5), but a direct comparison is less
821 informative about uncertainty in the magnitude of the trends. *Kent et al.* [2013] showed
822 similar temporal evolution of NMAT and SST in broad latitude bands in the northern
823 hemisphere and tropics. However there are differences of up to 0.4 K in the band from

824 55°S to 15°S between 1940 and 1960. Studies such as that by *Folland* [2005] can be used
825 to make more quantitative comparisons. *Folland* [2005] compared measured land air
826 temperatures with land air temperatures from an atmosphere-only climate model that had
827 observed SSTs (with and without bucket adjustments) as a boundary forcing. He found
828 much better agreement when the SSTs were adjusted. Atmospheric reanalyses also use
829 observed SSTs along with other observed meteorological variables to infer a physically
830 consistent estimate of land surface air temperatures. *Simmons et al.* [2010] showed that
831 land air temperatures from a reanalysis driven by observed SSTs were very close to those
832 of CRUTEM3 [*Brohan et al.*, 2006] over the period 1973 to 2008. *Compo et al.* [2013]
833 showed similar results for the whole of the twentieth century although the agreement was
834 not quite so close. Although their intention was to show that land temperatures were
835 reliable, their results indicate that there is broad consistency between observed SSTs and
836 land temperatures.

837

838 **3.3.6 Summary of Pervasive Systematic Errors and Biases**

839

840 The need to adjust SST data prior to 1941 to account for a cold bias associated with the
841 use of canvas and wooden buckets is well established. There is also good evidence for the
842 need to adjust data after 1941. Adjustments for these pervasive systematic errors have
843 been developed. There are, at all times, two different estimates of the bias adjustments,
844 which are in general agreement and give a first indication of the structural uncertainty.
845 Evidence for the efficacy of the adjustments comes from wind tunnel tests, comparisons
846 with coastal sites and consistency with subsurface ocean temperatures, marine air

847 temperatures and land air temperatures. Contrary evidence comes from a recent field
848 experiment in the Pacific. Uncertainty could be better understood by: improvements in
849 metadata; carefully designed fields tests of buckets and other measurements methods; the
850 creation of new independent evaluations of the biases; and continued comparison
851 between SST and related variables.

852

853 **3.4 Sampling Uncertainty**

854

855 The magnitude of the grid-box sampling uncertainty depends on the correlation and
856 variability of SSTs within the grid box, on the number of observations contributing to the
857 grid-box average and where in the grid box they are located. High average correlations
858 within a grid box, low variability and large numbers of observations lead to lower
859 uncertainty estimates. Conversely areas of high variability or low average correlation,
860 such as frontal regions or western boundary currents, tend to have higher grid-box
861 sampling uncertainties as do grid-box averages based on smaller numbers of
862 observations. The estimation of uncertainties arising from the sparseness of observations
863 at scales from grid box level to global has been approached in a number of ways.

864

865 **3.4.1 Grid-box Sampling Uncertainty**

866

867 *Weare and Strub* [1981] counted the number of observations needed to minimize
868 sampling uncertainty in a 5°x5° grid box by ensuring that the observations were evenly
869 split between all areas of the grid box, month and diurnal cycle. From this, they

870 concluded that even sampling could not be achieved with fewer than eleven observations,
871 but that in practice more than eleven, sometimes many more, would be needed.

872

873 *Rayner et al.* [2006] estimated a combined measurement and grid-box sampling
874 uncertainty by considering how the variance of the grid-box average changed as a
875 function of the number of observations. The technique picked up spatial variations in
876 grid-box sampling uncertainty associated with regions of high variability. *Rayner et al.*
877 [2009] showed results from an unpublished analysis by Kaplan, in which spatially
878 complete satellite data were used to estimate the variability within $1^\circ \times 1^\circ$ grid boxes. The
879 same features were seen as in the *Rayner et al.* [2006] analysis, allowing for differences
880 in resolution, although the uncertainties estimated by Kaplan tended to be higher. *She et*
881 *al.* [2007] also used sub-sampling of satellite data to estimate grid-box sampling
882 uncertainty for the Baltic Sea and North Sea. *Kent and Berry* [2005] showed that
883 separately assessing measurement and sampling uncertainties can help to decide whether
884 more, or better, observations are needed to reduce the average uncertainty in an
885 individual grid box.

886

887 *Morrissey and Greene* [2009] developed a theoretical model for estimating grid-box
888 sampling uncertainty that accounted for non-random sampling within a grid box. This
889 was an extension of the method used to estimate sampling uncertainties in land
890 temperature data and global temperatures by *Jones et al.* [1997]. Land temperatures are
891 measured by stations at fixed locations that take measurements every day. Marine
892 temperature measurements are taken at fixed times, but the ships and drifting buoys move

893 during a particular month. *Morrissey and Greene* [2009] do not provide a practical
894 implementation of their approach, only a theoretical framework. *Kennedy et al.* [2011b]
895 extended the concept of the average correlation within a grid box developed in *Jones et*
896 *al.* [1997] to incorporate a time dimension. *Kent and Berry* [2008] used a temporal
897 autocorrelation model that took account of the days within the period that were sampled,
898 and the days which were not, to estimate the temporal sampling uncertainty. An
899 alternative to the *Jones et al.* [1997] method for land data was provided by *Shen et al.*
900 [2007], but it has not yet been applied in SST analyses.

901

902 It is possible that the locations visited by ships and drifting buoys are related and, to an
903 extent, dictated by meteorological and oceanographic conditions. Ships have long used
904 the prevailing currents in the Atlantic to speed their progress and it is in the interest of
905 almost all shipping to steer clear of hurricanes and other foul weather. Bad weather is
906 also likely to have influenced how and when observations were made. Conversely, the
907 conditions in which a sail ship might become becalmed could lead to over sampling of
908 higher SSTs. Drifting buoys drift, and a drifter trapped in an eddy might persistently
909 measure temperatures that are representative of only a very limited area. Drifters also
910 tend to drift out of areas of upwelling and congregate in other areas.

911

912 The effect of uneven sampling can be reduced by the creation of ‘super observations’
913 during the gridding process [*Rayner et al.*, 2006], or data preparation stage [*Ishii et al.*,
914 2003], but such processes cannot readily account for the situations where no observations
915 are made at all.

916

917 As noted by *Rayner et al.* [2006], the grid-box sampling uncertainties are likely to be
918 uncorrelated or only weakly correlated between grid boxes so the effect of averaging
919 together many grid boxes will be to reduce the combined grid-box sampling uncertainty
920 by a factor proportional to the square root of the number of grid boxes. Consequently the
921 sampling component of the uncertainty will be of minor importance in the global annual
922 average (Figure 8).

923

924 **3.4.2 Large-scale Sampling Uncertainty**

925

926 Because *Rayner et al.* [2006] and *Kennedy et al.* [2011b] make no attempt to estimate
927 temperatures in grid boxes which contain no observations, an additional uncertainty had
928 to be computed when estimating area-averages. *Rayner et al.* [2006] used Optimal
929 Averaging (OA) as described in *Folland et al.* [2001] which estimates the area average in
930 a statistically optimal way and provides an estimate of the large-scale sampling
931 uncertainty. *Kennedy et al.* [2011b] subsampled globally complete fields taken from three
932 SST analyses and obtained similar uncertainties from each. The uncertainties of the
933 global averages computed by *Kennedy et al.* [2011b] were generally larger than those
934 estimated by *Rayner et al.* [2006]. *Palmer and Brohan* [2011] used an empirical method
935 based on that employed for grid-box averages in *Rayner et al.* [2006] to estimate global
936 and ocean basin averages of subsurface temperatures.

937

938 The *Kennedy et al.* [2011b] large-scale sampling uncertainty of the global average SST
939 anomaly is largest (with a 2-sigma uncertainty of around 0.15°C) in the 1860s when
940 coverage was at its worst (Figure 8). This falls to 0.03 °C by 2006. The fact that the
941 large-scale sampling uncertainty should be so small – particularly in the nineteenth
942 century – may be surprising. The relatively small uncertainty might simply be a reflection
943 of the assumptions made in the analyses used by *Kennedy et al.* [2011b] to estimate the
944 large-scale sampling uncertainty. Indeed, *Gouretski et al.* [2012] found that subsampling
945 an ocean reanalysis underestimated the uncertainty when the coverage was very sparse.
946 However, estimates made by *Jones* [1994] suggest that a hemispheric-average land-
947 surface air temperature series might be constructed using as few as a 109 stations. For
948 SST, the variability is typically much lower than for land temperatures though the area is
949 larger. It seems likely that the number of stations needed to make a reliable estimate of
950 the global average SST anomaly would not be vastly greater.

951

952 Another way of assessing the large-scale sampling uncertainty is to look at the effect of
953 reducing the coverage of well-sampled periods to that of the less-well-sampled nineteenth
954 century and recomputing the global average (see for example *Parker* [1987]). Figure 4
955 shows the range of global annual average SST anomalies obtained by reducing each year
956 to the coverage of years in the nineteenth century. So, for example, the range indicated by
957 the blue area in the upper panel for 2006 shows the range of global annual averages
958 obtained by reducing the coverage of 2006 successively to that of 1850, 1851, 1852... and
959 so on to 1899. The red line shows the global average SST anomaly from data that have
960 not been reduced in coverage. For most years, the difference between the sub-sampled

961 and more fully sampled data is smaller than 0.15K and the largest deviations are smaller
962 than 0.2K. For the large-scale sampling uncertainty of the global average to be
963 significantly larger would require the variability in the nineteenth century data gaps to be
964 different from that in the better-observed period.

965

966 **3.4.3 Summary of Sampling Uncertainty**

967

968 Uncertainties arising from under-sampling at a grid-box level are easy to assess if the
969 observations can be assumed to be randomly distributed within a grid box. However,
970 sampling is not random. The effect of this is reduced in most analyses by the calculation
971 of super-observations that combine nearby measurements; however, optimal methods to
972 minimize uncertainty are not generally applied. Simple estimates of large-scale sampling
973 uncertainty in the global-average SST from subsampling well-sampled periods suggest a
974 value of at most 0.2K even in poorly observed years. However, there are potential
975 limitations of these simple methods and they should be considered together with the
976 range of statistical reconstructions to get a more complete idea of uncertainty in large-
977 scale averages.

978

979 **3.5 Reconstruction Techniques and Other Structural Choices**

980

981 Creating global SST analyses is challenging because of the relative sparseness of
982 observations before the satellite era and the non-stationarity of the changing climate. A
983 large number of different SST data sets based on in situ data have been produced

984 employing a variety of statistical methods. The structural uncertainties associated with
985 estimating SSTs in data voids and at data-sparse times are therefore somewhat better
986 explored than structural uncertainties in the pervasive systematic errors. Data sets used in
987 this paper have been summarized in Table 5 and global averages for these data sets are
988 shown in Figure 5.

989

990 **3.5.1 Critique of Reconstruction Techniques**

991

992 The current generation of SST analyses are the survivors of an evolutionary process
993 during which less effective techniques were discarded in favor of better adapted
994 alternatives. It is worthwhile to ask how, as a group, they address the range of criticisms
995 that have arisen during that time.

996

997 One concern is that patterns of variability in the modern era which are used to estimate
998 the parameters of the statistical models might not faithfully represent variability at earlier
999 times [Hurrell and Trenberth, 1999]. The concern is allayed somewhat by the range of
1000 approaches taken. The method of Kaplan *et al.* [1998] which uses the modern period to
1001 define Empirical Orthogonal Functions (EOFs, see Hannachi *et al.*, [2007] for a review
1002 of the use of EOFs in the atmospheric sciences) tends to underestimate the long-term
1003 trend. This is particularly obvious in the nineteenth and early twentieth century. Rayner *et*
1004 *al.* [2003] extended the method by defining a low-frequency, large-scale EOF that better
1005 captured the long-term trend in the data. However, it is possible that a single EOF will
1006 fail to capture all the low-frequency changes. Smith *et al.* [2008] allow for a non-

1007 stationary low-frequency component in their analysis which contributes a large
1008 component of uncertainty in the early record, but their reconstruction reproduces less
1009 high-frequency variability at data-sparse epochs. *Ilin and Kaplan* [2009] and *Luttinen and*
1010 *Ilin* [2009, 2012] used algorithms that make use of data throughout the record to estimate
1011 the covariance structures and other parameters of their statistical models. The three
1012 algorithms use either large-scale patterns (VBPCA, GPFA) or local correlations (GP).
1013 Differences between the three methods are generally small at the global level, but they
1014 diverge during the 1860s when data are few. There is a caveat that despite using all
1015 available observations, such methods will still tend to give a greater weight to periods
1016 with more plentiful observations. *Ishii et al.* [2005] use a simply-parameterized local
1017 covariance function for interpolation. Their optimal interpolation (OI) method was
1018 assessed by *Hirahara et al.* [2013] to have larger analysis uncertainties and larger cross-
1019 validation errors than the EOF-based COBE-2 analysis. However, the use of a simple
1020 optimal interpolation method has the advantage that it makes fewer assumptions
1021 regarding the stationarity of large-scale variability.

1022

1023 Another concern is that methods that use EOFs to describe the variability might
1024 inadvertently impose spurious long-range teleconnections that do not exist in the real
1025 world [*Dommenget, 2007*]. *Smith et al.* [2008] explicitly limit the range across which
1026 teleconnections can act. *Ishii et al.* [2005] used a local covariance structure in their
1027 analysis. Analyses such as *Kaplan et al.* [1998] and *Rayner et al.* [2003] make the
1028 assumption that the EOFs retained in the analysis capture actual variability in the SST
1029 fields, but do not explicitly differentiate between variability that can be characterized

1030 purely in terms of local co-variability and large-scale teleconnections. *Karspeck et al.*
1031 [2012] note that there is not a clear separation of scales and that joint estimation of local
1032 and large scale covariances is the logical way to approach the problem.

1033

1034 Most, if not all, statistical methods have a tendency to lose variance either because they
1035 do not explicitly resolve small scale processes [*Kaplan et al.*, 1998; *Smith et al.*, 2008],
1036 because the method tends towards the climatological average in the absence of data [*Ishii*
1037 *et al.*, 2005; *Berry and Kent*, 2011], or because they tend to smooth the data. *Rayner et al.*
1038 [2003] used the method of *Kaplan et al.* [1998] but blended high-quality gridded
1039 averages back into the reconstructed fields to improve small scale variability where
1040 observations were plentiful. *Karspeck et al.* [2012] analyzed the residual difference
1041 between the observations and the analysis of *Kaplan et al.* [1998] analysis using local
1042 non-stationary covariances, and then drew a range of samples from the posterior
1043 distribution in order to provide consistent variance at all times and locations.

1044

1045 One assumption common to most of the above analysis methods is that SST variability
1046 can be decomposed into a small set of distinct patterns that can be combined linearly to
1047 describe any SST field. However, it is well known that phenomena such as El Niño and
1048 La Niña are not symmetric and that the equations that describe the evolution of SST are
1049 non-linear. Consequently, current analyses might not capture the full range of behavior in
1050 real SST fields [*Karnauskas*, 2013]. Current generation SST analyses are based on the
1051 assumption that individual measurement errors are uncorrelated and that errors are
1052 normally distributed. Analysis techniques that incorporate information about the

1053 correlation structure of the errors have not yet been developed. Such techniques are likely
1054 to be more computationally expensive and lead to larger analysis uncertainties.

1055

1056 **3.5.2 Other Structural Choices**

1057

1058 Analyses based on SST anomalies will also have an uncertainty associated with the
1059 climatological reference fields used to calculate the anomalies. Sub-surface analyses have
1060 been shown to be particularly sensitive to choice of base period [*Lyman et al.*, 2010], due
1061 in a large part to the relative sparseness of the data sets. Although the problem is likely to
1062 be less severe for the better-observed SST record, there are still regions – the Southern
1063 Ocean and Arctic Ocean – where observations are few. *Yasunaka and Hanawa* [2011]
1064 found that differences between long-term-average SSTs from different analyses were
1065 typically less than 0.5 K, but that they exceeded 1 K in places. The largest differences
1066 were at high latitudes and in regions with strong SST gradients. There are also likely to
1067 be pervasive systematic errors in the climatological averages [*Kennedy et al.*, 2011c].

1068

1069 Other structural differences arise from the way that SSTs are extended to the edge of the
1070 sea ice. SSTs can be estimated from measurements of sea-ice concentration [*Rayner et*
1071 *al.*, 2003; *Smith et al.*, 2008; *Hirahara et al.*, 2013]. Although their global impact is
1072 likely to be small, the uncertainties in these relationships and estimates need also to be
1073 factored into the uncertainty of SSTs in these regions. At the moment, the uncertainty
1074 associated with historical sea-ice concentrations is poorly understood.

1075

1076 **3.5.3 Comparisons of Reconstructions**

1077

1078 *Yasunaka and Hanawa* [2011] examined a range of climate indices based on seven
1079 different SST data sets. They found that the disagreement between data sets was marked
1080 before 1880, and that the trends in large scale averages and indices tend to diverge
1081 outside of the common climatology period. For the global average, the differences
1082 between analyses were around 0.2 K before 1920 and around 0.1-0.2 K in the modern
1083 period. Even for relatively well-observed events such as the 1925/26 El Niño, the detailed
1084 evolution of the SSTs in the tropical Pacific varied from analysis to analysis. The reasons
1085 for the discrepancies are not completely clear because each data set is based on a slightly
1086 different set of observations that have been quality controlled and processed in different
1087 ways, a problem that could be alleviated by running analyses on identical input data sets.

1088

1089 Combined with information about large-scale sampling uncertainties estimated in other
1090 ways, the spread between analyses suggests that the large-scale sampling uncertainty in
1091 global average SST anomaly is around 0.2 K in the late 19th century. For the large-scale
1092 sampling uncertainty of the global average to be much larger would require variability in
1093 the early record to have been different from variability in the modern period, which is a
1094 possibility. The resolution of such a question is most likely to be achieved via the
1095 digitisation of more observations from paper records.

1096

1097 Progress in assessing the differences between analysis techniques can also be made by
1098 studying the relative strengths and weaknesses of interpolation techniques on carefully

1099 prepared test data sets using synthetic data, or on ‘withheld’ data from well observed
1100 regions. By running each analysis on the same carefully-defined subsets and tests, it
1101 should be possible to isolate reasons for the differences between the analyses and assess
1102 the reliability of analysis uncertainty estimates. The International Surface Temperature
1103 Initiative (<http://www.surfacetemperatures.org/>) has been working on such benchmarking
1104 exercises for land surface air temperature data, building on work such as the COST
1105 ACTION project [*Venema et al., 2012*].

1106

1107 **3.5.4 Summary of Reconstruction Techniques and Structural Uncertainty**

1108

1109 A range of reconstruction techniques exist to make globally-complete or near globally-
1110 complete SST analyses. The spread in global mean SST between analyses is at worst
1111 around 0.2K. The analyses are based on a variety of different statistical models
1112 suggesting that estimates of global average SST are not strongly dependent on such
1113 choices. However, current reconstruction techniques do not account for systematic errors
1114 in the data – they assume errors are random and uncorrelated – and assume that SST
1115 fields can be simply parameterized in terms of limited numbers of patterns or simple
1116 covariance relationships. Objective comparison of different reconstruction techniques and
1117 their associated uncertainty estimates would be aided by the creation of standard
1118 benchmark tests which mimic the distribution and character of observational data.

1119

1120 **3.6 Comparing Components of Uncertainty**

1121

1122 Figure 7 shows individual components of the overall uncertainty estimated for three
1123 months. The components include: estimates of structural uncertainty (in lieu of a formal
1124 way to estimate this, it is calculated as the standard deviation of seven near-globally-
1125 complete analyses: COBE, Kaplan, ERSSTv3, HadISST, GPFA, GP and VBPCA),
1126 sampling uncertainty, combined random and systematic measurement error uncertainty,
1127 bias uncertainty (estimated from a 200-member ensemble described in section 4) and
1128 analysis uncertainties from ERSSTv3b [*Smith et al.* 2008].

1129

1130 At a monthly, grid-box level, the parametric uncertainty in the *Kennedy et al.* [2011c]
1131 systematic error estimates is typically the smallest uncertainty and is nearly always less
1132 than 0.2 K. The sampling uncertainty and measurement uncertainty both depend on the
1133 number of observations, so they are larger in areas with fewer observations. Of the two,
1134 measurement uncertainty is typically larger.

1135

1136 In well-observed periods, the spread between the different analyses is roughly what one
1137 might expect: closer agreement in well-observed regions, poorer agreement in data-sparse
1138 regions, principally the Southern Ocean and Arctic Ocean. At more poorly-observed
1139 times, the spread between analyses is narrower than the climatological standard deviation
1140 suggesting that the reconstructions are skilful in the sense that they are providing useful
1141 information in data voids. However, the narrow spread is in contrast to those areas where
1142 there have been changes in the input observations (see, for example, the Indian Ocean in
1143 Figure 7(b) and Figure 7(h)). A small number of observations, which are available to one
1144 analysis but not another, lead to a larger spread than is seen in data-free regions implying

1145 that, while there is diversity in the approaches, there may still be too little for the best
1146 estimates alone to effectively bracket the true uncertainty range.

1147

1148 The ERSSTv3 analysis uncertainties are largest in regions where there are consistent data
1149 voids. They show a similar pattern to the structural uncertainty estimate in 1944 and
1150 2003, but there is marked difference in 1891, with the analysis uncertainty being larger
1151 than the structural uncertainty in the poorly-observed western Pacific.

1152

1153 Figure 8 shows time series of the different components of uncertainty at different spatial
1154 scales from global to grid box. The bias uncertainty is relatively constant and is the
1155 smallest component of uncertainty at the grid box level for much of the record. The
1156 sampling uncertainty for a grid box is larger than the bias uncertainty when observations
1157 are few, but in the recent record they are comparable. In this example, the measurement
1158 uncertainty is larger than bias and sampling uncertainties at the grid box level, even when
1159 observations are numerous. However, in other grid boxes, characterised by strong SST
1160 gradients or high variability, such as the western boundary currents, the sampling
1161 uncertainty could be larger.

1162

1163 As the size of the area increases and more observations are included in the average, the
1164 sampling and measurement uncertainties decrease. Two estimates of the measurement
1165 uncertainty are included. In one, correlations between individual errors are taken into
1166 account. In the other, measurement errors are assumed to be random and independent. In
1167 the latter case, the measurement uncertainties become small relative to other sources of

1168 uncertainty at a basin scale early in the 20th century. However, the effect of correlated
1169 errors is such that measurement uncertainty remains a major source of uncertainty at all
1170 scales until the 1980s when the global VOS fleet reached its peak and the deployment of
1171 drifting and moored buoys began.

1172

1173 The largest component at the scales shown here is the structural uncertainty. In the grid
1174 box shown, the structural uncertainty is, at times, larger than the combined uncertainty
1175 from other components suggesting that some or all of the analyses are losing information.
1176 At a global level, where estimated analysis uncertainties are available for COBE, COBE-
1177 2, Kaplan and ERSSTv3b data sets, the structural uncertainty is comparable to the
1178 estimated analysis uncertainties. For example, in 1900, the ERSSTv3b analysis
1179 uncertainty is 0.03K, the COBE analysis uncertainty is 0.06K, COBE-2 gives 0.05K and
1180 Kaplan is around 0.05K.

1181

1182 Because of the nature of the uncertainties arising from the adjustments for pervasive
1183 systematic errors, the uncertainties become relatively more important as the averaging
1184 scale increases. At a global scale, bias uncertainties are comparable to or larger than all
1185 other uncertainty components from the 1940s to the present. There is a caveat: because
1186 the SSTs are expressed as anomalies, the size of the bias uncertainty depends on the base
1187 period used to calculate the anomalies. In Figure 8, the period used is 1961-1990, which
1188 is why there is a local minimum in the bias uncertainty centred on that period.

1189

1190 **3.7 Estimates of Total Uncertainty**

1191

1192 *Smith and Reynolds* [2005] attempted to combine all the different uncertainties described
1193 above to get a total uncertainty estimate. They combined their analysis uncertainty with
1194 measurement uncertainty, bias uncertainty and structural uncertainty. Uncertainty
1195 associated with pervasive systematic errors and structural uncertainty in the adjustments
1196 were estimated by taking the mean squared difference between the *Smith and Reynolds*
1197 [2002] and *Folland and Parker* [1995] bias adjustments in the prewar period. After
1198 World War 2, the bias uncertainty was estimated by calculating the average difference
1199 between engine room measurements and all measurements. Structural uncertainties were
1200 estimated by analysing the spread of three SST analyses.

1201

1202 Figure 9 shows the total uncertainty estimate from the latest version of the ERSST
1203 analysis, ERSSTv3b, in blue. A similar estimate was made based on the HadSST3 data
1204 set in the following way. Measurement uncertainties, grid-box sampling uncertainties and
1205 large-scale sampling uncertainties were estimated using the method of *Kennedy et al.*
1206 [2011b, 2011c]. To estimate the uncertainty associated with pervasive systematic
1207 errors, an ensemble of 200 data sets, comprising the 100 original ensemble members from
1208 HadSST3 and a 100-member ensemble generated by replacing the *Rayner et al.* [2006]
1209 bucket-correction fields with the fields from *Smith and Reynolds* [2002]. The adjustment
1210 uncertainties on individual months were assumed to be correlated within a year, giving a
1211 greater uncertainty range than in *Kennedy et al.* [2011c], particularly before 1941. During
1212 the war years 0.2 K was added to reflect the additional uncertainty during that period as

1213 described by *Kennedy et al.* [2011c]. As above, structural uncertainties were estimated by
1214 taking the standard deviation of area-average time series from seven analyses.

1215

1216 The total uncertainty estimates from these two assessments are comparable between 1880
1217 and 1915. Between 1915 and 1941, the ERSSTv3b uncertainty estimate is larger because
1218 the estimated bias uncertainty is larger. The difference is most obvious in the northern
1219 hemisphere where the differences between the *Smith and Reynolds* [2002] and *Folland*
1220 *and Parker* [1995] bias adjustments are largest. From 1941 to present, the HadSST3-
1221 based uncertainty estimate is the larger because the bias uncertainty is larger than in
1222 ERSSTv3b.

1223

1224 The obvious question that arises is “do these assessments span the full uncertainty
1225 range?” In this case, it probably pays to err on the side of caution. Although the structural
1226 uncertainty is based on a range of methods for infilling missing data, there are still
1227 commonalities in the approaches taken and there is little diversity in the approaches to
1228 bias adjustment. The lack of diversity is troubling because the differences between the
1229 median estimates of HadSST3 and ERSSTv3b are greater than the estimated uncertainties
1230 of the ERSSTv3b analysis at times during the period 1950-1970 suggesting that the
1231 uncertainties may have been underestimated in the earlier assessment.

1232

1233 **4 Presentation of Uncertainty**

1234

1235 At present, some groups provide explicit uncertainty estimates based on their analysis
1236 techniques [*Kaplan et al.*, 1998; *Smith et al.*, 2008; *Kennedy et al.*, 2011b, 2011c, *Ishii et*
1237 *al.*, 2005; *Hirahara et al.*, 2013]. The uncertainty estimates derived from a particular
1238 analysis will tend to misestimate the true uncertainty because they rely on the analysis
1239 method and the assumptions on which it is based being correct.

1240

1241 Comparing uncertainty estimates provided with analyses can be difficult because not all
1242 analyses consider the same sources of uncertainties. Consequently, a narrower
1243 uncertainty range does not necessarily imply a better analysis. One way that data set
1244 providers could help users is to provide an inventory of sources of uncertainty that have
1245 been considered either explicitly or implicitly. This would allow users to assess the
1246 relative maturity of the uncertainty analysis.

1247

1248 There is a further difficulty in supplying and using uncertainty estimates: the traditional
1249 means of displaying uncertainties – the error bar, or error range – does not preserve the
1250 covariance structure of the uncertainties. Unfortunately, storing covariance information
1251 for all but the lowest resolution data sets can be prohibitively expensive. EOF-based
1252 analyses, like that of *Kaplan et al.* [1998], could in principle efficiently store the spatial-
1253 error covariances because only the covariances of the reduced space of principal
1254 components need to be kept. For *Kaplan et al.* [1998], based on a reduced space of only
1255 80 EOFs, this is a matrix of order 80^2 elements for each time step as opposed to 1000^2
1256 elements for the full-field covariance matrix. The difficulty with this approach is that not

1257 all variability can be resolved by the leading EOFs and excluding higher-order EOFs will
1258 underestimate the full uncertainty.

1259

1260 *Karspeck et al.* [2012] drew samples from the posterior probability produced by their
1261 analysis. Each sample provides an SST field that is consistent with the available
1262 observations and the estimated covariance structure. Sampling has the added advantage
1263 that it can be combined easily with Monte-Carlo samples from the measurement bias
1264 distributions. However, production of samples is not always computationally efficient.

1265 *Karspeck et al.* [2012] were able to do it for the North Atlantic region, but the
1266 computational costs of extending the analysis unchanged to the rest of the world could be
1267 prohibitive. *Kennedy et al.* [2011c] provided an ensemble of 100 interchangeable
1268 realizations of their bias-adjusted data set, HadSST3. The ensemble spans parametric
1269 uncertainties in their adjustment method.

1270

1271 By providing a set of plausible realizations of a data set, or alternatively by providing
1272 plausible realizations of typical measurement errors [*Mears et al.*, 2011], it can be
1273 relatively easy for users to assess the sensitivity of their analysis to uncertainties in SST
1274 data. For example, individual ensemble members of HadSST3 were used in *Tokinaga et*
1275 *al.* [2012], along with other SST analyses, to show that their results were robust to the
1276 estimated bias uncertainties in SSTs.

1277

1278 Another approach [*Merchant et al.* 2013] is to separate out components of the uncertainty
1279 that correlate at different scales. Random measurement errors, such as sensor noise, are

1280 uncorrelated. Some uncertainties, for example those related to water vapor in a satellite
1281 view, are correlated at a synoptic scale. Yet others are correlated at all times and places.
1282 Grouping uncertainties in this way allows users to propagate uncertainty information
1283 more easily.

1284

1285 **5 Minimizing Exposure to Uncertainty**

1286

1287 Alternative approaches to using the SST data in a way that is less sensitive to biases and
1288 other data errors have been made. The following approaches make use of knowledge
1289 concerning the types of errors and uncertainties found in SST data and have been adapted
1290 to account for them. They highlight the importance of combining understanding of the
1291 measurements and their potential errors, as well as understanding of the phenomenon
1292 being analyzed. Perhaps the simplest example is *Schell* [1959] who suggested discarding
1293 grid-box averages (in that case Marsden squares) based on small numbers of
1294 observations.

1295

1296 *Thompson et al.* [2008] identified an abrupt drop in the observed global average SST
1297 anomaly in late 1945, which they attributed to a rapid change in the composition of
1298 ICOADS 2.0 [*Worley et al.*, 2005] from mostly US ships immediately before the 1945
1299 drop to mostly UK ships immediately afterwards. This hypothesis was lent further weight
1300 by *Kennedy et al.* [2011c]. In a follow-up paper [*Thompson et al.*, 2010], a drop in
1301 northern-hemisphere SSTs was identified. In order to show that the drop was not an
1302 artifact of the change in measurement method, they divided the ICOADS data into

1303 distinct subsets based on the country of the ships making the measurements, considered a
1304 range of different SST analyses, and looked at related variables such as NMAT and land
1305 surface air temperatures. The probability of a drop being due to a coincident change in
1306 the way that all countries measured SST, simultaneous with a sudden change in NMAT
1307 and land temperature bias, is small. The fact that the drop was seen in all the different
1308 data sets implied that the drop was real. *Tokinaga et al.* [2012] took a similar approach,
1309 using bucket measurements from ICOADS as a quasi-homogeneous estimate of SST
1310 change over the period 1950 to 2009.

1311

1312 In detection and attribution studies it is common to reduce the coverage of the models to
1313 match that of the data. Doing so reduces the exposure of the study to uncertainties
1314 associated with interpolation techniques, but it does not avoid the problem of systematic
1315 biases. Recent studies [*Jones and Stott, 2011*] have explicitly used a range of data sets to
1316 start to map out the effects of structural uncertainties on detection and attribution studies.

1317

1318 SST data sets are routinely compared to the output of climate simulations. Bearing in
1319 mind the discussion in section 2 on the definition of SST it might be necessary to ensure
1320 that the modeled output and the measured SST correspond to the same quantity. Many
1321 climate models employ a surface mixed layer that is several meters thick. However,
1322 models have been run with greater resolution in the near-surface ocean [e.g., *Bernie et al.*,
1323 2008] in order to simulate diurnal variability.

1324

1325 Another common use of SST data for which an understanding of the limitations of the
1326 data is important is in the calculation and interpretation of EOFs. In many studies EOFs
1327 are calculated from globally complete SST analyses because the lack of missing data
1328 makes calculating EOFs easy. However, it seems wise to bear in mind that a good deal of
1329 statistical processing has already been applied to the SST analyses to make them globally
1330 complete. Extracting EOFs from (or applying any other analysis technique to) what are in
1331 some cases EOF analyses already, could lead to difficulties of interpretation on top of the
1332 more general problems [*Hannachi et al., 2007; Dommenges, 2007; Karnauskas, 2013*].
1333 Techniques exist for estimating EOFs from gridded data sets with missing data and these
1334 can also incorporate uncertainty information though many assume that the errors are
1335 uncorrelated and will tend to underestimate uncertainty in the EOFs and their principal
1336 components. See for example, *Roweis [1998], Schneider [2001], Beckers and Rixen*
1337 [*2003*], *Rutherford et al. [2004], Housego-Stokes and Challenor [2004], Kondrashov*
1338 *and Ghil [2006], Ilin and Kaplan [2009]* and *Luttinen and Ilin [2009]*.

1339

1340 **6 Satellites**

1341

1342 Although the present review is principally concerned with in situ measurements of SST it
1343 is necessary to mention the important role that satellite data play in understanding SST
1344 variability and uncertainty. The advantages of satellite data are obvious; particularly the
1345 ability to measure large areas of the ocean using a single instrument, giving a more nearly
1346 global view of SST.

1347

1348 However, the first thing to note is that satellites monitor radiances and do not directly
1349 measure SSTs. The measured radiances are affected by the state and constituents of the
1350 atmosphere as well as variations in the state and temperature of the sea-surface. The
1351 wavelengths that are sampled are set by the design of the instrument. Retrieving SST
1352 from the radiances is a difficult inverse process and sensitive to biases and other errors
1353 [*Merchant et al.* 2008b]. The second thing to note is that satellite instruments are
1354 sensitive to the skin (upper few microns), or sub-skin (upper few millimeters)
1355 temperature depending on the wavelengths measured by the satellite. Because satellite
1356 instruments are sensitive to the topmost layer of the ocean, the diurnal range of retrieved
1357 SSTs is larger than for measurements made at depth. Thirdly, accurate SST retrievals
1358 from infra-red instruments are only possible when the view is not obscured by cloud.
1359 Microwave retrievals can penetrate cloud, but suffer from problems near to coastlines,
1360 and where precipitation rates are high. They also have coarser spatial resolution and
1361 higher measurement uncertainties [*O'Carroll et al.*, 2008].

1362

1363 The longest records of SST from satellite are derived from the AVHRR (Advanced Very
1364 High Resolution Radiometer) instruments. These instruments make nadir measurements
1365 using two infra-red channels. The retrievals are usually calibrated relative to in situ data.
1366 More recent re-processings use optimal estimation to obtain a retrieval that is
1367 independent of the in situ record [*Merchant et al.*, 2008b] but these have not yet been
1368 extended to calculating global averages. Furthermore, the AVHRR instrument is prone to
1369 systematic errors caused by aerosols in the atmosphere and the satellite orbits drift slowly
1370 altering the sampling of the diurnal cycle through time. Despite the numerous

1371 shortcomings of the AVHRR record, *Good et al.* [2007] showed that there was a long-
1372 term warming trend in SSTs as measured by AVHRR.

1373

1374 The Along-Track Scanning Radiometers (ATSR) [*Smith et al.*, 2012] were designed to
1375 meet the needs of climate monitoring. The satellite is a dual view instrument, taking nadir
1376 and forward views using three infra-red channels. The dual view configuration allows for
1377 more effective screening of aerosols and the three channels allow for accurate retrievals
1378 across a wider range of conditions. Furthermore, the onboard calibration system allows
1379 the stability of the radiance measurements from the instrument to be maintained. The
1380 ATSR data have been reprocessed in the ATSR Reanalysis for Climate (ARC) project
1381 [*Merchant et al.*, 2008a] and the resulting time series have been shown to have biases of
1382 less than 0.1 K and stability better than 5 mK/year since 1993 in the tropics where
1383 reliable long term moorings can be found [*Embury et al.*, 2012; *Merchant et al.*, 2012].
1384 The ARC reprocessing is almost independent of the in situ network therefore it can be
1385 used to corroborate trends seen in the in situ network. In a comparison between global
1386 average SST anomalies (at a nominal depth of 0.2 m) calculated using the ARC data and
1387 HadSST3, the two time series agree within the estimated HadSST3 uncertainties except
1388 for parts of the ATSR1 record in the early 1990s. The ATSR1 period is believed to be of
1389 lower quality as a result of the failure of one of the IR channels, failure of the satellite
1390 cooling system as well as the high stratospheric aerosol loadings following the eruption
1391 of Mount Pinatubo in 1991.

1392

1393 The nearly global, high-resolution view of the world's oceans provided by satellite
1394 instruments can be used as a way of improving and testing many aspects of SST analysis.
1395 By combining the more detailed fields produced by satellites with the long records of in
1396 situ measurements, more detailed reconstructions are possible over a wider area of the
1397 Earth [Rayner *et al.*, 2003; Smith *et al.*, 2008; Hirahara *et al.*, 2013]. Satellite data can
1398 also be used to assess the verisimilitude of reconstructions based on sparser in situ data.

1399

1400 **7 Concluding Remarks and Future Directions**

1401

1402 One of the chief difficulties in assessing the uncertainties in SST data sets is the
1403 impossibility of tracing individual observations back via an unbroken chain to
1404 international measurement standards. The creation of a global array of reference stations
1405 each making simultaneous redundant measurements of a variety of marine variables
1406 could solve some of the problems of SST analysis that have bedeviled the understanding
1407 of historical SST change and would provide a gold standard against which the *future*
1408 wider observing system – incorporating observations from ships, buoys, profiling floats
1409 and satellites – can be assessed. Even without such traceability a climate record could be
1410 more easily maintained by stricter adherence to the Global Climate Observing System
1411 [GCOS 2003] climate monitoring principles.

1412

1413 In the absence of such a network the estimation of uncertainties has depended heavily on
1414 redundancies in measurement systems and in analysis techniques. Full use of the
1415 redundancies is now being made in the modern period via comparisons of the many

1416 available satellite sources with each other and with in situ sources [*O'Carroll et al.*, 2008;
1417 *Merchant et al.*, 2012] and sub-surface data [*Gille*, 2012]. Analyses that ingest a variety
1418 of data sources can produce bias statistics for each of the inputs [*Brasnett*, 2008; *Xu and*
1419 *Ignatov*, 2010]. Such information can be exploited to assess their relative quality and, as
1420 the analyses are pushed further back in time [*Roberts-Jones et al.*, 2012], they will help
1421 assess uncertainties through a larger part of the record.

1422

1423 SSTs are physically related to other measurements including surface pressures and winds,
1424 salinity, air temperatures, sub-surface temperatures and ocean biology amongst others.
1425 Information from SST can be supplemented by analyses based on physical understanding
1426 of the climate system. It has already been shown that by combining information from
1427 night marine air temperatures with SST it was possible to greatly reduce uncertainties in
1428 early 20th and late 19th century SST. *Yu et al.* [2004] used a joint estimation method to
1429 minimize uncertainties in flux estimates based on a range of different variables mostly
1430 based on satellite data. Other studies [*Tung and Zhou*, 2010; *Deser et al.*, 2010] have used
1431 physical reasoning based on a host of variables to explore uncertainties in the long-term
1432 trends of tropical Pacific SSTs first raised by *Vecchi et al.* [2008]. It has even been
1433 suggested that proxy records such as isotope ratios from corals and ice cores could be
1434 used, with appropriate care, to understand uncertainties in the longest-term changes in
1435 SST [*Anderson et al.*, 2013]. The most advanced exemplars of physical and statistical
1436 synthesis are ocean and coupled reanalyses which will play an increasingly important role
1437 in understanding observational uncertainty and long-term climate change.

1438

1439 A key barrier to understanding SST uncertainty is a lack of appropriate metadata. Better
1440 information is needed concerning how measurements were made, which method was
1441 used to make a particular observation, calibration information, the depths at which
1442 observations were made, and even basic information such as the call sign or name of the
1443 ship that made a particular observation.

1444

1445 Some of this information can be inferred from data already contained in marine reports.

1446 Where reports in ICOADS cannot be associated with a particular ship, either because
1447 they have a missing ID, or a generic ID, there is much to be gained by grouping
1448 observations to give plausible ship tracks, or voyages. By using data association
1449 techniques to infer such metadata from the location information and other clues such as
1450 how frequently observations were made and which variables were observed, it should be
1451 possible to assess systematic and random errors on a ship-by-ship basis going back to the
1452 start of the record and even infer likely measurement methods based on characteristic
1453 variations of the measurements with the meteorological conditions.

1454

1455 A more systematic approach to the assessment of analysis techniques is needed to
1456 elucidate the reasons for the differences between analyses and to assess the verisimilitude
1457 of analysis uncertainty estimates. Approaches could include theoretical inter-comparisons
1458 of statistical methods, comparisons based on well-defined sets of common input
1459 observations, and benchmarks built from datasets (such as model output) where the truth
1460 is known a priori. Benchmark tests like those planned by the International Surface
1461 Temperature Initiative [*Thorne et al.* 2011b] provide an objective measure against which

1462 analysis techniques can be evaluated. Both analysis techniques and benchmarks will have
1463 to be tailored appropriately for the particular problems affecting SST measurements and
1464 the latest understanding of measurement uncertainties.

1465

1466 A key weakness of historical SST data sets is the lack of attention paid to evaluating the
1467 effects of data biases particularly in the post-1941 records. Further independent estimates
1468 of the biases produced need to be undertaken using as diverse a range of means as
1469 possible and the robust critique of existing methods must continue. Ideally, these would
1470 be complemented by carefully-designed field tests of buckets and other measurement
1471 methods.

1472

1473 Combining new analysis techniques that have been appropriately benchmarked with
1474 novel approaches to assessing uncertainty arising from systematic errors, pervasive
1475 systematic errors and their adjustments will give new end-to-end analyses that will help
1476 to explore the uncertainties in historical SSTs in a more systematic manner.

1477

1478 For long-term historical analyses, there is no substitute for actual observations and
1479 relevant metadata. Efforts to identify archives of marine observations and digitize them
1480 are ongoing [*Brohan et al.*, 2009; *Wilkinson et al.*, 2011]. Such programs are labor
1481 intensive, first in identifying and cataloguing the holdings in archives around the world,
1482 then in creating and storing digital images of the paper books and finally in keying the
1483 observations. The difficulty of decoding hand written entries in a variety of languages,
1484 formats and scripts means that optical character recognition technologies are of limited

1485 use. A number of popular crowd-sourcing projects have been started to key information
1486 from ships logs that have historical as well meteorological interest. OldWeather.org has
1487 keyed data from Royal Navy logs from the First World War [Brohan *et al.*, 2009] and is
1488 now working on logs from polar expeditions. Digitization of data also holds the
1489 possibility of extending instrumental records further back in time [Brohan *et al.*, 2010].
1490 New observations, with reliable metadata, can be used not only to reduce uncertainty in
1491 SST analyses, but also to test the reliability of existing interpolated products and their
1492 uncertainties.

1493

1494 The ultimate destination of newly digitized observations is the International
1495 Comprehensive Ocean Atmosphere Data Set (ICOADS) [Woodruff *et al.*, 2011]. The
1496 ICOADS repository of marine meteorological data has long been the focus of advances in
1497 the understanding of marine climatology. It provides a consistent baseline for a wide
1498 range of studies, providing a solid basis for traceability and reproducibility. The
1499 continued existence, maintenance and improvement of ICOADS are essential to the
1500 future understanding of the global climate.

1501

1502 Finally, the work of identifying and quantifying uncertainties will be pointless, if those
1503 uncertainties are not used. Uncertainty estimates provided with data sets have sometimes
1504 been difficult to use or easy to use inappropriately. As pointed out by Rayner *et al.*
1505 [2009], "more reliable and user-friendly representations of uncertainty should be
1506 provided" in order to encourage their widespread and effective use.

1507

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1520

1521 **Appendix A**

1522

1523 Figure 1 was calculated in the following way. Observations were separated into three
1524 groups – shallow, deep and unknown – using the metadata assignments of *Kennedy et al.*
1525 [2011c]. Bucket and buoy measurements were considered to be shallow. Engine intake
1526 and hull contact measurements were considered to be deep. Shallow measurements were
1527 assumed to exhibit a diurnal cycle equal to that measured by drifting buoys [*Kennedy et*
1528 *al.*, 2007]. Deep measurements were assumed to have no diurnal cycle. The two groups
1529 were assumed to measure the same temperature just before sunrise. The relative bias
1530 between the two was calculated by subtracting the minimum of the diurnal cycle from the

1531 daily average. This value varies by location and calendar month. The bias in each grid
1532 box was estimated by multiplying the relative bias by the fraction of shallow
1533 measurements. The bias was then normalized relative to the period 1961-1990, the
1534 anomaly period used for HadSST3. Figure 1 shows the global monthly average of the
1535 bias.

1536

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<i>Strong and McLean</i> [1984]	1.8K RMS difference between ship and AVHRR data
<i>Bernstein and Chelton</i> [1985] pg 11620	1.1 K
<i>Sarachik</i> [1984], <i>Weare</i> [1989] pg 359	1 K
<i>Wilkerson and Earle</i> [1990] pg 3381	3.5 K
<i>Cummings</i> [2005] Table 1, pg 3592	1.3 K (ERI) 0.6 K (Hull sensor) 1.2 K (bucket)
<i>Kent and Challenor</i> [2006] pg 484	1.2±0.4 K or 1.3±0.3 K depending on how measurements were weighted
<i>Kent et al.</i> [1999] abstract	1.5±0.1 K
<i>Kent and Berry</i> [2005] Table 2 pg 853	1.3±0.1 K and 1.2±0.1 K
<i>Reynolds et al.</i> [2002] pg 1613	1.3 K
<i>Kennedy et al.</i> [2011a] pg 83	1.0 K
<i>Ingleby</i> [2010] Table 10 pg 1487	0.9 K for automatic systems 1.2 K for manual measurements
<i>Kent and Berry</i> [2008] Table 5a pg 11	1.1 K
<i>Xu and Ignatov</i> [2010] pg 16 of 18	1.16 K

2158 **Table 1:** List of estimates of measurement error uncertainties for ships where random and
 2159 systematic errors were not dealt with separately.
 2160

References	Estimated measurement uncertainty for drifting buoy measurements
<i>Strong and Mclean</i> [1984]	0.6K RMS difference between drifter and AVHRR
<i>Reynolds et al.</i> [2002] pg 1613	0.5 K
<i>Emery et al.</i> [2001] pg 2393	0.3 K
<i>Cummings</i> [2005] Table 1, pg 3592	0.12 K
<i>O'Carroll et al.</i> [2008] abstract	0.23 K
<i>Kent and Berry</i> [2008] Table 5c pg 12	0.67 K
<i>Ingleby</i> [2010] Table 10 pg 1487	0.33 K
<i>Kennedy et al.</i> [2011a] pg 83	0.2-0.4 K
<i>Xu and Ignatov</i> [2010] pg 16 of 18	0.26 K
<i>Merchant et al.</i> [2012] Table 2 pg 8 of 18	0.15-0.19 K

2161 **Table 2:** List of estimates of measurement error uncertainties for drifting buoys where
 2162 random and systematic errors were not dealt with separately.
 2163

Reference	Estimated measurement uncertainty for moored buoy measurements
<i>Cummings</i> [2005] Table 1, pg 3592	0.05 K
<i>Kent and Berry</i> [2008] Table 5b pg 11	0.4 K

<i>Kennedy et al.</i> [2011a] pg 83	tropical moorings, 0.12 K; all moorings, 0.21 K
<i>Xu and Ignatov</i> [2010] pg 16 of 18	tropical moorings, 0.30 K; coastal moorings, 0.39 K
<i>Gilhousen</i> [1987] Table 6 pg 104	0.22 K

2164 **Table 3:** List of estimates of measurement error uncertainties for moored buoys where
2165 random and systematic errors were not dealt with separately.
2166

Reference	Platform type	Random	Systematic	Notes
<i>Kent and Berry</i> [2008] pg 11 Table 5a	Ship	0.7 K	0.8 K	From comparison with Numerical Weather Prediction fields provided with VOSCLim data
Pg 12 Table 5c	Drifter	0.6 K	0.3 K	
Pg 11 Table 5b	Mooring	0.3 K	0.2 K	
<i>Kennedy et al.</i> [2011a, 2011b] pg 86	Ship	0.74 K	0.71 K	From comparison with Along Track Scanning Radiometer SST retrievals
Pg 86	Drifter	0.26 K	0.29 K	
<i>Brasnett</i> [2008] values estimated for present study by	Ship	1.16 K	0.69 K	From comparison with interpolated fields

author				
<i>Xu and Ignatov</i> [2010] values estimated for present study by author	Ship	0.81 K	0.53 K	From comparison with multisensor satellite SST fields
<i>Kennedy et al.</i> [2011a, 2011b] method using <i>Atkinson et al.</i> [2013] whitelist	Ship	0.56 K	0.37 K	From comparison with multisensor satellite SST fields
<i>Gilhousen</i> [1987] Table 6 pg 104	Mooring	0.22 K	0.13 K	Comparison of moored buoys

2167 **Table 4:** List of estimates of measurement error uncertainties for all platforms for studies
2168 where the measurement error uncertainty is decomposed into random and systematic
2169 components.
2170

Data set	Input data set	Interpolation method	Resolution
ICOADS summaries [<i>Woodruff et al.</i> , 2011]	ICOADS 2.5	None	2°x2° monthly
HadSST2 [<i>Rayner et al.</i> , 2006]	ICOADS 2.1	None	5°x5° monthly

HadSST3 [<i>Kennedy et al.</i> , 2011b; <i>Kennedy et al.</i> , 2011c]	ICOADS 2.5	None	5°x5° monthly
TOHOKU [<i>Yasunaka and Hanawa</i> , 2002]	ICOADS 2.1	None	5°x5° monthly
HadISST1.1 [<i>Rayner et al.</i> , 2003]	Met Office Marine Databank and COADS, AVHRR satellite retrievals	Reduced Space Optimal Interpolation	1°x1° monthly
ERSSTv3b [<i>Smith et al.</i> , 2008]	ICOADS 2.1	Separate low and high frequency reconstructions. High frequency component based on EOTs	2°x2° monthly
COBE [<i>Ishii et al.</i> , 2005]	ICOADS 2.1 and Kobe collection	Optimal interpolation	1°x1° monthly
COBE-2 [<i>Hirahara et al.</i> , 2013]	ICOADS 2.5 and Kobe collection, AVHRR satellite retrievals	Multi scale analysis based on EOFs	1°x1° daily and monthly

Kaplan [<i>Kaplan et al.</i> , 1998]	Met Office Marine Databank	Reduced Space Optimal Smoothing	5°x5° monthly
NOCS [<i>Berry and Kent</i> , 2011]	ICOADS 2.5	Optimal Interpolation	1°x1° daily and monthly
VBPCA [<i>Ilin and Kaplan</i> , 2009]	ICOADS 2.5	Variational Bayesian Principal Component Analysis	5°x5° monthly
GPFA [<i>Luttinen and Ilin</i> , 2009]	ICOADS 2.5	Gaussian Process Factor Analysis	5°x5° monthly
GP [<i>Luttinen and Ilin</i> , 2012]	ICOADS 2.5	Gaussian Process	5°x5° monthly

2171 **Table 5:** List of datasets used and referred to in the review.

2172

2173 **Figure Captions**

2174

2175 **Figure 1:** (a) Estimated bias (with respect to the 1961-1990 average) on global average

2176 SST anomalies associated with measurement depth as a function of time (upper panel).

2177 (b) Global average SST anomaly from the HadSST3 [Kennedy et al. 2011b, 2011c]

2178 median before (black) and after (red) the measurement-depth bias has been subtracted.

2179 The two red lines reflect different assumptions concerning data that could not be

2180 definitively assigned to any particular measurement type. The large dip during World

2181 War 2 arises because the majority of observations were ERI measurements.

2182

2183 **Figure 2:** Time series of upper ocean temperatures (0-30 m) from nine moorings in the
2184 Tropical Ocean Atmosphere (TAO) array and the Subduction Array. The mooring and its
2185 location are given above each plot. The different coloured lines represent different depths
2186 and these are indicated by the legends in each panel. The Subduction Array data are
2187 described in *Moyer and Weller* [1997].

2188

2189 **Figure 3:** Distributions of estimated measurement errors and uncertainties from ships. (a)
2190 distributions of systematic measurement errors for all entries (2003-2007) in *Kennedy et*
2191 *al.* [2011a], *Brasnett* [2008], *Berry and Kent* [2008] and *Xu and Ignatov* [2010]. (b)
2192 distributions of random measurement error uncertainties (expressed as variances) from
2193 the same analyses as in the top left panel and *Atkinson et al.* [2013]. (c) as for top left
2194 except each ship now has only a single entry so the analyses are directly comparable. (d)
2195 scatter plot showing systematic measurement errors estimated by *Brasnett* [2008] and
2196 *Berry and Kent* [2008] showing the good correlation between the estimates.

2197

2198 **Figure 4:** (a) Estimated global average SST anomaly from HadSST3 [Kennedy et al.
2199 2011b, 2011c] (red) and for subsamples of the HadSST3 dataset reduced to 19th century
2200 coverage. The black line is the median of the samples and the blue area gives the range.
2201 (b) difference, on an expanded temperature scale, between the global average SST
2202 anomaly from the full HadSST3 data set and global averages calculated from the
2203 subsamples.

2204

2205 **Figure 5:** Global average sea-surface temperature anomalies and night marine air
2206 temperature anomalies from a range of data sets. (a) Simple gridded SST data sets
2207 including ICOADS v2.1 (red), 200 realizations of HadSST3 (pale grey), HadSST2 (dark
2208 green), TOHOKU (darker grey), ARC (*Merchant et al.* [2012] lime green) and the
2209 COBE-2 dataset sub-sampled to observational coverage (pale blue). (b) 8 Interpolated
2210 SST analyses including the COBE-2 dataset (pale blue), HadISST1.1 (gold), ERSSTv3b
2211 (orange), VBPCA, GPFA and GP (deep magenta), Kaplan (pink), NOCS (black). (c)
2212 shows the series in (a) and (b) combined. (d) NMAT: Ishii et al. (2005, red and blue),
2213 MOHMAT4N3 and HadMAT (*Rayner et al.* [2003], pink and orange), *Berry and Kent*
2214 [2009] (green), HadNMAT2 (*Kent et al.* [2013], gold).

2215

2216 **Figure 6:** Comparison between COBE-2 (black) and HadSST3 (red) metadata and bias
2217 estimates for the period 1920 to 2010. (a) Fraction of buckets assessed as being
2218 uninsulated. The two red lines indicate the earliest and latest switchover dates allowed in
2219 the generation of the HadSST3 ensemble. (b) Fractional contribution to the global
2220 average from buckets, buoys and engine room measurements. The total is less than unity;
2221 the remainder are either unknown (in the HadSST3 analysis) or uncategorized (COBE-2).
2222 (c) Estimated bias. There are 100 versions of HadSST3 and a single estimate from
2223 COBE-2.

2224

2225 **Figure 7:** Maps showing climatological standard deviation of SST (a, g, m), Structural
2226 uncertainty (b, h, n), Sampling uncertainty (c, i, o), measurement uncertainty (d, j, p), bias

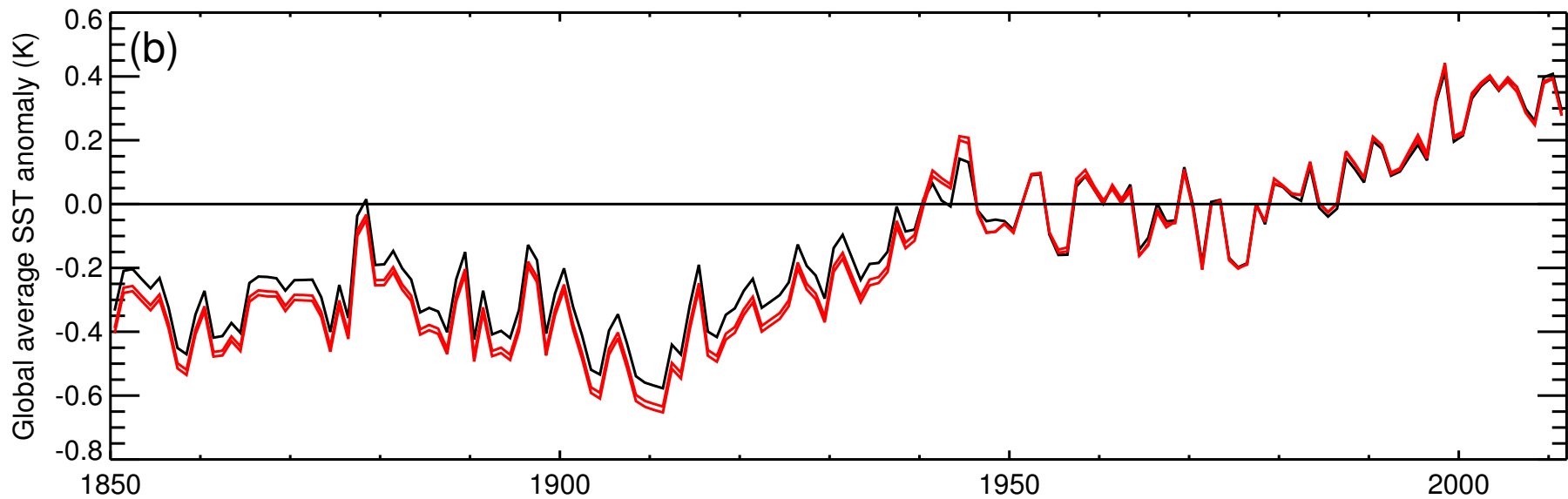
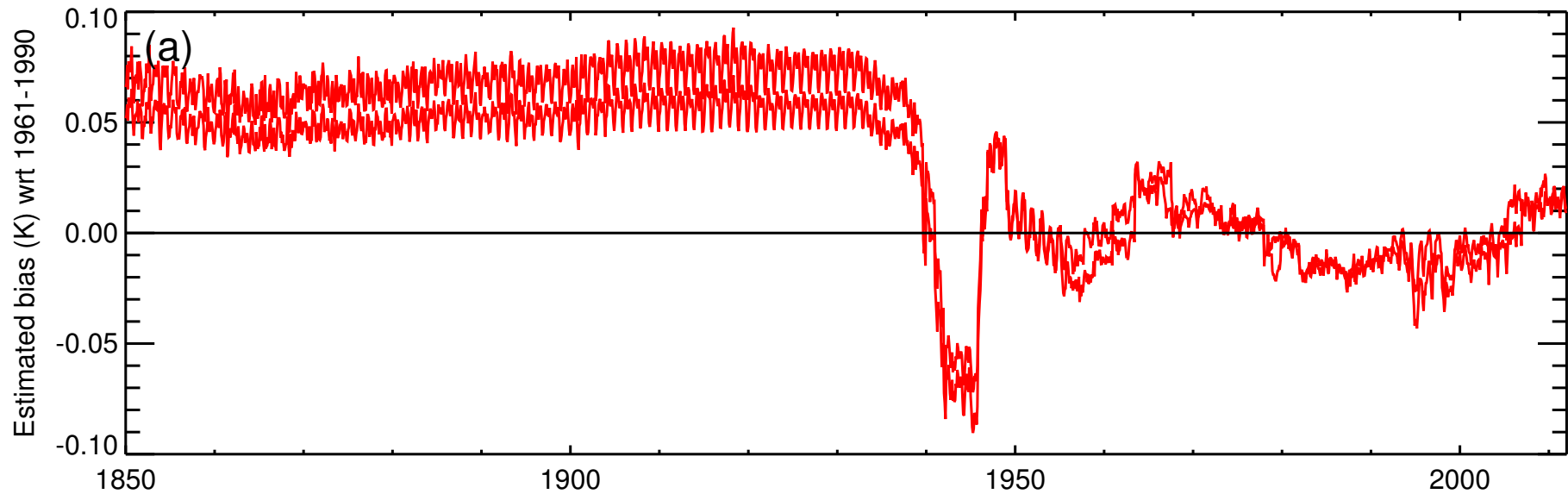
2227 uncertainty (e,k,q) and analysis uncertainty from ERSST (f, l, r). Three months are
2228 shown: (a-f) June 1891, (g-l) April 1944 and (m-r) August 2003.

2229

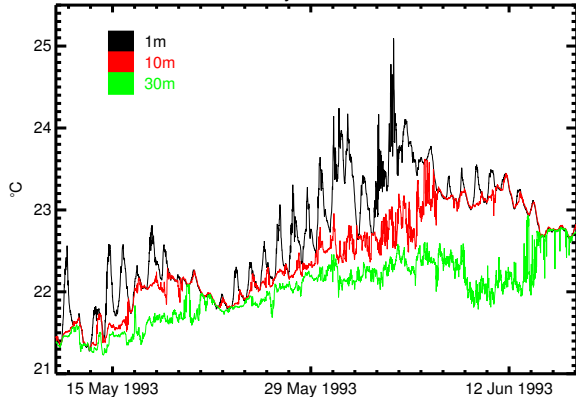
2230 **Figure 8:** Time series of estimated uncertainties arising from different sources in area-
2231 averages: (a) Global annual, (b) Northern hemisphere annual, (c) North Pacific annual,
2232 (d) North Atlantic annual and (e) a 5-degree grid box centered on 42.5°W, 27.5°N
2233 monthly. Uncertainty components shown are: (pale blue) grid-box sampling uncertainty,
2234 (green) uncorrelated measurement uncertainty, (red) correlated measurement uncertainty,
2235 (dark blue) parametric bias uncertainty from a 200-member ensemble based on HadSST3,
2236 (black) large-scale sampling uncertainty, and (magenta) structural uncertainty estimated
2237 by taking the range of the area-average calculated from seven near-globally-complete
2238 analyses.

2239

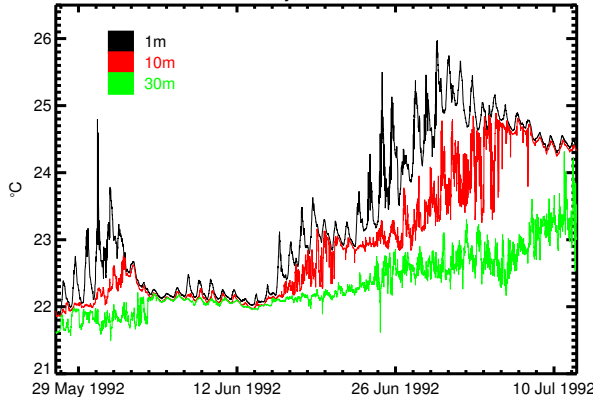
2240 **Figure 9:** (a) Global, (b) Northern Hemisphere, (c) Southern Hemisphere and (d)
2241 Tropical average sea-surface temperature anomalies with estimated 95% confidence
2242 range for ERSSTv3b (1880-2012 dark blue line and pale blue shading) and for the
2243 HadSST3 based analysis described in section 3.5 (1850-2011 red line and orange and
2244 yellow shading). The yellow shading indicates an estimate of the additional structural
2245 uncertainty in the HadSST3 series.



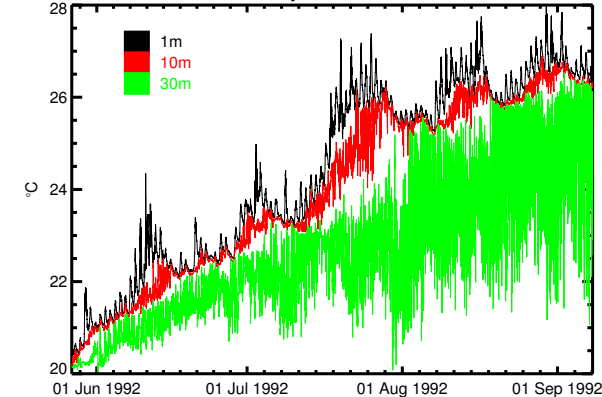
Subduction Array C3T 25.53°N 28.95°W



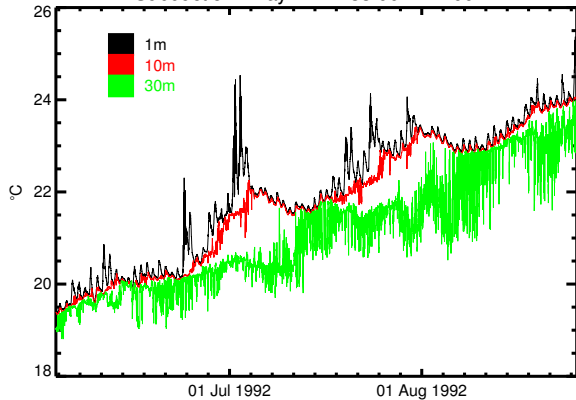
Subduction Array C2T 25.53°N 28.95°W



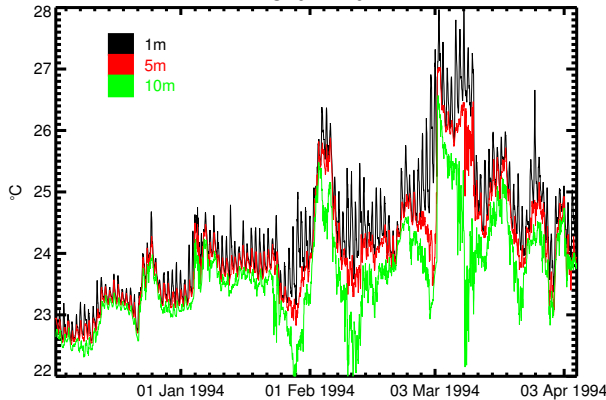
Subduction Array NW2T 32.91°N 33.89°W



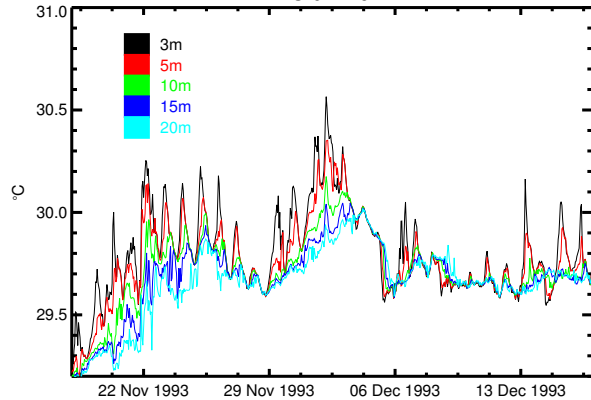
Subduction Array NE2T 33.00°N 22.00°W



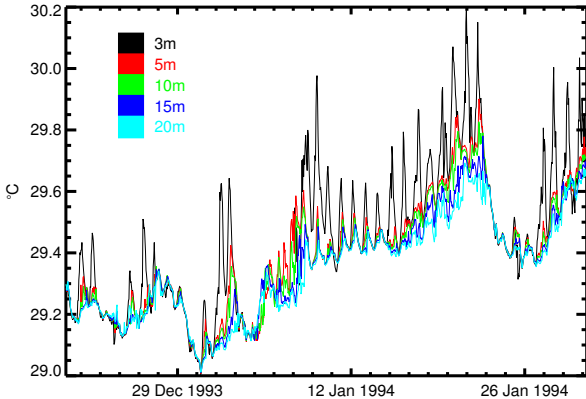
TAO 0°N 110°W



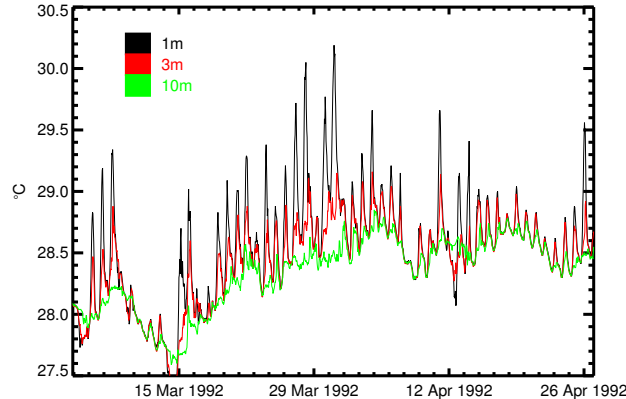
TAO 0°N 161°E



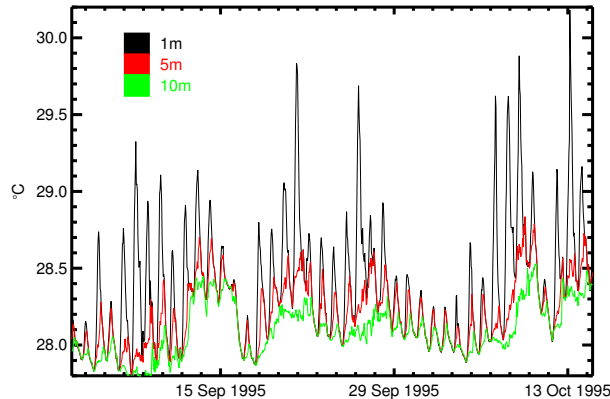
TAO 2°S 156°E



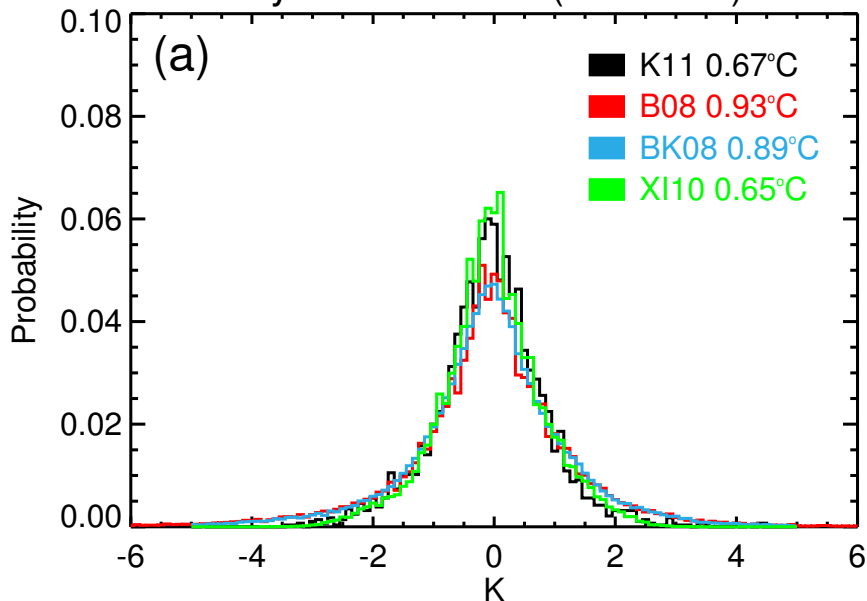
TAO 0°N 140°W



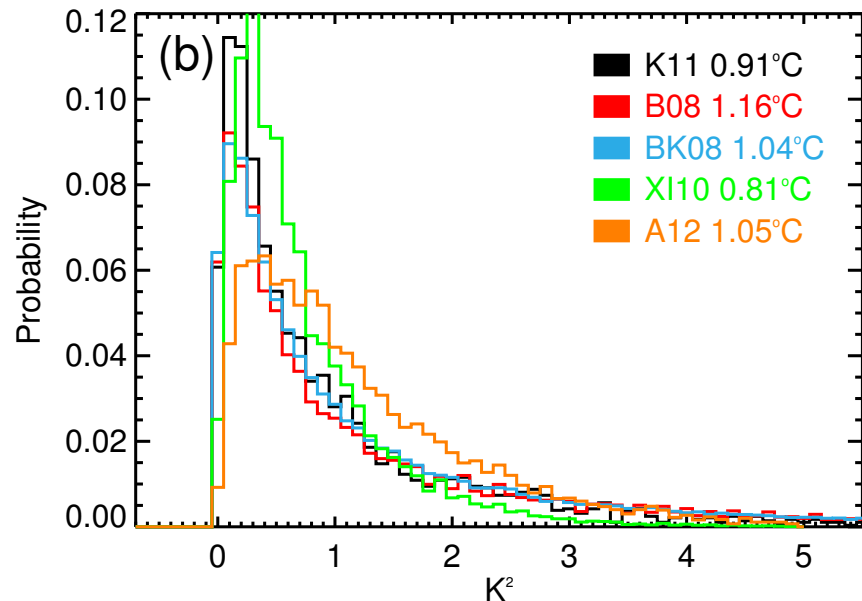
TAO 0°N 165°E



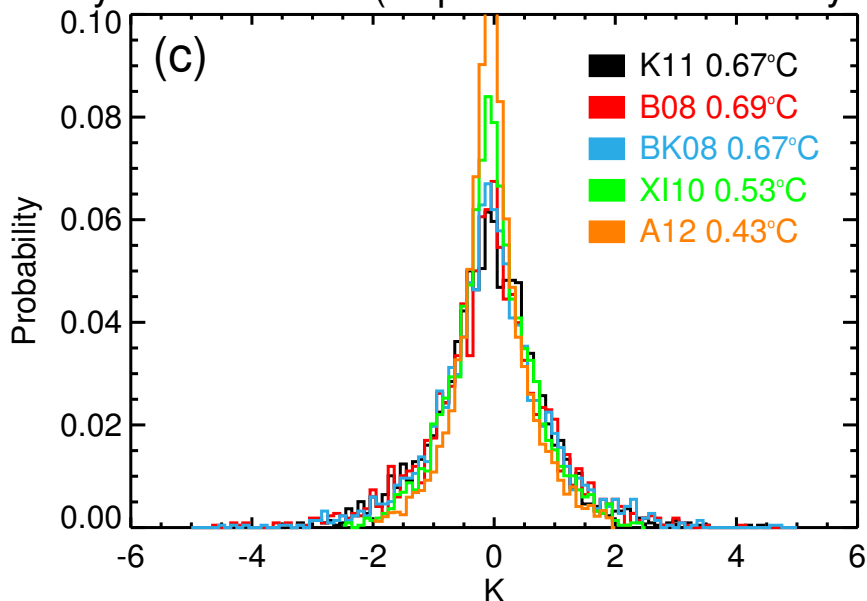
Systematic Error (all values)



Random Error Variance



Systematic Error (ships common to all analyses)



Systematic Error vs Systematic Error

