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Project : **SST CCI Phase-II**

Title : **User Requirements Document**

Abstract : This document presents the results of an exercise to gather requirements for the SST products to be developed by the CCI project.

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AMENDMENT RECORD

This document shall be amended by releasing a new edition of the document in its entirety. The Amendment Record Sheet below records the history and issue status of this document.

AMENDMENT RECORD SHEET

ISSUE	DATE	REASON FOR CHANGE
Phase-I		
1	29 Oct 2010	Initial Issue
2	30 Nov 2010	Revised following comments from Craig Donlon
Phase-II		
1	25 Apr 2014	Inclusion of requirements from the MyOcean User Requirements Document and the ESA SST CCI CAR (Simon Good)
C	20 Nov 2016	Revision based on new requirements gathering, amended following internal review
2	21 Nov 2016	Issued to ESA
2A	21 Dec 2016	Revision following ESA review
2.1	13 Jan 2017	Issued to ESA

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EXECUTIVE SUMMARY

The European Space Agency (ESA) Climate Change Initiative (CCI) Sea Surface Temperature (SST) project, SST CCI, aims to improve SST satellite data records to meet the requirements of the climate research community.

This document presents requirements from climate research users, which were gathered via six methods:

1) a literature review of relevant documents from bodies such as the Global Climate Observing System (GCOS),
2) review of 'lessons learned' information provided by other projects,
3) questionnaires, which asked about
    a) currently available SST data, and
    b) future needs for SST data, five years from now,
4) discussion sessions,
5) review of user requirements found in the ESA SST CCI Climate Assessment Report (CAR) from Phase 1, and the MyOcean Weather, Seasonal Forecasting and Climate User Requirements Document).
6) a user workshop on uncertainties

This document builds upon and updates previous User Requirements Documents [RD.171; RD.385]. Table 5 presents a full list of requirements from RD.171 and RD.385 and this analysis; if requirements have been superseded by our new analysis, we present only the latest version. For readability, we do not reproduce the full text of those documents here, but concentrate on the new information we have gathered in this analysis. In particular, this version includes results from a second survey (see Annex A), together with requirements gathered at a user workshop on uncertainties (see http://www.esa-sst-cci.org/PUG/workshop.htm).

1. INTRODUCTION

1.1 Purpose and Scope

The European Space Agency (ESA) Climate Change Initiative (CCI) [RD.155] aims to improve satellite data records for 14 essential climate variables (ECVs) to meet the requirements of the climate research community. This document presents the results of a survey of climate-user requirements for the sea surface temperature (SST) ECV, which was undertaken as part of the SST component of the CCI project, SST CCI during 2016.

The requirements were gathered via six methods:

1) a literature review of relevant documents from bodies such as the Global Climate Observing System (GCOS),
2) review of lessons learned information provided by other projects.
3) Questionnaires (the first in 2010 and the second in 2016), which asked about
    a) currently available SST data (in 2010 only), and,
    b) future needs for SST data, five years from now.
4) discussion sessions,
5) review of user requirements found in the ESA SST CCI Climate Assessment Report (CAR) from Phase 1 [RD.371], and the MyOcean Weather, Seasonal Forecasting and Climate User Requirements Document [RD.392]).
6) a user workshop on uncertainty

This document builds upon and updates previous User Requirements Documents [RD.171; RD.385]. Table 5 presents a full list of requirements from RD.171 and RD.385 and this analysis; if requirements have been superseded by our new analysis, we present only the latest version. For readability, we do not reproduce the full text of those documents here, but concentrate on the new information with have gathered in this analysis. In particular, this version includes results from a second survey (see Annex A), together with requirements gathered at a user workshop on uncertainties (see http://www.esa-sst-cci.org/PUG/workshop.htm).

Throughout and in Table 5, requirements are each given a unique identifier. The format of the identifier is SST_CCI-UR-SSS-n, where UR stands for User Requirement, SSS is the method of gathering (REF: through analysis of reference documents; QUF: from results of the first questionnaire; CAR: from the Climate Assessment Report of the Phase I products; LLP: from lessons learned from other projects; MYO: from the MyOcean User Requirements Document; UWU: through discussion at the User Workshop on Uncertainties; and QUS: from results of the second questionnaire), and n is the user requirement number.

The information contained here will be analysed and used as the basis for the specifications of the products to be produced by the project (the “SST CCI products”), which will be published in a separate document.

1.2 Referenced Documents

The following is a list of documents with a bearing on the content of this report. Where referenced in the text, these are identified as [RD.n], where 'n' is the number in the list below:

RD.74 Rayner, N. A., et al. (2003), Global analyses of sea surface temperature, sea ice, and night marine air temperature since the late nineteenth century, Journal of Geophysical Research-Atmospheres, 108(D14).

RD.76 Reynolds, R. W., et al. (2007), Daily high-resolution-blended analyses for sea surface temperature, Journal of Climate, 20, 5473-5496.

RD.150 Systematic Observation Requirements for Satellite-based Products for Climate: Supplemental Details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in support of the UNFCCC (GCOS-92)", ESA CCI SOW 1 issue 1.4 revision 1 - 09/11/2009 EOP-SEP/SOW/0031-09/SP GCOS-107, September 2006 (WMO/TD No.1338) Available online at http://www.wmo.int/pages/prog/gcos/index.php

RD.152 The Second Report on the Adequacy of the Global Observing Systems for Climate in Support of the UNFCCC, GCOS – 82, April 2003 (WMO/TD No. 1143) Available online at http://www.wmo.int/pages/prog/gcos/index.php

RD.155 The ESA Climate Change Initiative – Description issue 1 revision 0 - 30/09/09 EOP-SEP/TN/0030-09/SP Available online at: http://earth.esa.int/workshops/esa_cci/ESA_CCI_Description.pdf

RD.156 GCOS Climate Monitoring Implementation Principles, November 1999 Available online at: http://www.wmo.int/pages/prog/gcos/documents/GCOS_Climate_Monitoring_Principles.pdf

RD.159 Implementation Plan for the Global Observing System for Climate in support of the UNFCCC, GCOS-92, October 2004 (WMO/TD No.1219) Available online at http://www.wmo.int/pages/prog/gcos/index.php

RD.163 Guideline for the generation of datasets and products meeting GCOS Requirements, GCOS-143 (WMO/TD No.1530), May 2010; Available online at: http://www.wmo.int/pages/prog/gcos/index.php

RD.164 ESA Climate Change Initiative phase 1 – scientific user consultation and detailed specification – statement of work, Issue 1.4, Revision 1, 09/11/2009, Reference EOP-SEP/SOW/0031-09/SP; http://earth.eo.esa.int/workshops/esa_cci/ao6207SoW.pdf

RD.165 Annex G to RD.164, Sea Surface Temperature ECV (SST_cci)

RD.171 CCI Phase 1 (SST) (2010), User Requirements Document, Reference SST_CCI-URD-UKMO-001;

RD.187 Merchant C J, D Llewellyn-Jones, R W Saunders, N A Rayner, E C Kent, C P Old, D Berry, A R Birks, T Blackmore, G K Corlett, O Embury, V L Jay, J Kennedy, C T Mutlow, T J Nightingale, A G OCarroll, M J Pritchard, J J Remedios and S Tett (2008), Deriving a sea surface temperature record suitable for climate change research from the along-track scanning radiometers, Adv. Sp. Res, 41 (1), 1-11. doi:10.1016/j.asr.2007.07.041

RD.205 Kilpatrick, KA; Podesta, GP; Evans, R (2001) Overview of the NOAA/NASA advanced very high resolution radiometer Pathfinder algorithm for sea surface temperature and associated matchup database, JGR, 106, pp9179-9197

RD.371 ESA SST CCI CAR for version 1 of the products. Available online at http://www.esa-sst-cci.org/sites/default/files/Documents/public/SST_CCI-CAR-UKMO-001-Issue_1-signed-accepted.pdf

RD.385 SST_CCI User Requirements Document (URD), SST_CCI-URD-UKMO-201.

RD.390 Climate Modelling User Group (2015), Deliverable 1.1, Requirements Baseline Document

RD.391 Systematic observation requirements for satellite-based data products for climate, 2011 update: Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 Update)", December 2011, GCOS – 154

RD.392 MyOcean Service Weather, Seasonal Forecasting & Climate User Requirements Document, v3.0, 2011

RD.394 Wentz, FJ; Gentemann, C; Smith, D; et al. (2000) Satellite measurements of sea surface temperature through clouds, Science, 288, pp 847-850

1.3 Definitions of Terms

The following terms have been used in this report with the meanings shown.

Term	Definition
Analysis	In the sense of an "SST analysis" this means that the field has been interpolated or smoothed.
AOPC	Atmospheric Observation Panel for Climate
ATSR	Along Track Scanning Radiometer
AVHRR	Advanced Very High Resolution Radiometer
CAR	Climate Assessment Report
CCI	Climate Change Initiative
CDR	Climate Data Record
CF	Climate and Forecast
CMUG	Climate Modelling User Group
CliC	Climate and Cryosphere
CLIVAR	Variability and predictability of the ocean-atmosphere system
ECV	Essential Climate Variable
ESA	European Space Agency
GCOS	Global Climate Observing System
GHRSST	Group for High Resolution Sea Surface Temperature

GOOS	Global Ocean Observing System
HadISST	Hadley Centre Sea Ice and Sea Surface Temperature dataset
ICOADS	International Comprehensive Ocean-Atmosphere Data Set
In situ data	SST observations made *in situ* by drifting or moored buoys, Argo floats, Voluntary Observing Ships or ship-borne radiometers, etc
NetCDF	Network Common Data Format
NOAA	National Oceanographic and Atmospheric Administration
NWP	Numerical Weather Prediction
NRT	Near real time
OI	Optimal Interpolation
OOPC	Ocean Observations Panel for Climate
OSTIA	Operational Sea surface Temperature and sea Ice Analysis
SST	Sea Surface Temperature
TMI	TRMM Microwave Imager (TMI)
TRMM	Tropical Rainfall Measuring Mission
UNFCCC	United Nations Framework Convention on Climate Change
WCRP	World Climate Research Programme
WMO	World Meteorological Organisation

2. EXISTING SST REQUIREMENTS INFORMATION

2.1 Introduction

Before presenting the results of the SST CCI requirements gathering exercise, we first present requirements for SST data that have been gathered by other organisations and groups. These are provided as a comparison point for the reader for the requirements discussed in the rest of this document. Note that these requirements are not all exclusively for climate applications.

2.2 Climate Modelling User Group (CMUG) requirements

The climate modelling user group (CMUG) was established by ESA to provide links between the CCI projects that will generate data and climate modelling users. Part of their remit is to determine climate modellers' user requirements for each of the ECVs. The requirements they have determined for SST are shown in Table 1 (reproduced from Climate Modelling User Group Phase II Requirement Baseline Document, April 2015; RD.390).

This information updates and extends that available for previous URDs [RD.171 and RD.385]. In particular, needs for error covariance information are new and concur with our own analysis (see Section 4.2.2.24).

Also mentioned in the CMUG document are: the requirement for dynamical reanalysis to provide a 3-hourly update to the SST field as a boundary condition for the assimilation of the atmospheric and other oceanic variables; and a requirement to have reprocessed SST data within a month of real time to be able to put severe weather events into context for Government or media requests.

It is worth noting here that it would be impossible to demonstrate a stability of 0.01°C/decade anywhere on the globe with the current observing system.

	Horizontal resolution (km)	Temporal sampling	Precision (°C)	Accuracy (°C)	Stability (°C/ decade)	Uncertainty requirement (see caption)
Trend monitoring	10/1km	1 week	0.1	0.1	0.01	UNCERTL3
Seasonal forecasting	30	12 hours	0.1	0.1	0.05	ERRCOV
Decadal forecasting	30	1 month	0.1	0.1	0.1	ERRCOV
Climate quality analysis	30	12 hours	0.1	0.1	0.05	ERRCOV
Global Reanalysis	30	12 hours	0.1	0.1	0.01	ERRCOV
Regional Reanalysis	5	3 hours	0.1	0.1	0.01	ERRCOV
Climate Services	1	3 hours	0.1	0.1	0.01	UNCERTL3

Table 1. Requirements for SST gathered by the CMUG (reproduced from Climate Modelling User Group Phase II Requirement Baseline Document, April 2015). The accuracy and stability values assume global coverage for 100km spatial scales.

Uncertainty requirement is either for error covariance matrix for TCDR (ERRCOV) or L3 product merged accuracy (here referred to as UNCERTL3, rather than CMUG's original "ERRMERG").

2.3 Group for High Resolution Sea Surface Temperature (GHRSST) requirements

The Group for High-Resolution Sea Surface Temperature (GHRSST) provides SST data for operational oceanographic, meteorological, climate and other users. A set of requirements for SST data, principally in respect of use for numerical weather prediction, is provided on their webpage (https://www.ghrsst.org/science-and-applications/user-requirements/.). This is reproduced in Table 2. The "Accuracy" target here is thought to represent the SST standard uncertainty at the stated spatial scale, rather than bias.

	Horizontal resolution (km)	Delay (hours)		Accuracy (°C)
		Target	Threshold	
Coastal ocean	At least 1	3	6	<0.3
Open ocean	5-10	6	12	<0.4
Ultra-high resolution	2	3	6	<0.3

Table 2. User requirements for GHRSST data, reproduced from https://www.ghrsst.org/science-and-applications/user-requirements/. The target column contains the optimal requirements; threshold contains the limiting requirement beyond which the data are no longer useful.

2.4 Global Climate Observing System (GCOS) requirements for satellite-based data products for climate – 2011 update

The Global Climate Observing System (GCOS) have published a set of observation requirements for satellite-based data products for climate [RD.391]. The requirements listed in the 2011 update of the document are reproduced in Table 3 (note these are target requirements). The description of the meaning of the "Accuracy" target is similar to that of standard uncertainty.

Horizontal resolution	Temporal resolution	Accuracy	Stability
10 km	Daily	0.1 K over 100 km scales	Less than 0.03 K over 100 km scales

Table 3. GCOS target SST requirements, reproduced from [RD.391]

2.5 World Meteorological Organisation (WMO) requirements

The World Meteorological Organisation (WMO) maintains a list of user requirements, gathered by people and organisations such as the Global Climate Observing System (GCOS), the World Climate Research Programme (WCRP) and the Joint Technical Commission for Oceanography and Marine Meteorology (JCOMM). The requirements for SST are shown in Table 4.

These requirements are updated in some cases from those presented in previous URDs [RD.171 and RD.385].

Source	Application	Uncertainty (K)			Horizontal res. (km)			Observing cycle (h)			Timeliness (h unless otherwise stated)		
		Goal	B/T	T/H	Goal	B/T	T/H	Goal	B/T	T/H	Goal	B/T	T/H
AOPC	Climate-AOPC	0.25	0.4	1	10	50	500	3	6	24	3	6	12
WCRP	CLIVAR	0.1	0.2	0.3	10	20	50	3	4	6	24	36	3 d
WCRP	Climate modelling research	0.5	1	2	50	100	250	1	3	12	30d	45d	60d
J Eyre	Global NWP	0.3	0.5	1	5	15	250	3	24	120	3	24	5 d
JF Mahfouf	High res. NWP	0.3	0.5	1	1	5	20	1	2	6	0.5	1	6
P Ambrosetti	Nowcasting / Very short range forecasting	0.5	0.8	2	5	10	50	3	6	24	3	6	24
JCOMM	Ocean applications	0.1	0.5	1	10	25	100	1	3	24	5m	1	6
JCOMM	Ocean applications	0.1	0.5	1	1	10	25	1	3	24	5m	1	6
JCOMM	Ocean applications	0.1	0.2	0.5	10	50	100	1	3	24	12	24	3 d
JCOMM	Ocean applications	0.1	0.2	0.5	5	10	25	6	24	72	1	2	3
JCOMM	Ocean applications	0.1	0.5	1	0.5	1	10	0.5	1	3	0.5	1	6
JCOMM	Ocean applications	0.1	0.2	0.5	1	5	10	3	12	24	1	2	3
OOPC	Climate-OOPC	0.1	0.126	0.2	1	8	500	1	3	24	3	5	12
L Ferranti	Seasonal and inter-annual forecasts	0.1	0.2	0.5	50	85.5	250	3	6	12	3	6	24
WCRP	CLIC	0.5	0.8	2	25	39.7	100	24	30	48	30 d	38 d	60 d

Table 4. Requirements on horizontal resolution, observing cycle, timeliness and uncertainty of SST data for different user categories, as documented in the WMO Observing Systems Capability Analysis and Review (OSCAR) Tool http://www.wmo-sat.info/oscar/variables/view/134). T/H: the "threshold" is the minimum requirement to be met to ensure that data are useful. Goal: the "goal" is an ideal requirement above which further improvements are not necessary. B/T: the "breakthrough" is an intermediate level between "threshold" and "goal" which, if achieved, would result in a significant improvement for the targeted application.

3. REQUIREMENTS FROM REFERENCE DOCUMENTS

3.1 Introduction

A variety of documents hass been published by organisations such as GCOS that discuss the generation and provision of climate data. Although the SST CCI project is not concerned with making measurements, many of the principles described in these documents do apply. Similarly, there have been many projects in the past that aimed to generate data for climate applications. Some of the lessons learned in those projects can be translated into user requirements that are relevant to the SST CCI project. Part of the user requirements gathering exercise was to obtain and read these documents and extract requirements. These are detailed in the following sections.

3.2 Requirements from documents about generation and provision of climate data

Documents that are relevant to the generation of climate data records and to the SST CCI project were identified and requirements were extracted from them. In some cases, for example where the documents referred specifically to observations, the requirements were rephrased or adapted to apply to the CCI products. The requirements are listed below; each has three columns of information associated with them. In the first column a unique identifier for each requirement is specified. The requirement itself is in the second column. In the third column are any additional comments and references to the documents that informed the requirements (in square brackets). This format is used throughout this document.

SST_CCI-UR-REF-1	There is a continuing need for a timely flow of climate quality data to climate monitoring and analysis centres.	See SST_CCI-UR-QUS-43 for a definition of timely; the continuing need for data can be addressed by ensuring that the data record is extendable in the future when new instrumentation is available. [RD.159, RD.163, RD.164]
SST_CCI-UR-REF-2	Global coverage is required.	See also SST_CCI-UR-QUS-41. [RD.163, RD.164]
SST_CCI-UR-REF-3	Products are required that cover at least 30 years.	For example to aid study of climate change and variability. [RD.159]
SST_CCI-UR-REF-4	Uncertainties need to be characterised comprehensively.	This should include the full error budget of the translation from the input data to the products and the error covariance structure. [RD.152, RD.164, RD.390]
SST_CCI-UR-REF-5	Uncertainties need to be in the products.	[RD.165]

SST_CCI-UR-REF-6	Indicators of confidence in uncertainty estimates are required.	[RD.165]
SST_CCI-UR-REF-7	Uncertainty characteristics should be verified by comparison against independent observations.	[RD.152]
SST_CCI-UR-REF-8	Transition of the climate data record system from research to sustained routine production needs to be promoted.	[RD.151, RD.156]
SST_CCI-UR-REF-9	Feedback is required to producers of L0/L1 data used by the project to inform them of any issues that have been discovered with their data.	[RD.152, RD.156]
SST_CCI-UR-REF-10	The requirements of users with access to the least developed computing infrastructures need to be addressed.	[RD.159]
SST_CCI-UR-REF-11	All steps taken during production should be published.	Including algorithm selection and statements about accuracy, resolution and homogeneity. [RD.163]
SST_CCI-UR-REF-12	Data need to be easily accessible.	[RD.159]
SST_CCI-UR-REF-13	Data need to be free.	[RD.159]
SST_CCI-UR-REF-14	Data need to be unrestricted in their availability.	[RD.159]
SST_CCI-UR-REF-15	Standards should be followed for data storage and information sharing.	For example, in order to reduce operating costs. [RD.151]
SST_CCI-UR-REF-16	Standards and procedures for storage of metadata should be utilised.	[RD.159]
SST_CCI-UR-REF-17	Full information about input data and any processing applied needs to be archived.	To allow future reprocessing. [RD.152]
SST_CCI-UR-REF-18	There is a requirement to publish information about data and algorithm maturity.	For example which parts have undergone peer-review. [RD.163]

SST_CCI-UR-REF-19	A statement saying point by point which GCOS guidelines, applicable to product development, have been followed should be published.	[RD.163]
SST_CCI-UR-REF-20	Access to data, products and documentation needs to be provided.	[RD.163]
SST_CCI-UR-REF-21	Version control of code, documentation and data should be maintained.	[RD.163]
SST_CCI-UR-REF-22	Appropriate user groups need to be consulted systematically.	To establish requirements and to inspire global participation in use of data. [RD.151]
SST_CCI-UR-REF-23	A mechanism for feedback from users needs to be provided.	[RD.163]

3.3 Requirements from lessons learned from other projects

Lessons learned documents were sought from other projects that aimed to produce climate data records, during the writing of RD.171,. If these did not exist, projects were asked to comment on aspects of the project that worked, did not work, and what they would have done differently. Four replies were received at that time. Requirements that were identified from these replies are listed below.

SST_CCI-UR-LLP-24	It is beneficial to users to reduce as much as possible any barriers to obtaining and using data.	
SST_CCI-UR-LLP-25	Requests from users for support need to be dealt with quickly and thoroughly.	
SST_CCI-UR-LLP-26	It is important to foster good communication between the project, users and other interested parties.	
SST_CCI-UR-LLP-27	Users need to be kept informed of developments.	By providing information via email alerts, on the project website and by publishing results throughout the lifetime of the project.
SST_CCI-UR-LLP-28	The project should be made to feel open and inclusive to users and other scientists.	By making meeting reports, presentations and minutes available.

SST_CCI-UR-LLP-29	Users should have easy access to information, documents, products and contacts through a high quality website.

4. QUESTIONNAIRE

4.1 Introduction

Current and future users of SST data were invited to enter their requirements into an online questionnaire. The questions that were asked in the questionnaire are included as Annex A. Invites were sent to more than 1000 email addresses. Two methodologies were applied to generate this list of email addresses:

First, lists of peer-reviewed publications that cite published references for various SST datasets were downloaded from Web of Science (http://apps.isiknowledge.com). The datasets used are given below:

- Hadley Centre Sea Ice and Sea Surface Temperature (HadISST; Rayner et al, 2003; RD.74);
- National Oceanographic and Atmospheric Administration (NOAA) Daily Optimal Interpolation (OI) (Reynolds et al, 2007; RD.76);
- Advanced Very High Resolution Radiometer (AVHRR) Pathfinder v5 (Kilpatrick et al, 2001; RD.205);
- Tropical Rainfall Measuring Mission (TRMM) Microwave Imager (TMI, Wentz et al., 2000; RD.394);
- ATSR Reanalysis for Climate (Merchant et al., 2008; RD.187)

Email addresses and names were mined from the data.

Responses were received from 132 scientists from around the world. The results and user requirements presented here are based on these responses.

The number of responses, divided by continent, is shown in Figure 1. The location of responses is further broken down to the country level in Figure 2. This plot demonstrates that the most responses were received from the UK and USA, but that a good geographical spread was achieved.

The questionnaire asked users for their requirements for SST data five years from now.

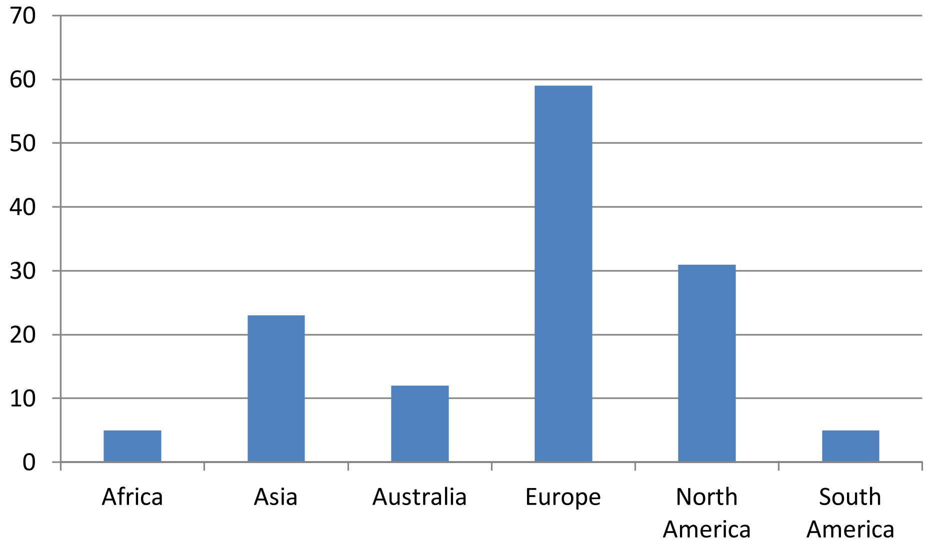


Figure 1. Number of respondents to the survey by continent.

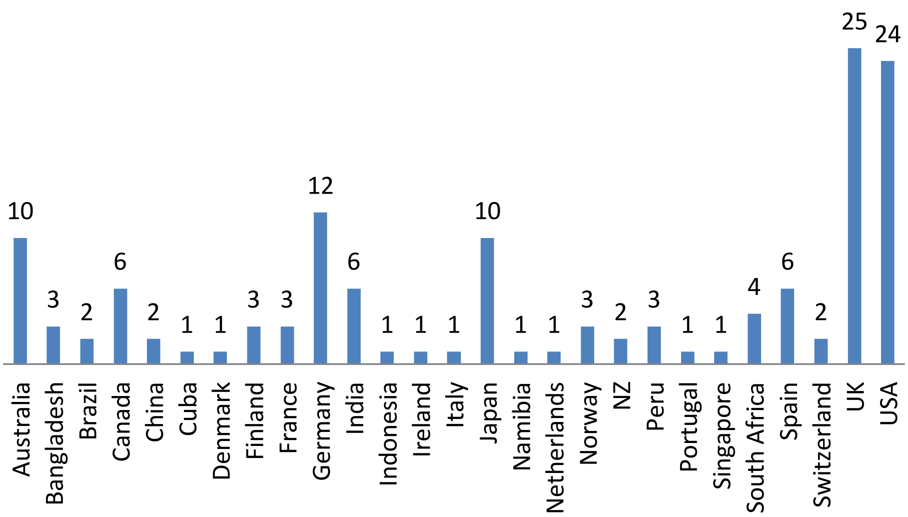


Figure 2. Number of respondents to the survey by country.

Respondents were asked to classify the application for which they currently use SST data (Figure 3). The 'Other' category includes: marine ecology; coupled data assimilation; atmospheric model forcing; climate feedbacks; air quality modelling; comparison to other SST data; interpretation and analysis of hydrographic data; fisheries; process studies; atmospheric chemistry; agricultural research; weather prediction; climate impact model evaluation; ocean heat content assessment; and calibration of proxy data.

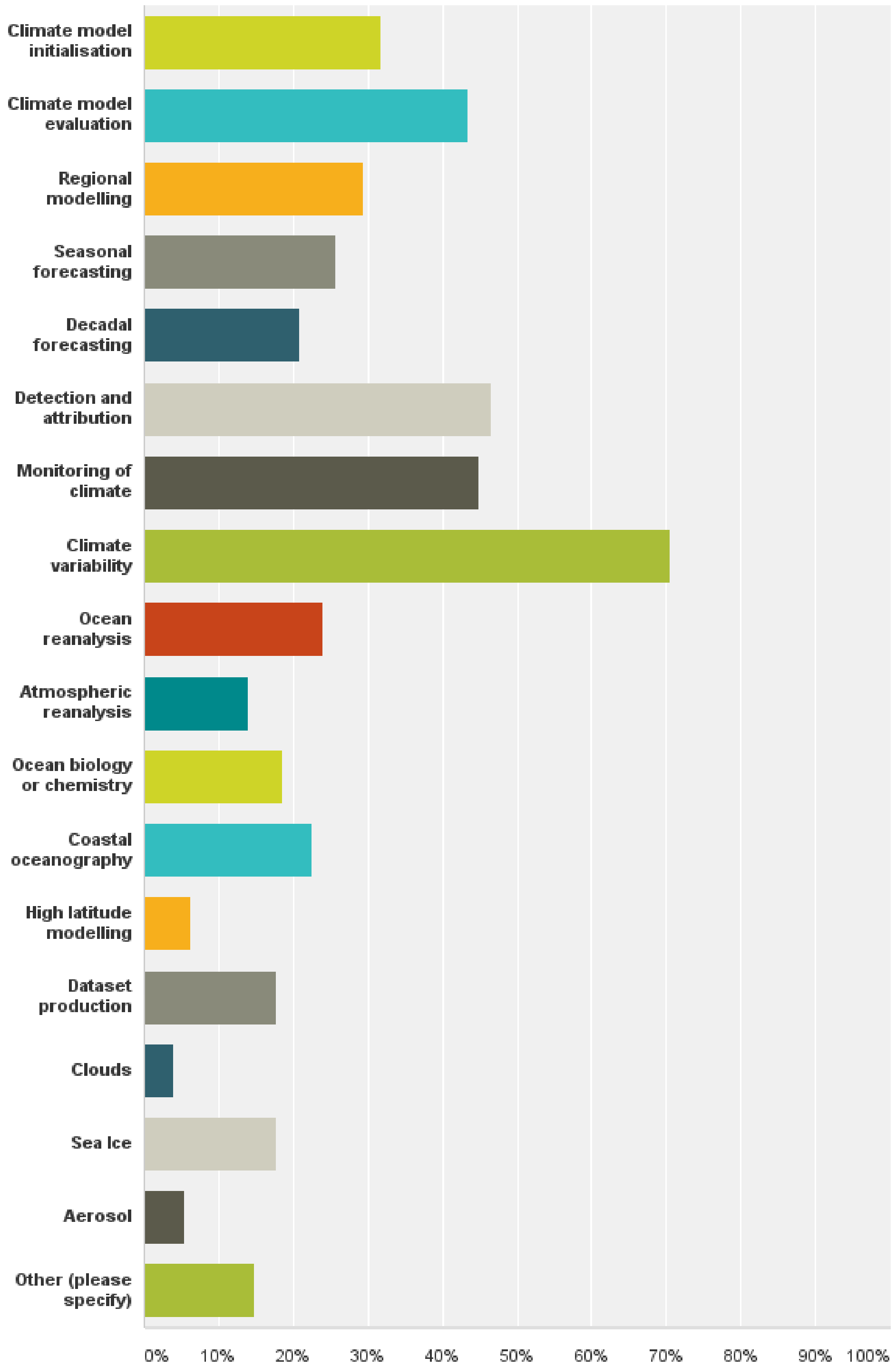


Figure 3. Distribution of responses in each application category in terms of the total numbers of respondents. Respondents were able to select more than one category.

4.2 Results of requirements gathering for future use of SST data

4.2.1 Introduction

Respondents were asked to think ahead up to 5 years in the future about their requirements for SST data in their particular applications. These may be applications that are currently only being planned and so some level of speculation is involved in the responses. For many of the questions, respondents were asked for three levels of requirement. These were aimed at understanding the range of performance levels that would be useful to the users. The levels were:

Threshold: the limit at which the observation becomes ineffectual and is no use for the application.

Breakthrough: the level at which a significant improvement in this application would be achieved.

Objective: the maximum performance limit for the observation, beyond which no significant improvement in the application would be achieved.

In the following, each question from the questionnaire is discussed in turn. Figures showing the responses are shown for each of the questions.

4.2.2 Responses to each question

4.2.2.1 Data level required

Respondents were asked whether their application required data on the original grid/swath of the instrument (level 2), gridded data (level 3) or analysed data (level 4). Results are shown in Figure 4. These show that level 4 data is the most commonly required, followed by level 3 and then level 2.

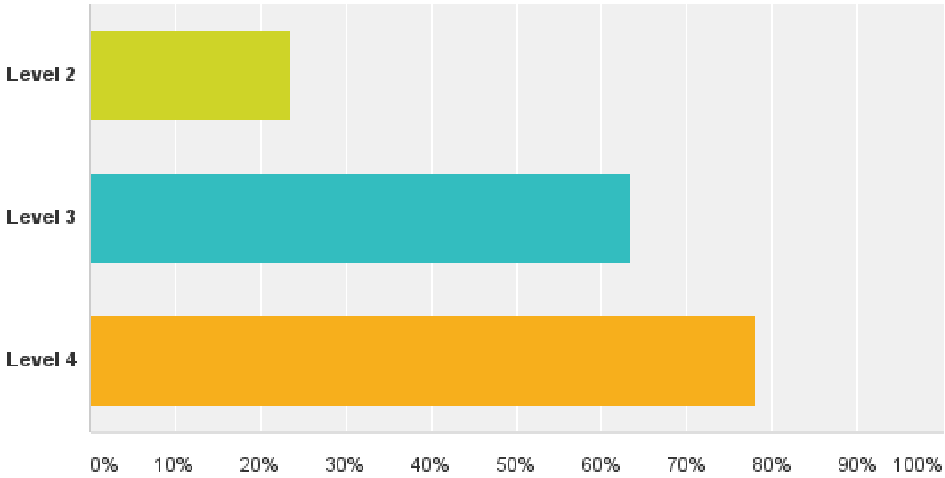


Figure 4. Data level required by the applications.

SST_CCI-UR-QUS-30	The most common requirement is for level 4 data (78%), with level 3 (63%) also required by the majority of respondents. Some also require level 2 data (24%).

4.2.2.2 Definition of grid

If respondents chose either level 3 or level 4 data in the previous question they were also asked about the grid they would like the data on.

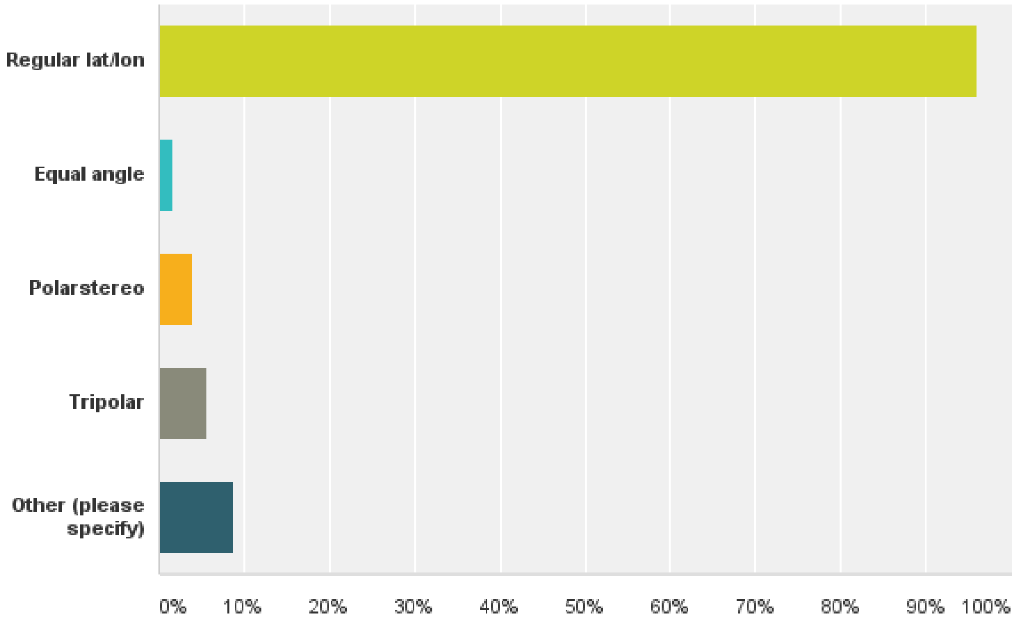


Figure 5. Grid to use for Level 3 or Level 4 data.

As shown in Figure 5, there was a strong preference shown for a regular latitude-longitude grid. A few users favoured alternatives such as a tripolar grid, or equal area.

SST_CCI-UR-QUS-31	Respondents have a clear preference that level 3 and level 4 data should be provided on a regular latitude-longitude grid.

4.2.2.3 Use of anomalies

In order to determine whether or not the SST CCI project should provide users with an anomaly product, i.e. deviations from a long-term average in each location, users were asked whether or not this was of relevance to their application. In 60% of cases, this was.

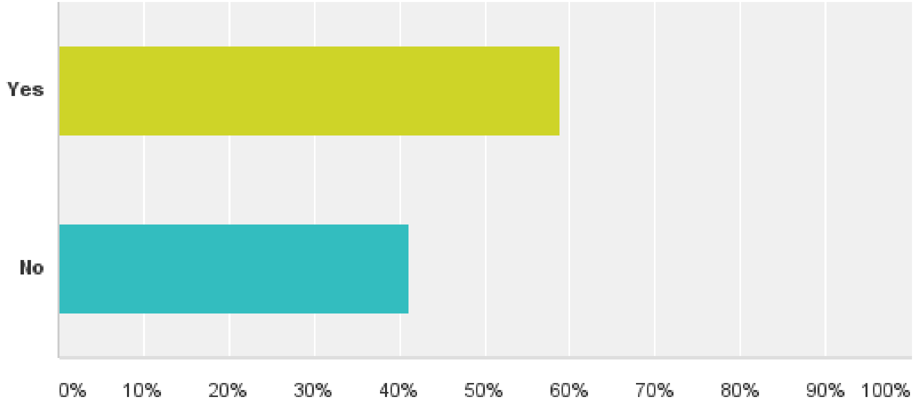


Figure 6. Does your application require the provision of anomalies?

SST_CCI-UR-QUS-32	An anomaly product should be provided to allow users to assess deviations from the long term average.

4.2.2.4 Land/sea mask

Users were asked whether they had a preference for continuity with operational updates (to the Met Office OSTIA product) or accuracy in the land/sea mask used for the level 4 analysis.

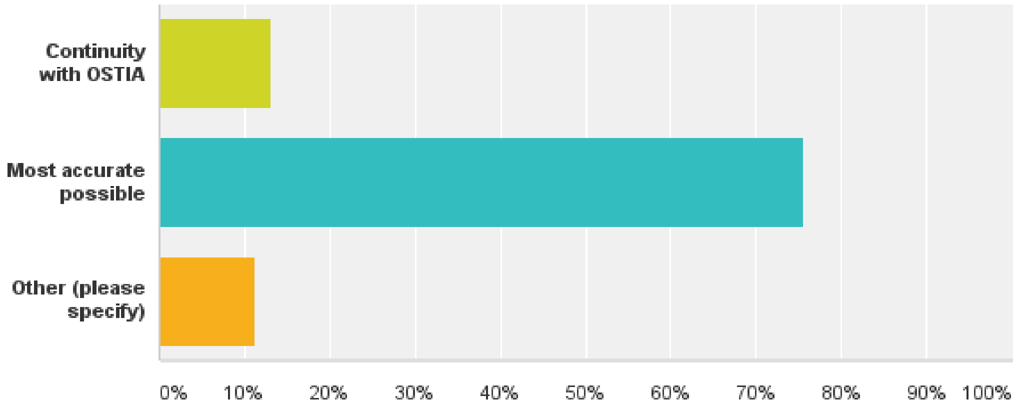


Figure 7. If you would use the L4 analysis product, what is the most important feature to your application of the land/sea mask used?

There was a clear preference for accuracy, but some users require continuity with the operational OSTIA product. Respondents were asked to explain their answers to this question.

For applications that value consistency, this was chosen because:

- For time series analysis it is crucial to have consistent data in time;

- Continuity would make life easier, but improvements in representation of any aspects would be good too;
- Our atmospheric applications rely on OSTIA SST, hence continuity with respect to that would be very helpful.

For those who primarily value accuracy, their reasons were:

- One respondent uses SST to pinpoint the discharge of groundwater into coasts and lakes; the more accurate this is, the better this data can guide more costly field campaigns;
- A focus on coastal, offshore areas, or shallow, near-shore systems requires an accurate land/sea mask;
- It would be state-of-the-art;
- Coarse land masks cause problems in doing coastal biology work;
- Coastal regions require correct specification and weighting;
- Wanting the most realistic representation of land/sea mask;
- Merging SST and (land) surface air temperature requires accurate land/sea masks;
- Use of near-shore *in situ* underwater temperature recorders requires accurate location;
- My work with SST data hinges directly around the SST products accuracy in knowing which pixels are land (coastline) and which are ocean. I want to be able to compare appropriately close ocean pixels to my coastal time series that are not affected by land bleed etc.;
- Operational OSTIA land/sea mask is not the best;
- We are interested in very coastal processes, and the geomorphological properties of the coast become important determinants of coastal thermal seawater properties;
- For performing simulations on a very fine resolution it is important to have the land/sea mask close to perfect;
- Working in a region with many islands, and strong contrasts on both sides of the islands; need to understand local variability and coastal currents;
- When adapting the land-sea mask to that of our model, the most accurate native land-sea mask is the best;
- Land sea masks vary significantly among different data products and the most accurate representation is preferable;
- Accuracy is of the utmost importance to my work;
- Regional Climate Models are set with different, high horizontal resolution. An SST dataset with the most accurate land/sea mask will surely improve the representation of SSTs along the coasts.

Other points raised were:

- I find it easier to use whatever is the coarsest land mask when analyzing between data sets. The finer resolution the land mask, the less of limiting factor this is with this data set;
- Ensure comparability with other products from different institutions;
- We need to see the land without masks to allow us to evaluate fog, low level clouds, smoke and other atmospheric interference;
- I am only interested in ocean areas for which a reasonable estimate of SST can be made. Estuaries, lagoons, rivers and lakes are of less interest if they are not well represented in the data set.

SST_CCI-UR-QUS-33	The most accurate land/sea mask possible should be used for the level 4 analysis to facilitate use in various application areas. However, this should also be consistent with data sets used to update the CDR to enable trend analysis.

4.2.2.5 Combining data

Respondents were asked for their opinion about whether it was acceptable to combine data from multiple similar instruments (for example the ATSR series) or from many different sensor types (such as ATSR and AVHRR together). Results are in Figure 8.

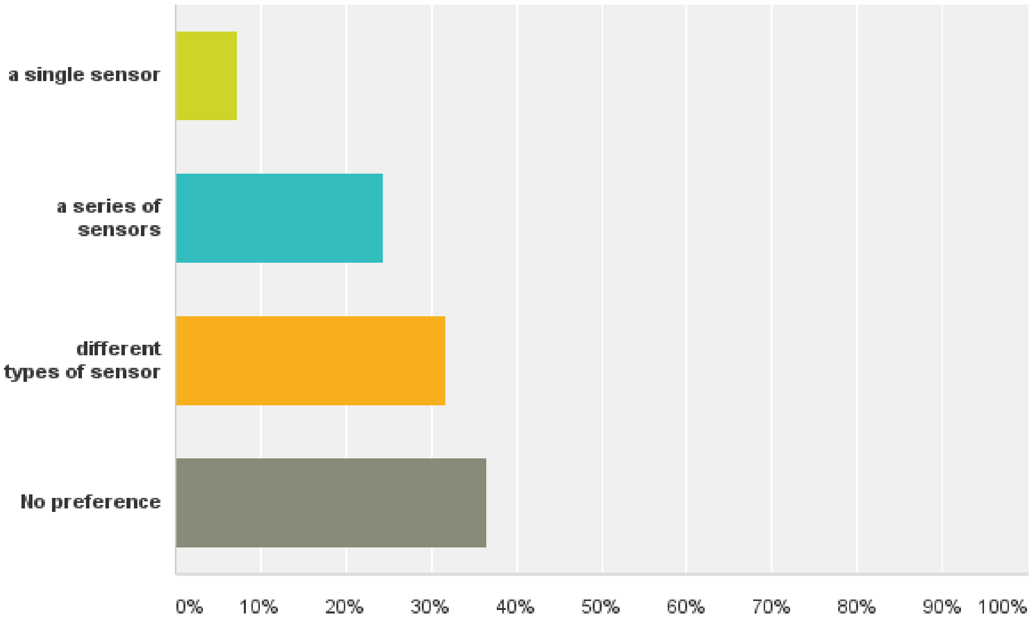


Figure 8. Is it acceptable to combine together different data for this application? Preference for number of sensors used.

The most common response to this question was 'no preference', with about a third of respondents electing this option. Of those expressing an opinion there were similar numbers for the two options for combining data. The relatively few responses asking for no combination of data were in the data set production, coupled data assimilation, climate variability, and atmospheric reanalysis categories. However there were also other responses in these categories for the other options.

SST_CCI-UR-QUS-34	The needs of different users can be met by making available single-sensor records, sensor-series datasets, and multiple-sensor analyses.

4.2.2.6 Spatial resolution

Respondents were asked what spatial resolution they require for their applications. They were asked to specify these in terms of breakthrough, threshold and objective requirements. The results are shown in Figure 9.

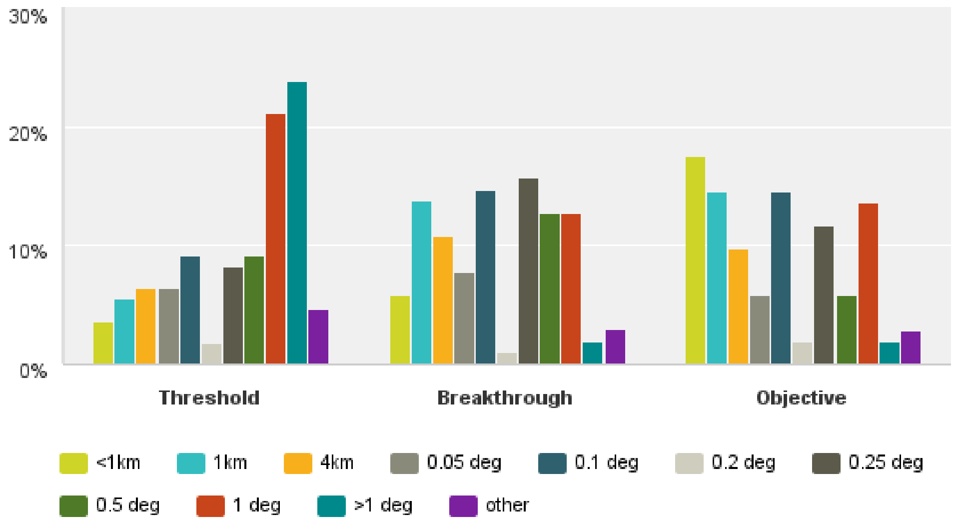


Figure 9. The spatial resolution required.

Even at the threshold level of requirements, respondents chose the full range of options presented to them. Particularly high resolution is required in the ocean biology or chemistry, and coastal oceanography categories, or for use in comparison with *in situ* measurements. Responses in other categories were quite mixed.

At the breakthrough requirement level, the distribution of responses was quite broad. 1km, 0.1 and 0.25 all received a high number of responses. Again, responses within categories were generally mixed.

At the objective requirement level there were peaks to the distribution of responses at <1 km, 1km and 0.1° resolution. However, responses were received across the whole range of options, and there was still a broad range of responses in many of the application categories.

SST_CCI-UR-QUS-35	Overall, the requirements for spatial resolution are mixed, but consistent with those articulated in RD.171.	Requirement from first survey will be used.

4.2.2.7 Local or universal time

Respondents were asked if they prefer data where all SSTs are at the same local time (such as provided by a polar orbiting satellite) or at the same universal time (as from a geostationary satellite). Results are in Figure 10.

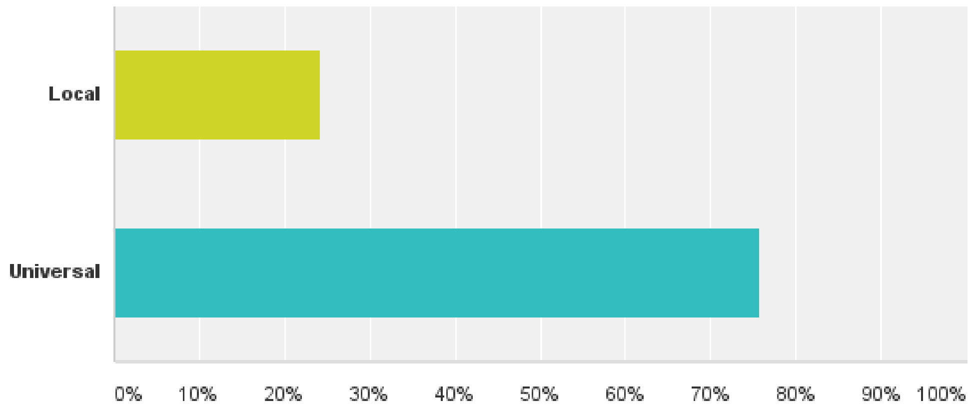


Figure 10. SSTs to be at the same local or universal time?

The preferred option was for SSTs at the same universal time, although there were also a significant number of responses for the alternative.

SST_CCI-UR-QUS-36	SST data corresponding to the same universal time is preferred to SSTs at the same local time by the majority of potential users of the SST CCI products.

4.2.2.8 Data frequency

Respondents were asked how frequently they required SST data at a location; results are shown in Figure 11.

The threshold requirement responses peak at monthly data, with a second peak at daily.

At the breakthrough level, the peak in response is at daily frequency. At the objective level it is also at daily, although the distribution now also has a peak at 3 hourly frequency.

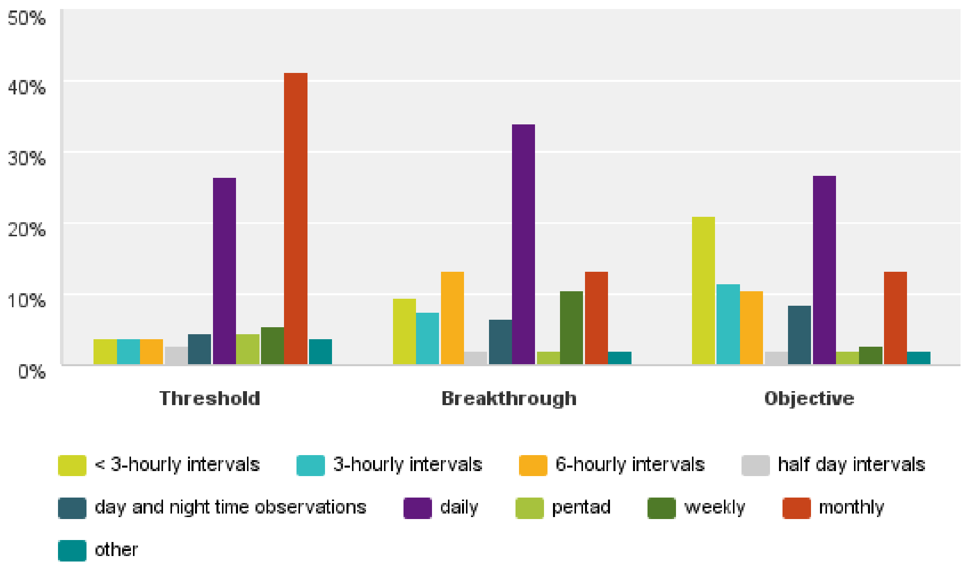


Figure 11. Requirements for frequency of SSTs at a location.

SST_CCI-UR-QUS-37	The most common requirements for data frequency at a location are monthly and daily (threshold), daily (breakthrough and objective), with 3 hourly or more frequent also yielding many responses (at objective).	There were also significant numbers of users who had more stringent requirements. For example almost a third of respondents selected 6 hourly or more frequent at the breakthrough requirement level.

4.2.2.9 Representation of diurnal variability

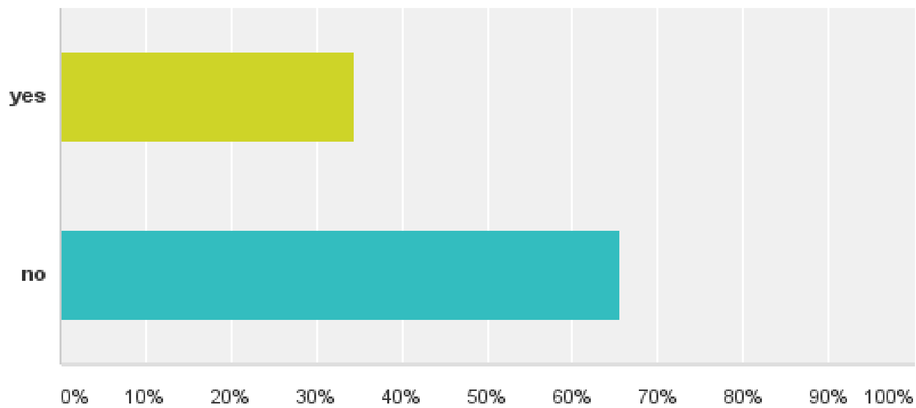


Figure 12. Does your application require information about the diurnal variability of SST?

The majority of respondents do not require information about the diurnal variability of SST for their application. However, a significant minority do. They were asked to explain further:

- Diurnal information on SST could inform on small scale physical forcing and could find application when studying diurnal variation of biological activities;
- It can be important for land/sea breeze formation;
- I would be interested in linking this variability to species patterns;
- Small scale and short time scale features, such as the diurnal cycle of SST and precipitation in the tropics, are important to understand since we believe we see too strong a link between both as compared to observations;
- To understand diurnal rainfall pattern;
- I am designing a ocean data assimilation system for a coupled GCM. With diurnal cycle included, I can match the timing of observational data with my model more accurately;
- To examine the diurnal cycle of convection over the oceans and its representation in models;
- To maximize the amount of data in the high latitudes;
- The effect of diurnal wind on local temperatures would be a beneficial investigation;
- Ecosystems may respond to brief extreme values in stressors, as well as lower-frequency trends. For this reason, having a reliable estimate of higher-frequency variability may be desirable. Shelf benthic ecosystems can ALSO be greatly impacted by the depth and temperature of the diurnal warm layer, vs. the surface. And diurnal variability over shallow water may differ significantly from that over deeper water nearby, particularly where wind- and wave-mixing are affected by adjacency to land;
- A large part of my work looks at comparing the differences in temperatures between *in situ* and SST data. Knowledge of diurnal variability allows me to use more of my *in situ* data for this comparison;
- Calculation of correlation coefficients is highly sensitive;
- The diurnal variability of turbulent heat fluxes is important in some places;
- SST diurnal heating is important as an indicator of rate of change. Also it better allows us to evaluate the imagery if 24 hour composites rather than night time and day time separate composites are made. Daytime is when we often see more aberrations in the data from the atmosphere or air-sea interface;
- Now that coupled models have coupling frequency less than daily, validation of the diurnal cycle magnitude (and its potential feedback on surface fluxes) is becoming of increasing interest;
- One of the main benefits from coupled data assimilation and coupled forecasting for NWP should come from improved modelling and analysis of the diurnal cycle of SST;
- Organism activity often varies diurnally e.g. organisms may migrate into the upper water column only at night or at dawn and dusk;
- The diurnal variability of SST might affect the atmospheric response, in particular, near coastal regions;
- The diurnal variability would allow us to assess the vertical extent of a thermal anomaly
- The atmospheric surface layer responds to these diurnal changes and it would be great to capture these effects;
- Diurnal variability constitutes a source of variability in SST data sets of all kinds. Characterising diurnal variability cleanly will (by reducing unexplained variance aka noise) help to diagnose biases and other systematic errors that affect the assessment of long term trends.

Other relevant information:

- Our scheme assumes that the SST is the foundation temperature and models daily variations via a skin-temperature scheme;
- Particularly for high-resolution NWP, it is becoming increasing important to follow diurnal variations in SST to improve weather forecasts. See WMO Statements of Guidance for more detail: http://www.wmo.int/pages/prog/www/OSY/GOS-RRR.html#SOG;
- One respondent interested in the Arctic wrote: when I'm interested there is either all day or all night.

SST_CCI-UR-QUS-38	It would be valuable for a number of different applications to provide information about the diurnal variability of SST

4.2.2.10 Temporal averaging

Respondents were asked the level of temporal averaging that would be acceptable to achieve the requirement in the previous question. The results are in Figure 13.

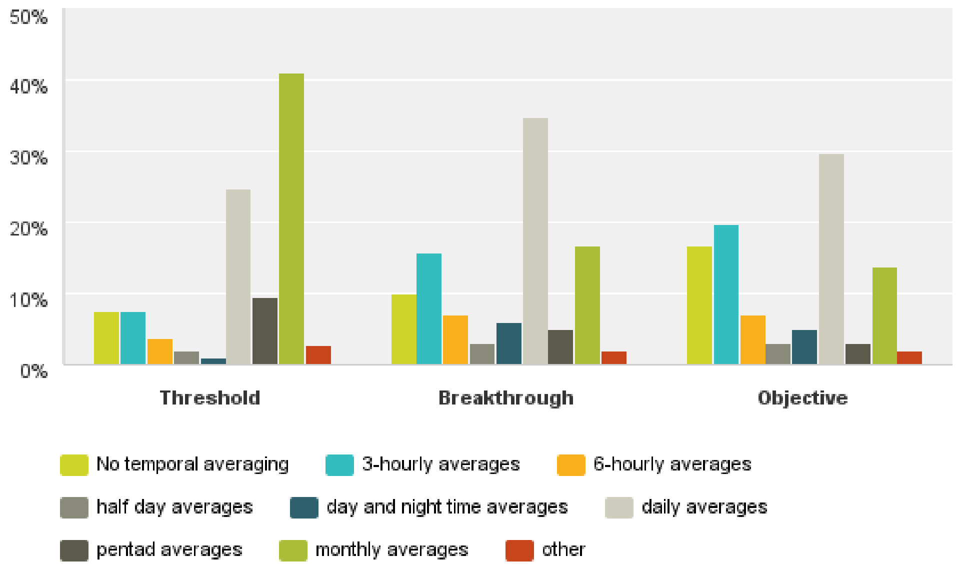


Figure 13. Requirements for temporal averaging of data.

Results closely mirror those of the question about data frequency. These results imply that the respondents are generally happy with temporal averaging, rather than requiring a snapshot of SSTs at a particular time. However, a significant minority (8%, 10%, and 17% at the threshold, breakthrough and objective levels respectively) of respondents chose the ‘no temporal averaging option’.

SST_CCI-UR-QUS-39	For the majority of respondents it is acceptable to use temporal averaging when building datasets.	However, it is not acceptable for a minority of respondents.

4.2.2.11 Data times

Respondents were asked for which times of the day they required SSTs.

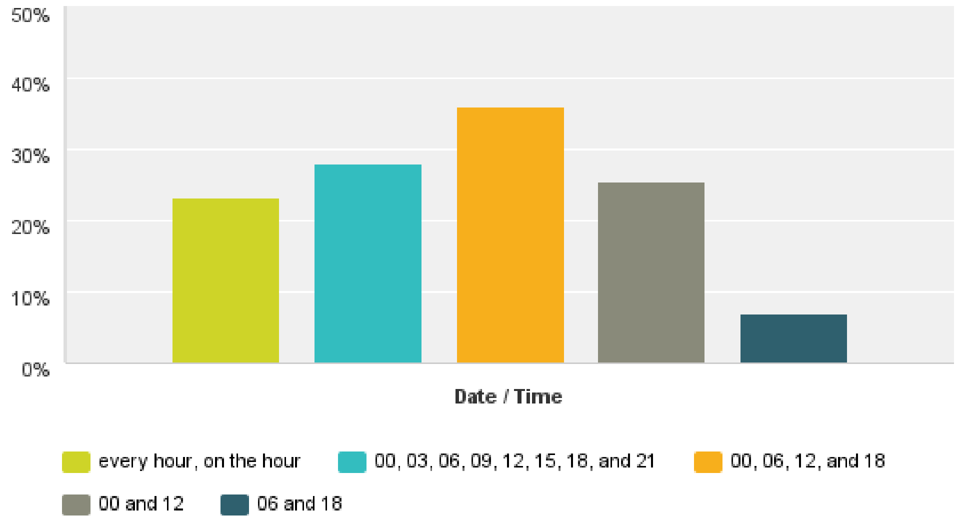


Figure 14. Times of the day when SSTs are required.

Overall, SST data is most required at midnight, 6 am, midday and 6 pm. “Other” responses included daily averages.

SST_CCI-UR-QUS-40	SSTs are most commonly required at midnight, 6 am, midday and 6pm. But a majority of respondents require observations more frequently, either every three hours or every hour.

4.2.2.12 Spatial coverage

This question asked about the coverage (global or regional) that is required.

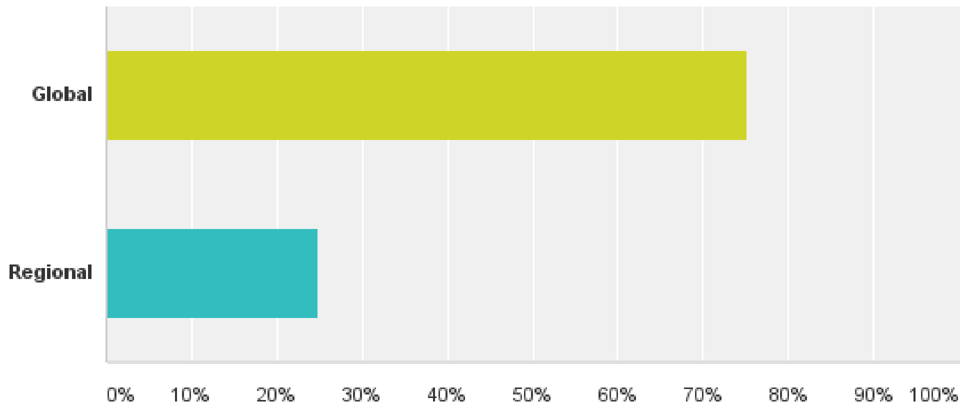


Figure 15. Spatial coverage required.

The majority of respondents require global coverage (Figure 15). However, some applications are regional. Individual regions specified by potential users covered a wide range of locations and spatial scales. These are listed below:

North Atlantic; Australia, including Northwest Australia, Western Australia, Coral Sea and Tasman Sea; Indian Ocean; Alaskan waters (Bering Sea, Gulf of Alaska, Chukchi Sea, Beaufort Sea); Indian Ocean; Indo-Pacific region; west of Scotland and around the UK; South Atlantic; Southern Ocean; southern Africa coastal region; insular and continental shelves in the tropics and sub-tropics (any location where reef-building corals are found); polar regions (Arctic and Antarctic); Arabian Gulf; tropical Pacific; and the Mediterranean.

SST_CCI-UR-QUS-41	Global coverage is required.	See also SST_CCI-UR-REF-2.

4.2.2.13 Temporal coverage

Users were asked what length of time series they require. Results are illustrated in Figure 16.

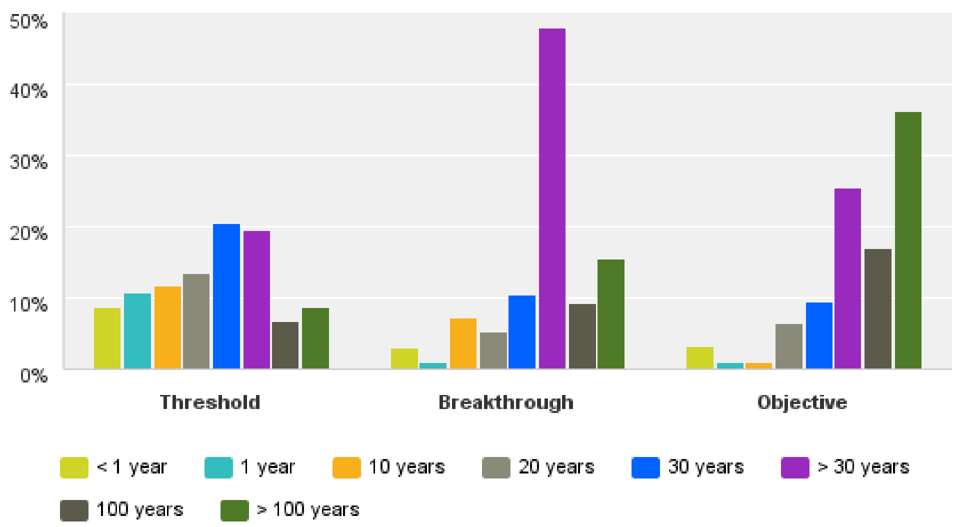


Figure 16. Requirements for temporal coverage.

Responses covered the full range of possible answers at threshold, breakthrough and objective levels of requirements. At the threshold level, the distribution of responses peaks at 30 years, although there is also a peak at >30 years. This is driven by applications such as the analysis of climate variability. At the breakthrough level, there is a clear indication that respondents want long >30 year data records, and this comes out even stronger in the objective requirements, where 100 years or more are needed. Clearly, satellite data are insufficient to achieve a record of 100 years or more and combination with historical *in situ* measurements is needed.

When asked why they needed long records, respondents replied:

- to analyse decadal variability;
- to get the historical climatology correct for a given reef system;
- I am interested in long-term climate variability and sometimes study phenomena with timescales of 50+ years. The more cycles we can capture the better;
- we are comparing SST trends to long-term time series of fish growth derived from otoliths. Some of our otolith datasets go back ~100 yrs;
- longer data sets give the ability to look a historical genetic/temperature changes;
- separation between global warming signal and other climate variability (e.g. PDO) needs more than 100 year records;
- trend detection;
- long-term consistent SST data sets are the most useful to climate variability studies, the longer the better. Less than 50 years is effectively useless for this purpose;
- I'm interested in climate extremes, and to define them it's good to have a long timeseries over which to average and to identify trends; and
- to distinguish trends from multidecadal variability.

SST_CCI-UR-QUS-42	The most common responses at the threshold requirement level are for temporal coverage of 30 or more years (40% of responses). At the breakthrough and objective requirements levels there is a clear requirement for data records longer than 30 years, with >100 years the most common requirement at objective level.

4.2.2.14 Interim climate data records

In this question, respondents were asked whether or not the concept of an interim climate data record (ICDR) was relevant to their application.

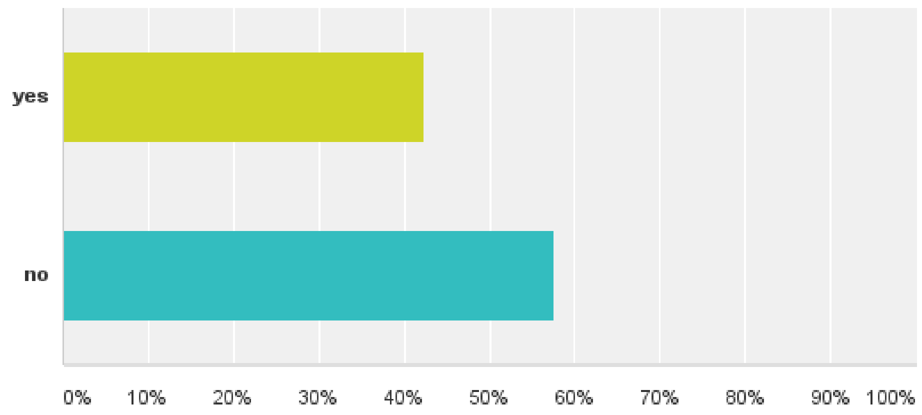


Figure 17. Is the concept of an interim climate data record important to your application?

For those who answered that an ICDR would be relevant to their application, they were also asked what delay between time of measurement and receipt would be acceptable. Answers ranged from less than a day to a year.

For respondents who require data within a day, reasons included:

- Assimilating real time L2 data on operational basis in our ocean models;
- Timeliness requirements are different for global and high-resolution NWP. We support the requirements for these two application areas as set out in WMO's OSCAR/Requirements database;
- Ideally the delay would be under one day so that an assessment of the day would be available the next day. For some products, which are produced monthly, a slightly longer delay - a few days - would be acceptable;
- A one day delay would be fine (for survey planning we need satellite pictures as soon as possible, to decide in real time where to sample during survey), but much more than that no.

For those who require data within a few days, their applications included:

- We would ideally like to be able to see for climate monitoring a one week (or one day) average up to yesterday inclusive, i.e. near-real time (e.g. like OSTIA), that can also be related to a long-term historical climatology (unlike OSTIA);
- 2 days would be acceptable (as there is substantial intra-seasonal variability), 1 day would be much better;
- 1-7 days for early detection of anomalies such as the marine heat wave;
- A week (for monitoring). It depends on the time scale of the data.

If over a week’s delay is acceptable, this is because:

- 10 day delay may be OK (for operational climate monitoring);
- Having the previous month's average available about 14 days after the month ends would be acceptable;
- 20 day delay acceptable to support operational attribution.

The majority of other respondents cited a month as an acceptable delay, but others still find a few months acceptable (e.g. for some event attribution studies). Production of time-bound international modelling intercomparison simulations (e.g. CMIP6 seasonal-to-decadal predictions) require data by certain specific times, rather than routinely updated.

SST_CCI-UR-QUS-43	ICDRs are relevant to many applications. Timeliness requirements of updates vary from within a day to a year later.	However, some users have much tighter requirements and need data as quickly as within half a day.

4.2.2.15 Depth that SSTs should correspond to

Users were queried about what depth the SST CCI products should correspond to. This question was motivated by the fact that there are a number of different definitions of SST. One of these is SSTfnd, which is defined as the SST free of diurnal variability i.e. the temperature at the first time of day when heat gained from solar absorption exceeds the surface heat loss.

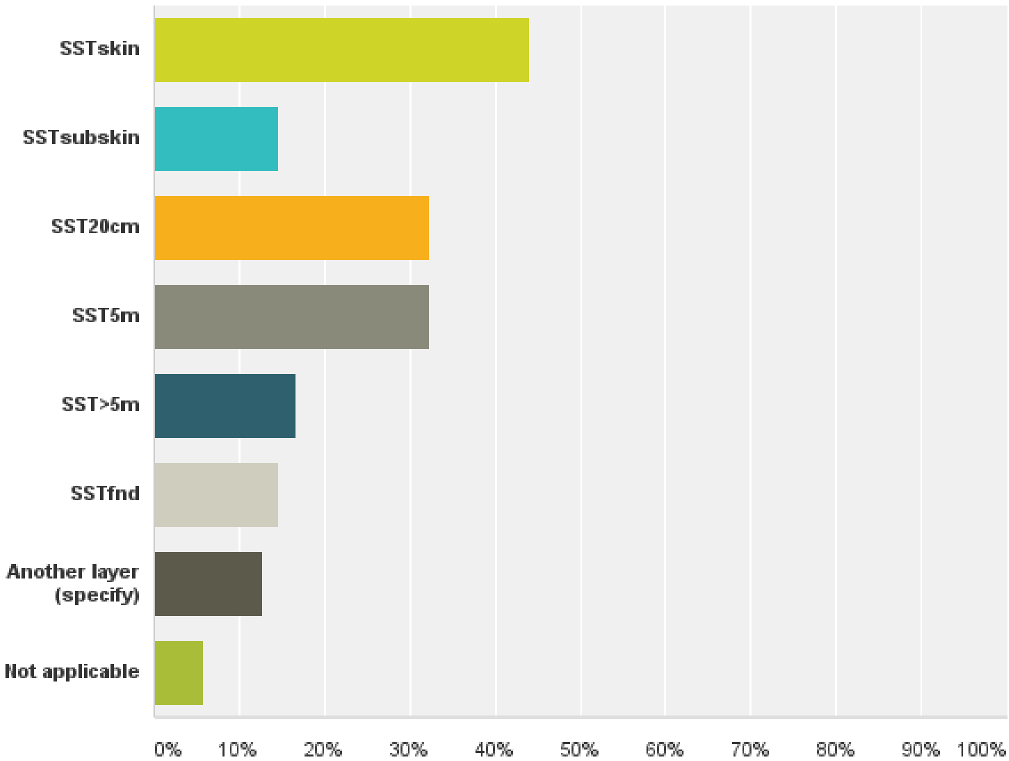


Figure 18. For your application, which type(s) of SST is (are) most relevant?

A range of responses were received, as shown in Figure 18. Overall, SSTskin, which is the depth sensed by infrared satellite instruments, had the most responses.

More detailed responses included:

- Top 1-2m would be much better than top 5m;

- We would like 'deeper' estimates of temperature because coral bleaching can occur 10s of meters deep; however, we also recognize that 1) the sensors can only see/model so deep, and 2) the upper 20 meters are normally well mixed in nearshore environments;
- Water temperatures at different depths are relevant for different species including bottom temperatures;
- Understanding the difference between the top ~20 cm and top ~10 m would be great;
- I'm investigating fish species spread throughout the water column, so the deeper the better;
- A 'top layer' would be that consistent with an upper ocean model level (1m thickness);
- Where necessary, we can apply cool-skin and warm-layer corrections to SST data using other products (from air-sea flux estimates, or from empirical wind and wave relationships). But we much prefer an "SST" product that reliably (more or less) does this for us. Ultimately, our "Objective" is to guess extremes in the sea temperature immediately above the shallow seafloor;
- Skin more likely useful for surface fluxes. 20cm more comparable to ocean model (top box thickness of ~1m);
- For diurnal SST analysis systems we'd like the skin SST;
- For some modelling applications we'd like SST at the top model layer, but this may change over time and from one system to another. The current models have a top box which is meant to represent an average over the top 1 metre;
- For some data assimilation applications, the assimilation is really only aiming to correct for errors in the foundation SST and will not attempt to correct for errors in the diurnal cycle and so foundation estimates may be more useful;
- Organisms probably more driven by deeper temperatures, but we recognise that subsurface data are more limited - in some cases one can estimate bottom temps using SST or from oceanographic models tuned with SST observations;
- Skin-depth difference models should be very well documented and transparent;
- Since I'm mostly comparing SSTs to the skin temperature of climate models, the first option is the most suitable;
- Provide whatever the satellite measures best, and leave it as a task for the SST analysis centre to deal with the problem of estimating SSTs at other depths;
- Ideally this would be comparable to the definition of SST in the climate model, but this may vary among climate models and it might generally not make much sense to adapt observational products to climate model setups;
- 1m layer for some applications;
- SSTskin is key for my applications but we are also working on the thermal structure of ship wakes which would benefit from knowing all the SST types;
- 5m would be optimal as it matches with the top ocean layer temperature relatively well.

SST_CCI-UR-QUS-44	SSTskin is the depth most commonly required by respondents, closely followed by SSTs at depths roughly corresponding to the range of traditional *in situ* observations (20 cm and 5 m).

4.2.2.16 Provision of simpler-to-use data

The SST CCI project will make L2 and L3C products available in a flexible format containing information enabling users to derive the SST and its uncertainty adjusted to different depths and times appropriate to their needs. We also propose to make available a standard product file which provides information in a simpler-to-use form. This standard file would contain SSTskin at the observation time, plus one other adjusted SST.

Respondents were asked whether or not they would you use such a simple standard file.

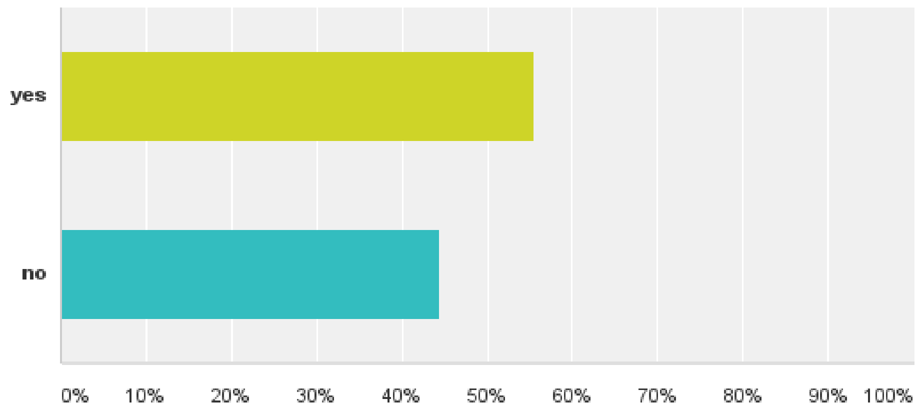


Figure 19. Would you use a simpler-to-use standard file with specific adjustments applied?

A small majority said yes. If yes, they were then asked which combination of adjustments is most relevant to their application.

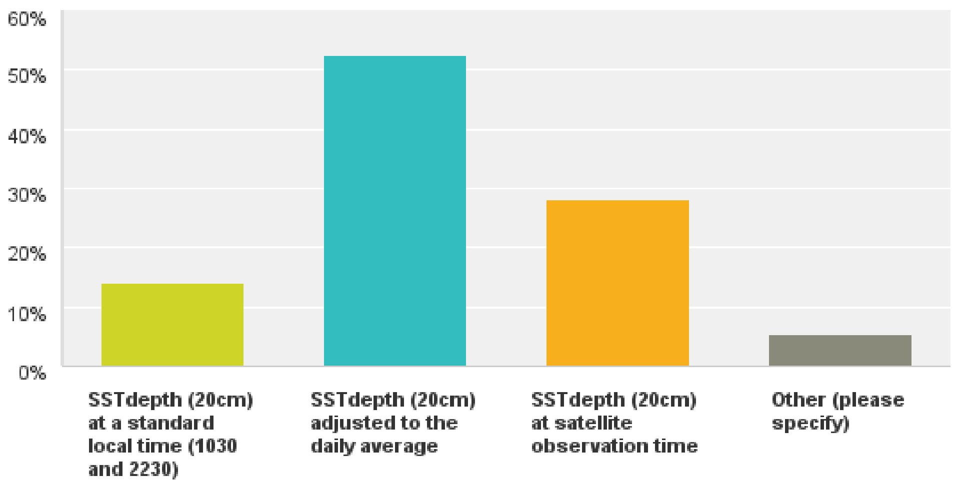


Figure 20. Preferred standard adjustments to be applied.

A clear preference for over half of respondents was a standard product file containing SST20cm, adjusted to the daily average. However, a significant minority required SST20cm at satellite observation time.

SST_CCI-UR-QUS-45	A standard product file of SST20cm adjusted to the daily average should be provided.

4.2.2.17 Information provided in locations partially covered by sea ice

Respondents were asked what should be reported in locations where there is sea ice partly or completely covering the ocean. Responses are shown in Figure 21.

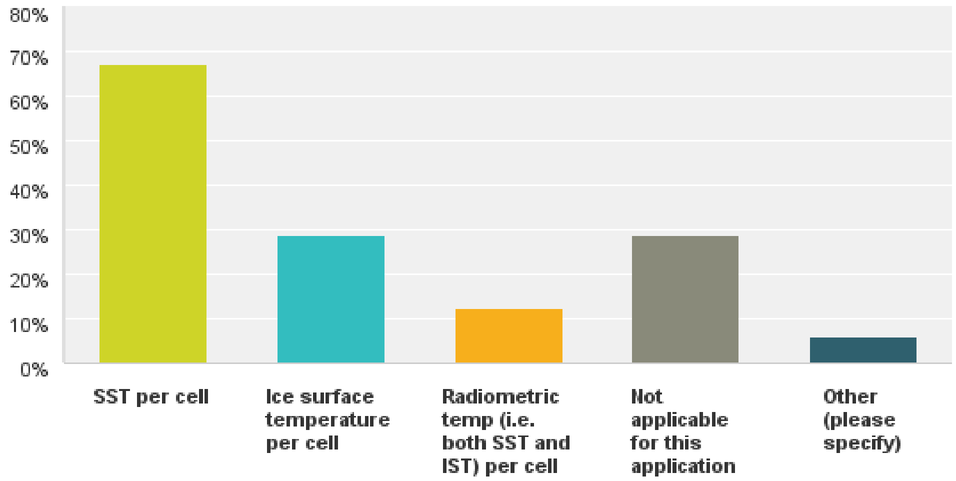


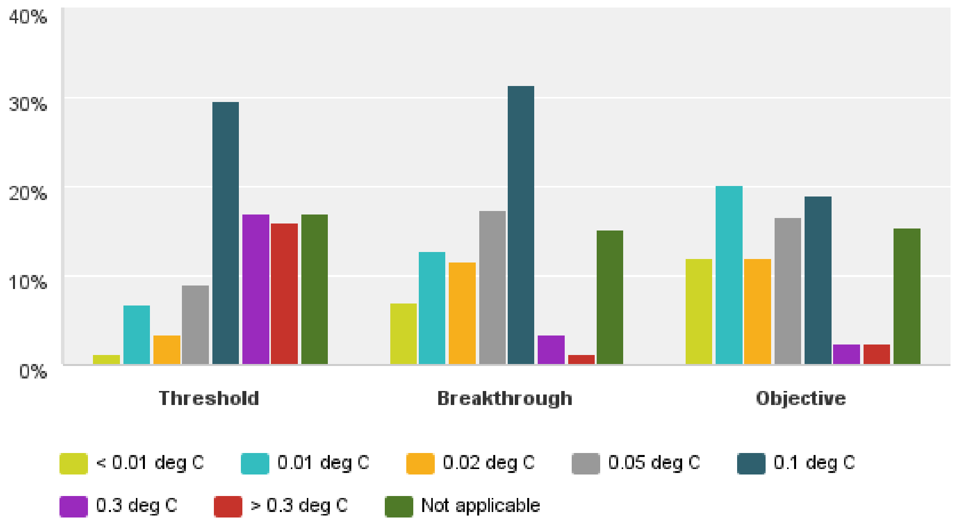
Figure 21. Responses to question about information provision in sea ice affected locations.

The most common response was SST, with a significant minority needing ice surface temperature. Suggestions under 'Other' were: percentage ice covered/ice concentration and a separate sea ice extension data set.

SST_CCI-UR-QUS-46	Reporting of SST is most commonly required for sea-ice affected areas.	However, 41% of respondents expressing a requirement favoured either ice surface or radiometric temperature.

4.2.2.18 Acceptable levels of bias

The respondents were asked for their requirements for the amount of bias in the data that would be acceptable. As well as selecting a value for the bias, they were also asked to specify the spatial scale for which the achievement of this level of performance should be demonstrated. Results are shown in Figure 22.



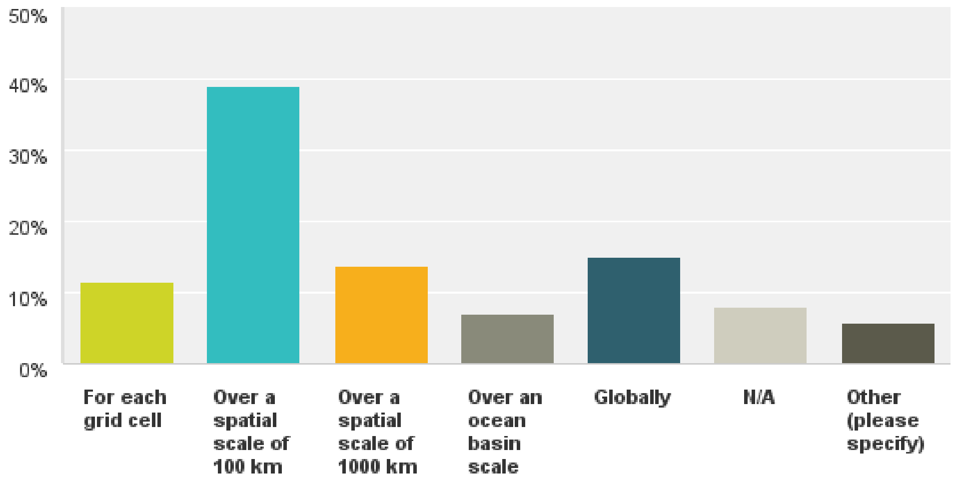


Figure 22. Requirements for amount of bias that is acceptable (top) and region over which this should be demonstrated (bottom).

At the threshold level, requirements for acceptable bias were largely 0.1°C or greater. At breakthrough level, the peak response was 0.1°C. At the objective level this was more evenly spread. The peak response for the spatial scale over which to demonstrate the achievement of this level of performance was 100 km. It is noted that availability of high quality *in situ* data will determine whether it is possible to demonstrate this at all times and locations.

SST_CCI-UR-QUS-47	The most common acceptable levels of bias were 0.1°C (threshold and breakthrough), and more evenly spread at values between 0.01 and 0.1°C (objective). The most common response was that the achievement of this should be demonstrated over a spatial scale of 100 km. Half of users would be satisfied by demonstration over a scale of 1000 km.

4.2.2.19 Required precision

Respondents were asked about the precision (the standard deviation of error due to random and pseudo-random effects that vary on sub-seasonal timescales) that is required for their application.

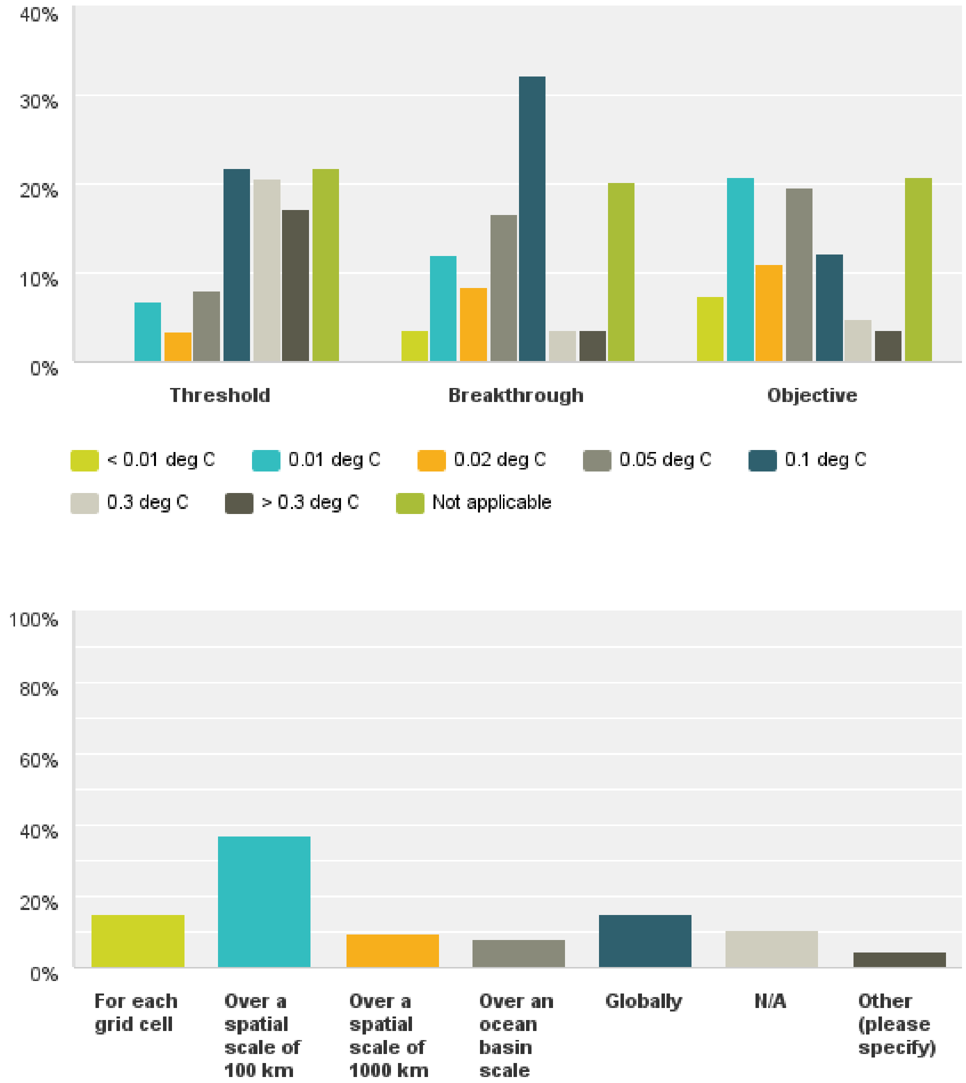


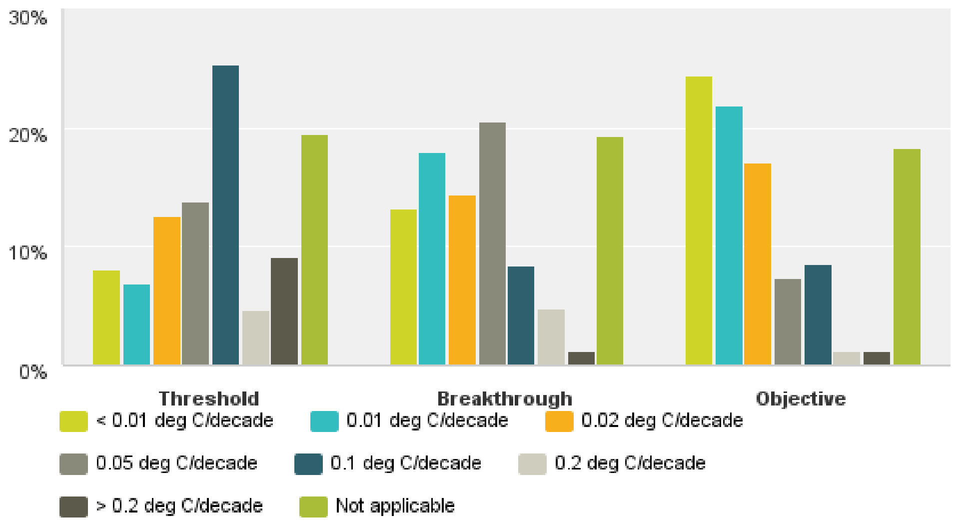
Figure 23. Requirements for precision.

The answers received (Figure 23) were very similar to those for bias and hence the conclusions are also similar.

SST_CCI-UR-QUS-48	The most common breakthrough response was that 0.1°C is the required precision and that the achievement of this should be demonstrated over a spatial scale of 100 km.

4.2.2.20 Acceptable levels of drift

This question asked for requirements for the acceptable amount of drift (change in bias over time) in the data. Results are in Figure 24.



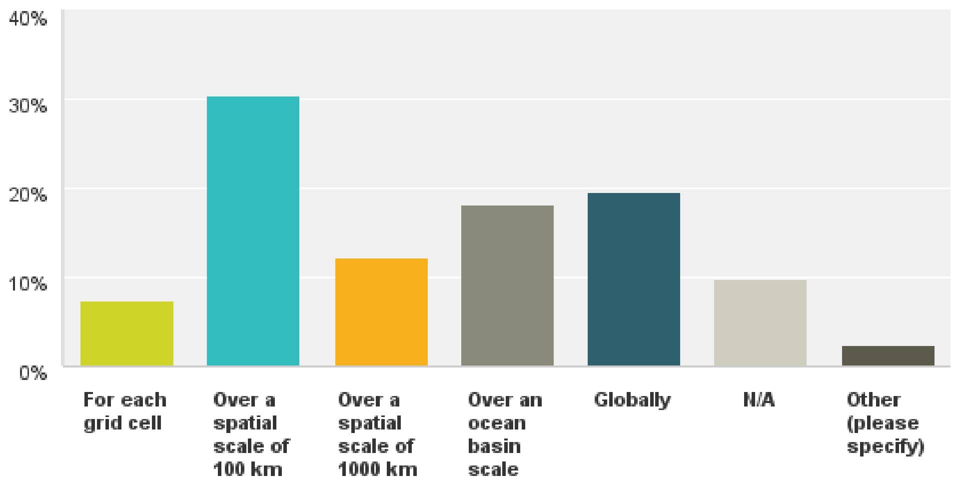


Figure 24. Requirements for the acceptable level of drift in the data.

Of those specifying a preference, at the threshold level the most common requirement was for a drift of no more than 0.1°C per decade. At breakthrough level this becomes

0.05°C per decade, with over half of users satisfied if this is achieved. At objective level, requirements become very challenging with a majority of users choosing a level in the range <0.01°C to 0.02°C per decade. Again, the most common response was that the achievement of this should be demonstrated over a spatial scale of 100 km, but as mentioned above, this level of stability is likely impossible to demonstrate with the current observing system. As with the requirements for bias and precision, the demonstration of this will depend on the availability of high quality *in situ* data.

SST_CCI-UR-QUS-49	At the threshold level, 0.1°C per decade was the most common response for the acceptable level of drift. At breakthrough level 0.05°C per decade was the most common response. At the objective requirement levels, most respondents state a requirement for stability of 0.02°C per decade or better. The most common response for the spatial scale that the achievement of this should be demonstrated over was 100 km.	However, a significant number of users have stricter requirements at both threshold and breakthrough levels.

4.2.2.21 Presentation of locally-correlated errors

This question enquired whether respondents' applications were sensitive to locally-correlated errors (e.g. errors that are correlated within synoptic scales and uncorrelated beyond).

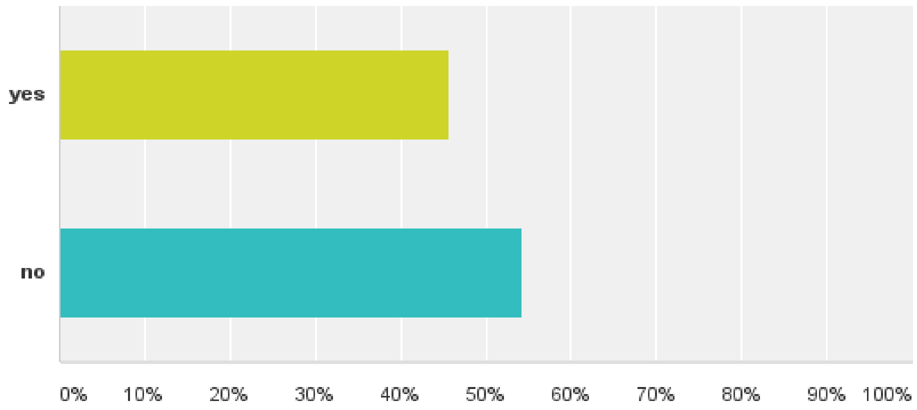


Figure 25. Result of question asking whether or not locally-correlated errors are an issue.

As shown in Figure 25, respondents were fairly evenly split as to whether or not this for an issue for them.

4.2.2.22 Acceptable change in bias between day and night SSTs

Respondents could optionally provide requirements for an acceptable change in relative bias between day and night SSTs. Figure 26 shows the results from those who entered requirements.

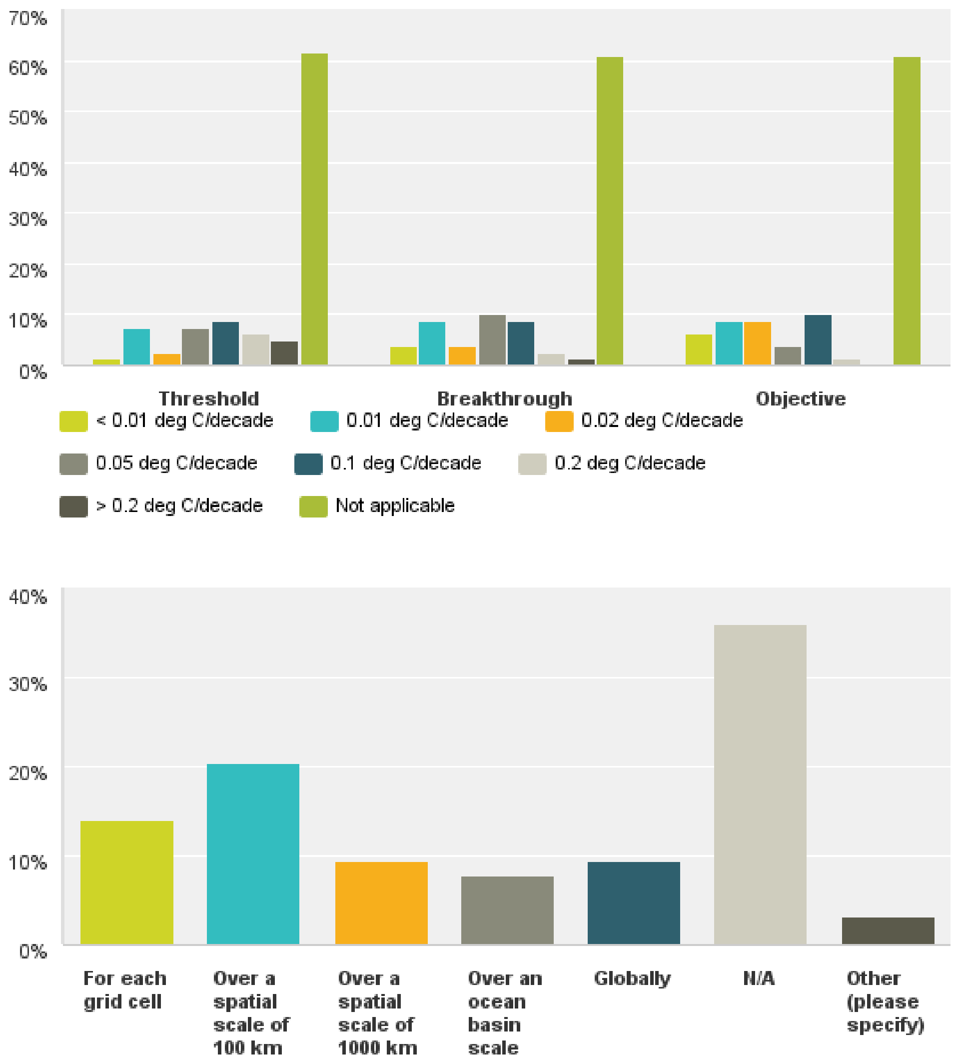


Figure 26. Requirements for acceptable level of drift in day-night differences.

Most respondents felt this was not relevant to their application. Of those who did consider it relevant, their responses were fairly evenly spread for all levels, with a tendency to increasing requirements at objective level, as would be expected. The most common requirement was for the achievement of this to be demonstrated over a spatial scale of 100 km. As with the previous similar questions, demonstration of this will depend on availability of high quality data to compare to.

4.2.2.23 Acceptable change in bias over the annual cycle

Respondents could also provide requirements for an acceptable change in bias level over the annual cycle. Figure 27 shows the results from those who entered requirements.

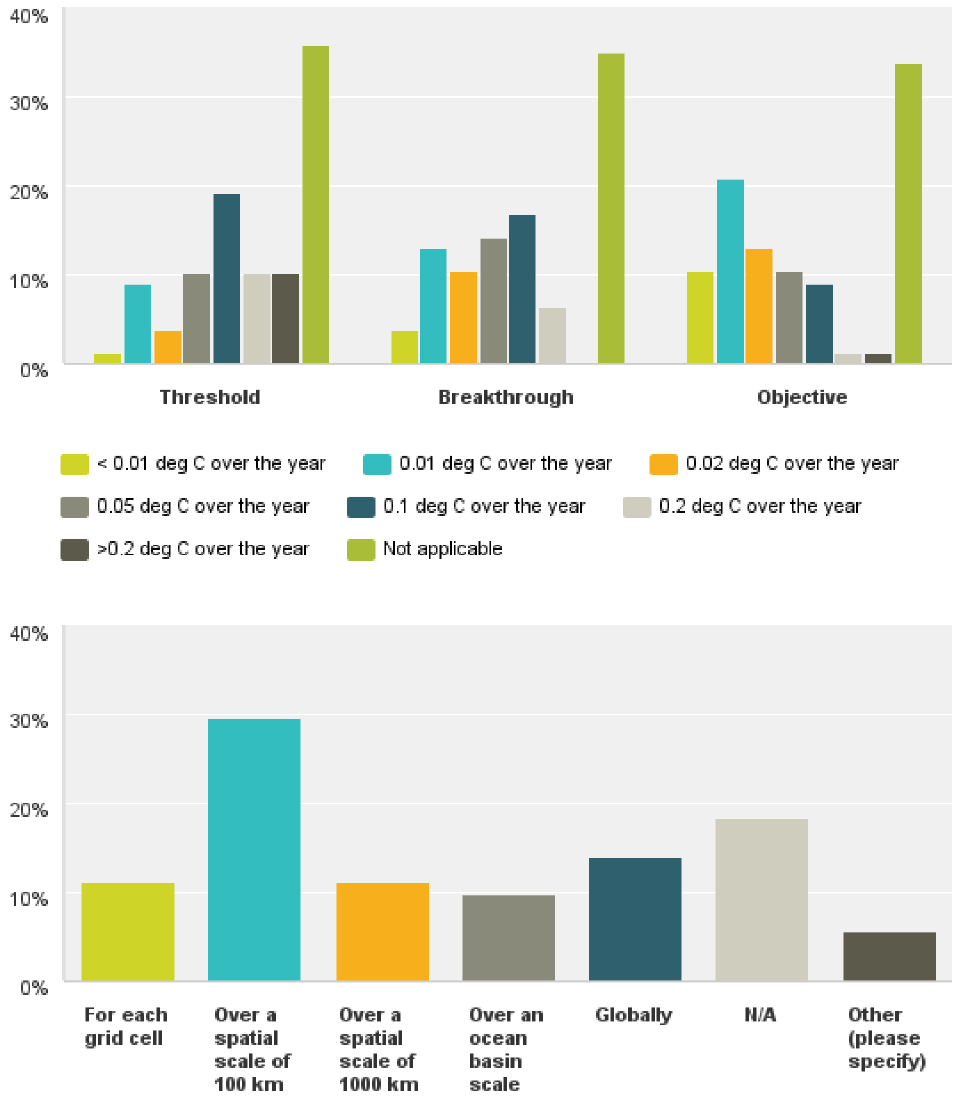


Figure 27. Acceptable change in bias over the annual cycle.

Again, the most responses were for 0.1°C over the year at threshold and breakthrough, changing to 0.01°C over the year at the objective level, and for the achievement of this to be demonstrated over a spatial scale of 100 km. It is noted again that demonstration of this will depend on availability of comparison data.

SST_CCI-UR-QUS-50	At all requirement levels, the most common response was that 0.1°C per decade is the acceptable change in bias over the annual cycle. The most common requirement was that the achievement of this should be demonstrated over a spatial scale of 100 km.

4.2.2.24 Uncertainty information

The User Workshop on Uncertainty (see Section 5) identified a significant interest within the user community of the provision of uncertainty information via an ensemble (a set of plausible realizations of each SST field which span the uncertainties in the data). To see if this appetite was shared by the wider user base, we asked if SST uncertainty information were to be represented by an ensemble, what size of ensemble would respondents need for their application (i.e. how many members)?

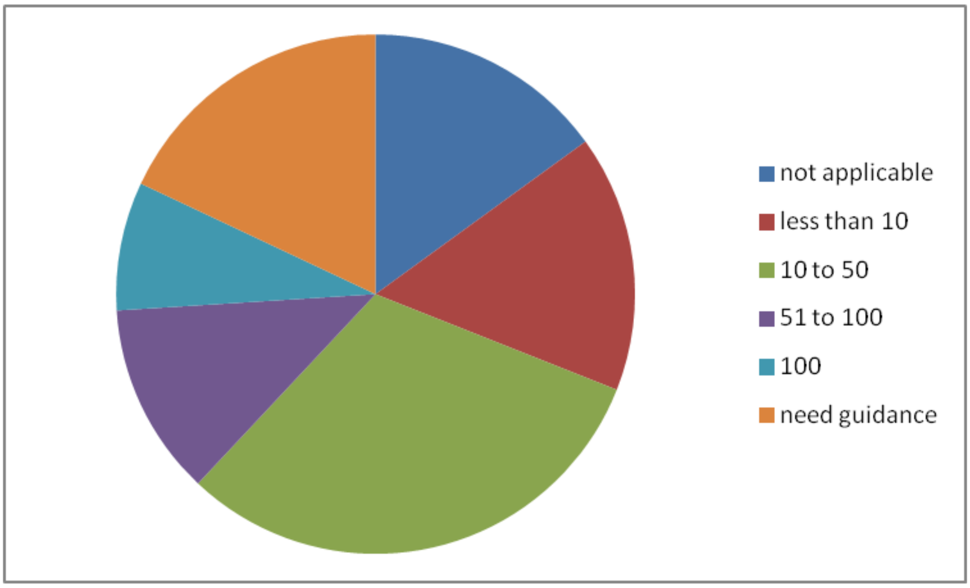


Figure 28. Number of ensemble members needed.

A clear appetite for an ensemble was indicated, with over half of respondents requiring more than ten ensemble members.

When asked why they preferred this number of ensemble members, they responded:

- Manageable number of realizations;
- The computation limit;
- Enough to establish the magnitude of the uncertainty well;
- Matches current number of simulations in GCMs;
- Based on my experience about ocean ensemble data assimilation, this might the smallest valid ensemble size;
- Operational ensemble is currently 80;
- It matches the number of simulations we generally need to get a handle on the model's internal variability using a single SST data set. A similar number of SST data sets would allow us to span obs and model uncertainty together - however, this relies on there being sufficient computing resources to do this number of simulations;
- I use LETKF with 56 ensembles. I might be able to use the ensemble data directly in our system;
- Threshold 2 - min and max (or 1st and 99th percentile). Breakthrough 4 - is ensemble bimodal? Objective 8 - what is skewness?;
- Comparable to standard model ensemble sizes for historical CMIP simulations
- We aren't currently running ensemble ocean forecasts but it is in our plans and we also have the underlying capability to make use of ensemble information in

the data assimilation. We would like this to be for the L2 data. In the medium term I don't expect we'll be able to afford computationally to run more than a few 10s of ensemble members;

- We run models with 30 ensemble members;
- With an ensemble > 100 we don't need to worry about sampling error anymore. Our operational ocean forecasting system use an EnKF with 100 members;
- I'm not an expert, but it should be as large as necessary to adequately characterise the error distribution;
- I'm afraid that less than 30 would not allow for estimating robust statistics of the error. But I'm aware that it is impossible to deliver 30 members for practical reasons;
- Sufficient to specify 10th & 90th percentiles.

SST_CCI-UR-QUS-51	Many users would benefit from the provision of information on uncertainty via an ensemble. This ensemble should have more than ten ensemble members.	Some users require as many as 100 ensemble members

4.2.2.25 Use of error covariance matrices

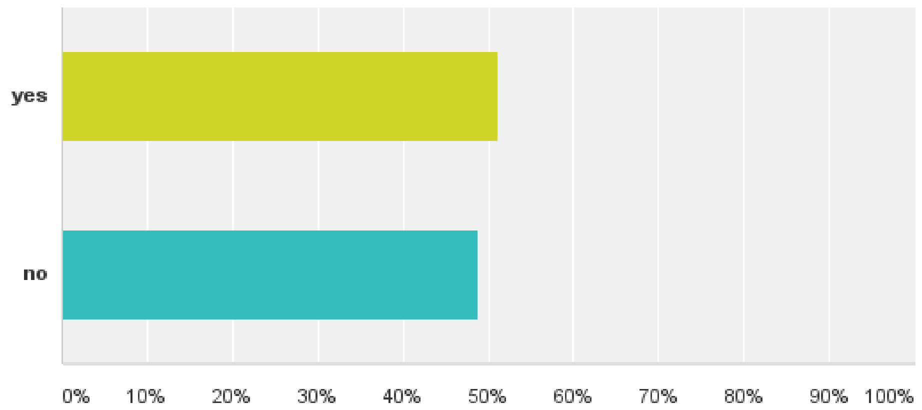


Figure 29. If SST uncertainty information were to be provided as a parametrised covariance matrix, would you use this?

The User Workshop on Uncertainties identified two preferences amongst users for means of providing information on the covariance structure of SST errors. As previously discussed, the provision of an ensemble was identified by many as their preferred option. The other option was use of a parameterised covariance matrix. Here too, amongst this independent sample, we see just over half of respondents would use this information.

SST_CCI-UR-QUS-52	Many users would benefit from the provision of information on uncertainty via a parameterised error covariance matrix.

4.2.2.26 Communication of quality information

Figure 30 shows preferences for how quality information should be communicated.

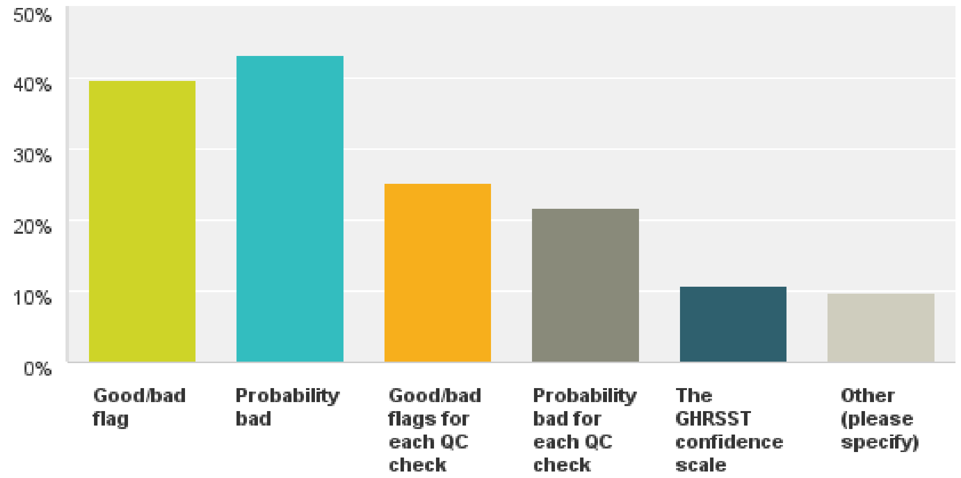


Figure 30. Preferences for how quality information should be communicated.

A roughly equal number of respondents chose to either have a binary good/bad flag for each SST value or to have a value for each SST to say the probability that it is bad. Other options, such as providing information about the quality control checks that had been failed, received fewer responses, but were still popular.

SST_CCI-UR-QUS-53	Quality information is needed for each SST and associated uncertainty estimate that is simple to use.	For example a single field indicating “good/bad” or the overall probability that a value is bad.

4.2.2.27 Other information to be provided in the data files

Respondents were asked what other information should be provided within the data files. The results are shown in Figure 31.

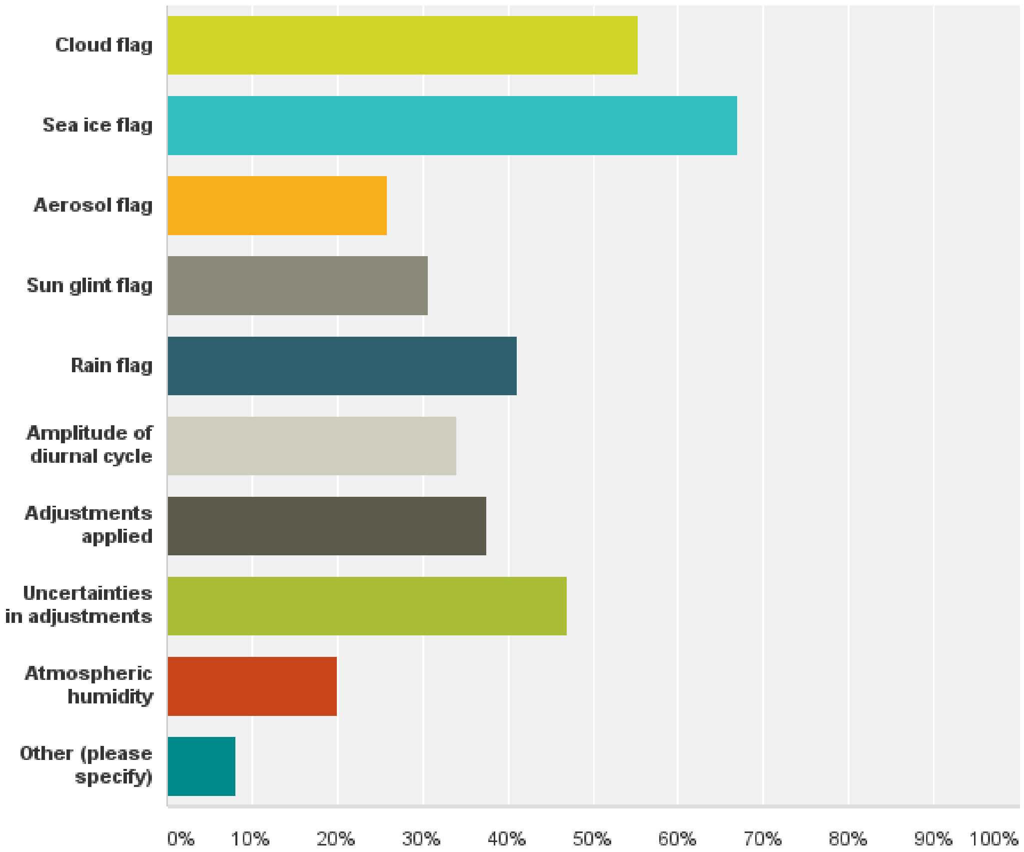


Figure 31. Additional information that should be provided in data files.

All the suggested information was of interest to some respondents. Information about cloud and sea ice locations was most commonly selected. However, all the options received a significant number of responses. Additionally, the following were suggested:

- Whether a location is gap filled or not gap filled and how (with which method) was it filled?
- Information on anomalously cold data points, data points that may contain extreme upwelling;
- Information about difference with respect to adjacent pixels. That is possibly useful in upwelling areas with steep SST gradients;
- Included information about adjustments as a safeguard (to be able to get at the data).

Respondents were also asked if they would like ancillary data to be provided, i.e. extra data that would complement the SSTs. The results (Figure 32) demonstrate that all options provided (aerosol optical depth, sea ice concentration and wind speed) would be valuable to at least some respondents. Solar radiation was also suggested.

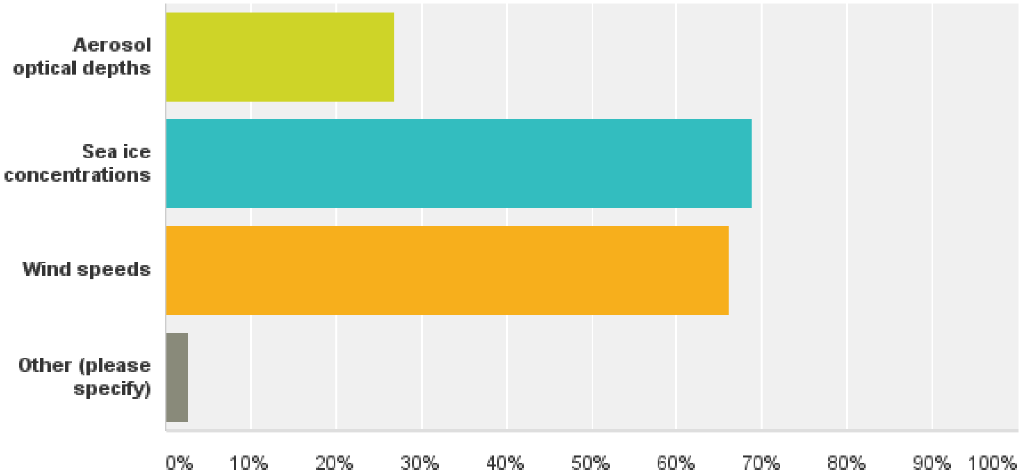


Figure 32. Preferences for what ancillary data to provide.

Requirements for other information to be provided in the data files:

SST_CCI-UR-QUS-54	Provision of locations of clouds.	Required by 55% of respondents.
SST_CCI-UR-QUS-55	Provision of locations of sea ice locations.	Required by 67% of respondents.
SST_CCI-UR-QUS-56	Provisions of aerosol locations.	Required by 26% of respondents.
SST_CCI-UR-QUS-57	Provision of sun glint suspected locations	Required by 31% of respondents.
SST_CCI-UR-QUS-58	Provision of rain suspected locations	Required by 41% of respondents.
SST_CCI-UR-QUS-59	Provision of the amplitude of diurnal cycle	Required by 34% of respondents.
SST_CCI-UR-QUS-60	Provision of information about adjustments applied to data	Required by 38% of respondents.
SST_CCI-UR-QUS-61	Provision of uncertainties in adjustments	Required by 47% of respondents.
SST_CCI-UR-QUS-62	Provision of information about atmospheric humidity	Required by 20% of respondents.
SST_CCI-UR-QUS-63	Provision of sea ice concentration ancillary data.	Required by 69% of respondents.
SST_CCI-UR-QUS-64	Provision of wind speed ancillary data.	Required by 66% of respondents.

SST_CCI-UR-QUS-65	Provision of aerosol optical depth ancillary data.	Required by 27% of respondents.
SST_CCI-UR-QUS-66	Provision of irradiance ancillary data.	Suggested by one respondent.

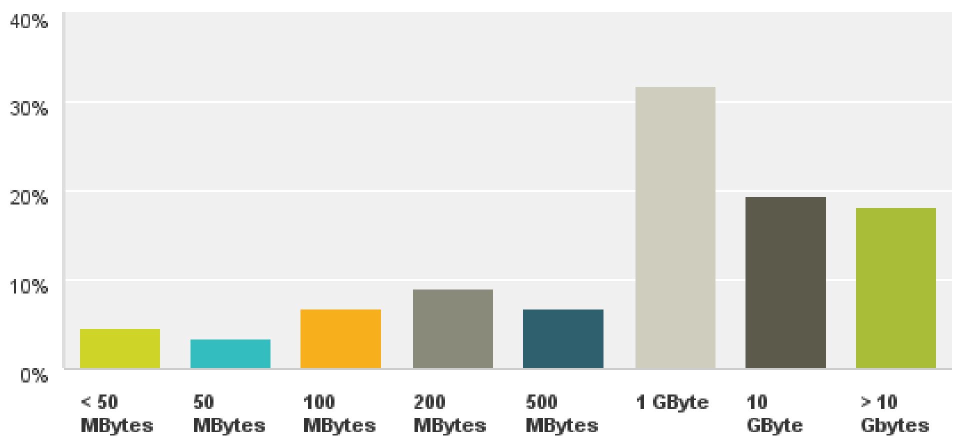
4.2.2.28 Dependence on other developments

Respondents were asked if their use of the data depends on other developments, i.e. would exploitation of the data for their application require development of models or other systems (such as observation operators) or tools? Suggestions were:

- Possibly medium-scale (5-10km) models and sparse repeat (0.5-2 months) *in situ* observations at sparse locations;
- KNMI Climate Explorer;
- Observation operators;
- An Agent Based Modeling framework;
- Developing new assimilation system for regional and global domain using LETKF;
- Expert systems based on expert opinion on geographically-specific environmental criteria for ecosystem impacts (e.g., additional criteria for bleaching beyond SST, such as mean wind speed, wave height, sun hours, or turbidity);
- More development / expansion of our coastal *in situ* seawater temperature monitoring system and coastal wind products for our area;
- Improved analysis methods, access to computing resource to take advantage of high quality satellite data and more complex error structures and ancillary information;
- Direct use of correlated observation error information is not currently possible in data assimilation schemes;
- A tool to interpolate from SST native grid to RCM grid, which could be easily obtained by modifying existing tools.

4.2.2.29 File formats and sizes

Respondents were asked for the limit of individual file size and total dataset size that they could handle. The distributions of responses are shown in Figure 33.



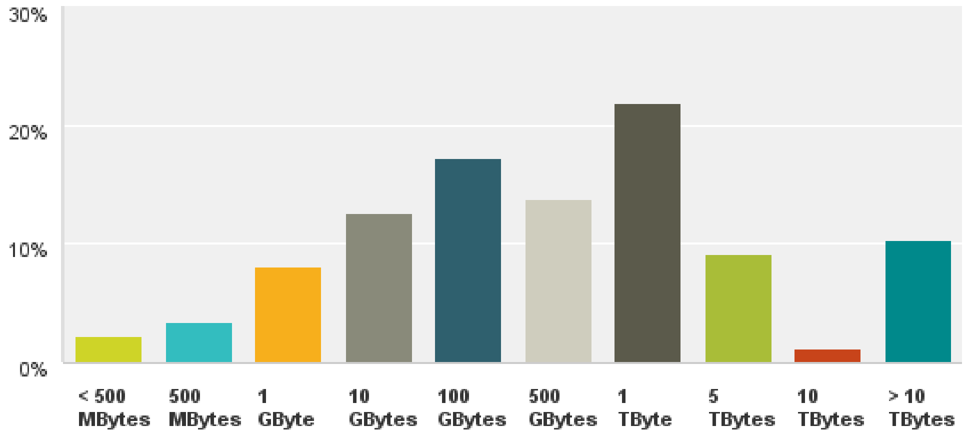


Figure 33. Limits to individual file size and total data size that users could handle.

A wide range of responses were received for both questions. For individual file size the maximum size that four respondents could handle was <50 MBytes. The mode of the distribution is at 1 GB.

Similarly a wide range of responses were received for total size of the data. Minimum response was <500 MB (two respondents), and maximum was >10 TB.

SST_CCI-UR-QUS-67	Respondents have widely varying capabilities in the size of individual files that they can handle.	Responses ranged between <50 MB and >10 GB.
SST_CCI-UR-QUS-68	Respondents have widely varying capabilities in the size of datasets that they can handle.	Responses ranged between <500 MB and >10 TB.

4.2.2.30 Format to be used for the data files

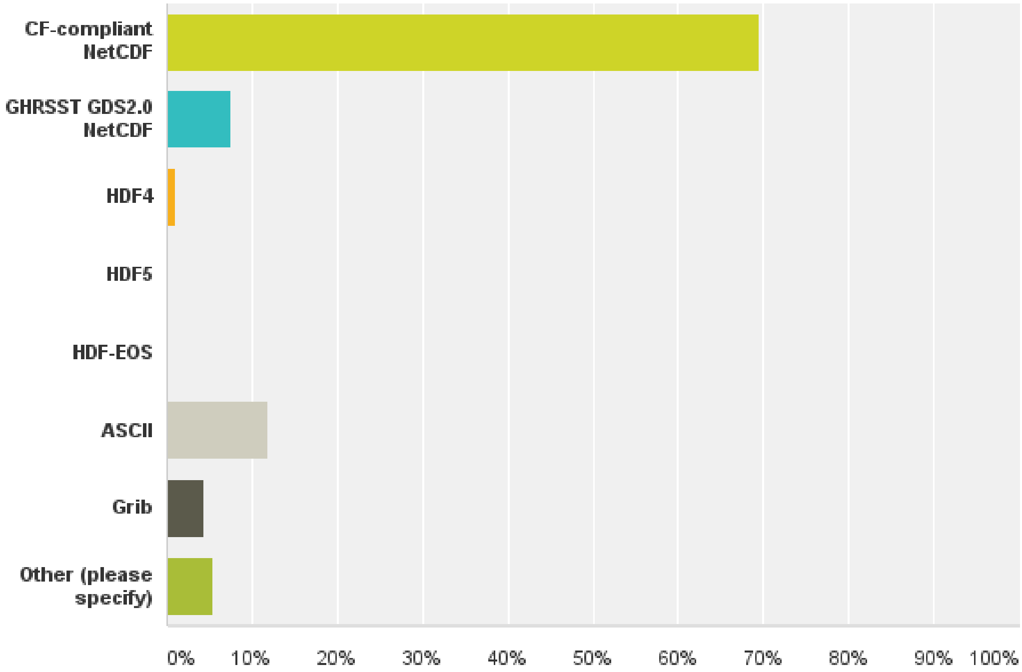


Figure 34. Format to be used for data files.

There was a clear preference shown in the responses for CF-compliant NetCDF to be used for the data files (Figure 34).

SST_CCI-UR-QUS-69	An overwhelming majority (78%) of respondents required data in CF-compliant NetCDF format.	Within that majority 8% specified the GHRSST GDS2.0 standard.

4.2.2.31 Data provision

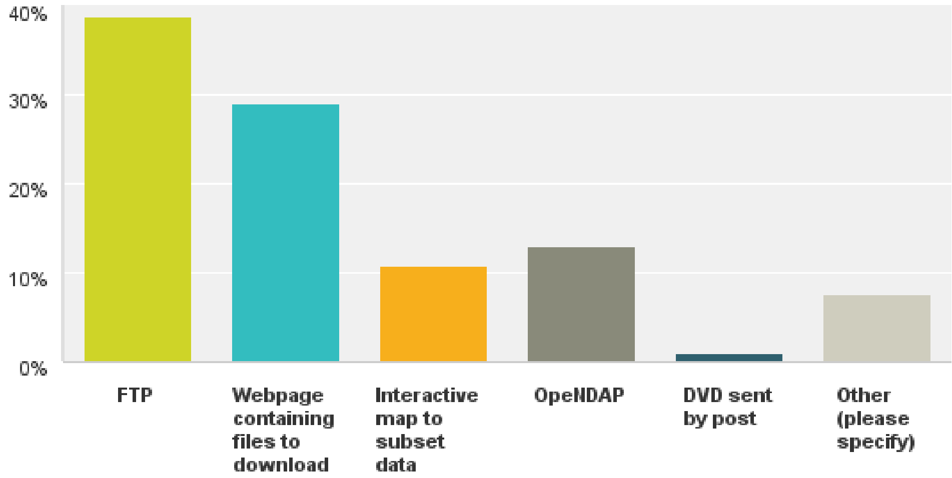


Figure 35. Method of transferring data

When asked which method of obtaining data they preferred, respondents gave a range of answers (Figure 35). The most popular method was File Transfer Protocol (FTP) but responses ranged all the way to having no local copy of the data at all.

Subsetting, whether using an interactive map, or not is required by some users. An automatable method was suggested by one respondent, as was provision on a shared resource, like the CEMS platform.

Options for obtaining data:

SST_CCI-UR-QUS-70	Provide facility to obtain data by FTP.	Chosen by 39% of respondents.
SST_CCI-UR-QUS-71	Provide facility to obtain data from a webpage.	Chosen by 29% of respondents.
SST_CCI-UR-QUS-72	Provide facility to obtain data using an interactive map.	Chosen by 11% of respondents.
SST_CCI-UR-QUS-73	Provide facility to obtain data using OPeNDAP.	Chosen by 12% of respondents.

4.2.2.32 Updating data

Respondents were asked how often they would like the data to be updated with improvements. The distribution of responses (Figure 36) contains two peaks; one for continuous incremental updates (23% of responses) and one for once a year (27% of responses.) It is therefore not possible to define a single user requirement from these results.

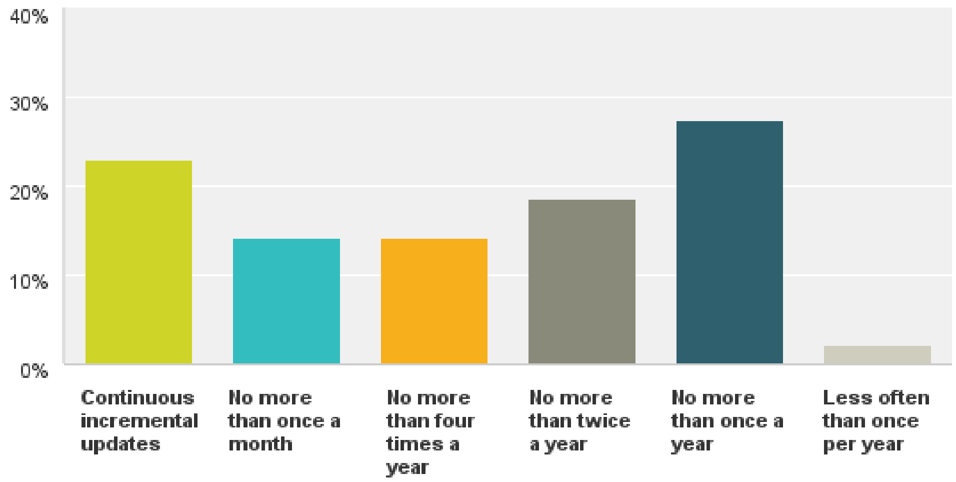


Figure 36. Preferences for frequency of improvements to the data.

4.2.2.33 Alerts

Figure 37. Preferences on how alerts about the data should be communicated.

Preferences were sought on how to receive updates about the data. As shown in Figure 37, by email and on the project webpage had the most responses.

Options for receiving alerts about the data:

SST_CCI-UR-QUS-74	Provide alerts by email.	Chosen by 59% of respondents. Implies facility for collection of e-mails associated with SST products by the data access systems such as CCI portal.
SST_CCI-UR-QUS-75	Provide alerts on the project webpage.	Chosen by 31% of respondents.

4.2.2.34 Software tools

Respondents were asked about the tools they currently use or plan to use to read in SST data. The tools suggested by more than one respondent are shown in Figure 38.

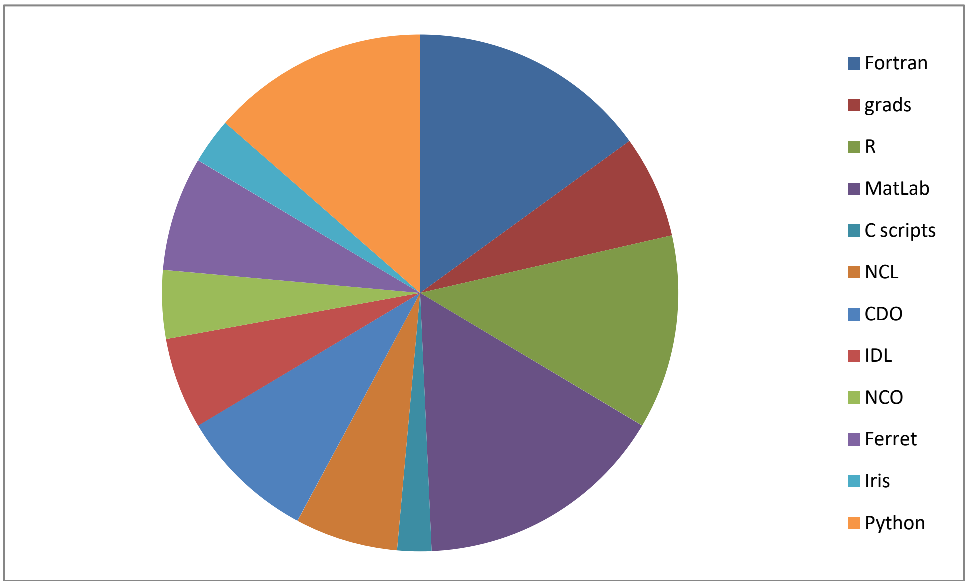


Figure 38. Tools currently used to read SST, or which will be used in future. Key applies clockwise.

Other tools included: UVCDAT; ESMValTool; Renux; ENVI; SEADAS; Windows; SAGA; SAS; GIS; Excel; BEAM.

SST_CCI-UR-QUS-76	SST CCI products should be made compatible with commonly-used methods of reading SST data, i.e. Fortran, Grads, R, Matlab, C, NCL, CDO, IDL, NCO, Ferret, Iris and Python.	Other tools are also used.

4.3 Additional comments

Respondents were given a final opportunity to provide further thoughts. Those not covered by earlier responses are reproduced here:

- Human-readable text files that can be parsed using the command line and a little python would be perfect. In the past, I've been frustrated by how complex it is to find, obtain, and parse the correct data for my needs since I am not primarily a climate scientist and these data are not my area of expertise;
- It would be appreciated if the data set comes along with a table listing all the raw data used;
- Please make sure errors are documented;
- The eastern Pacific (e.g. Niño 1+2 region) should be looked at with particular care when evaluating the new products. *In situ* measurements could be particularly valuable for this and I believe should be emphasised to the ongoing Tropical Pacific Observing System project (TPOS2020);

- Please provide a tool for error propagation to different temporal and spatial scales for L4 products;
- Uncertainty information on trends has heretofore been unavailable in a useful way. Information about the likely structure of correlated errors (be they local or large scale) has also been inaccessible. For some climate applications, it's the errors that correlate over a few years and thousands of kilometres that start to show up, but are hard to reconcile between instruments and aren't currently catered for. Maybe ensembles can fix this, but it would be useful to know something of the structure of these;

4.4 Summary

Users were invited to enter their requirements for SST data into an online questionnaire.

The results of the questionnaire have been presented. Wide ranges in responses were received for virtually all questions. This was also often the case when viewing responses from different people considering the needs of the same climate application. However, where possible, requirements have been formulated that reasonably represent the distribution of responses.

5. REQUIREMENTS OBTAINED FROM THE USER WORKSHOP ON UNCERTAINTIES

The workshop was held at the Met Office, Exeter, UK, on the 18th – 20th November 2014. Forty participants attended, spanning a range of interests, including climate research, numerical weather prediction, physical ocean modelling, ecological analysis, Earth system model evaluation and producers of SST datasets for both the satellite and historical eras. In line with the aim of the workshop for two-way dialogue, the event was structured with scene-setting presentations, a poster session, practical exercises applying uncertainty information, and break-out group discussions leading to plenary feedback and debate.

There are significant parallels between the priorities of a developer of a climate data record (CDR) and the priorities of a metrologist (metrology being the science of measurement and its uncertainty): both want measurements that are stable over time, insensitive to particular sensors and measurement methods, and are of uniform calibration and quality worldwide. Links were identified between Earth observation and metrology in day 1 of the workshop, via presentation and discussion. Good practice in tracing the uncertainty budget through satellite processing levels from instrumental measurement to geophysical product can be based on metrological norms encapsulated in documents such as the Guide to the expression of Uncertainty in Measurement (GUM; BIPM, 2008). In communicating about uncertainty, careful adherence to standard vocabulary can reduce ambiguity and increase understanding. In particular, it is useful to preserve the distinction between error ('mistaken-ness') and uncertainty ('doubt'). Uncertainty is typically quantified as the standard deviation of an estimated error distribution. In the case of Earth observation, uncertainty cannot be estimated from the dispersion of replicate measurements, as in a laboratory. Uncertainty modelling for EO relies heavily on understanding the instruments and retrieval processes, supporting error propagation by simulation and/or analytic techniques (Merchant and Embury, 2014). The metrological discipline of creating an uncertainty budget that is traceable (complete and defensible at each link the in the chain) can be used as a precedent for establishing the rigour and credibility of CDRs from EO.

The effects leading to errors in SST measurements of all sorts were reviewed in the workshop, it being clear that errors from different effects have very different correlations in space and time. Instrumental noise is usually modelled as independent random error between each SST measurement. Calibration drift over time, as an instrument ages, produces error that is highly correlated over global scales and years. EO datasets will usually also include errors on intermediate scales between these extremes, which may be termed locally systematic. In the case of SST, these effects are generally related to ambiguity arising from atmospheric variability, and therefore the errors correlate on synoptic scales. The current SST CCI approach is to specify components of uncertainty from random, locally systematic and systematic effects separately, and using these requires the user to engage with these concepts. In deriving uncertainty estimates for SSTs across the full range of scales needed by users, these different components of uncertainty need to be tracked and propagated separately, appropriate to their correlation structure.

Participants recommended that full characterisation and clear documentation of the error model was needed and either that these uncertainty components should be provided together with correlation information, or that their complex behaviour should be encapsulated in an ensemble as currently done by some providers of centennial-scale SST data sets. Since error covariance matrices can be large and difficult to use, it was recommended that these be parameterised to allow easy communication. It was therefore apparent in the workshop discussions that there is no simple answer to delivering uncertainty information to users, and that different users, for legitimate reasons, have different preferences amongst these options. The Climate Forecasting (CF) conventions require extension to accommodate more nuanced uncertainty information, in which effects and correlation structure can be specified. Participants recommended that use of uncertainty information would be facilitated by the provision of tools, for appropriate error propagation, ensemble selection or to create user-defined flags.

Even when provided with data producers' uncertainty estimates, users do not necessarily use these at face value. A discussion was held about what is required for SST users to trust uncertainty estimates attached to data as being realistic, and directly usable within their applications. Uncertainty validation and verification was welcomed, but more reference data is needed. The other two major influences were the scientific reputation of the data producers, established through the norms of peer reviewed publication, etc, and precedents where uncertainty information have been successfully exploited in applications. Formal mechanisms, such as publishing uncertainty traceability chains, were judged as less influential. However, this does not undermine the need for data producers to engage with uncertainty estimation in a rigorous, defensible manner, since this is part of building the necessary scientific credibility, as well as being good science practice.

Full outcomes from the meeting can be found at http://www.esa-sst-cci.org/PUG/workshop.htm.

All requirements have been copied into the table below, but only those more widely applicable are contained in the summary table of requirements, e.g. SST_CCI-UR-UWU-26 related very specifically to the User Workshop, so has not been carried forwards, but the requirement was actioned.

SST_CCI-UR-UWU-1	Information on uncertainties on specific/larger spatial scales, e.g. for ocean basin averages, and over longer temporal scales
SST_CCI-UR-UWU-2	A large, easy to use, fully-documented ensemble of sea surface temperature information, which samples the full error model and can be sub-selected according to need
SST_CCI-UR-UWU-3	A tool which allows the user to generate their own ensemble
SST_CCI-UR-UWU-4	A tool (perhaps web-based) to grid to any spatial/temporal scale (e.g. model grids) with full uncertainty propagation (and ensemble generation) from native resolution. This would include the ability to extract information for specific regions and to extract SST information for different depths
SST_CCI-UR-UWU-5	Quality flags as a proxy for uncertainty or a tool to create tailored flags for specific users/groups of users.
SST_CCI-UR-UWU-6	Full characterization and clear documentation of uncertainty, i.e.

	information on how uncertainty estimates were derived, what the contributing factors were, how to propagate them and what size to expect.
SST_CCI-UR-UWU-7	Quality flags should be well and prominently documented.
SST_CCI-UR-UWU-8	Indicator for the source of possible error (e.g. information on uncertainties from clouds to help to distinguish them from fronts)
SST_CCI-UR-UWU-9	Error covariance matrices
SST_CCI-UR-UWU-10	Error distribution
SST_CCI-UR-UWU-11	Median estimate, plus uncertainty
SST_CCI-UR-UWU-12	Validated uncertainties. (More high-quality reference data are needed.)
SST_CCI-UR-UWU-13	Quantified uncertainties back as far as possible in the historical record.
SST_CCI-UR-UWU-14	Coastal SSTs with uncertainties under all conditions.
SST_CCI-UR-UWU-15	Updates to the CF conventions (standard name tables) to provide sufficient vocabulary to describe all uncertainty components adequately.
SST_CCI-UR-UWU-16	Information content of analysed values, e.g. time of last measurement, number of contributing observations, or percentage coverage.
SST_CCI-UR-UWU-17	Operationally-available daily SST analyses together with uncertainty estimates for each value.
SST_CCI-UR-UWU-18	The ability to disentangle any retrieval bias from the systematic uncertainty term.
SST_CCI-UR-UWU-19	Consistent treatment/presentation of uncertainty components across ECVs.
SST_CCI-UR-UWU-20	Sufficient information, which is easily accessible, to make an informed choice about which data set to choose, including known limitations.
SST_CCI-UR-UWU-21	A PUG written by users.
SST_CCI-UR-UWU-22	Link to information in other fora, e.g.

	NCEP climate data guide, GHRSST multi-product ensemble.
SST_CCI-UR-UWU-23	Feedback mechanism, e.g. a forum or discussion group.
SST_CCI-UR-UWU-24	Code repository including, e.g. data readers and functions for common data manipulation tasks (in particular, how to use the time variable). Clear documentation of these.
SST_CCI-UR-UWU-25	Provision of SST variability within a given grid cell and its associated uncertainty.
SST_CCI-UR-UWU-26	Model answers to the practical activities from the SST user workshop on uncertainties.
SST_CCI-UR-UWU-27	Daily (or day/night) L3C products.
SST_CCI-UR-UWU-28	Rename the L4 analysis uncertainties to be more correct.
SST_CCI-UR-UWU-29	Clear documented examples of e.g. how to take products from the archive and use in applications.
SST_CCI-UR-UWU-30	Results from the uncertainty validation, along with their derivation, must be published in peer-reviewed literature.
SST_CCI-UR-UWU-31	Examples where the uncertainties have been used should be provided to show a demonstrable improvement in an application.
SST_CCI-UR-UWU-32	Validate product uncertainties at all scales e.g. global/regional/local/coastal.
SST_CCI-UR-UWU-33	Provide results from validating uncertainties in regions of known issues affecting satellite SST retrievals.
SST_CCI-UR-UWU-34	Clear advice should be given on interpretation of uncertainty verification maps, e.g. what to do where areas of high uncertainty cannot be validated.

6. CONCLUSIONS

This document has presented the results of a user requirements gathering exercise for the ESA SST CCI project.

Requirements were gathered through online questionnaires, discussion sessions, a user workshop, from reference documents, the Phase I Climate Assessment Report and from lessons learned from other projects.

A series of requirements was identified (designated [SST_CCI-REQ-n] below), largely based on overall responses to the questionnaire. These requirements are listed in Table 5. Using these requirements, specifications for SST CCI products will be developed and a description of whether and how these requirements will be met in this phase of the SST CCI project can be found in the Product Specification Document (PSD).

The format of the source identifiers used below is SST_CCI-UR-SSS-n, where UR stands for User Requirement, SSS is the method of gathering (REF: through analysis of reference documents; QUF: from results of the first questionnaire; CAR: from the Climate Assessment Report of the Phase I products; LLP: from lessons learned from other projects; MYO: from the MyOcean User Requirements Document; UWU: through discussion at the User Workshop on Uncertainties; and QUS: from results of the second questionnaire), and n is the user requirement number. In many cases, multiple statements have been merged together into one statement of requirement, which has been designated the identifier SST_CCI-REQ-n.

The table also includes a suggestion of how to validate these requirements to ensure that they have been met (TST: By test as specified in a test procedure; INS: Inspection by ESA; ANL: By analysis and preparation of a Technical Note describing the analysis and results).

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-1]	Provide products at levels 2, 3 (uncollated and daily collated) and 4.	The most common requirement is for level 4 data (78%), with level 3 (63%) also required by the majority of respondents. Some also require level 2 data (24%). L2P, L3U and L3C versions of data should be provided for all non-analysed data products. Versions of the data with gaps (if they exist) and versions without gaps are required.	SST_CCI-UR-QUS-77 / SST_CCI-UR-CAR-134 / SST_CCI-UR-QUF-39 / SST_CCI-UR-UWU-27	INS
[SST_CCI-REQ-2]	Provide single-sensor records, sensor-series data sets and multiple-sensor, gap-free analyses.	The needs of different users can be met by making available single-sensor records, sensor-series datasets, and multiple-sensor analyses. Data should be combined where this will allow weaknesses in individual datasets to be overcome. For those users who are happy with a multi-sensor SST record.	SST_CCI-UR-QUF-35 / SST_CCI-UR-QUS-78 / SST_CCI-UR-QUE-30	INS
[SST_CCI-REQ-3]	Provide some products which are a combination of infrared and microwave satellite data.	SSTs retrieved from infrared and microwave satellite data should be combined, in order to reduce biases and data gaps.	SST_CCI-UR-CAR-136	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-4]	Provide SSTskin	SSTskin is the depth most commonly required by respondents, closely followed by SSTs at depths roughly corresponding to the range of traditional *in situ* observations (20 cm and 5 m).	]SST_CCI-UR-QUS-44	INS
[SST_CCI-REQ-5]	Provide daily average SST20cm	A standard product file of SST20cm adjusted to the daily average should be provided, for those users interested in using a simpler-to-use standard product.	SST_CCI-UR-QUS-45	INS
[SST_CCI-REQ-6]	Provide SST20cm at the observation time	SST data are required that are adjusted to a standard depth but not adjusted to a standard local time.	SST_CCI-UR-CAR-135	INS
[SST_CCI-REQ-7]	Provide SST anomalies relative to a long-term reference climatology	An anomaly product should be provided to allow users to assess deviations from the long term average.	SST_CCI-UR-QUS-79	INS
[SST_CCI-REQ-8]	Provide SST in sea-ice affected areas	Reporting of SST is most commonly required for sea-ice affected areas. However, 41% of respondents expressing a requirement favoured either ice surface or radiometric temperature.	SST_CCI-UR-QUS-46	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-9]	Provide global coverage	Global coverage is required.	From questionnaire and [RD.163, RD.164]. SST_CCI-UR-REF-2 / SST_CCI-UR-QUS-41 / SST_CCI-UR-QUF-42	INS
[SST_CCI-REQ-10]	Provide level 3 and 4 data on a regular latitude-longitude grid	Respondents have a clear preference that level 3 and level 4 data should be provided on a regular latitude-longitude grid.	SST_CCI-UR-QUS-80	INS
[SST_CCI-REQ-11]	Provide level 4 data and temporal updates using the most accurate land/sea mask possible	The most accurate land/sea mask possible should be used for the level 4 analysis to facilitate use in various application areas. However, this should also be consistent with data sets used to update the CDR to enable trend analysis.	SST_CCI-UR-QUS-81	ANL

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-12] [SST_CCI-REQ-13]	Provide products of 30 or more years in length Provide products longer than 100 years by combining satellite retrievals with *in situ* measurements	The most common responses at the threshold requirement level are for temporal coverage of 30 or more years (40% of responses). At the breakthrough and objective requirements levels there is a clear requirement for data records longer than 30 years, with >100 years the most common requirement at objective level. This is to aid study of climate change and variability.	From questionnaire and [RD.159]. SST_CCI-UR-REF-3 / SST_CCI-UR-QUS-42	INS
[SST_CCI-REQ-14]	Provide data at least at 0.1° latitude by 0.1° longitude resolution	Overall, the most common responses for spatial resolution were 1° (threshold), 0.1° (breakthrough) and <1 km (objective). See also RD.390	SST_CCI-UR-QUF-36	INS
[SST_CCI-REQ-15]	Provide SST data at a particular universal time		SST_CCI-UR-QUS-36	INS
[SST_CCI-REQ-16]	Provide at least daily resolution		SST_CCI-UR-QUS-37 / SST_CCI-UR-QUS-40 / SST_CCI-UR-CAR-137	INS
[SST_CCI-REQ-17]	Provide information about the diurnal variability of SST		SST_CCI-UR-QUS-38	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-18]	Provide updates in a timely, ongoing manner	There is a continuing need for a timely flow of climate quality data to climate monitoring and analysis centres. See SST_CCI-UR-QUS-43 for a definition of timely; the continuing need for data can be addressed by ensuring that the data record is extendable in the future when new instrumentation is available. [RD.159, RD.163, RD.164] ICDRs are relevant to many applications. Timeliness requirements of updates vary from within a day to a year later. However, some users have much tighter requirements and need data as quickly as within half a day, e.g. seasonal forecasting requires daily, real-time (within hours) access to data. See also RD.390	SST_CCI-UR-REF-1 / SST_CCI-UR-QUS-43 / SST_CCI-UR-DIS-121	INS
[SST_CCI-REQ-19] [SST_CCI-REQ-20]	Provide SST with no more than a maximum of 0.1°C bias. Encourage reference data providers to enable assessment of bias on a spatial scale of 100km.	The most common acceptable levels of bias were 0.1°C (threshold and breakthrough), and more evenly spread at values between 0.01 and 0.1°C (objective). The most common response was that the achievement of this should be demonstrated over a spatial scale of 100 km. See also RD.390	SST_CCI-UR-QUS-47	ANL

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-21] [SST_CCI-REQ-22]	Provide SST with at least 0.1°C precision. Encourage reference data providers to enable assessment of precision on a spatial scale of 100km.	The most common breakthrough response was that 0.1°C is the required precision and that the achievement of this should be demonstrated over a spatial scale of 100 km. See also RD.390	SST_CCI-UR-QUS-48	ANL
[SST_CCI-REQ-23] [SST_CCI-REQ-24]	Provide SST with a maximum drift of 0.05°C/decade. Encourage reference data providers to enable assessment of drift on a spatial scale of 100km.	At the threshold level, 0.1°C per decade was the most common response for the acceptable level of drift. At breakthrough level 0.05°C per decade was the most common response. At the objective requirement levels, respondents require stability of 0.02°C per decade or better. The most common response for the spatial scale that the achievement of this should be demonstrated over was 100 km. However, a significant number of users have stricter requirements at both threshold and breakthrough levels. See also RD.390	SST_CCI-UR-QUS-49	ANL

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-25] [SST_CCI-REQ-26]	Provide SST with no more than a maximum change of bias of 0.1°C over the annual cycle. Encourage reference data providers to enable assessment of change in bias over the annual cycle on a spatial scale of 100km.	At all requirement levels, the most common response was that 0.1°C per decade is the acceptable change in bias over the annual cycle. The most common requirement was that the achievement of this should be demonstrated over a spatial scale of 100 km.	SST_CCI-UR-QUS-50	ANL
[SST_CCI-REQ-27]	Provide comprehensively characterised uncertainties in the products, together with indicators of confidence in uncertainty	Uncertainties need to be characterised comprehensively. Uncertainty estimates need to be in the products. Indicators of confidence in uncertainty estimates are required. Characterisation of uncertainties needs to be improved relative to current datasets. This should include the full error budget of the translation from the input data to the products and the error covariance structure. [RD.152, RD.164, RD.390]. See also [RD.165]	SST_CCI-UR-REF-4 / SST_CCI-UR-QUE-31 / SST_CCI-UR-UWU-6 / SST_CCI-UR-REF-5 / SST_CCI-UR-REF-6	ANL
[SST_CCI-REQ-28]	Verify uncertainty estimates by comparison against independent observations	Uncertainty characteristics should be verified by comparison against independent observations. See [RD.152]	SST_CCI-UR-REF-7 / SST_CCI-UR-UWU-12	ANL

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-29]	Provide information about the spatial and temporal correlation structure of errors	Information about the correlation structure of errors is essential or desirable for most respondents. Information on the temporal correlation of errors is required. For example information on correlations of analysis errors should be provided. See also RD.390 Users require information that allows the calculation of uncertainties on larger fields. For example to produce global or regional averages.	SST_CCI-UR-QUF-57 / SST_CCI-UR-CAR-138 / SST_CCI-UR-DIS-128	INS
[SST_CCI-REQ-30]	Provide a means to propagate uncertainty information to larger spatial scales	Information on uncertainties on specific/larger spatial scales, e.g. for ocean basin averages, and over longer temporal scales Some users prefer to have the uncertainty information propagated for them.	SST_CCI-UR-UWU-1	INS
[SST_CCI-REQ-31]	Provide advice on what users are to do where uncertainty cannot be verified	Clear advice should be given on interpretation of uncertainty verification maps, e.g. what to do where areas of high uncertainty cannot be validated.	SST_CCI-UR-UWU-34	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-32]	Provide an easy-to-use, fully-documented ensemble of SST, including an ensemble median and at least ten ensemble members	Many users would benefit from the provision of information on uncertainty via an easy to use, fully-documented ensemble. This ensemble should have more than ten ensemble members. Some users require as many as 100 ensemble members and should be able to be sub-selected according to need. For SST data in the form of an ensemble, the ensemble median should be provided, together with the uncertainty	SST_CCI-UR-DIS-127 / SST_CCI-UR-UWU-2 / SST_CCI-UR-QUS-82 / SST_CCI-UR-MYO-132 / SST_CCI-UR-UWU-11	INS
[SST_CCI-REQ-33]	Provide a parameterised error covariance matrix	Many users would benefit from the provision of information on uncertainty via a parameterised error covariance matrix.	SST_CCI-UR-QUS-83 / SST_CCI-UR-UWU-9	INS
[SST_CCI-REQ-34]	Provide probability distributions to convey information on uncertainty	Uncertainty information in the form of probability distributions is required by many.	SST_CCI-UR-QUF-56 / SST_CCI-UR-UWU-10	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-35]	Provide simple-to-use quality information for each SST value	Quality information is needed for each SST value that is simple to use. For example a single field indicating “good/bad” or the overall probability that a value is bad. An indicator should be available that can be used to determine if a particular grid cell contains a good quality SST without having to do any further checking of the data.	SST_CCI-UR-QUS-53 / SST_CCI-UR-CAR-139	INS
[SST_CCI-REQ-36]	Provide information on location of clouds	Provision of locations of clouds. Required by 55% of respondents.	SST_CCI-UR-QUS-54	INS
[SST_CCI-REQ-37]	Provide information on location of sea ice and its concentration	Provision of locations of sea ice. Required by 67% of respondents.	SST_CCI-UR-QUS-55 / SST_CCI-UR-QUS-63	INS
[SST_CCI-REQ-38]	Provide information on adjustments applied to the data and their uncertainties	Provision of information about adjustments applied to data. Required by 38% of respondents. Provision of uncertainties in adjustments. Required by 47% of respondents.	SST_CCI-UR-QUS-60 / SST_CCI-UR-QUS-61	INS
[SST_CCI-REQ-39]	Provide information on wind speed	Provision of wind speed ancillary data. Required by 66% of respondents.	SST_CCI-UR-QUS-64	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-40]	Consider users with the least developed computing infrastructures when designing product files and provision mechanisms	The requirements of users with access to the least developed computing infrastructures need to be addressed. [RD.159] Respondents have widely varying capabilities in the size of datasets that they can handle. Responses ranged between <50 MB and >10 GB for individual files. Responses ranged between <500 MB and >10 TB for total data volume.	SST_CCI-UR-REF-10 / SST_CCI-UR-QUS-67 / SST_CCI-UR-QUS-68	TST
[SST_CCI-REQ-41]	Provide easily accessible data in a free and unrestricted manner	Data need to be unrestricted in their availability. Data need to be easily accessible. Data need to be free. It is beneficial to users to reduce as much as possible any barriers to obtaining and using data. [RD.159]	SST_CCI-UR-REF-12 / SST_CCI-UR-DIS-117 / SST_CCI-UR-LLP-24 / SST_CCI-UR-REF-13 / SST_CCI-UR-REF-14	INS
[SST_CCI-REQ-42]	Provide data in CF-compliant NetCDF format	An overwhelming majority (78%) of respondents required data in CF-compliant NetCDF format. Within that majority 8% specified the GHRSST GDS2.0 standard. Data should be easy to use.	SST_CCI-UR-QUS-69 / SST_CCI-UR-DIS-118	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-43]	Provide users with the ability to select and download a subset or region of data	The ability to select and download a region of data should be provided. Users require the ability to select data for a particular time period.	SST_CCI-UR-CAR-142 / SST_CCI-UR-DIS-124	TST
[SST_CCI-REQ-44]	Ensure data can be downloaded quickly	The archive used to serve the data to users should provide sufficiently fast download speeds to make it viable for users to obtain the data within a short time frame. This might require mirror download sites in different countries.	SST_CCI-UR-CAR-141	TST
[SST_CCI-REQ-45]	Provide data alerts to users on the project website and by email if they provide their email addresses	Provide alerts by email. Chosen by 59% of respondents. Provide alerts on the project webpage. Chosen by 31% of respondents.	SST_CCI-UR-QUS-74 / SST_CCI-UR-QUS-75	INS
[SST_CCI-REQ-46]	Follow community standards for data and metadata storage and information sharing	Standards should be followed for data storage and information sharing. Standards and procedures for storage of metadata should be implemented. [RD.159] For example, in order to reduce operating costs. [RD.151]	SST_CCI-UR-REF-15 / SST_CCI-UR-REF-16	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-47]	Archive full information about input data and processing applied	Full information about input data and any processing applied needs to be archived. To allow future reprocessing. [RD.152]	SST_CCI-UR-REF-17	INS
[SST_CCI-REQ-48]	Publish results throughout the lifetime of the project	Users need to be kept informed of developments. By publishing results throughout the lifetime of the project.	SST_CCI-UR-LLP-27	INS
[SST_CCI-REQ-49]	Publish all steps taken during production	All steps taken during production should be published. Including data sources, algorithm selection and statements about accuracy, resolution and homogeneity. [RD.163]	SST_CCI-UR-REF-11	INS
[SST_CCI-REQ-50]	Provide information about data and algorithm maturity	There is a requirement to publish information about data and algorithm maturity. For example which parts have undergone peer-review. [RD.163]	SST_CCI-UR-REF-18	INS
[SST_CCI-REQ-51]	Provide clear documentation about derivation of uncertainty estimates, contributing factors to uncertainty and how to propagate uncertainty estimates	Clear documentation of uncertainty, i.e. information on how uncertainty estimates were derived, what the contributing factors were, how to propagate them and what size to expect.	SST_CCI-UR-UWU-6	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-52]	Provide clear documented examples of how to obtain products from the archive and use in example applications	Clear documented examples of e.g. how to take products from the archive and use in applications.	SST_CCI-UR-UWU-29	INS
[SST_CCI-REQ-53]	Consult appropriate users systematically	Appropriate user groups need to be consulted systematically. To establish requirements and to inspire global participation in use of data. [RD.151] It is important to foster good communication between the project, users and other interested parties.	SST_CCI-UR-REF-22 / SST_CCI-UR-LLP-26	INS
[SST_CCI-REQ-54]	Provide a user feedback mechanism	A mechanism for feedback from users needs to be provided. [RD.163]	SST_CCI-UR-REF-23	INS
[SST_CCI-REQ-55]	Provide a high quality website containing relevant information, documents, products and contact information	Users should have easy access to information, documents, products and contacts through a high quality website. The project should be made to feel open and inclusive to users and other scientists. By making meeting reports, presentations and minutes available.	SST_CCI-UR-LLP-28 / SST_CCI-UR-LLP-29	INS
[SST_CCI-REQ-56]	Provide documentation alongside the data on the data download site	Documentation should be made available alongside the data on the data download site.	SST_CCI-UR-CAR-140	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-57]	Provide a tool to quickly grid to any spatial/temporal scale with full uncertainty propagation, extract information for specific regions and extract SST information for different depths	A tool (perhaps web-based) to grid to any spatial/temporal scale (e.g. model grids) with full uncertainty propagation (and ensemble generation) from native resolution. This would include the ability to extract information for specific regions and to extract SST information for different depths Tools provided to process the data should run in real time.	SST_CCI-UR-UWU-4 / SST_CCI-UR-QUF-97 / SST_CCI-UR-CAR-144	TST
[SST_CCI-REQ-58]	Provide an open source code repository including data readers and functions for common data manipulation tasks with clear documentation	Code repository including, e.g. data readers and functions for common data manipulation tasks (in particular, how to use the time variable). Clear documentation of these. SST CCI products should be made compatible with commonly-used methods of reading SST data, i.e. Fortran, Grads, R, Matlab, C, NCL, CDO, IDL, NCO, Ferret, Iris and Python.	SST_CCI-UR-UWU-24 / SST_CCI-UR-QUF-98 / SST_CCI-UR-QUF-107 / SST_CCI-UR-QUS-76	TST
[SST_CCI-REQ-59]	Provide a tool which allows users to generate their own ensemble data set	A tool which allows the user to generate their own ensemble	SST_CCI-UR-UWU-3	TST
[SST_CCI-REQ-60]	Provide simple documentation	Provision of simple documentation. Chosen by 87% of respondents.	SST_CCI-UR-QUF-111	INS

Requirement identifier	Statement of requirement	Comments	Source	Validation
[SST_CCI-REQ-61]	Provide detailed documentation, including information about the algorithms used	Provision of detailed documentation. Chosen by 60% of respondents.	SST_CCI-UR-QUF-112	INS
[SST_CCI-REQ-62]	Provide feedback to producers of L0/L1 data used to inform them of any problems discovered with their data	Feedback is required to producers of L0/L1 data used by the project to inform them of any issues that have been discovered with their data. [RD.152, RD.156]	SST_CCI-UR-REF-9	ANL
[SST_CCI-REQ-63]	Maintain code under version control	Version control should be maintained. [RD.163]	SST_CCI-UR-REF-21	INS
[SST_CCI-REQ-64]	Provide a list of known gaps in the data	A list of known gaps in the data should be provided.	SST_CCI-UR-CAR-143	INS

Table 5. Full list of user requirements, organised into categories.

7. ANNEX A