Fiducial Reference Measurements for Satellite Ocean Colour Phase-2

FRM Requirements Document for Instrument Manufacturers (RMANU)

FRM4SOC2-RMANU

Title	Specifications of minimum requirements for qualification of OCR instrument as FRM instruments for manufacturers (RMANU)
Document reference	FRM4SOC2-RMANU
Project	EUMETSAT – FRM4SOC Phase-2
Contract	EUMETSAT Contract No. EUM/CO/21/460002539/JIG
Deliverable	D-27 FRM Requirements Document for Instrument Manufacturers (RMANU)
Version	1.1
Date issued	15.02.2023

Prepared By		Approved by	
Name:	Kevin Ruddick	Name:	Juan Ignacio Gossn
Organisation:	RBINS	Organisation:	EUMETSAT
Position:	FRM4SOC Phase 2 Task 1 Leader	Position:	FRM4SOC Phase 2 Project Officer
Date:		Date:	
Signature:	Kevin Ruddick (Signature) Digitally signed by Kevin Ruddick (Signature) Date: 2023.04.28 13:11:26 +02'00'	Signature:	Juan Ignacio Gossn Digitally signed by Juan Ignacio Gossn Date: 2023.05.15 15:46:26 +02'00'

Document Control Table

Title	FRM Requirements Document for Instrument Manufacturers (RMANU)
Document reference	FRM4SOC2-RMANU
Project	EUMETSAT – FRM4SOC Phase-2
Contract	EUMETSAT Contract No. EUM/CO/21/460002539/JIG
Deliverable	D-27
Version	1.1
Date Issued	15.02.2023

Document Change Record

Index	Issue	Revision	Date	Brief description	Issued by
1	1	0	27.01.2023	First draft partners	RBINS (Kevin Ruddick), including input from partners, esp. TARTU, and from discussions with instrument manufacturers at the FRM4SOC Workshop of Dec 2022. Section 3.2 here copied directly from section 5 of FRM4SOC2 deliverable D-12.
2	1	1	15.02.2023	Addition of Chapter 4 with recommendations to manufacturers and one sentence of Executive Summary	Viktor Vabson, Ilmar Ansko and Riho Vendt (TARTU)

Distribution List

Company/Organisation	Name	Format	No. of Copies
UT	Riho Vendt Viktor Vabson Karin Pai	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
ACRI-ST	Christophe Lerebourg Sébastien Clerc	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
Brockmann Consult	Carsten Brockmann Helge Dzierzon Uwe Lange	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
NPL	Agnieszka Bialek Madhu Mittra Sam Hunt Chris McLellan	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
PML	Gavin Tilstone Giorgio Dall'Olmo	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
RBINS	Kevin Ruddick	Electronic file – pdf and original (WORD) file	1 pdf 1 WORD file
EUMETSAT	Ewa Kwiatkowska Juan Gossn	Electronic file – pdf	1 pdf

Executive Summary

The objective of this document is to specify the minimum requirements to be fulfilled by OCR instrument manufacturers for an instrument to be accepted as suitable for a Fiducial Reference Measurement (FRM).

The main section 2 of this document is largely a subset from the wider FRM Requirements Document D-2 condensed to focus on the instrument-related requirements under responsibility of the manufacturer and excluding the other non-instrument requirements for a FRM.

The document's target public is an OCR instrument manufacturer whose customers may be interested to make Fiducial Reference Measurements.

While the FRM4SOC-2 project focuses primarily on the two models of TriOS-Ramses and SeaBird-HyperOCR, the present document is generic enough to cover both these two models and probably all present and future OCR models. The process for the inclusion of any new OCR models as FRM is simply to satisfy these requirements.

A checklist of 9 instrument-related requirements and 4 documentation-related requirements is provided for an OCR instrument (and the underlying calibration/characterisation) to be considered as suitable for Fiducial Reference Measurements. Detailed guidance on meeting these requirements is provided in FRM4SOC2 project deliverables D-11 and D-12.

Recommendations are also provided to manufacturers, particularly for the design of new OCR, with particular attention to thermal effects.

Conclusions on the feasibility of this approach and discussion of the challenges facing OCR manufacturers are provided, using feedback obtained from the FRM4SOC2 project workshop.

Table of contents

List of Figures

List of Tables

Acronyms and Abbreviations

Acronym	Description
AAOT	Acqua Alta Oceanographic Tower
AATSR	Advanced Along-Track Scanning Radiometer
AD	Applicable Document
ADUM	Architecture Design and User Manual document
AERONET-OC	The Ocean Color component of the Aerosol Robotic Network
AMT	Atlantic Meridional Transect
API	Application Program Interface
ARC	Assessment of In Situ Radiometric Capabilities for Coastal Water Remote Sensing Applications
BRDF	Bidirectional reflectance distribution function
Cal	Calibration
CEOS	Committee on Earth Observation Satellites
Char	Characterization
CLI	Command-Line interface
DP	Data Package
DR	Documentation-related Requirements
EO	Earth Observation
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FOV	Field of view
FRM	Fiducial Reference Measurements
FRM4SOC	Fiducial Reference Measurements for Satellite Ocean Colour
GEO	Group on Earth Observations
HQ	Headquarters
IOCCG	International Ocean-Colour Coordinating Group
IPR	Intellectual Property Rights
IR	Instrument-related Requirements
KO	Kick Off meeting
LUT	Look Up Table
MAVT	MERIS and Advanced Along-Track Scanning Radiometer Validation Team
MERIS	Medium Resolution Imaging Spectrometer
MVT	MERIS Validation Team
NASA	National Aeronautics and Space Administration
NERC	Natural Environment Research Council
NMI	National Metrology Institute
OC	Ocean Colour
OCDB	Ocean Colour Database
OCR	Ocean Colour Radiometer
PDF	Portable Document Format
MR	Protocol-related Requirements
QA	Quality Assurance

Acronym	Description
QA4EO	Quality Assurance framework for Earth Observation
QC	Quality Control
PMP	Project Management Plan
RSP	Remote Sensing and Products Division
RD	Reference Document
S3	Sentinel-3
S3VT-OC	Sentinel-3 Validation Team – Ocean Colour group
SeaWiFS	Sea-Viewing Wide Field-of-View Sensor
SIRREX	SeaWiFS Intercalibration Round Robin Experiments
SI	International System of Units
SOW	Statement of Work
SST	Sea Surface Temperature
TO	Tartu Observatory, University of Tartu
TR	Technical Report
TSM	Total suspended material
VAL	Validation
VIM	International Vocabulary of Metrology

Applicable documents

Table 0-1. Applicable documents

ID	Description
[AD-0]	Statement of Work for FRM4SOC phase2, EUM/RSP/SOW/19/1131157
[AD-1]	ESA's contract no 4000117454/16/I-SBo (https://frm4soc.org)
[AD-2]	D-70: Technical Report TR-2 "A Review of Commonly used Fiducial Reference Measurement (FRM) Ocean Colour Radiometers (OCR) used for Satellite OCR Validation" (available at https://frm4soc.org/index.php/documents/deliverables/)
[AD-3]	'Statement of Work for Database of Ocean Colour In Situ Fiducial Reference Measurement Collections for Calibration and Validation', EUM/OPSCOPER/SOW/17/956607.
[AD-4]	IOCCG Protocol Series (2019). "Protocols for Satellite Ocean Colour Data Validation: In Situ Optical Radiometry". Zibordi, G., Voss, K. J., Johnson, B. C. and Mueller, J. L. IOCCG Ocean Optics and Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation, Volume 3.0, IOCCG, Dartmouth, NS, Canada. (Available at https://ioccg.org/what-we-do/ioccg-publications/oceanoptics-protocols-satellite-ocean-colour-sensor-validation/)
[AD-5]	K. Ruddick et. al., "A Review of Protocols for Fiducial Reference Measurements of Water-Leaving Radiance for Validation of Satellite Remote-Sensing Data over Water", Remote Sens. 2019, 11(19), 2198; https://doi.org/10.3390/rs11192198
[AD-6]	K. Ruddick et. al., "A Review of Protocols for Fiducial Reference Measurements of Downwelling Irradiance for the Validation of Satellite Remote Sensing Data over Water", Remote Sens. 2019, 11(15), 1742; https://doi.org/10.3390/rs11151742
[AD-7]	International Network for Sensor Inter-comparison and Uncertainty assessment for Ocean Color Radiometry (INSITU-OCR), http://ioccg.org/wpcontent/uploads/2016/02/INSITU-OCR-white-paper.pdf.
[AD-8]	D-80a: Technical Report TR-3a "Protocols and Procedures to Verify the Performance of Reference Irradiance Sources used by Fiducial Reference Measurement Ocean Colour Radiometers for Satellite Validation" (available at https://frm4soc.org/index.php/documents/deliverables/)
[AD-9]	D-80b Technical Report TR-3b "Protocols and Procedures to Verify the Performance of Reference Radiance Sources used by Fiducial Reference Measurement Ocean Colour Radiometers for Satellite Validation" (available at https://frm4soc.org/index.php/documents/deliverables/)
[AD-10]	Białek, A.; Douglas, S.; Kuusk, J.; Ansko, I.; Vabson, V.; Vendt, R.; Casal, A.T. Example of Monte Carlo Method Uncertainty Evaluation for Above-Water Ocean Colour Radiometry. Remote Sens. 2020, 12, 780. https://doi.org/10.3390/rs12050780
[AD-11]	TR-9 Technical Report "Results from the First FRM4SOC Field Inter-Comparison Experiment (FICE) of Ocean Colour Radiometers" (available at https://frm4soc.org/index.php/documents/deliverables/)
[AD-12]	IOCCG Ocean Optics & Biogeochemistry Protocols for Satellite Ocean Colour Sensor Validation (https://ioccg.org/what-we-do/ioccg-publications/ocean-opticsprotocols-satellite-ocean-colour-sensor-validation/)

Reference documents

Table 0-2. Reference documents

ID	Description
[RD-1]	ESA's contract no 4000117454/16/I-SBo (https://frm4soc.org)

1 Introduction

1.1 Scope of the document

The objective of this document is to specify the minimum requirements to be fulfilled by OCR instrument manufacturers for an instrument to be accepted as suitable for a Fiducial Reference Measurement (FRM).

The main section 2 of this document is largely a subset from the wider FRM Requirements Document D-2 condensed to focus on the instrument-related requirements under responsibility of the manufacturer and excluding the other non-instrument requirements for a FRM.

The document's target public is an OCR instrument manufacturer whose customers may be interested to make Fiducial Reference Measurements.

While the FRM4SOC-2 project focuses primarily on the two models of TriOS-Ramses and SeaBird-HyperOCR, the present document is generic enough to cover both these two models and probably all present and future OCR models. The process for the inclusion of any new OCR models as FRM is simply to satisfy these requirements.

This document draws heavily on heritage from the work of the FRM4SOC-1 project, as documented by papers from the FRM4SOC Special Issue of *Remote Sensing* [1–8] and FRM4SOC Technical Reports [AD-2], as well as work of the international community within the IOCCG framework [AD-4, AD-7]. This document is specifically supported by the FRM4SOC2 deliverables which provides detailed guidelines on calibration laboratory practices and standards (D-11) and on specific processes for OCR calibration and characterisation (D-12).

1.2 Definition of Fiducial Reference Measurement

Within the current document we use the definition of Fiducial Reference Measurement provided by preface p xiii of [1], adapted from the original idea of [9] for Sea Surface Temperature measurements, whereby the defining mandatory characteristics of a "Fiducial Reference Measurement (FRM)" are:

The FRM must:

- have documented traceability to SI units (via an unbroken chain of calibrations and comparisons);
- be accompanied by a complete estimate of uncertainty, including contributions from all FRM instruments and all data acquisition and processing steps;
- follow well-defined protocols/community-wide management practices;
- be openly available for independent scrutiny and;
- be independent from the satellite retrieval process;

Of these five characteristics, only the first two (SI traceability and uncertainty estimation) are relevant for OCR instrument manufacturers.

1.3 FRMOCnet objectives

The FRMOCnet as proposed by EUMETSAT and illustrated in Figure 1-1 is envisaged as a network containing:

1. Databases with
    a. Serial number, calibration and characterization coefficients of individual OCRs (among other metadata),
    b. Measurements of Rrs with end-to-end uncertainty budget with relevant metadata.
    c. OCR users (institutions) that comply with FRM standards – to be defined in this document,
2. An "FRM community processor" software - interacting with the data described in 1 - outputting normalized water-leaving radiance and the corresponding end-to-end uncertainty budget from underwater/above water radiometric measurements and related needed metadata.
3. An information base of protocols, guidelines and tools to define, clarify and simplify FRM procedures.

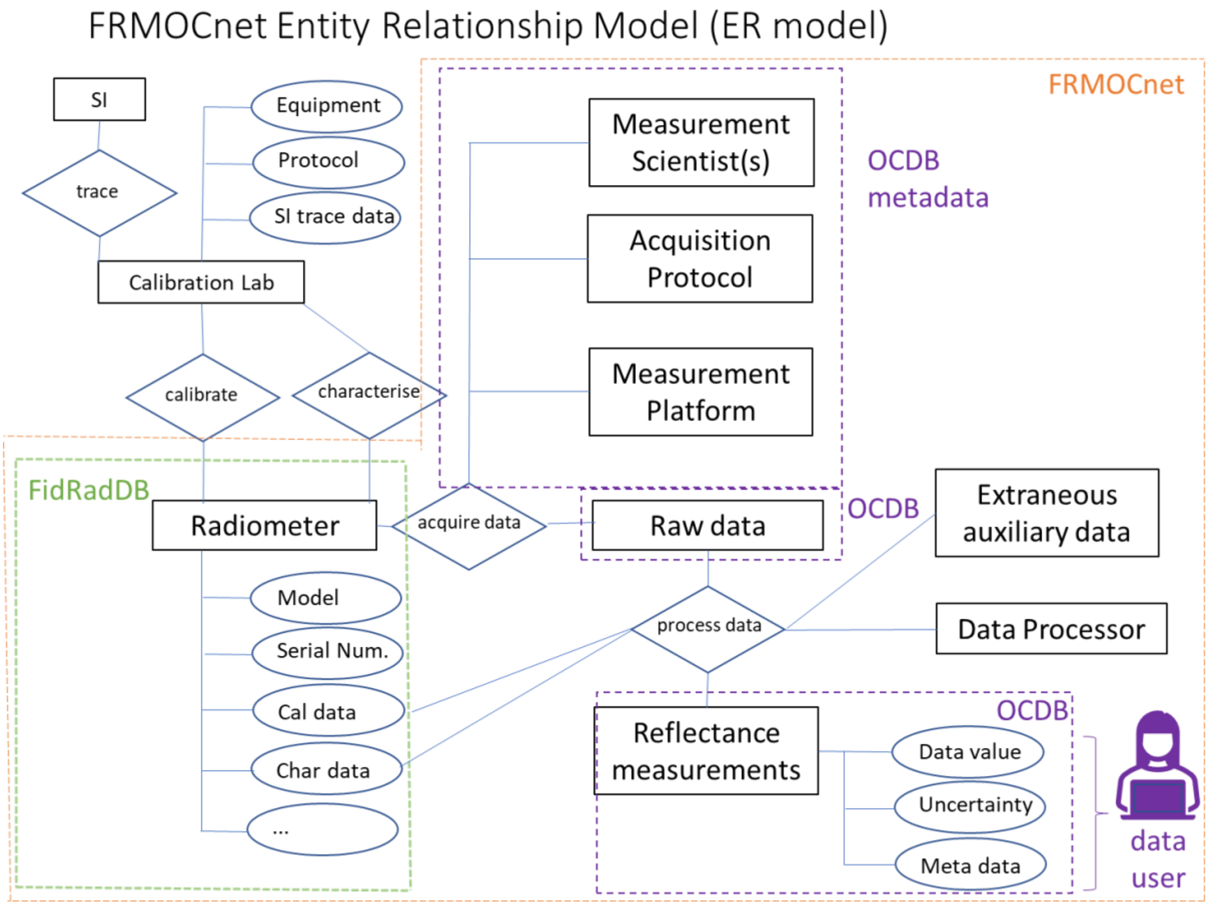

Figure 1-1 Heavily simplified proposal for a FRMOCnet Entity Relationship model ("ER model") following the notation of [Chen, 1976]. "Extraneous data" refers to data from other sources needed for processing, e.g. wind speed.

The current document is relevant for the FRMOCnet/FidRadDB box (Figure 1-1), where the calibration and characterisation data for each radiometer Serial Number (SN) is stored. In the absence of characterisation data at the SN level, uncertainty estimation can be "class-based", assuming that all SN from a OCR type/model have similar performance.

The "class-based" approach requires that the manufacturing process does not change significantly in time and has the consequence of higher uncertainty than the SN-based approach because of inter-SN variability within a class. As an example, a change of irradiance sensor cosine diffuser material, e.g. between fused silica and PTFE (Teflon), would significantly affect both cosine response and thermal sensitivity and a "class-based" approach would need to consider this as two distinct classes each with its own characterization data and uncertainty.

1.4 Calibration and characterisation of OCR

The Ocean Colour Radiometers (OCR) to be deployed in the field measure radiances and irradiances with an associated uncertainty. This uncertainty is separated here into "calibration" and "characterisation". Calibration (radiometric) refers to the conversion of Digital Numbers for each photodetector to a radiance or irradiance in SI units at a certain wavelength, generally by use of linear slope ("responsivity") and offset ("dark") coefficients, which may vary in time and may require special attention to immersion effects for in-water measurements [10,11]. A calibration result shall always include a statement on uncertainty. Characterisation refers to all other processes which modify the assumed linear calibration model, including [3,12,13]:

- Non-linearity
- Thermal sensitivity
- Angular sensitivity (especially imperfect cosine response for planar irradiance sensors)
- Spectral response function (including straylight for hyperspectral spectrometers, out of band response for filter radiometers)
- Polarisation sensitivity

- Temporal response
- Pressure effects

These instrument properties have been well-known for decades and corresponding characterisations are considered necessary already by the 2003 NASA Ocean Optics Protocols [12], with reinforcement of the need for such characterisations and updated review of the state of the art in the 2019 IOCCG Protocols [13]. In the FRM context, estimation of uncertainty related to all such instrument properties is needed to complete the total measurement uncertainty estimate … but is often lacking. The need for regular, e.g. annual, calibration of radiometers is well-understood and recognised by measurement scientists, who make appropriate preparations for the financial, down-time and transport/customs/logistical implications of such calibrations. The need for full characterisation of instruments is less well-established, presumably because of the high cost of such characterisations and the low availability of laboratories equipped to perform such characterisations. The FRM4SOC-1 review of radiometer instruments [AD-4] revealed a high diversity in the availability of information on and understanding of such characterisation from the instrument manufacturers. The possibility of performing such characterisations is beyond the capabilities of some instrument manufacturers and, if not required by their customers, is difficult to justify financially because of the high cost of both infrastructure and expertise.

It is noted that these radiometric characterisations are generally considered as independent, in view of the already considerable difficulties in establishing adequate corrections and quantifying residual uncertainties. However, there may be complex situations where two or more characteristics are related, e.g. thermal effects may affect responsivity, dark current *and* wavelength scale.

Because of the high cost of both infrastructure and expertise required for these instrument characterisations, there is also little knowledge on the possible time variation of such characterisations. The FRM4SOC and EU/HYPERNETS projects are considering the design of less expensive tests to identify any time variation of characteristics such as straylight distribution function and hence trigger, when necessary, an update laboratory re-characterisation. As an example, the MOBY system includes internal reference sources [14] to monitor continuously and validate the straylight distribution correction using the straylight distribution function from less frequent laboratory characterisations.

1.5 OCR calibration and characterization - review of precursor specifications

As regards *requirements* on radiometer performance, the NASA Ocean Optics Protocols Volume II, in Chapter 3 [15], already back in 2003 provided *insight* and *recommendations* on how instrument calibration and characterisation should be performed as well as, in Chapter 2, some minimum *specifications* or *requirements* for individual characteristics, e.g. (their Table 2.2) "straylight rejection of 10^{-6}", "signal:noise ratio of 1000:1 (at minimum)", etc. The 2019 IOCCG Ocean Optics Protocols adopted a similar approach, including *recommended specifications* (e.g. Table 1-1 reproduced from their Table 2.2) as well as a combination of limits beyond which characterisation and correction are required, e.g. "Sensors with temperature coefficients greater than 0.01% per °C should be characterized and a correction applied to the data to constrain residual temperature dependence below 0.01% per °C".

It is noted that some of the specifications provided in Table 1-1 may be difficult to achieve with current hyperspectral radiometers. E.g. correction of non-linearities to 0.1% may be very challenging. Straylight rejection of 10^{-5} may be difficult to achieve [16] and translation of the driving requirement of "residual after correction for this effect, below 1% in each band across the full spectral range" into requirements on the radiometer depends on the spectral composition of the (undefined) target. It is the ambition of the FRM4SOC-2 project to better understand how the final measurement uncertainty for water reflectance is affected by uncertainties from each such radiometer instrument characteristic, to assist in refining requirements on instrument characterisation.

Table 1-1. Recommended specifications for hyperspectral radiometers applied for validation activities. Reproduced from Table 2.2 of [13].

Optical Sensors	
Spectral Range	380 to 900 nm (an extension in the ultraviolet is desirable)
Spectral Resolution	3-10 nm (FWHM)
Spectral Sampling	1-3 nm (or at least 2 times the spectral resolution)
Wavelength Accuracy	10% FWHM resolution
Wavelength Stability	5% FWHM of resolution
Signal-to-Noise Ratio	1000:1 (at minimum)
Stray Light Rejection	10^{-5} (of the maximum radiometric signal at each spectral band)
FOV Maximum (full-angle)	5°, 20° (for above-water and in-water, respectively)
Temperature Stability	Specified for the range from 0 °C to 45 °C
Linearity	Correctable to 0.1%

The IOCCG protocols [13] also provide helpful guidance on the type and occurrence of calibrations and characterisations that are needed for validation activities - see Table 1-2 reproduced from their Table 3.1.

The FRMSOC2 consortium considers that [13] is a most comprehensive summary of former efforts during the last 20–30 years about cal/char activities, including recommendations on the regularity/type of the characterisation/calibration requirements. Calibration of OCR shall be performed regularly, once a year. All other characteristics of the FRM OCR instruments listed by [13] shall be determined at least once before its application for FRM purposes. Repeated characterisation of some parameters of OCR is needed after known significant constructional or other changes of the OCR instrument or in case of doubts. Such cases are detailed in FRM4SOC-2 D-8.

Table 1-2. Basic requirements on the type and occurrence of calibrations and main characterizations of field radiometers supporting ocean colour validation activities. Reproduced from Table 3.1 of [13].

	Regular	Occasional	Initial	Class-based
Radiometric responsivity	x			
Spectral response		x		
Out-of-band & stray light		x		
Immersion factor (irradiance)			x	
Immersion factor (radiance)				x
Angular response			x	
Linearity				x
Integration time				x
Temperature response				x
Polarization sensitivity				x
Dark-signal	x			
Temporal response				x
Pressure effects				x

2 Requirement of SI-traceability and existence of an Uncertainty estimate

FRM requirements of SI-traceability and the existence of an uncertainty estimate are detailed in the following subsections for the parts of the process that involve OCR instrument manufacturers. Other aspects of the FRM process, e.g. relating to field deployment and processing of measurements, can be found in the wider scope of FRM4SOC2 project deliverable D-2.

As will be seen, there are no requirements or constraints on the OCR instrument design. The requirements stated here are applicable to any generic OCR design, including both multispectral and hyperspectral sensors. The fundamental metrological requirement is that the OCR be calibrated and characterised such that any measurement result can have an associated uncertainty.

2.1 FRM Requirements for calibration and characterisation of Ocean Colour Radiometers

The full list of requirements for a Fiducial Reference Measurement (FRM4SOC2 project Deliverable D-2) includes a subset of instrument-related requirements ("IRx"), some of which are typically under the responsibility of the OCR manufacturer and/or its associated calibration laboratory, others are under the responsibility of the measurement scientist. The current section provides only the subset of these requirements ("IRxM") typically under the responsibility of the OCR manufacturer. Thus, as regards the calibration and characterisation of Ocean Colour radiometers to be used for Fiducial Reference Measurements:

IR1M. The uncertainty associated with radiometric responsivity of an OCR shall be estimated and delivered, including: the quantification of uncertainties from the radiometric calibration laboratory; and, for in-water measurements, (residual) uncertainties associated with immersion factors. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform these laboratory measurements.

IR2M. The uncertainty associated with straylight/out-of-band response of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements.

IR3M. The uncertainty associated with angular response of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.

IR4M. The uncertainty associated with non-linearity of an OCR shall be estimated and delivered, including any integration time response. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform these laboratory measurements.

IR5M. The uncertainty associated with thermal sensitivity of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.

IR6M. The uncertainty associated with polarisation sensitivity of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.

IR7M. The uncertainty associated with dark signal removal for an OCR measurement shall be estimated and delivered, including any possible temperature effects. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements.

IR8M. The uncertainty associated with temporal response (system transient response) for an OCR measurement shall be estimated and delivered. The project deliverable D-12 provides guidance on how to perform the laboratory measurements.

For new OCR models to be capable of performing a Fiducial Reference Measurement, they must provide the abovementioned IR1-IR8M laboratory characterisations.

In addition to the above requirements related to the measurement result, it is necessary to assign a value to the wavelength to which the measurement result refers. Like space and time coordinates, wavelength is an independent variable. When data is archived/used it is typical to have as metadata only the central wavelength and perhaps the bandwidth (as Full Width Half Maximum, FWHM). In the best cases the full spectral response function may be supplied.

It is proposed here that measurement results should be recorded for a central wavelength and bandwidth specific to each pixel or, for multispectral instruments, each spectral band on each OCR. The underlying spectral response function should be available in FRMOCnet/FidRadDB.

Thus, it is tentatively proposed here that:

IR9M. The uncertainty associated with wavelength scale for an OCR instrument shall be estimated (excluding factors such as straylight and out-of-band response already included in IR2M). This estimation shall be made relative to the central wavelength and bandwidth (assumed square or Gaussian) or to the full spectral response function. The FRM4SOC-2 project deliverable D-12, provides guidance on how to perform the laboratory measurements.

Again, for new OCR models to be included the FRMOCnet/FidRadDB, they must provide the abovementioned IR9 information.

Finally, for measurements to be included/flagged as "FRM" there should clearly be some documentation to describe traceably how these instrument-related requirements have been fulfilled. It is therefore suggested that inclusion of any measurement result as FRM should be subject to the documentation-related requirement ("DR") that:

DR1M. Each measurement result shall be linked to an OCR instrument, identified by serial number, and for which a document is available describing the SI traceable calibration and characterisation history.

and

DR2M. Each measurement result shall be linked to a document describing the detailed methodology used to estimate uncertainties IR1-IR9M, including all relevant equations, physical models and their associated parameters.

2.2 FRM Requirements for calibration laboratory standards and processes

The laboratories assigned to calibrate and characterise the Ocean Colour Radiometers (OCR) that are deployed in the field must themselves employ Secondary Optical Standards and processes ensuring traceability to SI units with an associated uncertainty. This upstream traceability, generally provided by National Metrology Institutes (NMIs), falls outside the scope of the 2003 NASA and 2019 IOCCG Ocean Optics Protocols, but was previously addressed by the NASA/SIRREX ("SeaWiFS Intercalibration Round Robin Experiments") activity, SIMBIOS program ("Second Intercomparison and Merger for Interdisciplinary Ocean Studies) [15], and the FRM4SOC-1 project Laboratory Calibration Experiment [Bialek et al, 2020].

As stated in section 5 of FRM4SOC2 deliverable D-12:

"A secondary laboratory performing calibration and characterisation of OCR instruments shall be able to provide to FRMOCnet, (ILAC) recognised accreditation certificate to ISO 17025 standard or self-declaration[1] documentation about conformance to this standard regarding their OCR calibration and characterisation activities.

The main issues required by ISO 17025 or equivalent involve (not a complete list; for full requirements, refer to ISO 17025):

- qualified personnel, with permanent monitoring of competence of personnel;
- facilities with a controlled environment (e.g. temperature and humidity control, dark rooms with low stray light level);
- permanent presence and redundancy of measurement standards and instrumentation;
- firm traceability to SI by regular calibrations and checks between calibrations of all significant instruments used for cal/char activities;
- defined cal/char procedures, including relevant protocols for characterisation of OCR;
- uncertainty budgets compiled and evaluated according to the cal/char procedures of the lab;
- periodic participation in relevant inter-comparison measurements.

This set of requirements must be present for each parameter for characterisation. Laboratories to be considered FRM compliant do not necessarily need to be formally accredited to ISO 17025. However, the principles of quality control as established by the standard must be fully followed for validated traceability and uncertainty budgets. Self-declaration shall include regularly updated documentation covering all issues listed in Table 51, which are presented clearly and with sufficient details."

Table 0-1. Minimum content of the self-declaration documentation for FRM labs. Reproduced from FRM4SOC-2 deliverable D-12.

Requirements for laboratories	Requirement in D-2
Requirements for the competence of personnel (qualification, training, supervision, authorisation, monitoring the competence)	Appendix B
Requirements for environmental conditions in a lab (suitability for lab activities, documented requirements, control/monitoring of conditions, access to lab)	IR1 – IR9
Access to principal measurement equipment needed for cal/char activities (documentation, handling, sufficient accuracy, validation of performance)	DR2
Calibration program for the measurement equipment, which shall be regularly reviewed and adjusted; labelling according to calibration status	DR2
Traceability charts for all relevant measurements ensure that results are traceable to SI units	DR3
Description of procedures, including detailed measurement models (appropriate updated documentation, validation, proper performance)	DR3
Relevant uncertainty budgets for all principal measurements	DR3
Reports of comparison exercises, analysis of comparison results	OR2
Description of internal quality procedures to maintain the conformance with requirements of the self-declaration to ISO 17025	DR4

In summary, as regards the calibration and characterisation laboratory standards and processes, inclusion of an OCR as FRM in FRMOCnet/FidRadDB should be subject to the documentation-related requirements ("DR") that:

DR3. The Secondary Laboratory performing calibration and characterisation of OCR instruments shall provide documentation describing the SI traceability of their in-house optical standards and calibration/characterisation processes. Guidelines for achieving this are provided in FRM4SOC2 deliverable D-11.

DR-3 may be achieved by suitably documented calibration/characterisation certificates provided together with any calibration/characterisation data.

Furthermore:

DR4. The Secondary Laboratory performing calibration and characterisation of OCR instruments shall be able to provide, (ILAC) recognised accreditation certificate to ISO 17025 standard or self-declaration documentation about conformance[1] to this standard regarding their OCR calibration and characterisation activities. Guidelines for achieving this are provided in FRM4SOC2 deliverable D-11.

3 Process for FRM "certification"

While section 2 of this document proposes a set of requirements "IRxM") and associated documentation-related requirements ("DR"), the question of how such requirements are checked or certified and by whom has not yet been decided. The topic of FRM "certification" requires further discussion – some preliminary ideas are provided in Appendix B of FRM4SOC2 deliverable D-2.

4 Recommendations for manufacturers

Whereas section 2 lists the *requirements* that must be met, this section provides some *recommendations* for manufacturers of OCR, particularly for the case of the design of new radiometers. These recommendations are based largely on lessons learned from the detailed analysis that has been made of the performance of the current generation of commercially-available OCR.

On the basis of recent experience it is recommended that:

Reference Measurements (FRM). FRM capability is precondition to use these OCRs for the Satellite Ocean Colour Validation. Therefore, the following recommendations for manufacturers are proposed:

[1] ISO "self-declaration" is not just a statement. All requirements of a standard (or other requirements document) apply. The conformance must be presented on a relevant forum or must have passed an external audit. The difference from accreditation is that the process is not done by a dedicated authorized (ILAC) body.

1. Materials used for the construction of principal parts of OCRs shall be optically and thermally stable in the full range of the operating conditions.

2. The internal optical, mechanical and electronic components shall continuously withstand the specified temperature limits.

3. Recommended operating conditions: from 0 °C up to 50 °C

4. Internal heat load of OCRs shall be as small as possible and shall not depend on operating mode

5. OCRs shall contain all construction elements needed for effective use of instruments:

a. Temperature control of the optical sensor (stabilized to a certain temperature in the range within 5 °C to 10 °C) or

b. Internal thermal sensor in vicinity of optical sensor (for OCRs without temperature control)

c. Reliable method for the measurement of the dark signal; for example, the entrance optics shall be occulted via a shutter or a cap

6. Maximum permissible errors of some parameters of OCRs shall meet the principal requirements of IOCCG Recommendations or equivalent, especially:

a. For the angular response (cosine collector)

b. For the accuracy of integration times

c. For the polarization sensitivity

7. The OCR specification shall include description of the complex effect of operating conditions in case inter-dependence of parameters is present -- e.g. dark signal shall be presented as a function of temperature and integration time. For long integration times the applicable upper temperature limit be lower than for the short times.

8. The provided calibration certificates and test protocols shall include the statement of uncertainties from the laboratory performing the radiometric calibration

9. Raw data from the sensor shall be available (all pixels, temperature, etc.) for instrument users

10. Instrument communication protocol shall be fully described

11. Teflon diffusers shall be avoided (because of temperature-dependent optical properties).

12. Cooperation between the manufacturers and users of OCR shall be initiated for preparation of unified protocol for collecting and handling of measurements data of the OCR.

5 Conclusions and Discussion

This document aims to specify the minimum requirements for qualification of individual OCRs as FRM instruments.

The requirements consist of instrument requirements under the manufacturers' responsibility ("IRx",) and associated documentation-related requirements ("DRx"). These have been explained in the preceding sections and are summarised in Table 5-1.

It is noted that the requirements stated here are already ambitious and some requirements may be difficult to reach for many instrument manufacturers in the short/medium term (3-5 year). The lack of radiometer characterisation information from many manufacturers is of particular concern.

This is the first version (v1) of a document that was presented, via the wider deliverable D-2, at the FRM4SOC-2 Project Workshop and will be further consolidated after review by the project Expert Review Board and by instrument manufacturers (if the latter have time to provide such comments).

Discussions at the FRM4SOC-2 with instrument manufacturers did include relevant feedback on these FRM requirements:

- While all instrument manufacturers have an associated calibration laboratory, either in-house or at a nearby dedicated subcontractor facility, such laboratories are not always ISO 17025 compliant.

- Very few instrument manufacturers are able to provide the required detailed characterisations although some may be available on request. These characterisations often require very specialised laboratory facilities and staff and the implementation can be extremely time-consuming and hence costly per instrument. If not required by the customer they will obviously not be performed. If not required by sufficient customers (in this very low volume market) they will not even be available on request.
- Support from major end-users such as space agencies may be necessary to overcome the significant economic barrier to achieving the required laboratory characterisations.
- The establishment of an equipment pool of OCR for which such characterisations have been performed may be a solution to ensure that FRM can be made by measurement scientists without the budgets needed to procure all required laboratory characterisations.
- It would be useful to understand which components of the uncertainty estimate contribute most to the total in order to prioritise cost effectively the related laboratory characterisations. This understanding may result from the end-to-end uncertainty estimations made within the FRM4SOC2 project.

Table 5-1. Summary of proposed instrument -related requirements under responsibility of the manufacturer ("IRxM") and associated documentation-related requirements ("DRx") for FRM usage.

Type	Description
IR1M.	The uncertainty associated with radiometric responsivity of an OCR shall be estimated and delivered, including: the quantification of uncertainties from the radiometric calibration laboratory; and, for in-water measurements, (residual) uncertainties associated with immersion factors. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform these laboratory measurements.
IR2M.	The uncertainty associated with straylight/out-of-band response of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 will provide guidance on how to perform the laboratory measurements.
IR3M.	The uncertainty associated with angular response of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.
IR4M.	The uncertainty associated with non-linearity of an OCR shall be estimated and delivered, including any integration time response. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform these laboratory measurements.
IR5M.	The uncertainty associated with thermal sensitivity of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.
IR6M.	The uncertainty associated with polarisation sensitivity of an OCR shall be estimated and delivered. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements themselves.
IR7M.	The uncertainty associated with dark signal removal for an OCR measurement shall be estimated and delivered, including any possible temperature effects. The FRM4SOC-2 project deliverable D-12 provides guidance on how to perform the laboratory measurements.
IR8M.	The uncertainty associated with temporal response (system transient response) for an OCR measurement shall be estimated and delivered. The project deliverable D-12 provides guidance on how to perform the laboratory measurements.
IR9M.	The uncertainty associated with wavelength scale for an OCR instrument shall be estimated (excluding factors such as straylight and out-of-band response already included in IR2M). This estimation shall be made relative to the central wavelength and bandwidth (assumed square or Gaussian) or to the full spectral response function. The FRM4SOC-2 project deliverable D-12, provides guidance on how to perform the laboratory measurements.
DR1M.	Each OCR instrument is identified by serial number, and has an associated document describing the SI traceable calibration and characterisation.
DR2M.	Each OCR instrument has an associated document describing the detailed methodology used to estimate uncertainties IR1-IR9, including all relevant equations, physical models and their associated parameters.
DR3M.	The Secondary Laboratory performing calibration and characterisation of OCR instruments shall provide documentation describing the SI traceability of their in-house optical standards and calibration/characterisation processes. Guidelines for achieving this are provided in FRM4SOC2 deliverable D-11.
DR4M.	The Secondary Laboratory performing calibration and characterisation of OCR instruments shall be able to provide, (ILAC) recognised accreditation certificate to ISO 17025 standard or self-declaration documentation about conformance to this standard regarding their OCR calibration and characterisation activities. Guidelines for achieving this are provided in FRM4SOC2 deliverable D-11.

6 References

1. Banks, A.C.; Vendt, R.; Alikas, K.; Bialek, A.; Kuusk, J.; Lerebourg, C.; Ruddick, K.; Tilstone, G.; Vabson, V.; Donlon, C.; et al. Fiducial Reference Measurements for Satellite Ocean Colour (FRM4SOC). *Remote Sens.* **2020**, *12*, 1322, doi:10.3390/rs12081322.
2. Białek, A.; Goodman, T.; Woolliams, E.; Brachmann, J.F.S.; Schwarzmaier, T.; Kuusk, J.; Ansko, I.; Vabson, V.; Lau, I.C.; MacLellan, C.; et al. Results from Verification of Reference Irradiance and Radiance Sources Laboratory Calibration Experiment Campaign. *Remote Sens.* **2020**, *12*, 2220, doi:10.3390/rs12142220.
3. Vabson, V.; Kuusk, J.; Ansko, I.; Vendt, R.; Alikas, K.; Ruddick, K.; Ansper, A.; Bresciani, M.; Burmester, H.; Costa, M.; et al. Laboratory Intercomparison of Radiometers Used for Satellite Validation in the 400-900 Nm Range. *Remote Sens.* **2019**, *11*, 1101, doi:https://doi.org/10.3390/rs11091101.
4. Vabson, V.; Kuusk, J.; Ansko, I.; Vendt, R.; Alikas, K.; Ruddick, K.; Ansper, A.; Bresciani, M.; Burmester, H.; Costa, M.; et al. Field Intercomparison of Radiometers Used for Satellite Validation in the 400-900 Nm Range. *Remote Sens.* **2019**, *11*, 1129, doi:https://doi.org/10.3390/rs11091129.
5. Ruddick, K.; Voss, K.; Banks, A.C.; Boss, E.; Castagna, A.; Frouin, R.J.; Hieronymi, M.; Jamet, C.; Johnson, B.C.; Kuusk, J.; et al. A Review of Protocols for Fiducial Reference Measurements of Downwelling Irradiance for Validation of Satellite Remote Sensing Data over Water. *Remote Sens.* **2019**, *11*, 1742.
6. Ruddick, K.G.; Voss, K.; Boss, E.; Castagna, A.; Frouin, R.; Gilerson, A.; Hieronymi, M.; Johnson, B.C.; Kuusk, J.; Lee, Z.; et al. A Review of Protocols for Fiducial Reference Measurements of Water-Leaving Radiance for Validation of Satellite Remote-Sensing Data over Water. *Remote Sens.* **2019**, *11*, 2198, doi:10.3390/rs11192198.
7. Tilstone, G.; Dall'Olmo, G.; Hieronymi, M.; Ruddick, K.; Beck, M.; Ligi, M.; Costa, M.; D'Alimonte, D.; Vellucci, V.; Vansteenwegen, D.; et al. Field Intercomparison of Radiometer Measurements for Ocean Colour Validation. *Remote Sens.* **2020**, *12*, 1587, doi:10.3390/rs12101587.
8. Białek, A.; Douglas, S.; Kuusk, J.; Ansko, I.; Vabson, V.; Vendt, R.; Casal, T. Example of Monte Carlo Method Uncertainty Evaluation for Above-Water Ocean Colour Radiometry. *Remote Sens.* **2020**, *12*, 780, doi:10.3390/rs12050780.
9. Donlon, C.J.; Wimmer, W.; Robinson, I.; Fisher, G.; Ferlet, M.; Nightingale, T.; Bras, B. A Second-Generation Blackbody System for the Calibration and Verification of Seagoing Infrared Radiometers. *J. Atmospheric Ocean. Technol.* **2014**, *31*, 1104–1127, doi:10.1175/JTECH-D-13-00151.1.
10. Hooker, S.B.; Zibordi, G. Advanced Methods for Characterizing the Immersion Factor of Irradiance Sensors. *J. Atmospheric Ocean. Technol.* **2005**, *22*, 757–770, doi:10.1175/JTECH1736.1.
11. Zibordi, G. Immersion Factor of In-Water Radiance Sensors: Assessment for a Class of Radiometers. *J. Atmospheric Ocean. Technol.* **2006**, *23*, 302–313.
12. Hooker, S.B. Characterization of Oceanographic and Atmospheric Radiometers (Chapter 5) - Stability Monitoring of Field Radiometers Using Portable Sources. In *Ocean Optics Protocols for Satellite Ocean Color Sensor Validation, Revision 4, Volume II: Instrument Specifications, Characterization and Calibration*; NASA/TM; 2003; pp. 50–57.
13. Zibordi, G.; Voss, K.; Johnson, B.C.; Mueller, J.L. *Protocols for Satellite Ocean Color Data Validation: In Situ Optical Radiometry (v3.0)*; Dartmouth, Canada, 2019;
14. Feinholz, M.E.; Flora, S.J.; Yarbrough, M.A.; Lykke, K.R.; Brown, S.W.; Johnson, B.C.; Clark, D.K. Stray Light Correction of the Marine Optical System. *J. Atmospheric Ocean. Technol.* **2009**, *26*, 57–73, doi:10.1175/2008JTECHO597.1.
15. Meister, G.; Abel, P.; Carder, K.; Chapin, A.; Clark, D.K.; Cooper, J.; Davis, C.; English, D.; Fargion, G.S.; Feinholz, M.; et al. *The Second SIMBIOS Radiometric Intercomparison (SIMRIC-2), March-November 2002*; 2003; pp. 1–76;.
16. Zong, Y.; Brown, S.W.; Johnson, B.C.; Lykke, K.R.; Ohno, Y. Simple Spectral Stray Light Correction Method for Array Spectroradiometers. *Appl. Opt.* **2006**, *45*, 1111–1119, doi:10.1364/ao.45.001111.
17. BIPM *International Vocabulary of Metrology – Basic and General Concepts and Associated Terms (VIM)*;
18. Bouvet, M.; Thome, K.; Berthelot, B.; Bialek, A.; Czapla-Myers, J.; Fox, N.P.; Goryl, P.; Henry, P.; Ma, L.; Marcq, S.; et al. RadCalNet: A Radiometric Calibration Network for Earth Observing Imagers Operating in the Visible to Shortwave Infrared Spectral Range. *Remote Sens.* **2019**, *11*, 2401, doi:10.3390/rs11202401.