

Template for Annual SCOR Working Group Reports to SCOR

1. Name of group

SCOR Working Group 148 (since April 2016)

International Quality Controlled Ocean Database: Subsurface temperature profiles (IQuOD)

2. Activities since previous report to SCOR (e.g., virtual or in-person meetings, email discussions, special sessions). Limit 1000 words

A brief summary of key activities:

- [Public release of first interim IQuOD dataset \(v0.1\)](#), including intelligent metadata for XBT instruments and uncertainty assignments (March 2018)
- [Peer-reviewed publication of intelligent metadata algorithm in Journal of Atmospheric and Oceanic Technology](#) (March 2018)
- [Annual IQuOD workshop was held at IODE in Ostende](#), Belgium during 16th-18th April 2018 (in conjunction with XBT Science Team meeting)
- Various email discussions around uncertainty and intelligent metadata assignments in the run-up to the v0.1 data release.
- Various data-checking activities around release of v0.1 dataset.
- Various progress made in IQuOD Task Teams – see IQuOD workshop link below for links to Task Team presentations.
- IQuOD members co-chaired a session at AGU Ocean Sciences 2018, including an invited presentation from Tim Boyer on IQuOD v0.1. More details available here: <https://agu.confex.com/agu/os18/meetingapp.cgi/Session/37001>
- IQuOD members co-chaired a session at the EGU annual general assembly, including an invited presentation from Steve Diggs on IQuOD v0.1. More details available here: <https://meetingorganizer.copernicus.org/EGU2018/orals/26551>

3. Documents published since previous report to SCOR (e.g., peer-reviewed journal articles, reports, Web pages) and should be limited to publications that resulted directly from WG activities and which acknowledge SCOR support

The first version (v0.1) of the IQuOD database has been published and is available to download from the NOAA National Centers for Environmental Information website:
<https://data.nodc.noaa.gov/cgi-bin/iso?id=gov.noaa.nodc:0170893>

This first data release includes provision of intelligent metadata for unknown XBT profiles (see Palmer et al, 2018 below) and uncertainty assignments. A description of the dataset is available here:

https://www.nodc.noaa.gov/archive/arc0118/0170893/1.1/data/0-data/IQuOD_v0.1_information.pdf

“An Algorithm for Classifying Unknown Expendable Bathythermograph (XBT) Instruments Based on Existing Metadata” M.D. Palmer, T. Boyer, R. Cowley, S. Kizu, F. Reseghetti, T. Suzuki and A. Thresher, Journal of Atmospheric and Oceanic Technology, published online 8th March 2018.

<https://journals.ametsoc.org/doi/abs/10.1175/JTECH-D-17-0129.1>

The agenda and presentations from the 2018 IQuOD workshop are available here:

https://iode.org/index.php?option=com_oe&task=viewEventRecord&eventID=2100

Workshop report (current draft version):

https://www.dropbox.com/s/xqx5kzib6w2uw0l/IQuOD_5th_workshop_report_draft_v03.docx?dl=0

Various updates have been published on the AutoQC GitHub code repository:

<https://github.com/IQuOD/AutoQC>

Progress on data formats on GitHub code repository:

<https://github.com/IQuOD/Formats>

4. Progress toward achieving group’s terms of reference. List each term of reference separately and describe progress on each one. Limit 1000 words

SCOR WG 148 proposal: [Copy](#)

1. To develop, implement and document algorithms for assignment of “intelligent” metadata – i.e. an informed guess as to likely values for missing information – for temperature profiles where crucial metadata is missing.

Palmer et al (2018) paper describing the IQuOD v0.1 intelligent metadata algorithm has been published in Journal of Atmospheric and Oceanic Technology. These metadata assignments have been included in the v0.1 IQuOD database (published March 2018).

2. To evaluate and document the most effective combination of automated quality control (AutoQC) procedures for temperature profile observations. International collaboration will be required for the design and coordination of benchmarking experiments using high quality reference datasets.

50 AutoQC tests from six different institutions have been implemented and are freely available from the GitHub repository: <https://github.com/IQuOD/AutoQC>

Progress has been made improving the software infrastructure and code to assess the performance of AutoQC combinations to yield best combination of tests for a given false positive rate. A first assessment of best combinations has been carried out on the QuOTA dataset.

3. To establish and implement a set of optimal automated quality control procedures, by reaching international community consensus and using the knowledge gained in the benchmarking tests from ToR-2 (above); to produce and publish a reference guide for best practices in automated quality control of ocean temperature profiles; and to develop and freely distribute an open-source quality control software toolkit to promote wide and rapid adoption of best practices by the oceanographic community.

All code continues to be made available in real-time via the GitHub repository. Analysis of AutoQC tests has begun and will form the basis of a scientific paper.

4. To examine and document the feasibility of machine learning and other novel computational methods for enhanced quality control, to potentially minimize labor costs associated with human expert quality control procedures.

Machine learning approaches are being used as part of the AutoQC benchmarking exercise (e.g. the CoTeDe “fuzzy logic” test). Machine learning approaches are also being investigated for future assignment of XBT intelligent metadata (iMeta). A paper on applying a neural network approach to iMeta is currently under revision at Journal of Atmospheric and Oceanic Technology with a more comprehensive intercomparison of various Machine Learning approaches underway at the UK Met Office.

5. To develop, implement and document internationally agreed best practice methods for assignment of uncertainty estimates to each temperature observation.

A first approach to assignment of uncertainty to each temperature observation has been devised and is incorporated into the IQuOD v0.1 dataset. Details are available here:

https://www.nodc.noaa.gov/archive/arc0118/0170893/1.1/data/0-data/IQuOD_v0.1_information.pdf

6. To freely disseminate (interim) versions of the IQuOD global temperature profile database (and added value-products) as it evolves over the next 3 years, in user-friendly file formats.

A first v0.1 IQuOD dataset has been released, using the World Ocean Database file format, which is widely used by the international community. There are ongoing discussions on the file format for the first complete IQuOD release (including AutoQC flags), which will be based upon the widely-used Argo NetCDF format. More details are available here: <https://github.com/IQuOD/Formats>

7. To share knowledge and transfer skills in instrumentation, regional oceanography, quality control procedures and data stewardship with international scientists in both developed and developing nations.

Knowledge transfer activities are reflected in the strong representation from at the AGU Ocean Sciences meeting in February 2018 and the EGU general assembly meeting in April 2018. The 2018 IQuOD workshop was well attended with participants from a range of different countries. More details here: https://iode.org/index.php?option=com_oe&task=viewEventParticipants&eventID=2100

5. WG activities planned for the coming year. Limit 500 words

The main focus for the coming year is working towards a full release of the IQuOD database, including an optimal set of automated QC checks. We also expect to deliver incremental improvements in provision of intelligent metadata for XBT instruments and uncertainty estimates.

We expect to submit a paper on the automated QC comparisons and document the set of checks that have been used for the IQuOD v1.0 data release (expected during 2019).

6. Is the group having difficulties expected in achieving terms of reference or meeting original time schedule? If so, why, and what is being done to address the difficulties Limit 200 words

It may be necessary to entrain more effort into the AutoQC comparison work.

7. Any special comments or requests to SCOR. Limit 100 words.

We are planning to submit a 4-year IQuOD-related project proposal for the Australian Research Council – Linkage Projects in December 2018. We will need to have cash (max. AUS 30 K/year) and in-kind contributions, from international and national (potential) partners. Technical focus will be on data rescue and Expert Quality Control activities.

Additional information can be submitted and will be included in the background book for the SCOR meeting at the discretion of the SCOR Executive Committee Reporter for the WG and the SCOR Secretariat.