QuinCe: An online tool for processing and quality control of surface ocean CO$_2$ measurements

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Scientists collecting surface ocean CO$_2$ measurements must perform data reduction and quality control (QC) prior to further usage of the data. The tools for these tasks are typically developed by the scientists themselves, leading to dozens of different software programs in use across the community. Different interpretations of protocols lead to inconsistent data handling, and since these self-developed tools are rarely published there is little transparency and traceability for users of the data – increasing the overall uncertainty of these observations.

The Ocean Thematic Centre (OTC) of the pan-European Research Infrastructure Integrated Carbon Observation System (ICOS) is developing online software to provide data reduction and QC tools for all members measuring surface ocean CO$_2$. Scientists submit the raw data from their instruments, which will be processed to calculate surface fCO$_2$ using a fully open source set of algorithms based upon internationally agreed and defined criteria. A suite of automated QC tools, based on those developed for the Surface Ocean CO2 Atlas (SOCAT), will identify basic issues such as out-of-range data, outliers, date/time issues etc., and flag them for later verification by the scientist. Plotting and mapping tools will allow detailed inspection of the data to locate further potential issues. Each data record will be assigned a WOCE flag stating the quality (Good, Questionable or Bad). Once this QC has been completed, the data can be exported in a variety of formats, and/or submitted directly to central data archives such as the ICOS Carbon Portal or SOCAT.

Metadata will be integrated into this process using internationally approved protocols and schemas which are currently being developed in conjunction with partner institutions and projects[1], thus rendering the handling of data processing, quality control and metadata from collection to publication fully operational within the sphere of ICOS.

Data provenance will be recorded in a number of ways. Data sets published through the ICOS Carbon Portal will include both the quality-controlled data and the original data files as they were uploaded to QuinCe. For other projects, these files will be available on demand. The metadata for each data set will include a note stating that processing was performed using QuinCe, with version numbers so the exact code used can be traced in future (all versions of QuinCe will be archived in a public version control system). Records of every quality control flag set by the automatic and manual quality control processes will be kept in QuinCe. These can be made available as required, but protocols for standardising and automating such features have not yet been developed.

Unified tools like QuinCe will streamline data processing, helping to reduce delays in data publishing. This is becoming ever more important as demand for up-to-date climate data grows (e.g. the United Nations Sustainable Development Goals 14.3 [Ocean Acidification]). Planned features such as accepting near real time data streams transmitted directly from the instruments themselves and more sophisticated automatic QC checks will allow even greater time savings. Easy-to-use data inspection tools will reduce the effort required to perform additional manual QC. Data centres will be assured that data submitted via QuinCe will have undergone a minimum level of QC, with records of both the automatic and manual QC providing complete transparency and improved stewardship. QuinCe will also ensure automatic data conversion to formats required by data centres, reducing the incidence of

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[1] NOAA Ocean Acidification Project, NOAA PMEL, and NOAA NCEI OCADS

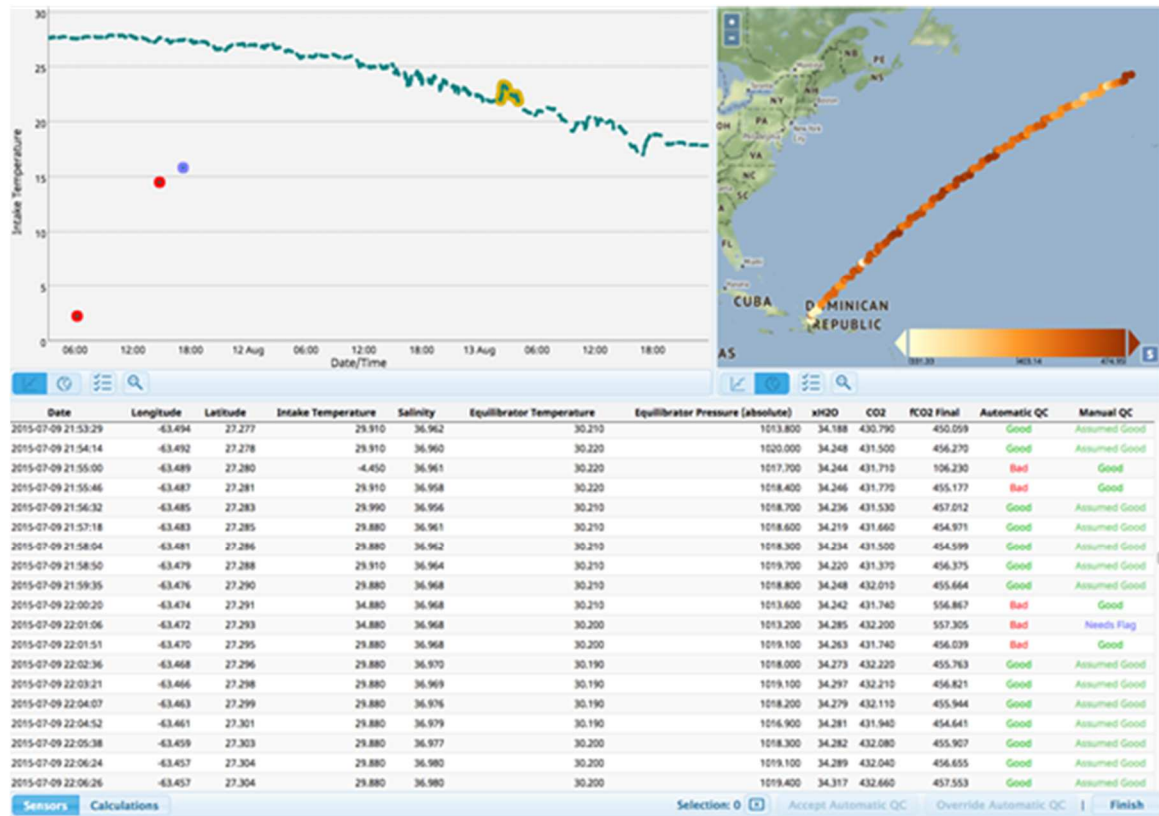data transmission and formatting errors and also reducing the workload of both the scientists and data managers.

Figure 1: Example of the Quality Control screen in the QuinCe software