PAPA
Design of common protocols
for
data collection, transmission and quality control

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Deliverable D3.1

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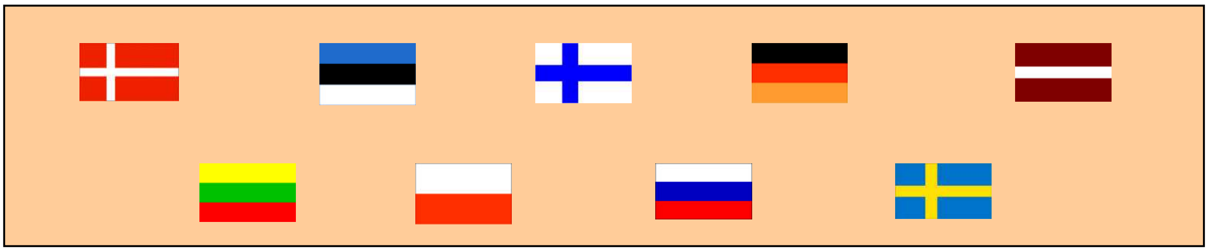
www. boos.org/papa/papa.html



Deliverable D3.1

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A web based on-line questionnaire and MYSQL database is an essential part of this deliverable. It is installed under http://www.io-warnemuende.de/papa (user: papa, pwd: apap).

Contents

Executive Summary

"Operational oceanography includes a routinely collection, interpretation and presentation of data from the ocean and atmosphere with the purpose of:

- Giving an reliable description of the actual conditions of the sea including its living resources
- Providing prognoses for the future developments of the conditions in the sea
- Establishing a marine database from which time series and statistical analysis can be obtained for descriptions of trends and changes in the marine environment including consequences for the living conditions in, on and around the sea."

[BOOS Plan, Buch and Dahlin 2000]

In order to attain this goal, an over-all quality assurance for operational real-time measurements is of great importance. Therefore, the following tasks were carried out in the framework of the PAPA OBS sub project:

- Improvement of Quality Assurance (QA) protocols for operational real-time measurements in the Baltic Operational Oceanographic System (BOOS)
- Development of a web based questionnaire with a MYSQL database system to obtain an inventory of the existing quality assurance protocols in BOOS
- Set up of the QA database as a living system for the evaluation and sustainable on-line use as inventory for the other PAPA work packages
- Development of new protocols and strategies for comprehensive quality assured operational real time data around the Baltic Sea

1 Introduction

The upgrade of an operational observing and forecasting system in the Baltic Sea is the overall task of the PAPA project. Within the scope of BOOS, high quality data sets and long time series are needed. In order to obtain high quality data, common protocols for quality control are essential.
Within PAPA OBS (WP3) task 3.2 and task 3.3 common protocols have been developed. They are based on the evaluation of basic data pre-processing procedures and existing quality assurance (QA) protocols.

The main objective of quality control for operational data is to ensure data consistency for each measured parameter within a collection of operational data. One of the most important goals must be to assure that the quality and errors associated with the data are transparent to the user. Therefore, additional quality assurance procedures have to be applied and meta data must be collected regularly as quality assurance information. Data quality assurance information notifies users of the data about the way in which they were gathered, checked, and processed. It also provides information about the types of algorithms used, the kinds of errors that occurred, and how these errors were corrected or flagged.

Therefore, the following tasks were focussed on in the implementation plan of PAPA OBS:

Task 3.2: Evaluation of basic data pre-processing procedures
(Feb 2003 – Oct 2003)

(Extract from the implementation plan)
The methodology (software) used by each partner for data pre-processing procedures will be compared … Although there is considerable experience on data quality assurance in the processing stage, common protocols for quality performance will be stated. Its application will be the first step towards establishing procedures for the assurance of comparability and compatibility of data acquisition, transmission and exchange systems by each institution.

Implementation:
The sensor depending processing SW converting raw data to physical data will not be dealt with. The main purpose is to compare the first procedures controlling the data-flow from sensor to real data.

Task 3.3: Evaluation of the quality assurance protocols
(Feb 2003 – Oct 2003)

(Extract from the implementation plan)
The quality of the data is assured by a series of protocols driving the operational activity from collection design, to fieldwork, data transmission, quality control and dissemination practices. All these aspects will be evaluated in order to define common protocols and achieve a defined 'minimum performance level' for operational systems.

Implementation:
Parallel to task 3.2 the pre-processing SW is analysed to get some common methods to define common protocols in achieving a 'minimum performance criterion' for operational systems.

In the context of this sub work package, the understanding of 'common protocols' is the following**:**

Common protocols include all steps, which are necessary to collect quality controlled operational data:

1. Inspection of sensors / instruments at a laboratory by using reference standards
2. Regular reference measurements during a measuring period
3. Calculation / conversion algorithms
4. Overall data transmission
5. Data processing
6. Storage and flagging (including all quality assurance procedures)

In order to fulfil the implementation plan in a first step, it was necessary to get an overview of the participants' operationally measured parameters and the established standards for quality assurance (QA). Therefore, a questionnaire and QA inventory had to be developed.
After the first project meetings, it became clear that the questionnaire and inventory had to be strictly parameter orientated.

A timetable of the development and implementation of the questionnaire and QA database system for quality assurance is added in annex table 1.

2 QA protocols and pre-processing procedures

Description of the web based questionnaire and database system

An accelerated collection of the participant's QA meta information in accordance with the project time schedule necessitated the build up of a web-based questionnaire and database as a living and sustainable system. The established questionnaire is based on a php interface combined with a MYSQL database. It is divided into three main sections:
1. General information on participants
2. Input forms
3. Export of database content.

The structure of the questionnaire is clearly parameter type orientated. The current version consists of four parameter types:

Hydrography	[2.1]	Table 3
Meteorology	[2.2]	Table 4
Biology	[2.3]	Table 5
Chemistry	[2.4]	Table 6

For each of these parameter types, separate input forms are provided. The input forms include a list of parameters (e.g. temperature [2.1.1], salinity [2.1.2], oxygen [2.1.4] etc.) which can be attributed to either of the following measuring locations: moorings / mixed stations, ship borne measurements and other locations (e.g. a temperature measurement from a fixed station has the number [2.1.1.1]).The project participants have the opportunity to extend the list of parameters according to their data sets. An inventory of the current parameter types is listed in the annex table 2.

The web-based questionnaire and database system was installed on a web server the project partners having access via a password.
The project's participants filled in the questionnaire input forms according to the following procedure:
(1) All participants were requested to provide general information on:
Institute, contact person, expert person for quality assurance, and contact address
(annex table 2)
(2) Participants could then complete the input forms of the quality assurance questionnaire according to the above described structure.
Each input form is based on a list of thirteen questions (measuring instrument, accuracy, calculation / conversion algorithms, QA-reference, sensor calibration (laboratory pre / post), field reference measurements, post correction (validation), and QA-algorithms). The information obtained from the questionnaire is automatically submitted to the QA MYSQL database. The results are immediately available on the web page of the system. The design of the questionnaire facilitates substantial changes and updates of the database.
(3) A web-based data export from the database is available for every project participant. Field orientated summary reports (institute, parameter, location etc.) can also be presented on the web page.
For individual use (e.g. other PAPA work packages, BOOS products etc.) all information of the MYSQL-database is transferred into the ftp-box of the IOW on a regular basis.

3 Results of the QA database

A preliminary version of the web-based questionnaire was released and made available to all project partners on July 31, 2003. In August, September, and October 2003 several parameters were added to the questionnaire due to feedback and comments from a number of participants. All project partners were asked to complete the questionnaire until the beginning of November 2003. The results of this questionnaire were reported and discussed at the annual PAPA meeting in Gdansk (November 28, 2003). Information on quality assurance is now available from all participants.

3.1 General results from questionnaire

Until November 4, 2003, 438 logins to the questionnaire web page were recorded. The distribution among the different parameter types within the database is as follows:

103 Hydrographical parameter sets
48 Meteorological parameter sets
52 Chemical parameter sets
21 Biological parameter sets

The following list includes some details on the number of institutes which filled in the questionnaire and the number and types of measuring locations.

General	[1]:	***14 / 15 Institutes*** (November 4) ***15 / 15 Institutes*** (December 4)
Hydrographical parameters	[2.1]:	***14 / 15 Institutes*** 103 parameter sets (62 station / mooring, 31 ship, 10 other locations)
Meteorological parameters	[2.2]:	***10 / 15 Institutes*** 47 parameter sets (35 station / mooring, 12 ship, 0 other locations)
Biological parameters	[2.3]:	***14 / 15 Institutes*** 21 parameter sets (2 station/ mooring, 16 ship, 3 other locations.)
Chemical parameters	[2.4]:	***6 / 15 Institutes*** 52 parameter sets (10 station/mooring, 34 ship, 8 other locations)
Export function used	[3]:	121 times

Thus, a considerable amount of information is now available for the evaluation of common quality assurance protocols of operational oceanographic data for the Baltic Sea community.

3.2 General evaluation of basic data pre-processing procedures

According to the implementation plan, the software used by each partner for data pre-processing procedures had to be compared. Within this task the sensor depending processing software had not to be dealt with (extract implementation plan). In order to find a suitable solution, section 3.2.1 was extended to “overall data processing algorithms for operational measurements”.

The comparison also had to consider each partner’s requirements for common protocols controlling the operational collection and transmission of data. An extended understanding of ‘common protocols’ was developed for this subtask and includes now all steps, which are necessary to ensure the quality of operational data. Equal procedures and methods for the assurance of comparability and compatibility of data acquisition, transmission and exchange systems by each institution still need to be established.
These topics are discussed in section 3.3.

3.2.1 Data preprocessing algorithms

The web based questionnaire and the database system include the established algorithms, which drive the pre processing software.
As an example the algorithms for temperature, salinity and oxygen are discussed briefly. A complete list of algorithms established among the project partners is attached under annex table 7.

3.2.2 Development of common protocols

In this project, the term ‘common protocols’ was defined as “all steps which are necessary to assure the quality of operational data” (3.3.).
According to the topic of data transmission protocols a detailed evaluation was carried out already under the scope of the EU-project FIESTA (FIESTA EUROMAR-PROJECT, 1993). FIESTA recommends using modern conversion and communication facilities for oceanographic data transmission. During the last decade, modern digital data transmission facilities have become much easier to use and more secure, reducing the error rates significantly. Error correction methods have been and will be introduced. For this reason, no further investigations were carried out in this sub task.

Experiences from previous projects have shown that strict definitions of data formats need to be avoided. Therefore, BOOS allows almost free data formats to be submitted by the participants. Formats are restricted to the ASCII-Format only (3.2.3). The conversion to joined formats will be done by tools developed under WP 7 (PAPA INFO).

3.2.3 Dissemination of information and results

The ftp-box system, previously developed in BOOS has been significantly improved by PAPA OBS and INFO (WP3 and 7). All partners are obliged to use the individual ftp-box (read only by the other partners) for filling in operational data, meta data, disclaimer, header and format information.
The only restriction is the use of the ASCII-format. Using the ASCII-format individual data sets are formed and available for all partners (e.g. real time data and the inventory of the QA database are available via the IOW-ftp-box in ASCII format, too.)

3.3 Evaluation of Quality assurance protocols

Within this project, the quality of the data is assured by a series of protocols driving the operational activity from collection design, to fieldwork, data transmission, quality control and dissemination practices. All these aspects will be evaluated in order to define common protocols and achieve a defined 'minimum performance level' for operational systems (extract from implementation plan).

3.3.1 Inventory of existent quality assurance (QA) protocols

The necessary inventory was derived from the web based QA questionnaire and database system (available via the IOW-ftp-box).
According to the structure of the QA questionnaire and database system an evaluation for hydrographical, meteorological, biological and chemical parameters was carried out.

In order to depict the evaluation procedure and results, a detailed analysis of three selected parameters (temperature, salinity and oxygen) are presented.

Hydrographical parameters

- Most of the operational hydrographical data are available in real time.
- The quality standards between the different parameter vary.
- Quality assurance for sea level measurements is generally warranted (ISO standard and local certification).
- QA is generally assured for measurements of temperature, conductivity (salinity), and oxygen water samples (bottles).
- QA for wave direction and height measurements, as well as QA for current measurements is carried with algorithms from the equipments’ producers.
- There is a lack of general common protocols for hydrographical operational real-time measurements.
- For real time data presentation only a few and simple algorithms are already applied.
- QA flags to assure QA for database archiving are not yet standardised.
- High performance WOCE-standards are available for CTD – profiling.

Meteorological parameters

- Generally, the atmosphere is a less aggressive environment.
- The instruments applied by the partners are simple and stable.
- Regular calibrations are carried out by either the producers or weather services.
- There is considerable long term experience in operational real time measurements.
- Problems with QA for optical sensors not solved.

Chemical parameters

- Only a few operational real time measurements are available (nutrients), most are shipboard or near shore bottle measurements for monitoring purposes.
- For data derived from bottle samples, QA standards and algorithms are generally used.
- Inter calibrations between the institutes and reference laboratories are carried out regularly.
- Standard protocols are defined by HELCOM and ICES.
- Standard laboratory calibration procedures are assured by e.g. QUASIMEME.

Biological parameters

- Only a few operational real time measurements are available (bio-optical measurements), most are shipboard or near shore bottle measurements for monitoring purposes.
- Protocols are well defined by HELCOM and ICES.

Most of the participating groups are associated with their hydrographical departments. Therefore, most of the information of the QA inventory is related to physical oceanography. Hydrographic measurements dominate real-time operational measurements. A gap was detected in the acceptance of common protocols for QA operational real-time hydrographic measurements.
As an example in the following paragraph, a detailed compilation is done for temperature, conductivity (salinity) and oxygen.

Evaluation for Temperature

Institutes (14):	BSH, CMR, DMI, FIMR, IMWM, IOPAS, IOW, LHMA, MIG, MSI, RDANH, SMHI, SYKE, UL
Instruments:	Seabird (SBE): SeaCat, Sealogger, MicroCTD; Pt100; Thermometer 3-MT; FSI; Aanderaa C/T/D Seabird: SBE911, SBE19-03, SBE49; GO Mark III; CTD ECO; FSI CTD; Thermistor sensor , Hg Thermometer
Pre calibration:	3 lab calibration, 4 by manufacture, 7 no calibration
Ref measuring:	6 regularly, 8 no measuring
Post correction / validation:	6 post val., 8 no val.
Calculation algorithm:	6 ITS-90, 8 no information
Quality reference:	3 accreditation, 2 local certification, 9 no

Quality flags:	6 yes, 8 no	
Quality algorithm:	5 spike, limit control 1 adaptive limits filter, 8 no information	
System* accuracy of measurement:	shipboard	3 x 0.005K, 3 x 0.01K, 3 x 0.05K
	fixed station	3 x 0.01K, 2 x 0.05K, 2 x 0.1K
System* stability (drift):	shipboard	between 0.1 and 0.001K/month
	fixed station	between 0.01 and 0.001K/month
System* resolution:	shipboard	between 0.01 and 0.001K
	fixed station	between 0.1 and 0.001K
Sensor accuracy (from producer):	shipboard	between 0.01 and 0.001K
	shipboard	between 0.1 and 0.001K

Evaluation for Salinity (Conductivity)

Institutes (12):	BSH, CMR, DMI, IMWM, IOPAS, IOW, MIG, MSI, RDANH, SMHI, SYKE, UL	
Instruments:	Aanderaa C/T/D, Autosal Seabird: SBE911, SBE49 SEACAT; CTD ECO; Valeport Model Mark III	
Pre calibration:	9 yes, 3 no calibration	
Ref measuring:	7 yes, 5 no	
Post correction / validation:	6 post val., 6 no val.	
Calculation algorithm:	8 x pss-78, 4 x no information	
Quality reference:	5 x certification, 7 no	
Quality flags:	4 yes, 8 no	
Quality algorithm:	4 x spike, limit control, 8 no	
System* accuracy of measurement:	shipboard	between 0.01 and 0.001psu
	fixed station	between 0.01 and 0.005psu
System* stability (drift):	shipboard	between 0.1 and 0.001psu
	fixed station	between 0.1 and 0.001psu
System* resolution:	shipboard	between 0.01 and 0.001psu
	fixed station	between 0.01 and 0.005psu
Sensor accuracy (from producer):	shipboard	between 0.05 and 0.001psu
	shipboard	between 0.01 and 0.001psu

Evaluation for Oxygen

Institutes (7):	BSH, CMR, IOW, MSI, SMHI, SYKE, UL BSH, IOW (fixed station)
Instruments:	Water sample (Winkler Titration); Zuellig; Seabird: SBE911, YSI; SAIV205; Autoburette
Pre calibration:	2 yes, 5 no calibration
Ref measuring:	3 yes, 4 no
Post correction / validation:	3 post val., 5 no val.
Calculation algorithm:	2 x Owens and Millard 1985, 5 no information
Quality reference:	3 x certification, 4 no
Quality flags:	1 yes, 6 no
Quality algorithm:	3 spike, limit control, 4 no information
System* accuracy of measurement:	between 0.01 and 0.5 ml/l
System* stability (drift):	between 0.01 and 0.5 ml/l
System* resolution:	between 0.01 and 0.1 ml/l
Sensor accuracy (from producer):	between 0.01 and 0.5 ml/l

3.3.2 Definition of common protocols for a 'minimum performance criterion'

Common protocols for bottle data (ship borne / near shore measurements of biological and chemical parameters), meteorological- and profiling hydrographical measurements are well defined and established (ICES/HELCOM Advisory Committee on the Marine Environment , 2002, ICES/HELCOM Advisory Committee on the Marine Environment , 2002, IOC CEC: DG-XII, MAST and IOC: IODE,1993 Manual and Guides 26, MILLARD, R., 1993, GRASSHOFF, K., K. KREMLING UND M. EHRHARDT, 1999, UNESCO, 1978, WEISS, R. F., 1970). For these types of measurements, well-defined and established QA protocols have to be fulfilled as 'minimum performance criteria'.
In the Baltic operational observing and forecasting system fixed offshore stations, moorings etc. with real time data transmission are of growing importance. However, the number of offshore automatically operating stations is still low. Most of the platforms are equipped with hydrographical and meteorological sensors only. Until now, very few biological and chemical instruments are used on real-time observation platforms. Bio-fouling, corrosion and damages in heavy seas are the outstanding problems. All of these cause slightly larger drifts of the sensors.
To apply reference measurements and established QA methods regularly is difficult due to the remoteness of the offshore stations and high costs.
There is a real lack of special biological and chemical QA methods for off shore operational platforms and the well developed laboratory QA methods can not be used in most cases.
For this reasons, new common protocols for QA for operational real-time measurements have been and have still to be developed.

The inventory obtained from the QA questionnaire and database system shows the following results:

Pre deployment check

67 of 115 hydro	35 of 47 met	5 of 22 bio	44 of 66 che

During deployment comparison

53 of 115 hydro	29 of 47 met	8 of 22 bio	31 of 66 che

Data pre- and post processing

61 of 115 hydro	15 of 47 met	3 of 22 bio	30 of 66 che

Flagging

21 of 115 hydro	5 of 47 met	0 of 22 bio	10 of 66 che

Generally, three common protocols for the quality assurance of operational real time measurements for the BOOS community were derived. The following section briefly exemplifies criteria for best, good and minimum performance protocols.

Common Protocols for operational real time measurements

A) Best performance QA protocol for operational oceanographic measurements

10 steps to get high accuracy quality controlled datasets

1. **Pre-conditions -**
   - use of accurate, low drift sensors (e.g. with fouling protection) and digital outputs.
   - digital data transmission protocols meet modern common standards with error protection.

2. **Pre deployment calibration** -
   - brand -new calibration from producer.
   - Sensor / instrument check and calibration with reference standards at laboratory.
   - documentation of calibration parameters.
   - test of data transmission, processing performance and recording facilities.

3. **Pre deployment check** -
   - check and comparison before deployment (e.g. ship borne CTD / water sample).

4. **Deployment documentation** -
   - recording of parameters (location, instrument information, meta information, sampling scheme etc.).

5. **During deployment comparison** -
   - reference measurements during deployment / measuring period (e.g. every month with ship borne CTD and water samples or as often as possible).

6. **Post deployment check** -
   - comparison measurements after deployment (e.g. ship borne CTD / water sample).

7. **Post deployment calibration -**
   - sensor- / Instrument check and calibration with reference standards at laboratory.
   - documentation of calibration parameters.

8. **Data pre-processing** -
   - Automatic quality control of data (e.g. corrupted data, spikes, identification gaps etc.).
   - transfer to database.
   - flagging.

9. **Data post processing** -
   - correction and validation by using reference / comparison measurements.
   - application of quality flags to the database (including meta data and validation steps).

10. **Data presentation** -
    - user-friendly presentation of data, meta data and graphics via the web.

B) Good performance QA protocol for operational oceanographic measurements

8 steps to get high accuracy quality controlled datasets

1. **Pre-conditions** -
   - use of accurate, low drift sensors (e.g. with fouling protection).
   - analog/digital data transmission protocols.

2. **Pre deployment calibration** -
   - current calibration from producer.
   - sensor / instrument check.
   - documentation of calibration parameters.
   - test of data transmission, processing performance and recording facilities.

3. **Deployment documentation** -
   - recording of parameters (location, instrument information, meta information, sampling scheme etc.).

4. **During deployment comparison -**
   - reference measurements during deployment / measuring period (e.g. with ship borne CTD and water samples as often as possible).

5. **Post deployment check** -
   - comparison measurements after deployment (e.g. ship borne CTD / water sample).

6. **Data pre-processing** -
   - quality control of data (e.g. corrupted data, spikes, identification of gaps etc.).
   - transfer to files/databases.
   - flagging.

7. **Data post processing** -
   - correction and validation by using reference / comparison measurements.
   - application of quality flags to files / databases (including meta data and validation steps).

8. **Data presentation** -
   - user-friendly presentation of data, meta data and graphics.

C) Minimum performance QA protocol for operational oceanographic measurements

6 steps to get high accuracy quality controlled datasets

1. **Pre-conditions** -
   - use of accurate, low drift sensors (e.g. with fouling protection).
   - analog/digital data transmission protocols.

2. **Pre deployment calibration** -
   - calibration from producer.
   - sensor / instrument check and documentation.

3. **Deployment documentation** -
   - recording of parameters (location, instrument information, meta information, sampling scheme …).

4. **During deployment comparison -**
   - reference measurements during deployment / measuring period for sensors/ instruments with noticeable drift.

5. **Post deployment check** -
   - comparison measurements after deployment (e.g. ship borne CTD / water sample).

6. **Data processing** -
   - correction and validation by using reference / comparison measurements.
   - flagging /labelling of data (including meta data and validation steps).

4 Recommendations

1. New guidelines for common protocols for quality assurance of operational real-time measurements are defined in PAPA OBS, task 3.3.2 A)-C). This guidelines have to be adopted in the Baltic Operational Oceanographic System (BOOS). They have to be further developed for new parameters.

2. It is strongly recommended to use additionally the following well established guidelines for the quality assurance and to combine them with the new common quality assurance protocols:

   IOC CEC: DG-XII, MAST and IOC: IODE,1993 Manual and Guides 26
   - Manual of Quality Control Procedures for Validation of Oceanographic Data
   ICES/HELCOMAdvisory Committee on the Marine Environment , 2002
   - ICES/HELCOM Steering Group on Quality Assurance of *Chemical* Measurements
   - ICES/HELCOM Steering Group on Quality Assurance of *Biological* Measurements

3. New protocols for QA documentation and quality flags for operational real-time measurements have to be developed, adopted and used as standard tools.

4. The quality assurance methods for operational real-time measurements have to be generally improved by:
   - regular inter-calibrations among the partners,
   - the establishment of a joined calibration laboratory in the Baltic countries for cost effective calibration of sensors and instruments with the same standards.

5. In the future, new projects have to be launched also to introduce a new phase of “scientific QA methods” for operational real-time measurements. “Scientific QA methods” mean that the data have been scrutinized according to the “best practice” and “best scientific understanding”.

5 References

BADEWIEN, T. H., 2002: *Horizontaler und vertikaler Sauerstoffaustausch in der Ostsee*, No. 53, Meereswissenschaftliche Berichte, Warnemünde.

BUCH, E. and DAHLINH., 2000, BOOS Plan - Baltic Operational Oceanographic System 1999-2003, in *EuroGOOS Publication NO. 14*.

CULBERSON, C. H., 1991, Rev. 1994: Dissolved Oxygen, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-15.

FEISTEL, R., G. NAUSCH UND E. HAGEN, 2003: The Baltic inflow of autumn 2001, in *Festschrift zum 65. Geburtstag von Wolfgang Matthäus*, Hg. W. Fennel und B. Hentzsch, Meereswissenschaftliche Berichte, Warnemünde, No. 54, S. 55-68.

FIESTA EUROMAR-PROJECT, 1993: *Rules of Field Data Quality Standardisation - Summary Report*, EUREKA Project EU 449.

ICES/HELCOMAdvisory Committee on the Marine Environment , 2002, Ref. C+E+H: Report of the ICES/HELCOM Steering Group on Quality Assurance of **Biological** Measurements in the Baltic Sea, in *International Council for the Exploration of the Sea*, ICES CM 2002/ACME:03.

ICES/HELCOMAdvisory Committee on the Marine Environment , 2002, Ref. C+E+H: Report of the ICES/HELCOM Steering Group on Quality Assurance of **Chemical** Measurements in the Baltic Sea, in *International Council for the Exploration of the Sea*, ICES CM 2002/ACME:02.

IOC CEC: DG-XII, MAST and IOC: IODE,1993 Manual and Guides 26 Manual of Quality Control Procedures for Validation of Oceanographic Data, in *SC-93/WS-19*, UNESCO .

FOFONOFF, N. P. UND R. MILLARD, 1991, Rev. 1994: Calculation of Physical Properties of Seawater, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-26.

GRASSHOFF, K., K. KREMLING UND M. EHRHARDT, 1999: *Methods of Seawater Analysis*, Bd. Third, Completely Revised and Extended Edition, WILEY-VCH Verlag.

LASS, H. U., V. MOHRHOLZ UND T. SEIFERT, 2003: On the pathways and mixing of saltwater plumes in the Arkona Sea, in *Festschrift zum 65. Geburtstag von Wolfgang Matthäus*, Hg. W. Fennel und B. Hentzsch, Meereswissenschaftliche Berichte, Warnemünde, No. 54, S. 38-54.

MATTHÄUS, W. UND G. NAUSCH, 2001: *The hydrographic-hydrochemical state of the western and central Baltic Sea in 1999/2000 and during the 1990s*, No. 45, Meereswissenschaftliche Berichte, Warnemünde.

MATTHÄUS, W., G. NAUSCH, H. U. LASS, K. NAGEL UND H. SIEGEL, 2000: *Hydrographisch-*

chemische Zustandseinschätzung der Ostsee 1999, No. 39, Meereswissenschaftliche Berichte, Warnemünde.
MILLARD, R., 1993, Rev. 1994: CTD Oxygen Calibration Procedure, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-30.

SAUNDERS, P. M., K.-H. MAHRT UND R. T. WILLIAMS, 1991, Rev. 1994: Sandards and Laboratory Calibration, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-11.

STALCUP, M. C., 1991, Rev. 1994: Salinity Measurements, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-9.

STIEGEBRANDT, A., 2003: Regulation of vertical stratification, length of stagnation periods and oxygen conditions in the deeper deepwater of the Baltic, in *Festschrift zum 65. Geburtstag von Wolfgang Matthäus*, Hg. W. Fennel und B. Hentzsch, Meereswissenschaftliche Berichte, Warnemünde, No. 54, S. 69-80.

TAYLOR, P. UND R. WELLER, 1991, Rev. 1994: Meteorological Measurements from WOCE Research Ships, in *WOCE Operations Manual*, Hg. WHP Operations and Methods, WOCE, Bd. WHP Office Report WHPO 91-1, S. 1-26.

UNESCO, 1978: The definition of a Practical Salinity Scale, pss-78, *Unesco technical papers in marine science*, **30**, 1-32.

WEISS, R. F., 1970: The solubility of nitrogen, oxygen and argon in water and seawater, *Deep-Sea Res.*, **17**, 721-735.

WINKLER, L. W., 1888: Die Bestimmung des im Wasser gelösten Sauerstoffes, *Berichte d. dtsch. chem. Gesellschaft*, **21**, 2843-2854.

QA Links

QUASIMEME Quality Assurance Laboratory Performance Studies for Environmental Measurements in Marine Samples. *http://www.quasimeme.marlab.ac.uk*

HELCOM Baltic Marine Environment Protection Commission (Helsinki Commission) *http://www.helcom.fi*

WOCE WHP WHP 91-1 : WOCE Operations Manual Revision: November 1994 (Calibrations and Standards, Methods for Water Sampling, Underway Measurements, CTD Methods), *http://whpo.ucsd.edu/manuals.htm*

WOCE WHP International Oceanographic Data and Information Exchange (IODE), Quality control *http://ioc.unesco.org/oceanteacher/resourcekit/*

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All PAPA participants

Annex

Table 1 Timetable of the development for the quality assurance

Feb. 2003 – Nov. 2003

Feb.	meeting with IOW QA experts
May	design concept of questionnaire (Riga meeting)
May	discussion of the concept with BSH & IOW experts
June	development of web based questionnaire php / MYSQL
July	1st version uploaded to IOW web page
Aug./Sep.	2nd version with updated parameter list
Oct.	first results are discussed at the Warnemuende PAPA expert meeting
Oct.	3rd version uploaded with changes after expert meeting: export function, adding new parameter
Nov. 4	closing of the questionnaire for report, data set export into IOW ftp-box
Nov. 28	report and discussion of the result at the annual PAPA meeting Gdansk

Table 2 General Information on Participant

An additional person/expert for QA is written in *italic*

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Table 3 Hydrographical Parameter List

Parameter	Number	Forms
Temperature	[2.1.1]	[2.1.1.1] Mooring / Fixed Station [2.1.1.2] Shipboard (CTD, flow through) [2.1.1.3] other, please specify
Salinity	[2.1.2]	[2.1.2.1] Mooring / Fixed Station [2.1.2.2] Shipboard (CTD, flow through) [2.1.2.3] other, please specify
Conductivity	[2.1.3]	[2.1.3.1] Mooring / Fixed Station [2.1.3.2] Shipboard(CTD, flow through) [2.1.3.3] other, please specify
Oxygen	[2.1.4]	[2.1.4.1] Mooring / Fixed Station [2.1.4.2] Shipboard CTD [2.1.4.3] other, please specify
Currents	[2.1.5]	[2.1.5.1] Mooring / Fixed Station [2.1.5.2] Ship mounted current meter [2.1.5.3] other, please specify
Radioactivity	[2.1.6]	[2.1.6.1] Mooring / Fixed Station [2.1.6.3] other, please specify
Pressure	[2.1.7]	[2.1.7.1] Mooring / Fixed Station [2.1.7.2] Shipboard CTD [2.1.7.3] other, please specify
Water level	[2.1.8]	[2.1.8.1] Fixed Station / Gage [2.1.8.3] other, please specify
Wave height	[2.1.9]	[2.1.9.1] Mooring / Fixed Station [2.1.9.3] other, please specify
Wave direction	[2.1.10]	[2.1.10.1] Mooring / Fixed Station [2.1.10.3] other, please specify
other Parameter	[2.2.11]	please send an email

Table 4 Meteorological Parameter List

Parameter	Number	Forms
Air Temperature	[2.2.1]	[2.2.1.1] Mooring / Fixed Station [2.2.1.2] Shipboard [2.2.1.3] other, please specify
Humidity	[2.2.2]	[2.2.2.1] Mooring / Fixed Station [2.2.2.2] Shipboard [2.2.2.3] other, please specify
Wind Speed	[2.2.3]	[2.2.3.1] Mooring / Fixed Station [2.2.3.2] Shipboard [2.2.3.3] other, please specify
Wind Direction	[2.2.4]	[2.2.4.1] Mooring / Fixed Station [2.2.4.2] Shipboard [2.2.4.3] other, please specify
Air Pressure	[2.2.5]	[2.2.5.1] Mooring / Fixed Station [2.2.5.2] Shipboard [2.2.5.3] other, please specify
Solar Radiation	[2.2.6]	[2.2.6.1] Mooring / Fixed Station [2.2.6.2] Shipboard [2.2.6.3] other, please specify
other Parameter	[2.2.7]	please send an email

Table 5 Biological Parameter List

Parameter	Number	Forms
Fluorescence Chl a	[2.3.1]	[2.3.1.1] Mooring / Fixed Station [2.3.1.2] Shipboard [2.3.1.3] other, please specify
Fluorescence Phyco	[2.3.2]	[2.3.2.1] Mooring / Fixed Station [2.3.2.2] Shipboard [2.3.2.3] other, please specify
Turbidity	[2.3.3]	[2.3.3.1] Mooring / Fixed Station [2.3.3.2] Shipboard [2.3.3.3] other, please specify
PAR	[2.3.4]	[2.3.4.1] Mooring / Fixed Station [2.3.4.2] Shipboard [2.3.4.3] other, please specify
Yellow Substances	[2.3.5]	[2.3.5.1] Mooring / Fixed Station [2.3.5.2] Shipboard [2.3.5.3] other, please specify
Phytoplankton	[2.3.6]	[2.3.6.1] Mooring / Fixed Station [2.3.6.2] Shipboard [2.3.6.3] other, please specify
Zooplankton	[2.3.7]	[2.3.7.1] Mooring / Fixed Station [2.3.7.2] Shipboard [2.3.7.3] other, please specify
Secchi disc depth	[2.3.8]	[2.3.8.1] Fixed Station / Gage [2.3.8.2] Shipboard [2.3.8.3] other, please specify
other Parameter	[2.3.9]	please send an email

Table 6 Chemical Parameter List

Parameter	Number	Forms
Total Phosphorous	[2.4.1]	[2.4.1.2] Shipboard [2.4.1.3] other, please specify
Phosphate (PO_4^{3--})	[2.4.2]	[2.4.2.1] Mooring / Fixed Station [2.4.2.2] Shipboard [2.4.2.3] other, please specify
Total Nitrogen	[2.4.3]	[2.4.3.2] Shipboard [2.4.3.3] other, please specify
Nitrate (NO_3^{--})	[2.4.4]	[2.4.4.1] Mooring / Fixed Station [2.4.4.2] Shipboard [2.4.4.3] other, please specify
Nitrite (NO_2^{--})	[2.4.5]	[2.4.5.1] Mooring / Fixed Station [2.4.5.2] Shipboard [2.4.5.3] other, please specify
Ammonia (NH_4^{+})	[2.4.6]	[2.4.6.1] Mooring / Fixed Station [2.4.6.2] Shipboard [2.4.6.3] other, please specify
Silicate (SiO_4^{4--})	[2.4.7]	[2.4.7.1] Mooring / Fixed Station [2.4.7.2] Shipboard [2.4.7.3] other, please specify
PH	[2.4.8]	[2.4.8.1] Fixed Station / Gage [2.4.8.2] Shipboard [2.4.8.3] other, please specify
CO_2	[2.4.9]	[2.4.9.1] Mooring / Fixed Station [2.4.9.2] Shipboard [2.4.9.3] other, please specify
Heavy Metals	[2.4.10]	[2.4.10.2] Shipboard [2.4.10.3] other, please specify
DDT and Metabolites	[2.4.11]	[2.4.11.2] Shipboard [2.4.11.3] other, please specify
HCH Isomers	[2.4.12]	[2.4.12.2] Shipboard [2.4.12.3] other, please specify
Hydrocarbons	[2.4.13]	[2.4.13.2] Shipboard [2.4.13.3] other, please specify
other Parameter	[2.4.14]	please send an email

Table 7 Used conversion and calculation algorithms

Hydrographical	Meteorological	Biological	Chemical

ITS-90	22x from producer	Lorenzen 67	24x by Grasshoff et al.,1999
given by manufacturer	no	calculation according to HELCOM manual by L. Edler	4x from producer
Lonquet-Higgins et al. 1963		acc. to HELCOM COMBINE manual)	
Owens and Millard, 1985			
saturation by Weiss 1970			
pss-78			
S [pss-78], T [ITS-90]			
UNESCO algorithms			
SBE-algorithm matched to ITS-90			