Research for Policy support

Contract n° 022603 (SSPI)

EAQC-WISE

European Analytical Quality Control in support of the Water Framework Directive via the Water Information System for Europe

Specific targeted Research Project
Scientific Support to Policies (SSP)

Deliverable N°: D33

Current state of the art and existing gaps in the communication of QA/QC information for the Water Framework Directive – Recommendations for QA/QC reporting and supervision (Work package 3)

Due date of deliverable: October 2008 Actual submission date: Juillet 2008

The deliverable authors are responsible for the content

Start date of the project : 1 December 2005 Duration : 36 months

AUTHOR:	Mike Gardner[1]
AFFILIATION:	[1]WRc
ADDRESS:	Frankland Road, Blagrove, Swindon, SN5 8YF, UK.
TEL.:	+44 1793 865204
EMAIL:	gardner_mj@wrcplc.co.uk
FURTHER AUTHORS:	Heather Leslie[2], [3] Anne Morin, [3] Valeria Dulio [2]IVM, [3]INERIS

DELIVERABLE D33

FINAL REPORT ON RECOMMENDATIONS OF WP3

CONTENTS

APPENDICES

LIST OF TABLES

LIST OF FIGURES

SUMMARY

Assessments of environmental quality made under the Water Framework Directive (WFD) must be based on monitoring data that are of appropriate quality. Two conditions have to be met in order that the fitness for purpose of data can be established. Firstly, analytical systems of appropriate performance must be developed and implemented. Secondly, steps must be taken to provide a robust demonstration that such analytical systems meet use-based data quality requirements. That is, adequate performance in monitoring must be both achieved and shown to have been achieved.

The EAQCWISE project is a response to this need to provide the necessary demonstration of data quality. Workpackage 3 has the goal of showing how to implement an approach to the capture and communication of quality assurance/quality control (QA/QC) information – in relation to data reported under the requirements of the WFD. There is a need for information on data quality to be collected as part of the monitoring process. Different institutional frameworks and different approaches to monitoring in different countries preclude the practical implementation of a uniform approach to quality control. It is recommended that Member states and Competent Authorities should use existing institutions to aim towards a common goal of fitness for purpose of WFD monitoring.

This report presents the principal recommendations of Workpackage 3 on data quality and QA/QC in the data reporting chain. The focus of attention has been on the monitoring of chemical contaminants – though, in relation to aspects of data communication, the main principles discussed here and recommendations presented will generally be relevant to other fields of monitoring (eg ecological and biological). The main recommendation is that Competent Authorities should establish Expert Groups with the responsibility of working within existing frameworks to meet WFD data quality requirements. The activities of such quality control expert groups should impact on all aspects of monitoring including:

- Promoting communication between data producers and data users re QC procedures and requirements;
- Establishing a clear link between QC data and the corresponding monitoring data;
- Defining monitoring specifications, including aspects of sampling programme design and methodology;
- Collating and recording key QC information used to support the validity of data for the WFD;
- Undertaking an annual assessment of data quality to determine compliance with defined performance criteria. This includes the identification of data that cannot be shown to meet requirements;
- Prioritising necessary improvements in analytical quality;

Each Group should have its own clear terms of reference that are appropriate to the way in which the relevant Competent Authorities manages data quality. Groups may serve several river basins or federal or local government bodies, though it is expected that Groups will be organised predominantly national lines. Group members should have a sound appreciation of current and potential analytical capabilities, be familiar with the principles and practice of QA/QC and appreciate the needs of the data user in order to be able to assess matters such as fitness for purpose and to prioritise actions that might be needed to improve data quality. The activities of the various expert Groups should be subject to coordination with respect to overall objectives and the assessment criteria used.

1. INTRODUCTION

The EAQCWISE project is a response to the need to ensure that data of adequate and demonstrable quality are used in assessments made under the Water Framework Directive (WFD).

Workpackage 3 has the goal of showing how to implement an approach to the capture and communication of quality assurance/quality control (QA/QC) information – in relation to data reported under the requirements of the WFD. An effective approach must promote a wider appreciation of the principles of quality control and of how data of appropriate quality are generated and validated for their intended use. It is also important for quality control activities to be recorded and their outcomes communicated to those who interpret data on environmental status.

Current activity in assessing communication of QA/QC information along the data reporting chain has been divided into three tasks: (1) information gathering, (2) discussion of findings at a workshop and (3) the production of recommendations for future approaches and actions.

This report present the recommendations required as the output of task 3.

As an introduction, the main requirements for the workpackage 3 tasks are summarised below.

1.1 Summary of the tasks of workpackage 3

1.1.1 Task 3.1 Information on the current position

This task investigated current practice across Europe with respect to the communication and flow of QA/QC information from laboratory practitioners through to regulatory bodies and authorities that constitute the users of monitoring data. The investigation included the following aspects with respect to the implementation of the Water Framework Directive (WFD):

- The level and type of QA/QC information provided by environmental laboratories to regulatory bodies and other third parties;
- The analytical method validation, internal QA/QC procedures and performance in PT schemes;
- The level of awareness about QA/QC of the practitioners (laboratory staff) who produce the data and of those who use the data - existing communication channels provided to the labs about QA/QC tools and services;
- Expectations of the different categories of data users regarding the quality of data and the QA/QC information that should be provided to them (and level of QA/QC information that is perceived to be needed as part of the final application of the data).

Information gathering carried out as part of the overall survey exercise undertaken was one of the key components of the whole project.

1.1.2 Task 3.2 Workshop

The output of the survey has been discussed with project participants and main stakeholders from different fields (i.e. monitoring laboratories, competent authorities at regional, national and EU level involved in the implementation of the WFD, European accreditation bodies, co-ordinators of RTD projects and networks focussing on QA/QC aspects in environmental monitoring).

A draft report (EAQCWISE Deliverable 32) describing the current position in QA/QC communication and probable future needs was compiled and presented at a workshop, held in June 2007 at Geel in Belgium.

1.1.3 Task 3.3: Defining a recommended approach for an EU system for effective and clear communication of QA/QC information throughout the data reporting chain

The results of the investigation in task 3.1 and discussions at the workshop have been used as a basis of recommendations for the communication of QA/QC information along the data reporting chain, at the EU, national and river basin levels. Proposals are based on information about current practices collected in task 3.1. Issue considered in formulating recommendations have included:

- The level and extent of communication concerning QA/QC;
- How basic technical principles relating to analytical measurement (traceability, uncertainty, validation) and supporting educational material are communicated to end users;
- The extent to which QA/QC issues are appreciated and acted upon by data users.

This report summarises these recommendations.

1.2 <u>Communication/data flow: current issues</u>

Responses to the EAQCWISE survey raised a number of points in relation to data quality and how the quality-related issues noted above are dealt with in the data flow from laboratories, via the Competent Authorities to WISE. These points are summarised below.

- The need to address the topic of data quality is not always clearly defined, particularly at the level of the data user. QC data are frequently not regarded as an essential part of the interpretation of a monitoring programme, so they are rarely requested or used. In many cases, it is perceived that data quality can be addressed at the earliest stages of monitoring – for example, at the stage when laboratories tender for analytical contracts – and then not taken into account subsequently. This is considered to be a serious defect because it fails to take account of the need for an ongoing assessment of data quality against project requirements.

- Even when quality is recognised as an important aspect of data production and interpretation, it is sometimes unclear who is responsible for data gathering and the assessment of data quality. Often the generation, storage and interpretation of quality-related information is left to the analytical laboratory. This can lead to a lack of a clear link between the monitoring data and the supporting, associated quality information, making it less easy (or impossible) for data users to review fitness for purpose at the data interpretation stage. Furthermore, reliance on laboratory-based systems for the storage and retrieval of quality information is inadvisable because laboratories can fail to record and store QC important information for reasons such as closure, relocation etc.

- There is little guidance or agreement on what QA/QC features are essential for different monitoring purposes (eg for the WFD programmes of operational/surveillance, investigative monitoring). There are no minimum criteria on how to capture QA/QC metadata, such as information concerning recovery correction, if to apply a recovery correction, how to do it, how to indicate whether or not it has been done;

- End-users are often unclear what to do about QA/QC or what to do with relevant information when it is provided.

In summary, there is need for a commonly accepted, reliable and consistent source of expertise/advice on technical/scientific issues about data quality. The ways in which this requirement can be addressed are discussed in the following chapter.

2. DISCUSSION AND RECOMMENDATIONS

The definition of measures to address the quality of quality control itself is one of the significant gaps in the management of data quality (Gardner (2007)). There is a need to address the power of any given QC regime to detect important error and to understand the reliability of individual approaches to QC. It is also important to consider how a reliable assessment of the quality of quality control can be captured, recorded and compared between different laboratories or different data sets. This information is also a key factor in the way in QC and monitoring data should be incorporated into the information chain that links the production and use of monitoring data.

In general terms, it is considered that harmonisation of practices in QA/QC across Member States should concentrate on assisting all Member States to achieve a basic common minimum standard, both in terms of <u>what is done</u> (QC practices) and <u>how much of it is done</u> (the intensity with which QC tools are applied). The aim should be to define a minimum level of QC effort. Questions that need to be addressed include:

- What validation tests are needed for analytical systems, under different circumstances (and what these different circumstances might be)? It can be easily appreciated that the methods such as ISO methods that have been tested extensively and defined clearly as part of their development might be more robust and more readily established in a laboratory than a method that might have been developed in only one laboratory and subsequently described in a literature paper. This might lead us to assume that a lower standard of validation might be needed for Standard Methods. The question is how much lower? Additionally, it is crucial to recognise that, regardless of the origin of a method, some degree of testing is needed at the place where it is used. This should have the minimum aim of showing that the method has been implemented (incorporated into an analytical system) satisfactorily and that its performance in use at that location is consistent with the published performance data. If this cannot be demonstrated, the implementation of the method is called into question, along with the quality of the results produced;

- What types and frequencies of routine controls should be required? Current practice with respect to these issues varies widely. One laboratory might analyse a control standard solution once in every 10 real samples, whereas another laboratory might carry out a determination on an in-house reference material once on every run of 20-30 samples. The former operates a relatively high frequency control regime; the latter might be considered to use a more realistic control material, albeit at lower frequency. The relative merits of different approaches will vary - depending on the type of analysis being undertaken (the concentration range of interest the susceptibility of the methodology to different categories of analytical error), the way in which analysis is conducted (frequency and size of analytical runs) and the inherent performance and robustness of the analytical system in relation to use-based targets;

- What are the specifications for the type, frequency and minimum acceptable performance in proficiency tests? The overall pass rate achieved by laboratories in a proficiency test (PT) programme is a complex interaction between PT scheme design/difficulty (sample types, levels, error targets etc) and laboratory capability. Nowadays laboratories often take part in many different PT programmes, involving the tens or hundreds of determinations each year. Given there potentially large numbers of samples and the use of 95%ile, z-score acceptability criteria, it is unrealistic to expect a 100% pass rate. Gardner and Dobbs (2004) suggest that an overall pass rate of 75% or more appears to be achievable routinely. General failure amongst participating laboratories to meet this 75% threshold appears to indicate that the analytical task is unduly difficult with respect to capability and an improvement programme may be needed. At the individual lab level, a proficiency test pass rate of greater than 75% might be seen as a minimum target for routine analysis.

The philosophy of aiming for a minimum common standard of QA/QC is in accord with the advice provided by Hund *et al* (2000) who suggest that, to improve quality in general, it would be most efficient to help laboratories with less sophisticated approaches to quality assurance, rather than devoting effort to the achievement of comparatively slight improvements in existing, relatively well-developed systems operated by the most experienced laboratories. This point is also made in articles by Quevauviller *et al* (1999 (a) and (b)).

Hence it is recommended that the dissemination of good practice in quality control should take precedence over initiatives that might seek either to develop new approaches to QA/QC or to seek rigorous uniformity of activity. Nevertheless, even in the more experienced laboratories there are usually relatively simple improvements that can be made to QC practices. Gardner (2007) has discussed the most common shortcomings in laboratories' QC activities, - the areas in which there might be the most serious discrepancies in the implementation of QC between one laboratory and another. These include the use of appropriate routine quality control materials (ie more relevant to the samples of interest in terms of determinand concentration and sample matrix), poor practice in the management and interpretation of control charts and the absence of QC for sampling procedures.

2.1 Expert Groups

Considerations and discussions of the requirement for guidance and harmonisation on QA/QC for the WFD, with special reference to the aims of workpackage 3, prompted the proposal for the establishment of a coordinated network of expert groups that might meet current needs. The strategy of using expert groups was seen as a rational compromise between the *laissez faire* approach of allowing laboratories to supervise data quality (and thereby running the risk of inadequate control and possible major disparities between Member States) and the highly bureaucratic, costly and labour intensive option of establishing control, storage and interpretation of QA/QC data at a centralised EU level

The establishment of expert review groups to oversee the collection of summary QC information, its compilation and interpretation has the advantage that it fosters a highly desirable sense responsibility for data quality on the part of the data user. It also makes use of individuals that have the interest, competence and expertise to do the job of managing data quality thus eliminating the need to train supervisory staff or to involve users with little interest or background in data quality. It will ensure that quality information can be captured in summary form from the laboratory and can be clearly associated with the monitoring data to which it refers. This means that data users would not need to place long-term reliance on laboratories' quality systems. Although this approach is not without resource requirements, it should be a relatively cost-effective and sustainable strategy that can play an important role in forging clear links between environmental monitoring data and their associated quality information.

The use of expert groups was also seen as offering the flexibility to accommodate different organisational models for data quality control that have grown up in different Member States. Different countries have developed different approaches to the supervision and assessment of data quality. This state of affairs has arisen for a number of reasons, including differences in:

- The local or regional government structure (eg federal or centralised) with respect to funding and the overall responsibility for monitoring;

- The extent to which responsibility for carrying out analysis is devolved (eg centralised with a national reference laboratory or shared amongst different agencies or organisations);

- The way in which responsibilities for environmental protection are apportioned (eg with a national environmental protection agency or with local government bodies);

- The requirements of current national data quality schemes (eg MCERTS);

- The availability and varied nature of PT schemes in different countries and regions. Just because a PT scheme might have been established does not mean that a given laboratory will either be able to or wish to take part in it. Laboratories are constrained by cost not to participate in all PT programmes. Furthermore, all may not be directly relevant or they may not be open or generally available. The choice of PT programme in which to participate is often determined by the preferences of different clients, with participation in one scheme sometimes having to serve a number of purposes. The ways in which the results of different PT programmes are assessed can be markedly different, perhaps as a consequence of slightly differing aims or differing philosophies. Thus the interpretation of PT outputs may need to be considered carefully before comparisons are made between laboratories taking part in different schemes;

- The needs and levels of participation in transnational monitoring programmes, each of which may have its own individual data quality protocols and requirements. This is particularly relevant to marine monitoring (eg OSPAR, MEDPOL) but also applies to freshwater monitoring in transnational river basins (e.g. the Rhine and the Danube).

These aspects are considered to be particularly important if any proposed approach to QC for the WFD is to be implemented across Europe, where there is a need to fit in with well-established, highly effective but differing methods of working that have been adopted in different countries.

It is envisaged that he responsibility of establishing an appropriate QC Review Group should be assigned to the relevant CA, to which the Group should be answerable. This is consistent with the idea that the CA would be the body most likely to have the resources to identify suitable Group members and to support the Group's activities. It might also be expected that a Group that is controlled and funded by a CA is likely to command the CA's attention.

2.2 Expert Groups - Key Issues

Experience in coordination of QA/QC for large monitoring programmes (e.g. by ICES in the field of marine monitoring) indicates that there are a number of critical points that need to be addressed:

- It is essential to ensure that the role of the QC Expert Group (QCEG) is well defined and integrated into the overall programme of data assessment and interpretation and that it has the power to influence the use of data; otherwise there is the danger that it may be ignored;

- In order that the data quality review process should not become mired in unnecessary detail a compromise must be struck between the desire to collect as much data as possible about data quality and the difficulty and expense of data collection and review. It is important to obtain enough QC information to allow a worthwhile comparison between the performance achieved in monitoring and relevant fitness for purpose criteria, but it is also important to be realistic about the level of detailed information that can be readily supplied and assessed (see proposals in section 2.4, below). The difficulty of getting laboratories to understand what is required and to provide the correct data in the desired format should also not be underestimated;

- Reporting of QC data can be a cause of delay; hence strict deadlines for information provision may need to be set. It may be necessary to apply sanctions in order to prompt provision of QC information that is timely and complete. For example, failure to report QC data by the deadline might lead to monitoring data not being used in assessments of environmental quality;

- Information should be collected on a rolling basis (it is proposed annually) so that up to date and relevant QC data are available;

- QCEGs need to have their own clear terms of reference. They will also need to be coordinated or provided with co-operating guidelines, in order that different CAs operate to similar principles. It is envisage that although CAs will convene their own Expert Groups some degree of coordination at an EU level will be needed – though this should not be taken to be a call for total harmonisation – the flexibility mentioned in section 2.1 is seen as essential to effective implementation. The role of coordination at the eu level is discussed further in the Appendices to this report;

- An important role of the QCEG would be to act as a focus for initiatives intended to provide awareness of QA/QC in the reporting chain from laboratory to CA and beyond to the DG-Environment;

- The selection of Group members should be made by the parent body (presumably part of the CA) and should aim to involve individuals who:

    - Have a sound appreciation of current and potential analytical capabilities;

    - Understand the principles and practice of QA/QC;

    - Appreciate the needs of the data user in order to be able to assess matters such as fitness for purpose and to prioritise actions that might be needed to improve data quality.

The exact nature and dynamic of any given QCEG need not be defined. As noted above, the way in which any given group operates will have to be determined by the local circumstances. In one case there might be an authoritative source of guidance, such as a National Reference Laboratory, which might take a steering role with less experienced monitoring laboratories. In other cases, the group might be composed of representatives of laboratories who were equally experienced and who could be expected to act more collaboratively.

2.3 QC Expert Groups – roles

The role of the QCEGs might be seen as being divided into activities prior to monitoring and after data collection.

Prior to monitoring

Before monitoring commences the Expert Group should be involved in:

- Facilitation of communication between data producers and data users about the basic requirements for QA/QC for physico-chemical monitoring undertaken for the Water Framework Directive;

- Definition of monitoring specifications, following Article 3 of the Commission Decision, (Commission Decision Dec. 2007) including performance targets and QA/QC guidance. These definitions should include a specification of required performance for each parameter, for each substance, – based on fitness for purpose – see section 2.4 below. The resulting performance criteria should be proposed by the QCEG to the competent monitoring authorities as a means of identifying suitable contracting laboratories;

- Determination of issues relating to analysis and monitoring of technically feasibility and disproportionate cost;

- Provision of guidance on topics including:

    - Sampling scheme design;

    - Procedures for sampling, sample handling and preservation and sample processing (e.g. digestion, extraction);

    - Suitable analytical techniques and appropriate specific methods;

    - Collection of QA/QC and metadata.

After data collection

QC information should be collected in summary form (see proposals below) and then reviewed with respect to the planned data use by a designated QC Expert Group (QCEG?). This Group would be responsible to the ultimate data user (e.g. the CA) for assessing fitness for purpose of the data, for identifying areas where improvement is needed and for confirming the aspects of data interpretation (e.g. trend detection) that are directly related to quality issues.

The Group would also be responsible for provision (based on the assessment of QC information) of advice to the competent monitoring authority regarding:

- The compliance of the data with respect to the defined performance criteria;

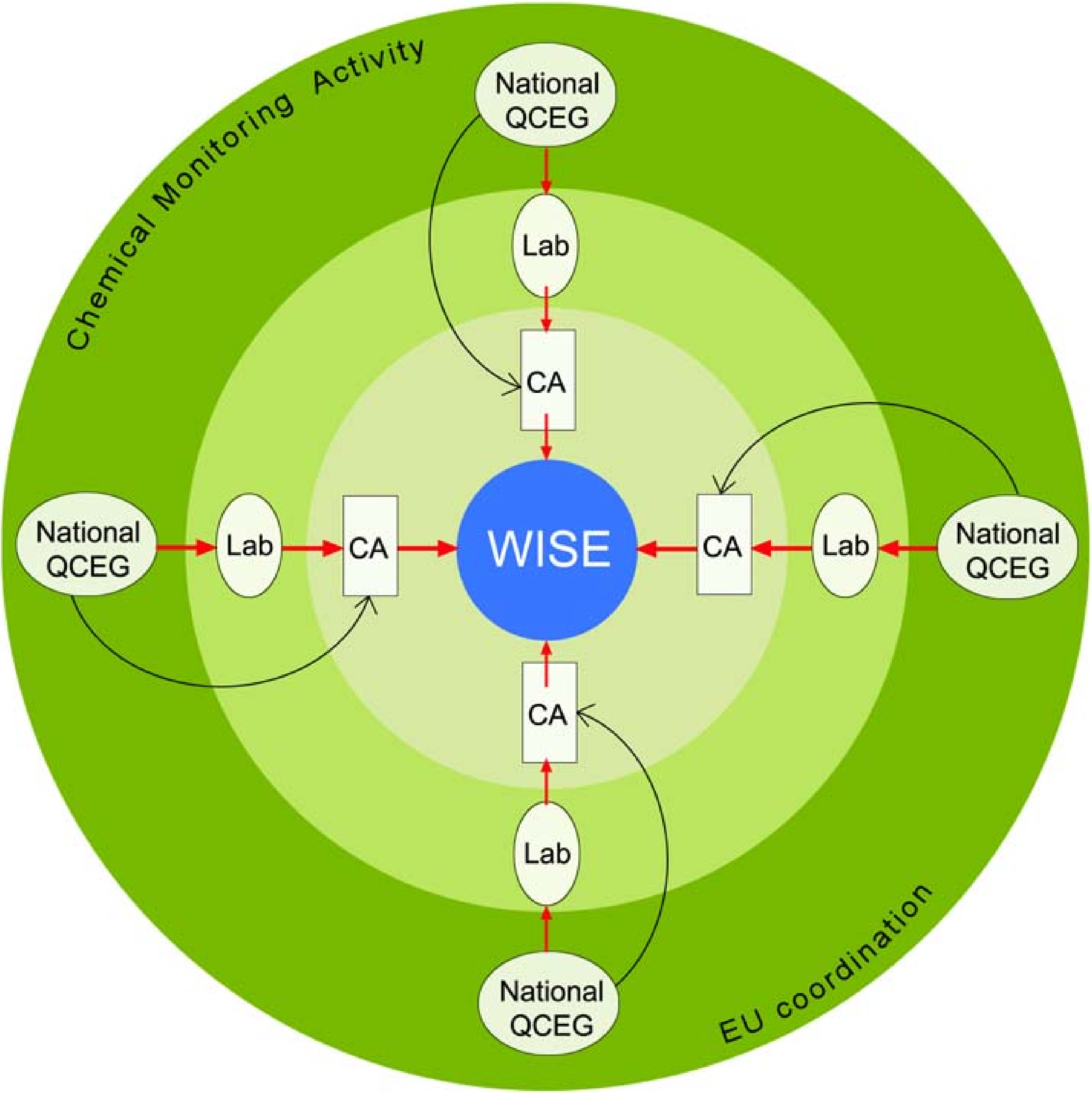
- The application of data screening techniques including those based on an assessment of relevant QC information as well as the more familiar “plausibility checks”;

- Measures required for improvement in performance (from gaps that are identified as part of the continuing QC programme).

It is recommended that the Expert Groups should have a role in advising on the subject of data collection (with respect to QC information and its links with monitoring data). It is proposed that the EAQC-WISE blueprint should include an input to the common template developed by DG ENV and EEA for WISE. This might help to ensure that data are collected to a common and complete format, that suitable links are established between data and QC information and that the profile of data quality issues is kept to the forefront in the gathering and interpretation of WFD data.

2.4 Overall Coordination of QCEGs

In spite of the main recommendation that different CAs are likely to need their own QCEGs, it is also true that the activities of different QCEGs will need some coordination. Furthermore, the flow of quality-related information must be managed in such a way that different users are provided with the level of detail that they require - that they are neither given insufficient QC information nor overloaded with detail that they do not need and which they might not be able to review or comprehend. Certainly, coordination of the way in which QC requirements are defined – and what is defined – is needed to form the basis of a common approach by QCEGs. Then, at the end of the assessment process, harmonisation of the way in which QC results are assessed and the response to poor performance would be necessary in order that Member States can be shown to be operating to a common and equitable set of criteria. The interaction between laboratories, CAs, QCEGs and WISE are illustrated in Figure 2.1.



QCEG activity

Formulate requirements on behalf of CAs Coordinate laboratory QC activity to meet requirements (validation, routine QC, CRMs, PT) Provide guidance on sampling and methodology Coordinate improvement plans	Collect and summarises key QC measures Assess demonstration of data quality – determine QC status Interpret QC activity for CAs	Link with other QCEGS via EU coordination to harmonise overall approach

Figure 2.1 QC and Reporting Information Flow

One of the most important aspects of quality assessment requiring agreement is the action to be taken when QC data are found not to provide an adequate demonstration that monitoring data meet quality requirements. Are such data to be deleted, recorded but marked as not to be used, flagged as of potentially poor quality (but without guidance on what use might be made of them)? If data quality assessment is worth anything at all, one thing that must not happen is for such monitoring data to be accepted as of equal status with fully quality assured data. This means that some method of identifying data of less than satisfactory QC status has to be devised and rigorously implemented. This level of decision is an example of one that has to be taken at EU level in order to ensure a common method of dealing with these issues that can affect the utility and comparability of assessments of European environmental quality. .

The proposed quality data flow must also be consistent with current procedures used (or planned) within the WISE framework. Current practice within WISE is to carry out an assessment of reported data. This is somewhat confusingly termed a "quality check" or "plausibility check" and comprises inspection of reported data with the aim of eliminating obvious errors such as reporting in incorrect units or the misplacement of decimal points. Whilst such checks involving a critical examination of the reported data are of value they cannot provide assurance of adequate control over measurement error. They can only be done with confidence once the basic criteria of fitness for purpose have already been met by satisfactory completion of

These considerations prompt the recommendation of a tiered approach to the establishment of a data quality assessment and review process as illustrated in Figure 2.2 below. The intention should be that important quality-related criteria should be defined and addressed during the measurement process. This does not mean that all QC information has to be available at all times. Instead, as the Figure shows, each time critical information is reviewed and found to meet requirements, less detail needs to be transmitted along the information chain. Thus the most detailed examination of QC data will be at the time measurement takes place. Subsequently, a summarised version of QC data will be assessed by the QCEG which will then forward relatively simple information relating the fitness for purpose of reported data to CAs. This sequence of assessment and approval is intended to provide the appropriate assurance of fitness for purpose.

The intention should be that detailed QC information and other meta-data should be stored predominantly at a local level, under supervision of the national QCEGs. Of course this aim should also take account of any data reporting requirements that might be specified for WISE. Where minimum data reporting requirements for QC – such as limit of detection, limit of quantification, uncertainty etc. and other supporting information have been defined these should be adhered to. These requirements are designed to provide summary information as a check on basic comparability and probably would not suffice for an assessment of data quality against a totally new requirement. For such an assessment it would usually be necessary to access more detailed information held at a local level.

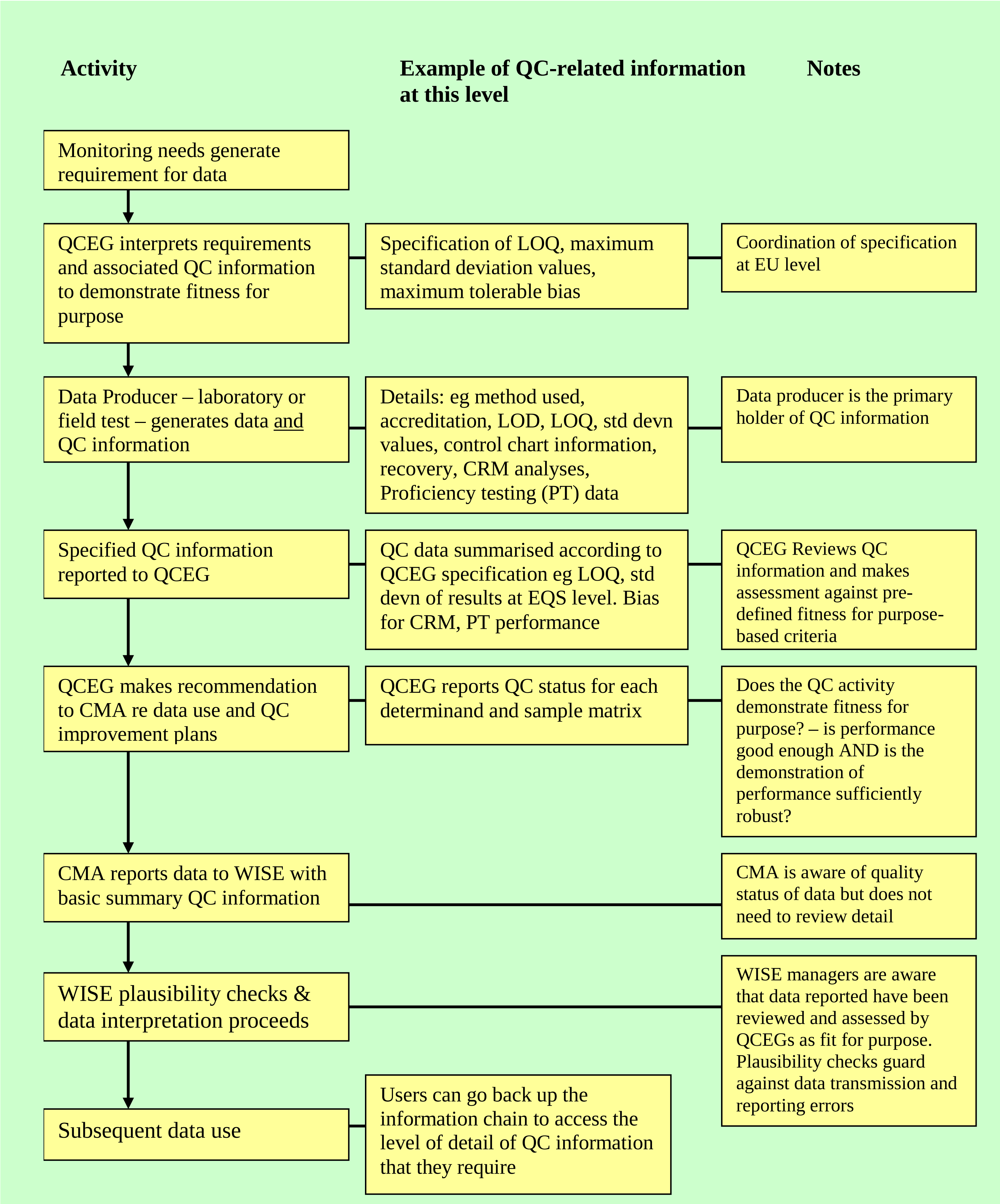


Figure 2.2 Illustration of the data quality information hierarchy

2.5 QC data to be requested and assessed

QC data and associated information (metadata) – The main question is how to identify the essential information and how to use it in exploiting results. What QC data (and other associated information) relevant to monitoring programmes should be stored in such a way as to be associated with the data on environmental quality?

Key metadata relevant to monitoring programmes include overall monitoring objectives, details of how the sampling programme was designed, why specific sites and sampling frequencies were chosen, who was responsible for aspects of design and execution of the programme (particularly sampling), analytical targets and how they were defined etc. Metadata serves several important purposes, including alerting data users to the existence and purpose of the data and of promoting data accessibility and applicability. It is important in preserving the value of data and can be used to organise and manage the knowledge collected in a sound, efficient manner.

QC summary data might be considered to include numerical data on at least some – though for this purpose, probably not all - of the following:

a) Analytical technique – either a reference to the method, if a standard method is used or the method's title plus a short description of its basis, if an in-house method or modified Standard Method is employed. (It is suggested that methodology should be available on request rather than making the Expert Group responsible for storing and scrutinising every full written procedure),

b) Concentration range of use (without the use of sample dilution)

c) Limit of detection (3x within-run standard deviation of blank sample)

d) Limit of quantification (10x within-run standard deviation of blank sample – ISO 13530)

e) Estimates of control over systematic error (recovery data, analyses of reference materials, for different sample types at concentration values near to the Environmental Quality Standard or other critical level of interest

f) Summary data on performance in PT programmes.

g) Information on control samples used routinely (serial number if relevant, concentration level and sample matrix)

h) Within-run standard deviation of results (for different sample types, at least at the EQS value and other points in the range of use)

i) Between-run standard deviation of results for different sample types, at least at the EQS value and other points in the range of use)

j) Overall standard deviation of results (combining within and between run components, for different sample types, at different points in the range of use)

It is proposed that a minimum of items (a) to (f), above, should be requested. QC data should be submitted as relevant to a specified set of monitoring data – eg annually from January to December inclusive. Once a set of required QC parameters has been settled upon, it is essential that that Expert

Group goes on to define clear numerical performance criteria for each of them. For example, for items (a) to (f) above definition and clear guidance on the following would be needed:

> (a) which determinations are defined as empirical and which therefore require a specified method;
>
> (b and c) the required LOD (LOQ) (and the minimum number of degrees of freedom that should be associated with the relevant measure of standard deviation).
>
> (d) maximum tolerable uncertainty at the EQS level (and how and with what precision such uncertainty is to be estimated);
>
> (e) Which control sample types are adequately representative to provide an appropriate demonstration of control.
>
> (f) acceptable performance in PT (e.g. z score of <2 for no less than 70% of samples analysed plus analysis of at least 80% of relevant available samples)

Examples of what might be proposed are shown in Table 2.1 below for several Priority Substances. It is stressed that this is an example of what an Expert Group might propose and not a definitive recommendation.

Table 2.1 Illustration of specification of analytical requirements

Name of priority substance	EQS as AA inland surface (µg/l)	(a) Operationally defined determinand requiring mandatory method?	(c) LOQ (µg/l)	(b) LOD (µg/l)	(d) Maximum tolerable uncertainty at the EQS concentration (µg/l)*	(e) Recommended reference materials	(f) PT performance**	Recommended PT schemes
Alachlor	0.3	na	0.10	0.03	0.15	to be completed	see note below	to be completed
Anthracene	0.1	na	0.03	0.01	0.05			
Atrazine	0.6	na	0.20	0.07	0.3			
Benzene	10	na	3.33	1.11	5			
Pentabromodiphenylether	0.0005	na	0.0002	0.00006	0.00025			
Cadmium	0.08	na	0.03	0.01	0.04			
C10-13-chloroalkanes	0.4	ISO ref(xxx)	0.13	0.04	0.2			
Chlorfenvinphos	0.1	na	0.03	0.01	0.05			
Chlorpyrifos	0.03	na	0.01	0.003	0.015			
1,2-Dichloroethane	10	na	3.33	1.11	5			
Dichloromethane	20	na	6.67	2.22	10			
Di(2-ethylhexyl)phthalate (DEHP)	1.3	na	0.43	0.14	0.65			
Diuron	0.2	na	0.07	0.02	0.1			
Endosulfan	0.005	na	0.0017	0.0006	0.0025			
Fluoranthene	0.1	na	0.03	0.01	0.05			
Hexachlorobenzene	0.01	na	0.003	0.001	0.005			
Hexachlorobutadiene	0.1	na	0.03	0.01	0.05			
Hexachlorocyclohexane	0.02	na	0.007	0.002	0.01			
(gamma-isomer, Lindane)	0.02	na	0.007	0.002	0.01			
Isoproturon	0.3	na	0.100	0.033	0.15			
Lead	7.2	na	2.40	0.80	3.6			
Mercury	0.05	na	0.017	0.006	0.025			
Naphthalene	2.4	na	0.80	0.27	1.2			

Nickel	20	na	6.67	2.22	10
Nonylphenols	0.3	na	0.100	0.033	0.15
Octylphenols	0.1	na	0.033	0.011	0.05
Pentachlorobenzene	0.007	na	0.00	0.00	0.0035
Pentachlorophenol	0.4	na	0.13	0.04	0.2
(Benzo(a)pyrene),	0.05	na	0.02	0.01	0.025
(Benzo(b)fluoranthene),	0.03	na	0.01	0.003	0.015
(Benzo(k)fluoranthene),		na			
(Benzo(g,h,i)perylene),	0.002	na	0.0007	0.0002	0.001
(Indeno(1,2,3-cd)pyrene)		na			
Simazine	1	na	0.33	0.11	0.5
Tributyltin compounds	0.0002	na	**0.0002**	**0.0001**	**0.0002*** **
(1,2,4-Trichlorobenzene)	0.4	na	0.13	0.04	0.2
Trichloromethane (Chloroform)	2.5	na	0.83	0.28	1.25
Trifluralin	0.03	na	0.01	0.003	0.015

* Uncertainty limits stated here refer to "intermediate" uncertainty **(1)** - ie that estimated on a within-laboratory basis (Hund *et al*. 2001.) Laboratories should aim to estimate and, where necessary, eliminate significant **(2)** systematic error (bias) - either by using methodology of demonstrably low bias or by determining bias (with suffficient precision) for the sample type of interest and applying a correction.

(1) The standard deviation value (minimum of 10 degrees of freedom) relating to this uncertainty is the within laboratory medium term standard deviation - accounting for within-run and between run sources of variation over a period of at least two weeks at the laboratory concerned. It can be calculated as

$\sqrt{(sd_{withinrun})^2 + (sd_{betweenrun})^2}$ (ISO/DIS 13530).

(2) Significant bias at the EQS value is defined as greater than 10% of the EQS - at which a maximum tolerable standard deviation of 20%of the EQS value is considered to apply.

** A medium term proficiency test pass rate of greater than approximately 75% is set as a minimum target for routine analysis to demonstrate fitness for purpose. This pass rate is proposed as a practical yardstick to be used by QA managers and accreditation bodies. This recommendation is contingent on a laboratory's continued and largely uninterrupted participation in a PT programme. Where performance falls below this level, laboratories are expected to establish a formal improvement plan.

*** Interim analytical targets for LOD, LOQ and Uncertainty have been set at higher values than those implied by the EQS because current capability is insufficient to meet the more stringent targets.

2.6 Illustrative examples of current good practice to be used as a reference and to show how different models can work.

OSPAR / ICES (and marine monitoring in general) – setting QC criteria and reviewing activity and performance and methodology – see Appendix A.

Germany - coordinating approach to marine monitoring – see Appendix B.

UK – National Marine Advisory Group - reviewing (marine) data quality and advising on performance targets – see Appendix C.

France – role of national reference laboratory. (providing guidance and policy) - see Appendix D.

Danube ICPDR - coordinating focus on data quality – see Appendix E.

3. CONCLUSIONS

There is a need for information on data quality to be collected as part of the monitoring process. This information is essential to programmes such as those serving the Water Framework Directive in order that monitoring can be shown to be of a quality that is fit for its intended purpose.

At present, although QA/QC activity does generate such information, there is not always a reliable link between quality related data and the corresponding monitoring data. Furthermore, data end-users are often unclear what to do about QA/QC or how to use relevant information when it is provided.

The principal recommendations of Workpackage 3 on data quality and QA/QC in the reporting chain are as follows.

CAs should establish Expert Groups with the following responsibilities:

- To facilitate communication between data producers and data users about the basic requirements for QA/QC for physicochemical monitoring undertaken for the Water Framework Directive;
- To define detailed monitoring specifications, for parameters such as limit of detection and control over random and systematic error;
- To determine issues of technically feasibility and disproportionate cost where current analytical performance is not likely to be adequate;
- To advise on sample programme design, analytical methods, QC practices and sampling techniques;
- To supervise the annual collection and collation of QC information that can be used to support the validity of data for the Water Framework Directive;
- To make an annual assessment of data quality and to determine compliance of the QC data with respect to the defined performance criteria;
- To identify data that can be shown to meet stated quality criteria (and those that, for one reason or another, cannot);
- To advise on the fitness for purpose of all data reported under the Water Framework Directive;
- To recommend and prioritise where improvements in analytical quality should be made;
- To advise on the subject of data collection (with respect to QC information and its links with monitoring data);

Each Group should have its own clear terms of reference that are appropriate to the way in which the relevant CA manages data quality. Groups may serve several river basins or federal or local government bodies, though it is expected that Groups will be organised predominantly national lines.

Group members should have a sound appreciation of current and potential analytical capabilities, be familiar with the principles and practice of QA/QC and appreciate the needs of the data user in order to be able to assess matters such as fitness for purpose and to prioritise actions that might be needed to improve data quality. The activities of the various expert Groups should be subject to central coordination with respect to overall objectives and the assessment criteria used. Differences in methodology would be acceptable in response to different methods of operation within various CAs.

REFERENCES

Commission Decision (Dec. 2007) of [version 17/12/2007] laying down, pursuant to Directive 2000/60/EC of the European Parliament and of the Council, technical specifications for analysis and monitoring of water status

EAQC-WISE Deliverable No. 32 - Final Report on the current state of the art of WP3

Gardner, M.J. (2007). Quality Control Techniques for Chemical Analysis – Some Current Shortcomings and Possible Future Developments. Accreditation and Quality Assurance (2007), 12 653–657.

Gardner, M.J. and Dobbs, A.J. How Well Should Laboratories Perform in Proficiency Tests? Journal of Environmental Monitoring, (2004) 6, 559 – 562.

Hund, Edelgard, Massart, D. Luc., Smeyers-Verbeke, Johanna. (2000) Inter-laboratory studies in analytical chemistry Analytica Chimica Acta 423 145–165.

Hund, Edelgard, Massart, D. Luc., Smeyers-Verbeke, Johanna. (2001). Operational definitions of uncertainty. Trends in analytical chemistry, vol. 20, no. 8, 394-404.

ISO/DIS 13530, Water quality – Guidance on analytical control for chemical and physico-chemical water analysis

Quevauviller, Philippe, Cámara, Carmen, Kramer, Kees J.M. (1999a) EC initiatives for quality assurance training in analytical chemistry Trends in Analytical Chemistry, 18 (9+10) 644-649.

Quevauviller, Philippe, Nieto de Castro, Carlos, Morabito, Roberto, Valcárcel, Miguel, Voulgaropoulos, Anastasios, Walsh, Máire. (1999b) Needs for improvement of the measurement infrastructure in Europe. Trends in Analytical Chemistry, 18 (9+10) 650-655.

Glossary of abbreviations

AA	annual average
AQC	analytical quality control
CA	competent authority
CMA	chemical monitoring activity
CRM	certified reference material
EQS	Environmental Quality Standard,
LOD	limit of detection
LOQ	limit of quantitation
MAC	maximum admissible concentration
Na	not applicable,
PT	proficiency test
QA	quality assurance
QC	quality control
QCEG	quality control expert group
Std dev	Standard deviation
WFD	water framework directive
WISE	water information system for Europe

APPENDIX A. OSPAR / ICES (AND MARINE MONITORING IN GENERAL) – SETTING QC CRITERIA AND REVIEWING ACTIVITY AND PERFORMANCE

The OSPAR Joint assessment and monitoring programme sets guidelines for the selection of data for use in assessments of environmental quality. Further arrangements for data-handling have been established to ensure consistency, efficiency and effectiveness both within OSPAR and with other international organisations. Guidance and coordination of the collection and use of quality-related information is provided via ICES. This includes specific instruction on:

- Use of data and acknowledgment of sources;
- Quality control procedures;
- The need to provide meta-data, including details of analytical / Measurement technique, accuracy and precision, performance data in PT schemes, details of routine controls including reference materials, Quality information such as flags or other indicators. Although the ICES Data Centre may perform some data quality control, the data source always retains responsibility for data quality;
- The policy for data collection and storage;
- Procedures for feedback concerning any problems encountered by data users with ICES-provided data.

Data and information are provided to ICES from many data sources. They are of variable quality and can be obtained using a variety of methodologies. Three types of data are differentiated;

- Detail data are individual measurements or observations. In order to interpret detail data, related attribute data such as type of date, location, time and unit of measurement are also required;
- Aggregate data are summarized detail data;
- Meta-data - data about data. That is, they provide information about detail or aggregate data sets. Examples of meta-data include accuracy, precision or method of measurement, and location, structure or ownership of the data. In order to maximize the usability of data and thereby their value, data sources must supply meta-data and, if available, data quality indicators. All data including meta-data and quality indicators should be submitted using standard coding formats and protocols to the extent possible.

It is recognised that in order to indicate the quality controls that have been applied to a specific data set, ICES' systems should accommodate quality flags. The system allows re-submission of data throughout the quality control process, and thus also allow for accelerated submission of data. For example, preliminary data can be submitted immediately after collection and replaced later by cleaned data. The reporting of suspected errors in the data is facilitated, and relevant information is relayed to the respective data source so corrections can be made.

ICES has the aim of developing quality control tools to ensure documented data quality.

And to provide expert advice on data usability (fitness for different purposes).

Particular attention has been paid to the ability to flag data with respect to their quality. It is noteworthy that a large number of flag designations have been devised to indicate different status levels – see below.

Examples of ICES Quality Flags

Note that apparently good data remain unflagged.

Flags that can be set by the analyst

- ? Questionable data - The question mark is used as a general quality flag or warning on data that appear to be wrong, but where no obvious reason has been found.
- I Interpolated manually - Used on data that have not been measured, but calculated manually from other data.
- Z Zero by definition- Used where no measurement has been made, for example of oxygen or nitrate in the presence of hydrogen sulphide, but where the concentration has to be zero.
- M Missing value - Used when a sample has been taken but no data have been reported, usually due to analytical problems.
- < Below the detection limit of the analytical method
- > Above the range of the analytical method

Further flags that can be set at the automated or manual validation and data assessment stage

- C Corrected value - used on data that have been recalculated due to, e.g., re-calibration.
- B Bad data - This flag is used on obviously bad data, or data which have been proven wrong.
- ! Exceptional, but should be correct - This flag is used on data that at first glance appears to be very dubious, but which have been checked and verified.
- N Not quality controlled - Mainly used to flag old data that have not gone through quality checks.

HELCOM, or other data users, are advised to require the submission of proficiency test results from all data providers (as well as results from the internal quality control and the use of certified reference materials), and to react if the laboratories fail to deliver. Furthermore, the submission of poor results, or the failure to submit results, is taken as a reason for downgrading the importance of data in data interpretation. Data sets not supported by the appropriate QC information for the regularly conducted assessment work are generally severely down-weighted.

APPENDIX B GERMANY - COORDINATING APPROACHES TO MARINE MONITORING

The following is a survey of the German contribution to the initial Global Ocean Observing System (GOOS) and of some GOOS supporting services in the years 2001 and 2002.

German Marine Monitoring Programme (BLMP)

Germany's contribution to the coastal module of GOOS is the German Marine Monitoring Programme (BLMP) which is constituted as a pool of different Federal and regional coastal authorities responsible for monitoring and assessment of the German marine environment. The BLMP represents Germany in different international forums dealing with monitoring and assessment in the sea, i.e. OSPAR, HELCOM and the EU. Collection of environmental data and information is carried out for all relevant problems in the sea, such as eutrophication, hazardous chemicals and radioactivity.

The following variables are determined in German territorial waters:

- Hydrographic measurements [temperature, salinity]
- Harmful substances
- Trace metals
    - sea water
    - sediment
    - organisms
- Organic trace substances
    - sea water
    - sediment
    - organisms
- Biological effects
- Nutrients, oxygen, hydrogen sulphide
- North Sea
- Baltic Sea
- Marine communities
- submarine communities
- sea birds

Agencies and institutions which presently co-operate in the BLMP are the following:

- Bundesforschungsanstalt für Fischerei (BFA-Fi)
- Bundesamt für Seeschifffahrt und Hydrographie (BSH)
- Bundesanstalt für Gewässerkunde (BfG)
- Umweltbundesamt (UBA)
- Biologische Anstalt Helgoland (BAH) im Alfred-Wegener Institut
- Landesamt für Umwelt, Naturschutz und Geologie, Mecklenburg-Vorpommern (LUNG)
- Staatliches Amt für Umwelt und Natur, Mecklenburg-Vorpommern (StAUN)

- Landesforschungsanstalt für Landwirtschaft und Fischerei, Mecklenburg-Vorpommern (LFA)
- Niedersächsisches Landesamt für Ökologie (NLÖ)
- Landesamt für Natur und Umwelt des Landes Schleswig-Holstein (LANU)
- Institut für Ostseeforschung Warnemünde an der Universität Rostock (IOW)

Quality Assurance

The German Federal Environmental Agency organises a Quality Assurance (QA) Panel to support the national Marine Monitoring Programme of the North and Baltic Sea. Its activities include an ongoing programme of quality control for biological measurements comprising ring tests and training workshops on all aspects of biological monitoring.

For chemical testing, the German authorities participate in and contribute to the coordinated approach to QC that is used by ICES (ICES (2005)) to validate monitoring data. Amongst other quality related topics ICES publishes detailed guidance on routine quality control and relevant aspects of methodology.

ICES. 2005. ICES/HELCOM Steering Group on Quality Assurance of Chemical Measurements in the Baltic Sea 24 pp.

APPENDIX C UK NATIONAL MARINE ADVISORY GROUP - REVIEWING (MARINE) DATA QUALITY AND ADVISING ON PERFORMANCE TARGETS AND METHODOLOGY

The description below has been adapted from: The UK National Marine Chemistry Advisory Group UK NMCAG

Terms of Reference

Aim

The aim of the group is to co-ordinate and advise on requirements for UK marine monitoring for chemistry determinands - with respect to methodology, techniques, quality assurance and associated research.

Context

The group has developed from the National Marine Chemistry Analytical Quality Control Group to have a wider remit covering all aspects of the monitoring of contaminants and supporting determinands in the UK marine environment. This is carried out to meet the needs of "drivers" such as OSPAR, WFD, etc and covers, for example, survey design, sampling protocols, sample analysis including QC, data quality assessment and reporting.
The group does not generate standard analytical methodologies, but it will provide guidance on:

- valid analytical approaches that are capable of generating data that are fit for purpose; and,
- the means by which fitness for purpose is to be demonstrated.

Reporting

The group reports both to the Clean and Safe Seas Evidence Group and to the Protocols Group, as different aspects of the remit of the group dictate.

Membership

The membership of the group consists of technical representatives of the Competent Authorities which are responsible for implementing the UK Clean Seas Environmental Monitoring Programme in relation to the UK Marine Monitoring and Assessment Strategy. The membership of the group will also include representatives from any and all other organisations carrying out monitoring or developing analytical techniques applicable to the monitoring of contaminants in the UK or wider European marine environment, and to experts as appropriate.

The terms of reference of the group are as follows:

1. Ensure that all marine chemistry analytical data is quality assured and assessed as fit for purpose using tools such as the Data Filter.
2. Provide guidance on appropriate approaches to with- and between- laboratory quality control, including input to the definition of required standards of analytical accuracy for different applications.
3. Interpret the outputs of QC programmes in the context of UK marine monitoring requirements.
4. Ensure that, wherever possible, marine analytical chemistry data is subject to external QC in the form of proficiency tests.
5. Liaise closely with appropriate PT schemes to ensure that they meet UK needs.

6. Advise the Clean and Safe Seas Evidence Group (1) on OSPAR/JAMP/CEMP/WFD chemical monitoring requirements and how best to implement these.
7. Advise the Clean and Safe Seas Evidence Group on priorities for the application and implementation of existing and new analytical chemistry monitoring techniques.
8. Advise the Clean and Safe Seas Evidence Group on the time scales over which each technique can be implemented in the AQC programme.
9. Recommend appropriate monitoring methods and procedures, including sampling, sample processing and analysis, for marine monitoring manuals.
10. Organise training workshops and/or interlaboratory exercises for participants as appropriate, and widen the experience of end users with each of the recommended techniques.
11. Liaise with focus group on aspects of data submission and storage on the national marine database, including links with quality.

Notes

[1] the "Clean and Safe Seas Evidence Group" is one of the coordinating groups that control UK marine monitoring. Its remit includes chemical m

APPENDIX D DANUBE ICPDR - COORDINATING FOCUS ON DATA QUALITY

The International Commission for the Protection of the Danube (ICPDR) has a role of facilitating co-operation amongst Danube basin countries with respect to water management. The ICPDR sprang from the adoption by basin countries in 1994 of the Danube River Protection Convention, an acknowledgment of the river's importance to the region. One of the principal activities is the coordination of a transnational monitoring network (TNMN) which also has links with WFD reporting. In order to ensure the quality of the TNMN data an inter-laboratory comparison exercises are organised on an annual schedule since 1992. The National Reference Laboratories and other national laboratories taking part in the monitoring activities of the TNMN, as well as laboratories responsible for pollution monitoring in the Black Sea area, participate in the QualcoDanube proficiency testing organized by VITUKI.

The QC programme is continuously revised to achieve consistency with the changing aims of the TNMN. The intention is that each determinand relevant to the TNMN should be covered by the inter-laboratory test programme at least once a year and that the concentration ranges in both the water and the sediment performance testing samples should be relevant to ambient concentrations. The test programme incorporates, in any one year, the option of additional exercises for determinands showing poorer accuracy and comparability. Such poor performance is defined as where the incidence of unsatisfactory z-scores rises above approximately 30%.

The incorporation of biological determinands into AQC programme is under consideration.

At the end of the yearly distributions, an Annual AQC Report is prepared.

Criteria for method validation have been defined as follows.

Before routine application of methodology the issues below should be considered carefully. definition of the method objective and field of application,

- description and optimization of the method (undertaken before validation)
- definition of the parameters for validation and required uncertainties,
- definition of the most significant criteria for accepting the results (Criteria of acceptance),
- verification of specific equipment used in the method or its validation ,
- specification of chemicals, reagents and standards,
- document control for the optimized method,
- operational documentation, procedure for method to be applied in routine work,
- definition of criteria for revalidation,
- definition of the frequency and range for routine checks on the suitability of the system,
- documentation and recording of the results of validation.

Status				Confidentiality				Accessibility	
S0	Approved/Released	x		PU	public	x		Work-space	x
S1	Reviewed			PP	Restricted to other programme participants (including the Commission Services)			Internet	
S2	Pending for review			RE	Restricted to a group specified by the consortium (including the Commission Services)			Paper	
S3	Draft for comments			CO	Confidential, only for members of the consortium (including the Commission Services)				
S4	Under preparation								