Intergovernmental Oceanographic Commission

Workshop Report No. 122

IOC-EU-BSH-NOAA-(WDC-A) International Workshop on Oceanographic Biological and Chemical Data Management

Hamburg, Germany
20-23 May 1996

UNESCO

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SUMMARY REPORT

ANNEXES

1. INTRODUCTION AND BACKGROUND

A knowledge of the global distribution of biological and chemical parameters pertinent to the ocean carbon system is critical to understanding the role of the world ocean as part of the earth's climate system. Global Change involves a diverse and complex set of scientific problems related to the biology and chemistry of our planet, as well as its physics. By compiling and archiving available biological, physical and chemical data, we can further our understanding of oceanographic processes (e.g., the variability in ocean productivity, fluxes between the ocean and atmosphere, oceanic biodiversity) and better design programmes for pollution monitoring and remediation, and coastal and fisheries resource management. In addition, to study Global Change issues, scientists need access to the most complete digital oceanographic databases possible.

The problems of archiving oceanographic data magnify when the scope of the archive extends through the geochemical to the bio-geochemical. A challenge is to develop the database, data analysis and data visualization structures which will enable widely distributed, multi-disciplinary investigators to work with each other's data and to collaborate with each other. In view of the need for oceanographic biological and chemical data, and of the problems in managing these data, it was decided to convene an International Workshop on Oceanographic Biological and Chemical Data Management to discuss the issues involved and identify ways to solve existing problems.

In part, the Workshop was an outgrowth of the Ocean Climate Data Workshop held in Greenbelt, Maryland, USA during February 1992. This Workshop made a number of recommendations, among them the need for a follow-on workshop which "*should be more narrowly focussed with some specific recommendations*".

The International Workshop on Oceanographic Biological and Chemical Data Management held in Hamburg, Germany, 20-23 May 1996, was a result of the decision of the Fifteenth Session of the IOC Committee on IODE to convene a meeting in recognition of the role of historical, digital archives of oceanographic biological, chemical and carbon dioxide data in understanding the World Ocean's bio-geochemical cycles. It was recommended that the Workshop bring together representatives from both government institutions (including data centres) and academic communities. The Workshop concentrated on a few parameters to ensure that progress is made in understanding how best to manage this data.

2. ORGANIZATION AND ADMINISTRATIVE ARRANGEMENTS

Mr. S. Levitus, the Chairman of the Workshop, opened the Meeting at 09:30 on 20 May 1996 and introduced Prof. W. Ehlers, the President of the Bundesamt für Seeschiffahrt und Hydrographie (BSH), who welcomed the participants and briefly informed them of the activities of his Institute and the attention being paid by Germany to oceanographic research, monitoring, data collection and management. He highlighted the achievements of BSH in oceanographic biological and chemical data management and contributions made to meet JGOFS, GOOS and the Helsinki Commission objectives. He wished the Workshop participants all success and a pleasant stay in Hamburg.

Mr. Levitus welcomed the participants on behalf of the Workshop Organizing Committee, recalled the efforts made in favour of the organization of the Meeting, emphasized the economic and environmental importance of oceanographic, biological and chemical data collection and management, including historical data, and identified objectives as presented in Chapter 3 of the Summary Report. He clearly signalled his hope for the success of the workshop and his expectation that the Workshop will produce recommendations for improving oceanographic biological and chemical data management. Mr. Levitus then asked the local organizer, Mr. F. Nast and the IOC Technical Secretary, Dr. I. Oliounine to review the arrangements for the Meeting.

The programme of the Workshop was adopted as presented in Annex I. The Meeting designated Dr. L. Stathoplos and Mr. T. O'Brien, both from the USA, as co-Rapporteurs for the Workshop. The programme consisted of 4 sessions and Prof. T. Platt (Canada), Prof. T. Dickey (USA), Dr. W. Balch (USA) and Dr. G. Paterson (UK) kindly agreed to be conveners of the Session.

Discussions on the various items were introduced through presentations by invited speakers representing the scientific community, data centres, interest groups and users working on topics related to the objectives of the Workshop. The 32 presentations covered the topics identified by the Organizing Committee and are presented in Annex I. Each presentation was followed by round table discussions and at the end of each day, working groups formulated conclusions and recommendations under the guidance of a convener. The recommendations are included in different sub-items of Chapter 4.

In all, more than 40 experts from 15 countries and 3 international organizations (ICES, the Helsinki Commission, the Sir Alistair Hardy Foundation for Ocean Science) registered for the Workshop. The complete List of Participants is given in Annex II.

Regarding the presentations, a volume of proceedings of the Workshop will be published by the end of 1996, which will allow for the careful review and revision process.

3. OBJECTIVES

Scientists need access to quality controlled digital oceanographic datasets of chemical and biological parameters to: (i) monitor and assess marine pollution phenomena, both chronic as well as catastrophic; (ii) conduct research studies on bio-geochemical cycles of the earth's ocean-atmosphere system.

The overall goal of the workshop is to improve the quantity and quality of chemical and biological data available to the scientific community. The specific purpose of the workshop is to provide recommendations to guide management of chemical and biological oceanographic data by the IOC/IODE system.

The topic "*Biological and Chemical Data Management*" encompasses so many parameters (from bacteria to large mammals and from trace gases to complex organic compounds) that the workshop was planned to focus on a few variables routinely sampled by oceanographers and use these as the fulcrum from which to address solving some of the problems associated with biological and chemical data management (see Annex III for the list of the variables).

Specific objectives:

Determine the requirements for managing oceanographic chemical and biological data, for example:

- Identifying parameters that the IOC/IODE system can effectively handle.
- Describing minimum meta data requirements that make the data useful for future users of the data.
- Identifying problems that may limit the usefulness of historical data.
- Identifying users of these data and their requirements.

We identified the following problems as starting points from which to address the issues of data management:

- Most biological data, and to a lesser extent chemical data, exist only in manuscript form.

- The archive of biological data is far smaller than for physical/chemical parameters because of the labour intensive nature of data collection.

- Data are in multiple formats.

- Availability of meta data is critical.

- Data containing taxonomic information requires taxonomic data management.

- The quality of existing data and meta data needs to be evaluated.

4. ISSUES OF DISCUSSION

A number of issues were discussed through presentations and the Workshop working groups. Many of these will require action by the IOC and other groups represented at the Workshop. These issues are listed in the order they were discussed (not prioritized or ranked) and are summarized as follows:

A. Need for Biological and Chemical Oceanographic Data

The Workshop considered the need for and stressed the importance of reliable biological and chemical oceanographic data to a wide scope of human activity and scientific studies. For example, global distributions of biological and chemical parameters pertinent to the ocean carbon system are critical in understanding the impact the world ocean may play in the Earth's climate system. Carbon reservoirs exist in several organic and inorganic forms in the ocean with fluxes between them. By coupling available biological, physical and chemical data, we can further our understanding of the spatial and temporal variability in ocean productivity, and fluxes between the ocean, atmosphere and land. Proper data management plays a crucial role in enabling this coupling.

The Workshop noted several areas in which historical archives of *in situ* biological and chemical oceanographic data may provide crucial information:

(i) To extend the usefulness of satellite data by providing surface marine data in persistently cloud-covered regions.

Example: *In situ* marine surface data can supplement satellite imagery of the Southern Ocean, with a persistent band of circumpolar cloudiness centered at 60° South.

(ii) To support biological resource management and assessment.

Examples:

a) Data will help understand ecological system replacement of fisheries (e.g., the cod collapse within George's Bank, the pollack to herring transition in the NW Pacific).

b) Data will help understand the impact of hydrological activities changing nutrient compositions (e.g., in the Black Sea, this event may have influenced Mnemiopsis ledeyi replacing fish in the Black Sea).

c) Fisheries management requires definition of carrying capacity, and better understanding of ENSO-type effects on up welling regions (in fact, climatic understanding was improved by the study of the collapse of the fish stocks as an indicator of a characteristic operating mode).

(iii) To support sustainable management of coastal regions.

Example: Discharge of untreated and/or partially treated urban and industrial waste water could create changes in the pelagic ecosystem, leading to intensive phytoplankton blooms, appearance of toxic phytoplankton species, and so forth. These changes could harm, for example, tourist and mariculture activities. This happened in Italy several years ago due to an intensive phytoplankton bloom in the Northern Adriatic.

(iv) To support studies and assessments of ocean biodiversity.

Example: While tremendous attention has been focused on terrestrial biodiversity, marine biodiversity has only recently received attention, despite the fact that marine systems are larger, older, and support nearly twice as many phyla of animals as do terrestrial systems (Hay & Fenical, Oceanography, 9 (1):1996).

(v) To support studies of the earth's bio-geochemical cycles.

Example: Changes of CO_2-related variables such as dissolved organic matter (DOM), pH, calcium carbonate dissolution ratios, and dissolved organic carbon (DOC), may be reflected in the temporal variability of plankton.

(vi) To help evaluate the impact of anthropogenic activities on ocean ecosystems.

Example: Calibration studies of primary productivity measurements suggest that open ocean species may be much more sensitive to pollution than coastal species.

(vii) To differentiate anthropogenic effects from natural variability.

Example: Work based on plankton measurements from the CPR programme strongly suggests that some plankton variability in the North Atlantic Ocean is related to ocean variability linked with the atmospheric forcing known as the North Atlantic Oscillation in sea level pressure.

B. Standardization of Biological Data Collection

The workshop agreed that special efforts should be made to standardize the methods used for biological data collection and to encourage monitoring programmes to take advantage of the protocols and expertise of existing programmes. In this context the following actions have been proposed:

(i) The UNESCO manuals on primary production, zooplankton and phytoplankton methodologies were published more than two decades ago. Revised versions of the primary production, phytoplankton and zooplankton manuals are urgently needed and should include recommended international standard methodologies for use in field studies. IOC is asked to request that UNESCO identify a timetable and editorial structure to produce a revised second edition of these manuals. Existing programme manuals, such as those for the UK JGOFS, should be taken advantage of in this update.

(ii) An international Quality Control programme should be established to provide accreditation to plankton analysts and laboratories. Such programmes should include exchange and inter-calibration of samples, training workshops, and include a structure to coordinate the production of improved technical manuals and identification keys for different regions of the world.

C. Development of Chemical and Biological Oceanographic Data Management

Recurrent themes of the Workshop included the critical need to improve data acquisition and archiving procedures and protocols. The Workshop agreed that the following actions should be implemented:

At the project level:

(i) Member States are encouraged to have their scientists submit data within the agreed-upon time frames to authorized data centres. Within each project, participants must agree on a time frame for data submission and adhere to it. Delayed submissions of data have been shown to lead to data loss. Submission of biological and chemical data is critical because their acquisition is both labour intensive and expensive. Closer liaison between data centres and funding managers could help monitor progress. Data must be archived at an authorized world, regional, or national data centre. Distribution of data via the Internet is not equivalent to archiving the data at an authorized data centre. Simply because these data are available at a project's Internet *Homepage* does not means these data, or the *Homepage*, will be available in the future.

The examples of data centre activities in the field of biological and chemical data management clearly showed that the best results have been achieved when oceanographic scientific programmes had a focus on data management issues as one of their core activities and when data managers were involved in the programme development from the early planning stage. Scientists trained in the discipline of the information being gathered should manage the data.

In addition, the results of data management are best when the scientific community is involved and co-operating with data managers on a continuing basis. Such integration of data management professionals with scientists has the advantage that experts within the project can help with the quality control and quality assurance before data are archived (Annex IV is an example of quality control protocols developed in this way for the EuroGOOS programme).

British Oceanographic Data Centre (BODC) activities in the UK-JGOFS programme were brought to the attention of the workshop. As the national data centre for the UK-JGOFS programme, the BODC took care that they were seen as 'honest brokers' of the data, granting equal access to all project participants, and have subsequently received approximately 95% of all collected UK-JGOFS data.

(ii) Taxonomic identifications need to have a system of quality control comparable to the physical sciences, i.e., publishing the sources used in identifications. Also, it is essential for traceable standards, that vouchers (e.g., representative specimens, micrographs, tissue samples or other appropriate representations of the taxa collected) be deposited in appropriate institutions such as museums.

(iii) Operational definitions of terms and standards are a recurrent problem in many areas within biological and chemical sciences. It is recognized that traceable standards are necessary but often not available. At a minimum, it is desirable for many variables that definable standards are used, i.e., analytical grade reagents be used for standard preparation. The participants also recommend that inter-calibration exercises be an integral part of project data collection and management.

At the data archiving level:

(i) Information flow between data holding institutions will be an increasing feature of global scale research. To maximize this flow, communication links between data centres and other biological and chemical information sources, e.g., natural history museums, need to be established through the Internet, joint working groups, and collaborative programmes.

(ii) Recognizing the importance of the Cruise Summary Report (CSR) as a source of information in marine biological and chemical data, but noting that only a fraction of cruises are reporting via the CSR, chief scientists should be strongly encouraged to use their efforts in utilizing the CSR system.

In any future revision of the CSR, special attention should be given to the chemical and biological parts of this form to ensure that current needs are being met.

The Workshop appreciated the efforts made by ICES in CSR monitoring and agreed that the compilation of information about the existence of marine chemical and biological and chemical data should jointly make use of the information already available from CSR.

(iii) There is an essential need to provide meta data when submitting data to a data centre. Meta data are information about the data. For example, a description of the data sampling methodology (e.g., ship speed, wire angle of the net tow, filter type and size, etc.). Acceptable data submissions must at a minimum include the meta data listed in Annex V. Data managers should emphasize the meta data requirement.

(iv) Greater cooperation between national, regional, and world data centres in the exchange and flow of data should be encouraged by funding agencies and project leaders (e.g., WOCE and JGOFS).

It is already possible to assimilate some biological and chemical oceanographic data into global databases. Submission of these data to data centres was actively encouraged. To make this process more effective, it was proposed that an inventory of biological and chemical oceanographic datasets be made at all marine institutions in Member Nations to determine available biological and chemical oceanographic data. The IOC/IODE Committee was recommended to identify a centre which will take the responsibility for creating a referral database and play a continuing role as the referral centre. The Workshop acknowledged the progress achieved by the IOC/JGOFS CO_2 Advisory Panel in CO_2 data inventory development and recommended to take the Panel's experience into account when developing the biological data inventory (The CO_2 Panel Strategy is presented in Annex VI).

D. Future Technology

The Workshop considered current and future *in situ* technology in relation to the management of marine biological and chemical data (Annex VII). The advancement of technologies in the ocean sciences has increased several fold the measurement precision, ranges, and coverage in space and time of biological and chemical data. To make preparations for future changes in instrumentation and data, the workshop noted that:

(i) Future changes in data type and data volume will place increased demands on data managers. Data managers need to be prepared for new data types (e.g., ADCP, multi-frequency acoustics, video, etc.) and larger volumes of data which will result from:

(a) increasing numbers of observations from platforms such as non-research vessels (e.g., fisheries vessels, ships-of-opportunity, oil rigs, etc.) that will be used to accommodate acoustical, bio-optical, and geochemical sensors.

(b) the addition of multi-disciplinary sensor suites to existing and future research and monitoring platforms (AUV's, autonomous profilers, expendable probes, etc.).

(ii) Data managers and scientists will need to:

(a) collaborate to insure that the introduction of new technologies and methodologies do not result in systematic bias shifts.

(b) interact on issues such as under sampling and aliasing which are inherent in biological sampling (e.g., from vertical migration of zooplankton, diurnal insolation and fluorescence effects).

(iii) Be able to make data available in flexible formats. Some users may desire individual video images, for example, whereas others may wish to utilize only estimated biomass derived from these images. Some future users may want raw acoustic backscatter data whereas others may desire estimated size distributions.

(iv) End-users and data managers should communicate on issues such as desired data presentation. For example, it is anticipated that visualization using video media will grow in demand.

E. Capacity Building

The Workshop agreed that efforts should be made and measures taken to disseminate knowledge and expertise in biological and chemical data collection and management. Developing countries should receive assistance in developing the skills needed to manage these data effectively. In this context the following actions have been proposed:

Capacity building through training:

(i) Training courses implemented in the framework of IOC-OSLR, GIPME, HAB and other related programmes should contain data management as an important component. IODE data managers should assist the programmes in providing necessary knowledge.

(ii) IODE training courses should become more data type (discipline) oriented. Biological and chemical oceanographic data management training courses should be given priority and be implemented in cooperation with related scientific programmes.

(iii) We encourage funding of projects, particularly by junior scientists, that utilize existing datasets.

Through computer and technical support:

(iv) Common software containing data handling tools should be expanded to include biological and chemical data, and should be included in *OceanPC* to expand the range of possible users.

(v) Hardware and software support, to help Member States in handling biological and chemical data, should become a component of all data rescue operations. Assistance in establishing and linking to modern communication facilities should be explored.

Through data management:

(vi) Collaboration between data centre personnel and scientific experts should be encouraged through sabbatical visits, fellowships and joint projects, especially for validating historical data.

F. Funding

An obligatory prerequisite of a successful programme is availability of resources for its implementation. The need to attract resources for biological and chemical data management was the subject of many presentations and prompted lengthy discussions at the plenary and working group sessions. This may be summarized as follows:

(i) Member Nations need to provide necessary resources to accomplish the projects recommended by the Workshop (e.g., development of an inventory of available biological and chemical data, provision of the necessary biological and chemical scientific expertise, development of projects using existing data sets, etc.).

(ii) Member Nations need to commit themselves to long-term support for data management of chemical and biological (including taxonomic information) data. Due regard should be made to fund the curation and integration of vouchers.

(iii) Funding agencies should support development of data systems that effectively and efficiently link diverse kinds of data (a process known as data fusion).

(iv) Member Nations should provide support through the IOC Trust Fund arrangements for capacity building activities.

(v) Member Nations need to provide support for biological and chemical data rescue activities, exemplified by the GODAR project.

5. CONCLUSIONS AND CLOSURE

The participants of the Workshop were of the general view that the goals had been achieved and the Meeting was a success. In a certain way it proved to be an important landmark, not only in IODE development, but also in establishing close links with other IOC programmes and international organizations involved in oceanographic biological and chemical data collection and management.

To further reinforce the inter-programme and international co-operation in the framework of the Workshop problem area, it was strongly recommended that a special body be created through relevant IOC programmes, e.g., GIPME, HAB, OSLR and programmes of other organizations, to bring together scientists, data managers and users to jointly tackle the problems related to oceanographic biological and chemical data.

The Workshop was of the opinion that the organization of these type of workshops should be continued on a regular basis and the next one be envisaged in 3 years when the requirements for biological and chemical data of GLOBEC, GOOS, and CLIVAR will be better identified.

In closing the Workshop, the Chairman, Mr. S. Levitus, expressed on behalf of the participants their appreciation for the facilities and hospitality provided by the BSH and commended all attendees and invited speakers on their active participation.

The Meeting was closed at 16:00 on 23 May 1996.

ANNEX I

WORKSHOP PROGRAMME

VENUE

The Workshop was held in Hamburg, Germany, in the Bundesamt für Seeschiffahrt und Hydrographie, BernhardNocht.Strasse 78, Room: Grosseer Sitzungssaal.

SPONSORS

- National Oceanographic Data Center of the United States of America/World Data Centre A for Oceanography;

- Intergovernmental Oceanographic Commission of UNESCO;

- European Union MAST Programme;

- Bundesamt für Seeschiffahrt und Hydrographie.

GENERAL OBJECTIVES

In order to conduct research studies on bio-geochemical cycles on the earth's ocean-atmosphere system, scientists need access to quality controlled digital oceanographic datasets of chemical and biological parameters. With the advent of new technology in the measurements of biological and chemical parameters, the precision of instruments has increased several fold. Despite the increase in precision, we should not automatically eliminate earlier measurements from historical archives.

The overall goal of the workshop is to improve the quantity and quality of chemical and biological data available to the scientific community. The specific purpose of the Workshop is to provide recommendations to guide management of chemical and biological oceanographic data by the IOC/IODE system.

The topic 'Biological and Chemical Data Management' encompasses many parameters, from bacteria to large mammals and from tracer gases to complex organic compounds. However, in order to focus on data management issues, case studies will be limited to parameters routinely sampled.

SPECIFIC OBJECTIVES

Determine the requirements for managing oceanographic chemical and biological data, for example:

- Identify parameters that the IOC/IODE system can effectively handle;
- Describe minimum metadata requirements that make data useful for future users;
- Identify problems that may limit the usefulness of historical data;
- Identify the users and their requirements.

The following problems have been identified as starting points from which to address the issues of data management:

- Most biological data, and to a lesser extent chemical data, exist only in manuscript form;
- Data exists in diverse formats;
- Availability of metadata is critical;
- Data containing taxonomic information requires taxonomic data management;
- The scientific evaluation of historical biological and chemical data and metadata needs to be supported by governmental and nongovernmental agencies.

METHODS

A mixture of scientific and data management presentations will be used to stimulate discussion. Three discussion topics have been selected as a vehicle to meet the Workshop objectives. They are:

- Application of historical biological and chemical measurements;
- International co-operation in data management of biological and chemical oceanographic data;
- Biological and chemical data management - how can the problems be tackled?

The Workshop will be introduced by speakers who will give attendees a broad overview of both on-going and planned activities. It is hoped that these speakers, as well as representatives of each of the topical areas, will lead a final panel discussion bringing together suggestions made during the meeting into requirements for future actions.

WORKSHOP PROGRAMME

Day 1: 20 May 1996

08.30 - 09.00	Registration
09.00 - 09.30	Opening Remarks Chairman: S. Levitus BSH President: P. Ehlers
SESSION I:	**OVERVIEW**
	Convener: T. Platt (Canada) Rapporteurs: L. Stathoplos, T. O'Brien (USA)
09.30 - 10.15	*Bio-geochemical Cycles:* T. Platt (Canada)
10.30 - 11.15	*Managing the Biodiversity of Marine Biological Data Perspective from a European Union Project:* G. Paterson (UK)
11.30 - 12.00	Coffee Break
12.00 - 12.45	*Data Archaeology and Rescue of Historical Oceanographic Data:* S. Levitus (USA)
13.00 - 14.00	Lunch
SESSION II:	**APPLICATION OF HISTORICAL BIOLOGICAL AND CHEMICAL MEASUREMENTS**
	Convener: T. Dickey (USA) Rapporteurs: L. Stathoplos, T. O'Brien (USA)
14.00 - 14.20	*Use of Time-series Chlorophyll Data:* Y. Dandonneau (France)
14.30 - 14.50	*Objective Analysis of Historical Chlorophyll Data:* M. Conkright (USA)
15.00 - 15.30	Coffee Break
15.30 - 15.50	*The Spatial and Temporal Variability of the CO_2 System in the Upper Waters of the Ocean:* P. Makkaveev (Russia)
16.00 - 16.20	*Interannual Variability of the World Ocean:* S. Levitus (USA)
16.30 - 16.50	*Bio-geochemical Modelling:* W. Gregg (USA)
17.00	Working Groups

Day 2: 21 May 1996

SESSION III:	**INTERNATIONAL COOPERATION IN DATA MANAGEMENT OF BIOLOGICAL AND CHEMICAL OCEANOGRAPHIC DATA**
	Convener: W. Balch (USA) Rapporteurs: L. Stathoplos, T. O'Brien (USA)
09.00 - 09.20	*Current and Past ICES Activities in Chemical and Biological Oceanographic Data:* H. Dooley (ICES)
09.30 - 09.50	*Management of Biological and Chemical Data within the JGOFS Project:* P. Machin (UK)
10.00 - 10.30	Coffee Break
10.30 - 10.50	*Management of Biological, Physical and Chemical Data within the GLOBEC Project:* R. Groman (USA)
11.00 - 11.20	*SeaWiFS Requirements for Biological Data:* W. Gregg (USA)
11.30 - 11.50	*Management of the HELCOM BMP Biological and Chemical Data:* J. Rissanen (Helsinki Commission)
12.00 - 13.00	Lunch
13.00 - 13.20	*Management of CO_2 Data at CDIAC:* A. Kozyr (USA)
13.30 - 13.50	*CO_2 Parameters: towards the Databases:* A. Poisson (France)
14.00 - 14.20	*Examples of Availability of Biological and Chemical Data:* F. Nast (Germany)
14.30 - 15.00	Coffee Break
15.00 - 15.20	*Emerging Technologies in Biological Sampling:* T. Dickey (USA)
15.30 - 15.50	*Status of Chemical Oceanographic Data in Russia:* V. Sapoznikov (Russia)
16.00 - 16.20	*Data Bank Management System of German NODC with a Focus on Chemical Data:* K. Motamedi, R. Schwabe (Germany)
16.30 - 16.50	*An Application of Distributed Object Technologies of Standardization and Automation of Queries from Diverse Marine Datasets:* M. Ostrowski (Norway)
18.00	Social Event (sponsored by BSH)

Day 3: 22 May 1996

SESSION IV:	**BIOLOGICAL AND CHEMICAL DATA MANAGEMENT**
	Convener: G. Paterson (UK) Rapporteurs: L. Stathoplos, T. O'Brien (USA)

09.00 - 09.20	*Accuracy of Historical Measurements of Nutrient Data:* C. Garside (USA)
09.30 - 09.50	*Accuracy of Historical Measurements of Primary Productivity Data:* W. Balch (USA)
10.00 - 10.30	Coffee Break
10.30 - 10.50	*Quality Control of Historical Chlorophyll Data:* M. Conkright (USA)
11.00 - 11.20	*Nutrient Data from the South Pacific: Synthesis of the WOCE and Historical Data:* V. Gouretskii (Russia)
11.30 - 11.50	*Accuracy of Historical Measurements of Plankton Data:* C. Reid (UK)
12.00 - 12.20	*Management of Biological Oceanographic Databases:* A. K. Ghosh (India)
12.30 - 13.30	Lunch
13.30 - 13.50	*Metadata Requirements for Plankton Data:* L. Stathoplos (USA)
14.00 - 14.20	*Metadata Requirements for Zooplankton Biomass Studies:* J. Rudjakov (Russia)
14.30 - 15.00	Coffee Break
15.00 - 15.20	*Taxonomic Code Systems and Taxonomic Data Management:* L. Stathoplos (USA)
15.30 - 15.50	*Taxonomic Identification:* R. P. Heijman (Netherlands)
16.00 - 16.20	*Long Time-series of some Hydro biology from the Eastern Mediterranean:* S. Lakkis (Lebanon)
16.30	Working Groups

Day 4: 23 May 1996

09.30 - 09.50	*Taxon Manager:* J. Reich (Switzerland)
10.00 - 12.20	Round table discussions led by the Workshop Chairman and Conveners of Sessions
12.30 - 13.30	Lunch
13.30 - 15.00	Formulation of conclusions and recommendations.

ANNEX II

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ANNEX III

LIST OF VARIABLES

The oceanographic variables discussed by the Workshop:

- Temperature;
- Salinity;
- Oxygen;
- Nutrients (e.g., Nitrate, Phosphate, Silicate, etc.);
- Chlorophyll;
- Primary Productivity;
- Other pigments (e.g., Phaeophytin, Fucoxanthin, Peridinin, etc.);
- Carbonate System (e.g., pH, alkalinity, etc.);
- Particulate Organic Carbon (POC);
- Dissolved Organic Carbon (DOC);
- Presence of pelagic taxa (plankton);
- Biomass (weight or volume) of pelagic taxa;
- Abundance of pelagic taxa.

ANNEX IV

QUALITY CONTROL PROCEDURES FOR CHEMICAL OCEANOGRAPHIC DATA MANAGEMENT

A. Standard Tests

(i) Test that the geographical co-ordinates of the observation do not plot on land. Comparison can be made with one of the standard high-resolution global coastline maps.

(ii) If there are a series of observations at different depths, and a maximum depth reading for the location, check that none of the observation data points are deeper than the maximum depth.

(iii) Check successive co-ordinates of geographical position of soundings (profiles), and mean velocity of ships between observations. This should not exceed a reasonable maximum velocity for the ship. Also check for stations which occur significantly off the cruise-track of the ship.

(iv) Where there are a series of samples or observations in descending and ascending sequence on a CTD rosette, or other sampling system, check that depths progressively increase and decrease in sequence, without reversals.

(v) Check the identifier code for ship or platform.

(vi) Check that the date and time fields are consistent.

(vii) Check that header information contains contact address for laboratories responsible for the analysis, and a reference number or identifier for chemical standards used and people responsible for the analysis.

B. Parameter-specific Tests

(i) Check that the data header contains information on the standard analytical procedures, calibration of equipment, and quality control of original data. This information can be in a compressed form referring to standard procedures. No details are required, but the information should allow the data user to go back to the original laboratory or project organizer and check the information if necessary.

(ii) Check that header information states that the data fields to follow contain numerical data referring to chemical parameters such as nitrate, phosphate, silicate, CO_2, oxygen, or chlorophyll. For any particular quality control system there should be a list of variables which are acceptable to that QC procedure, and others should be excluded.

(iii) Include header information to describe standard climatology or reference datasets which have been used for comparison in detecting anomalies and outliers.

(iv) Check that header information and data cycle labels include definition of units which are consistent with the variable being observed.

C. Variable-specific Tests

(i) Check that the values in each data column or series are consistent with the heading information. It is possible that column headings and values have become switched?

(ii) Check maximum range of numbers indicating variable concentrations. Is it physically or chemically possible that the number could be so high or so low?

(iii) Check rate of change of variable. Comparing one data value with the preceding and succeeding values in the series, is it conceivable that the change could be so large?

(iv) Detection of constant values. If 3 or 4 or more successive values are identical, or nearly identical, is this an error? Is it conceivable that so many successive values could be identical?

(v) Total range of the dataset. Is it reasonable that the highest value in the dataset and the lowest value in the dataset should occur? Check against the climatology for the region at that time of year.

(vi) Check single values of the dataset against the climatology for that time of year, location, and depth.

(vii) Compare departure from mean of climatology with standard deviation, and agreed multiple of standard deviation before flagging as an outlier.

(viii) If the sampling station is in the open ocean, does the profile go down to an ocean depth below the mixed layer, and produce a deep ocean value? If so, is this accurate in comparison with known climatology?

(ix) If location is in coastal or shelf waters, are the vertical and horizontal variabilities consistent with the climatology expected?

(x) Does this chemical analyte have a known relationship to salinity? If so, calculate ratios to salinity values, and flag data points failing outside acceptable range.

(xi) Do two or more of the analytes in the dataset have a predictable relationship to each other? If so, check that the ratios are acceptable, and that the trend or change in successive values of the two analytes are in the correct direction.

(An extract from a letter by Nick C. Flemming of EuroGOOS)

ANNEX V

METADATA REQUIREMENTS

Current global-scale research is being hampered by a lack of metadata associated with archived datasets. A recurrent theme of the workshop was the need to provide metadata with data submitted for archive, particularly for future assessment of data now being measured and banked. As a result minimum requirements for a number of variables were produced by experts at the Meeting, to provide examples of the information needed. It is clear from these examples that there can be no standard format and, therefore, it will be difficult to produce reliable check-lists. It must be the responsibility of the data producer to ensure that sufficient metadata is included to enable third parties to understand how and why the data was generated.

General Requirements:

- Position (latitude, longitude, operating area);
- Date and Time (signify if GMT or local);
- Range of Data Values (desirable);
- Ship;
- Cruise;
- Programme or Project;
- Institution;
- Principal Investigator(s).

Additional Requirements for:

Nutrients:

1. Sampling Method
    - Nansen Cast
        - Discrete bottles
        - Rosette
        - Bottle type
    - Continuous Samplers
        - Sampler description & rate
        - Pump
        - Profile or Underway

2. Storage Method
    - Container Size and Material
    - Storage Conditions
        - In light or dark
        - At room temperature/refrigerated/frozen
    - Duration (hrs - months)

3. Analysis
    - Location (ashore or at sea)
    - Reference to a published methodology
        - or -
    - Method description
    - Manual or automated CFA/FIJA
    - Chemical reaction
    - Standard - source/provenance
    - Linear range checked
    - Analyst and responsible person

4. Data Reduction
    - Reference to published methodology
        - or -

7. Method description
    - Raw data correction - blank/baseline
    - Calibration
        - range, # standards
        - manual graph, regression, turnkey software
    - Precision - from calibration/regression
    - Accuracy - relative to what?

5. Reporting
    - Chemical units (e.g., ug-at/l, mg/m^3, etc.)
    - Value representation (individual values, replicate averages, interpolated std z, etc.)
    - QA/QC flags and what they mean

6. Archival
    - Are data archived with author, institution, in another database
    - Relevant bibliography (desirable)

pCO_2:

1. Depth of seawater intake

2. Design of equilibrator

3. Method of CO_2 measurement (GC, IR, etc.)

4. Information on the calibration gases used
    - Manufacturer
    - Date of certification
    - Traceability of certification (if known)
    - Expected accuracy of certification
    - Concentrations of calibration gases used
    - Frequency of calibration

5. Information about calibration of the pressure and temperature measuring instruments that were used. In particular, an estimate of the quality of the sea surface temperature measurements.

6. Data corrections (e.g., sea temperature) - how many?

7. Precision and accuracy estimates of the overall measurements

In addition the following information should be archived:

1. $x(CO_2)$ - mole fraction of CO_2 - in dry air at equilibrium with sea surface water at the sea surface temperature at 1 atmosphere pressure.

2. Calculated fugacity of CO_2 in equilibrium with the surface sea water

3. Temperature sea surface

4. Salinity - sea surface

5. Atmospheric pressure

6. Actual equilibrium pressure

7. Measured wind speed and direction

For further information see http://cdiac.esd.ornl.gov/cdiac

Primary Production:

1. Depth/irradiance/incubation start and end times

2. Methodology protocols
   - Was chlorophyll measured on the same samples?
   - Were sampling bottles tested for toxicity?
   - Were filters used in C14 determinations, what type, pore size?
   - Was the C14 that passed the filters determined?
   - Were the filters treated to drive off the bicarbonates?
   - Was any carbonate C14 used in the primary production values?
   - Was C14 bicarbonate solution prepared in glass ampules?
   - Was non metallic hydro-wire used (e.g., Kevlar)?
   - Were bottles closed electronically or with coated messengers?
   - Were samples exposed to black rubber (e.g., O-rings or tubing)?
   - Was a time-zero sample subtracted?
   - Was a dark bottle subtracted?
   - Were samples pre-filtered to eliminate grazers?
   - What was the volume of the incubation bottles?
   - What instrument was used to measure light?
   - What kind of light collector (Cosine, scalar, etc.)?
   - Bottle cleaning protocol (e.g., acid soaking, water rinses)?
   - Type of incubation (on deck, simulated *in situ*)?
   - Type of scintillation counter used to measure C14?
   - Type of scintillation cocktail used?
   - Number of replicates?
   - How were incubations stopped (formalin, glutaraldehyde or filtration)?
   - What was E CO_2 concentration used in calculation?

3. Actual C14 values
   - Units of data
   - Light bottle C fixed per experiment (replicate 1...replicate N)
   - Light bottle C fixed per time (replicate 1.....replicate N)
   - Dark bottle C fixed per time (replicate 1.....replicate N)
   - Difference average light bottle - dark bottle

Chlorophyll and other Pigments:

1. Sample depth

2. Percentage light - from secchi disk, PAR

3. Method
   - Fluorometric
   - Spectrophotometric
   - High performance liquid chromatography

4. Material concentrated on a filter?

5. Filter type
   - Glass fibre
   - Millipore-type membrane
   - Nucleopore-type membrane

6. Filter pore size

7. Pigments analyzed

Chlorophyll a	Phaeophytin
Chlorophyll b, c1, c2	Fucoxanthin
Neofuxanthinol	Diatoxanthin

Dnoxanthin	Peridinin
Lutein	Zeaxanthin
Flavoxanthin	Violaxanthin
Neoxanthin	Alloxanthin
Astaxanthin	Monodoxanthin
Crocoxanthin	Myxoxanthin
Myoxoxanthophyll	Anthraxanthin
Siphoaxanthin	Phycoerythrin
Phyocyanin	Phycourbilin
19'- hexanoyl fucoxanthin	19'- butanoyl fucoxanthin
Diadinoxanthin	Diatoxanthin
Echinenone	Phaeophorbide-a
Chlorophyllide-a	Alpha-carotene
Beta-carotene	Gama-carotene

8. Concentration unit (e.g., ug/l, nanograms/l)

9. Concentration of pigment

PAR/Light Field:

1. Light Instrument
   - Spherical (scalar irradiance)
   - Cosine (downward vector irradiance)

2. Wave lengths measured of "PAR" (e.g., 350nm - 700nm or other?)

3. Manufacturer (e.g., Li-Cor, Biospherical, etc.)
   - Model
   - Serial number

4. Calibration methods and data of last calibration

5. Conversion algorithm with immersion factor (e.g., volts output to PAR)

6. PAR units for calibration/data reported (may be different)

7. Ship shadowing or buoy or drifter; shadowing ship effects/comments. Also note whether PAR sensors are used on ship deck, buoys or at depth. For deck/buoy measurements metadata should include information concerning possible contamination from ship lights, e.g., shadowing, reflected light contamination.

Considerable attention has been devoted to the points made above particularly for spectral data for the SeaWiFS programme.

Further information: US JGOFS Planning Report Number 18, Bio-optics in US JGOFS, December 1993, eds. T. Dickey and D. Siegel, 180 pp. US JGOFS Planning and Co-ordination Office, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, USA.

Plankton (biomass & taxon-based studies):

1. Sampling protocols
   - Upper and lower depth
   - Tow information
     - Type
     - Duration and speed
     - Distance
   - Gear type (Reference)
     - Type
     - Mouth area

Mesh size
Water volume sampled

2. Sorting protocols (Reference if available)
   Sieve mesh (if used)
   Fixative and preservative used
   Time between fixation and biomass estimate
   Large plankter protocol
      Are they removed?
      Minimum length or volume removed

3. Zooplankton biomass estimate protocols (Reference if available)
   Weight protocol (wet, dry, ashfree, etc.)
   Volume protocol (displacement, settled, etc.)
   Counting protocol (by aliquot, total enumeration, etc.)

4. Taxonomic Analysis
   Investigator
   Taxonomic literature used (e.g., references to keys, papers, etc.)
   Voucher material (e.g., specimens, tissue samples, etc.)
      Location (Museum, Laboratory, DNA database, etc.)

5. Remarks (e.g., plankton bloom present, etc.)

For further details of zooplankton biomass metadata see Dr. Rudjakov's paper in the Proceedings of the International Workshop on Marine Biological and Chemical Data Management.

Bacteria (abundance and production):

1. Start-time and end-time of incubation (local time or GMT)

2. What production technique was used (tritiated thymidine, tritiated leucine or other)

3. What abundance technique was used (epifluorescence microscopy, flow cytometry or other)

4. Sampling protocols:
   General:
      Was non-metallic hydro-wire used, coated messengers, any black rubber?
      What depths/irradiances were sampled?
      Was bacterial production and abundance measured on the same samples?
      What else was measured on these samples (e.g., primary production, chlorophyll)?

   Abundance Estimates by Epifluorescence Microscopy:
      Reference: JGOFS protocols
      Sample subdivision method:
         What volume was filtered to yield approx 100 cells per field of view?
         What filters used? recommended - 0.2um Nucleopore stained with Irgalan Black
         Fixative (glutaraledehyde or other)
         Stains used (DAPI, acridine orange or other)
            What were their final concentrations?
         Counting technique: should be approximately 100 cells per field of view.
         Microscope technique:
            Type of microscope
            Were filter sets appropriate to the stain used?
            Number of fields counted
            Time lapsed between sampling and filtering/staining.
            Any retrospective conversions applied?
            Counts calibrated against fluorescent microspheres?
         Units: how were number of cells/field of view converted to cells/litre?

Other techniques used?
details of filters,
pre-filtering,
number of fields counted,
approximate no. of cells per field,
operative size range of flow cytometer,
were the counts calibrated against fluorescent microspheres
any time delays between sampling and counting.

Production Protocols:

a) Incorporation of methyl-tritiated thymidine:
How were incubations terminated - by formalin?
Filters used:
Type, Pore size;
Was filtering carried out using vacuum pressure of 70mm Hg or lower?
What liquid scintillation analyzer was used,
What was the counting error?
Were quench corrections applied?
What liquid scintillation cocktail was used?
What incubation bottles were used,
How were they treated, acid cleaned, etc.?
Was the incubation at *in situ* temperature?
Was a time-zero bottle subtracted?
Conversion factors used from DPM to uptake rates
Units (e.g., picomoles of thymidine uptake/litre/hour)
Are the uptake rates averages of replicates?
If so, what is standard deviation?

b) Incorporation of tritiated leucine:
Reference: JGOFS protocols
How were incubations terminated, by 5% trichloroacetic acid (TCA)?
Filters used:
Type
Pore size
Was filtering carried out using vacuum pressure of 150 mm Hg or lower?
What liquid scintillation analyzer was used?
What was the counting error?
Were quench corrections applied?
What liquid scintillation cocktail was used?
What incubation bottles were used?
How were they treated, acid cleaned etc.?
Were samples handled with plastic gloves to avoid amino acid contamination?
Was the incubation at *in situ* temperature?
At what temperature was the incubation extracted into TCA (should be 80 deg C)?
Was a time-zero bottle subtracted?
Conversion factors used from DPM to uptake rates
Units (e.g., picomoles of leucine uptake/litre/hour)
Are the uptake rates averages of replicates?
If so, what is standard deviation?

Other Techniques:
What incubation bottles were used?
How were they treated, acid cleaned, etc.?
How was incubation terminated?
Was it at in situ temperature?
Details on analysis (e.g., scintillation counting), conversion factors, replicates, filters used, any time-zero bottles?

ANNEX VI

STRATEGY FOR CARBON DIOXIDE INVENTORY DEVELOPMENT

1. **Compile an international list of people** that might be expected to have knowledge of carbonate chemistry measurements.

2. **Compile an inventory** requesting the identified scientists to provide the dates and locations of their carbonate chemistry measurements with particular emphasis on $P(CO_2)$ measurements.

3. **Identify a suitable internationally recognized data centre** to act as the host for this archive of underway $P(CO_2)$ measurements.

4. **Collect the measurements together with associated "metadata"** from the individual scientists and build a homogenous database to be archived and made available from this data center.

5. Once the database is in place, initiate discussions with the $C0_2$ community to **identify any derived data products** such as gridded maps, etc. that should be developed and made available together with the primary data.

6. **Plan to incorporate future $P(CO_2)$ measurements** into this database.

(An extract from the IOC/JGOFS CO_2 Advisory Panel)

ANNEX VII

TABLE OF INSTRUMENTS FOR BIOLOGICAL AND CHEMICAL OCEANOGRAPHIC DATA COLLECTION

Sensor System	Measurements Made by Sensing System	Sampling Mode	Time-Scale Min:Max	Resolution Vertical:Horizontal
CTDs	Temperature Conductivity Pressure Dissolved O_2 pH	Profiled Moored, yo-yo, tow-yo Towed	1 hr:1 mon 1 min:1 yr 1 sec:1 day	0.5m:1 km 10m:10 km 0.5m:1 m
Current Meter	Water Velocity, Speed, & Direction	Moored	1 min:1 yr	10m:10 km
Water Bottles	Water for Shipboard or Laboratory Analysis	Profiled	1 hr:1 mon	10m:1km
Bio-Optical	Beam Attenuation Stimulated Fluorescence PAR Upwelling Radiance Down welling Irradiance Optical Plankton Counter	Profiled Moored Towed	1 hr:1 mon 1 min:1 yr 1 sec:1 day	1 m:1 km 10m:10 km 1 m:1 m
In situ chemical analyzer	Inorganic nutrient: O_2	Profiled Moored Towed	Continuous 2hr:2-3 mon	2m:100 km
In situ microbial rates (SID)	Primary production: tracer uptake	Moored Surface drifter	3-9hr: 1-3 mon (100 samples max)	10m:100 km
Optical Imaging	Video Images of Number, Size, Taxa & Biomass	Moored Towed	<1 sec:3 mon	1 pm:10 km 1 m:10 km
Nets	Species, Number & Size	Towed	1 hr:1 day	1 m:100 m
ADCP (300kHz)	Current Profiles Acoustical Backscattering	Moored Towed	1 min:1 yr 1 min:1 mon	1 m:10 km 1 m:10 m
SODAR	Wind Velocity Profiles	Moored Shipboard	10 min:1 yr 10 min:1 yr	10m:100 m
Lagrangian Drifters	GPS Position CTD & Bio-Optical	Drifting	1 hr:6 mon	10m:100 m
Acoustical Imaging	Acoustical Backscattering Numbers & Target Strength	Profiled Moored Towed	1 hr:1 mon 1 min:1 yr 10 sec:1 day	1 m:1 km 1 m:10 km 1 m:30 m

(Adapted from US Globec Report 6: 1992)

ANNEX VIII

LIST OF ACRONYMS

ADCP	Acoustic Doppler Current Profiler
AUV	Autonomous Underwater Vehicle
BODC	British Oceanographic Data Centre (United Kingdom)
BSH	Bundesamt für Seeschiffahrt und Hydrographie (Germany)
CDIAC	Carbon Dioxide Information Analysis Center
CLIVAR	Climate Variability & Predictability Programme
CPR	Continuous Plankton Recorder
CSR	Cruise Summary Report
CTD	Conductivity-Temperature-Depth Probe
DOM	Dissolved Organic Matter
ENSO	El Niño South Oscillation
EU	European Union
EUROGOOS	European Programme for the Global Ocean Observing System
GIPME	Global Investigation of Pollution in the Marine Environment
GLOBEC	Global Ocean Ecosystems Dynamics
GMT	Greenwich Mean Time
GPS	Global Positioning System
GODAR	Global Oceanographic Data Archaeology & Rescue Project
GOOS	Global Ocean Observing System
GTSPP	Global Temperature Salinity Pilot Project
HAB	Harmful Algal Bloom
HELCOM BMP	Helsinki Commission Biological Monitoring Programme
ICES	International Council for Exploration of the Sea
IFREMER	Institut Français de Recherche pour l'Exploitation de la Mer
IOC	Intergovernmental Oceanographic Commission
IODE	International Oceanographic Data & Information Exchange
JGOFS	Joint Global Ocean Flux Study
LODYC	Laboratoire d'Océanographie Dynamique et de Climatologie (France)
MAST	Marine Science & Technology
NASA	National Aeronautics & Space Administration (USA)
NESDIS	National Environmental Satellite, Data & Information Service (USA)
NOAA	National Oceanic & Atmospheric Administration, USA
NODC	National Oceanographic Data Center
OCEANPC	Ocean Personal Computer Project
OSLR	Ocean Science in Relation to Living Resources

PI	Principal Investigator
POC	Particulate Organic Carbon
QC	Quality Control
RAS	Russian Academy of Sciences
SeaWiFS	Sea-viewing Wide Field-of-view Sensor
SISMER	Systemes d'Information Scientifiques pour la Mer (France)
TCA	Tri-Chloroacetic Acid
UNESCO	United Nations Educational, Scientific & Cultural Organization
VNIRO	All-Russia Research Institute of Marine Fisheries & Oceanography
WDC	World Data Centre
WOCE	World Ocean Circulation Experiment

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