PARENT

Underway
Data Documentation

Introduction

This document describes the continuously sampled surface underway data from the PRIME cruise (Discovery cruise 221, June-July 1996). It includes measurements made from near-surface (approximate depth 4.5m) seawater taken from Discovery's "non-toxic supply", measurements made in air (meteorology), navigation and bathymetry.

Binary Merge File Structure

All parameters measured underway have been merged into a binary file, using time as the primary linking key. N.B. because this file is *binary*, it cannot be viewed directly by an editor**. On NO ACCOUNT try to print this binary file directly**.

The sampling resolution of the file is 1 minute. In the binary merge file, each parameter is identified by a single character; this is given in parentheses following each channel name.

Windows users may view the underway data, or convert them to ASCII, using the Underway Explorer program supplied on the CD-ROM. Users of other platforms who wish to use the underway data should contact BODC for assistance (bodcmail@ccms.ac.uk)

Underway Parameters

Navigation

N.B. Oceanographic convention dictates that ship's direction refers to the direction the ship is **going to**.

Parameter	Units	Instrument
Latitude (A)	Degrees North	Calculated by dead reckoning from GPS position fixes
Longitude (B)	Degrees East	Calculated as for latitude
Distance along track (K)	Km	Calculated using spherical geometry
Ship's heading ')'	Degrees (True)	Ship's Gyro compass
Bathymetry (J)	Metres	Echo-sounder (corrected by Carter's tables)

Meteorology

N.B. According to meteorological convention, wind direction is given as the direction the wind is **coming from**.

Parameter	Units	Instrument
Barometric pressure (1)	Millibars	Aneroid barometer
Dry bulb air temperature (a)	degrees Celsius	Port and starboard psychrometers
Wet bulb air temperature (b)	Degrees Celsius	Port and starboard psychrometers
PAR (L)	W/m^2	Port and starboard 2-pi PAR sensors
Solar radiation (O)	W/m^2	Port and starboard Vector solarimeters
Wind speed (Y)	Knots	Young Anemometer (corrected for ship's velocity and heading)
Wind direction (Z)	Degrees	Young Anemometer.

Hydrography and Optics

N.B. salinity was calculated from temperature and conductivity according to the formula given in Fofonoff (1973)

Parameter	Units	Instrument
Sea surface temperature (C)	degrees Celsius	TSG 103 thermosalinograph
Sea surface salinity (F)	PSU	TSG 103 thermosalinograph
Attenuance (I)	m^{-1}	SeaTech 25cm transmissometer (670nm)

Sea Surface Chemistry and Biology

Parameter	Units	Instrument
Chlorophyll (!)	$mg.m^{-3}$	Aquatrakka fluorometer
Nitrate (T)	µM	Technicon AutoAnalyser
Nitrite (U)	µM	Technicon AutoAnalyser
Phosphate (V)	µM	Technicon AutoAnalyser
Silicate (W)	µM	Technicon AutoAnalyser
Dissolved SF6 (x)	femtomolar	Electron Capture Detector
Ammonia (v)	nanomolar	Nanomolar ammonia

Sampling Protocols and Data Acquisition

Water was pumped continuously into the ship's "wet lab" from the non-toxic pump (approximate depth of intake, 4.5m) via a header tank which acted as a debubbler. The fluorometer and transmissometer were located in the header tank and thus sampled water which had come directly from the ship's hull. The thermosalinograph was also housed in a tank which received water directly from the hull; any warming of the water as it passed through the ship's hull was corrected for as the temperature was measured both at the point of intake and at the thermosalinograph housing. Various tubing supplied the other instruments such as the AutoAnalyser.

All instruments were logged by the ship's Level A computer system at 30 second intervals. The Level B passed the time-stamped data to the Level C Sun system where they were logged. The Level C data were submitted to BODC for processing at the end of each cruise.

At BODC each data stream was merged into a binary file using time as the primary linking key. The data were reduced to 1 minute sampling resolution at this point, to keep the binary merge files a manageable size.

Calibration and Quality Control Procedures

All underway data were screened using the in-house graphical editor SERPLO. A number of basic checks were made to begin with:

- unrealistic ship speeds or incursions onto land due to gaps or jumps in the navigation;
- unreasonable ranges of values according to climatology;
- lack of correspondence between related parameters or unreasonable ratios of chemical constituents.

The graphical editor was then used to time-step through the data in more detail, considering each data point. Instrument spikes and malfunctions were identified and "flagged" accordingly. An instrument spike was defined as a single value or small number of values which showed an inexplicable variation of more than the recommended target precision. "Flagging" involved setting a single character quality control flag to denote the status of the data; no values were deleted or changed. The following quality control flags were used:

- G good data
- I interpolated data (navigation and bathymetry only)
- S suspect data (instrument spike or malfunction)
- N null data (not measured)

Calibration procedures either involved applying algorithms supplied by the instrument manufacturers or comparing the continuous (raw) output against discrete calibration samples taken concurrently. Particular care was taken to ensure maximum temporal coverage of calibration samples, in order that any time-dependent instrument drift could be fully corrected. Errant calibration points were rejected only if sampling occurred over a considerable gradient and there was reasonable doubt that the underway instrument was sampling different water to the discrete calibration sample. Simple linear regression or multiple linear regression was used to establish the calibration algorithms, apart from in the case of the Aquatrakka fluorometer where the voltage was regressed against log-transformed chlorophyll concentrations.

Navigation

Three-dimensional Global Positioning System (3D-GPS) was used as the main form of ship's navigation with dead-reckoning applied between the satellite-derived position fixes. The GPS fix was only used as the definitive position when the Positional Dilution of Precision (PDOP) was less than 5. Where the PDOP became unacceptably high, alternative means of navigation were used (TX1107 satellite navigation, Decca in inshore waters). After initial screening using SERPLO to check for incursions onto land or jumps in navigation, any gaps in the navigation files of longer than 15 minutes were filled by manual position fixes taken by the ship's officers. A Fortran program was then run to re-interpolate the navigation between position fixes, incorporating the manual fixes. The output from this was then checked again using SERPLO and the ship's speed was computed; where this apparently exceeded 14 knots, further checks were made on the navigation data, which was re-interpolated if necessary.

During both cruises, the Level B on the ship's computer reset the distance run to zero partway through the cruise. The cleaned up navigation data were used to recalculate the distance run for the entire length of each cruise.

The bathymetry data are generally good for the latter part of the cruise. They are not available for the first part as the logging software was not initiated until partway through the cruise. Carter's table corrections were applied to compensate for latitude and temperature-dependent variations in the speed of sound through water.

DATA QUALITY : the ship's navigation and bathymetry instruments worked very well throughout the cruise and there were very few gaps in the navigation file, so excessive interpolation was not a problem. The quality of all the navigation data is therefore thought to be very good.

Meteorology

The MetPac instruments worked well and only minor flagging in SERPLO was necessary for all channels. The absolute wind velocity appeared to be totally independent of changes in the ship's heading, implying that the correction of the relative wind speed and direction for the ship's velocity and heading had been done properly. Comparison of port and starboard sensors showed good correspondence for air temperatures, PAR and solar radiation, with little evidence of shadowing.

The following calibrations (all from manufacturer's specifications) were applied :

Barometric Pressure	calibrated pre-cruise; logged as millibars absolute
Air temp (port and stbd)	calibrated pre-cruise; logged as degrees Celsius
Wind speed and direction	converted from relative to absolute
PAR - masthead	calibrated by Level C
PAR - port	calibrated by Level C
PAR - starboard	calibrated by Level C
Solar - port	calibrated by Level C
Solar - starboard	calibrated by Level C

DATA QUALITY - the PAR calibration algorithms are slightly out of date - light intensities went slightly negative at night, or failed to reach zero. Generally, these problems were minimal (i.e. offsets of no more than 5 W/m^2).

Hydrography and Optics

A SeaTech TSG 103 thermosalinograph was used to measure sea surface temperature and conductivity. Salinity - calculated from temperature and conductivity using the algoriths of Fofonoff and Millard (1982) - was calibrated against discrete samples taken off the non-toxic supply. The discrete samples were allowed to equilibrate to room temperature for 24 hours before salinity was determined on the shipboard Guildline Autolab salinometer, scaled to seawater ampoules of known salinity.

The calibration algorithms were found to be significantly different for leg 1 and leg 2 and the corrections to be added to the raw salinities were determined in segments as follows:

Cruise	Start Time	End Time	Correction	Standard Deviation
DI221 (leg 1)	11/06/96 05:00:00	01/07/96 21:13:00	-0.005417	0.012178
DI221 (leg 2)	01/07/96 21:14:00	22/07/96 15:46:00	-0.15933	0.01726

Temperature was calibrated against the top 5 metres of the calibrated CTDs, which were themselves calibrated/compared against SIS digital reversing thermometers (see CTD data document). The following calibration was determined:

DI221 : calibrated temperature = thermosalinograph temperature - 0.02792; s.d. = 0.002

A 25cm pathlength SeaTech transmissometer was used to measure water transparency. The light received at the end of the 25cm path was logged as a voltage, scaled from 0 to 5. This was then corrected for decay in the light source of the transmissometer, scaled to transmittance and finally converted to attenuance as follows:

Correction for light decay = (mmv - mz) / (av - zz)

where :

mmv = manufacturer’s maximum voltage = 4.738
mz = manufacturer’s zero = 0.0
av = voltage recorded in air = 4.670-4.675, throughout the cruise
zz = blocked transmission voltage = 0.0

Transmittance = corrected voltage * 20.0/ 100.0

Attenuance = -4.0 loge (transmittance).

The attenuance was screened and shown to correspond well with the chlorophyll concentration, which is reasonable for open ocean conditions.

DATA QUALITY - good. No known problems.

Sea Surface Chemistry and Biology

A Chelsea Instruments Aquatrakka flow-through fluorometer was used to measure fluorescence as a voltage (proportional to the natural log of the chlorophyll concentration). This was changed over part way through the cruise; the two-part calibration is a reflection of this. Calibration was against discrete samples taken from the non-toxic supply which were analysed by fluorometry. The log chlorophyll concentrations were regressed against the fluorometer voltage and log PAR, but the light term was found to be not significant. Thus, the calibration algorithms are just expressed in terms of the fluorometer voltage as follows:

DI221 : 11/06/96 05:00-18/07/96 22:27 : log chlorophyll = 0.001555*voltage – 3.28;
DI221 : 18/07/96 22:28-22/07/96 15:46 : log chlorophyll = 0.00249*voltage – 6.72;

All 5 dissolved nutrient species were measured using a Technicon AA2 AutoAnalyser connected to the pumped seawater supply by a continuous filter block (Morris et al, 1978) and calibrated against known standards after Armstrong et al. (1967)

- Nitrate was measured as the sum of dissolved nitrate and nitrite concentrations. The nitrate was reduced to nitrite by a copper/cadmium coil and then reacted with sulphanilamide in acidic conditions to form a diazo compound. This was coupled with N-1-naphthylethylenediamide- dihydrochloride to form a reddish-purple azo dye.

- Nitrite was analysed as for nitrate, but without the initial reduction step.

- Phosphate was analysed by reduction of a phosphomolybdate complex in acid solution to form ‘molybdenum blue’. Ascorbic acid was used, enhanced by the catalytic action of antimony potassium tartrate.

- Silicate was given by the reduction of a silicomolybdate solution to ‘molybdenum blue’ by ascorbic acid. Oxalic acid was added to eliminate interference from phosphates.

- Ammonia was analysed by a semi-continuous fluorescence analytical technique.

Processing the nutrient data involved screening the raw voltages to distinguish on-line measurements from baselines and standards. The baselines used were when Milli-Q was run through the system; nutrient-deplete seawater “baselines” were not used here, but were necessary to calculate the total standard concentrations. The time series was then split into internally consistent segments (according to changes in gain, baselines or instrument performance generally) and each segment was corrected for baseline drift using a linear regression of the baseline voltage as a function of time.

Each segment was then calibrated to convert the voltages into micromolar nutrient concentrations. The standard concentrations were calculated as the sum of the nominal concentration, plus the recorded concentration of the nutrient-deplete seawater in which the standards were made up. The linear regression for the recorded voltage expressed as a function of the standard concentration was carefully checked for each segment. Once this was completed, the whole time-series was again screened with particular attention paid to the concentrations obtained for the standards.

Finally, time corrections were applied to the whole time-series. This was done to compensate the time taken for water from the non-toxic supply to travel through the tubing of the AutoAnalyser. These times varied according to the nutrient species being measured thus:

Nitrate	-13 minutes
Nitrite	-8 minutes
Phosphate	-9.5 minutes
Silicate	-12.5 minutes

Dissolved sulphur hexafluoride (SF_6) was measured by electron capture detection (ECD) following sparging and trapping. Water was injected into the sparge tower of the gas chromatograph under a vacuum (500mm Hg) and mixed with sparge gas (oxygen-free nitrogen). Degassing of SF_6 from the sample was accelerated by the drawing in and rapid expulsion of the sample through 0.5mm orifices. The sparged SF_6 was then passed through magnesium perchlorate followed by a Nafion drier to absorb any water vapour and then directed through a cryogenically cooled Porapak Q trap (Upstill-Goddard et.al. 1991) to be stripped. The trap containing the sparged SF_6 was then isolated and raised out of the propanol, being heated from -70°C to 80°C in 25 seconds and the sparged SF_6 was transported to the chromatographic column where it was eluted after 50 seconds and passed to the electron capture detector. Oxygen and similar eluents were retained by molecular sieve columns.

Calibration was by reference to standards prepared by pressure dilution (Upstill-Goddard et.al., 1991) of 0.1% SF_6 in nitrogen mixture (Spantech Products Ltd., UK) in 9.4 litre bottles. Calibration precision for each GC unit showed a mean standard deviation of 2.5% or better.

References

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The BODC Underway Explorer

The BODC Underway Explorer is a *Windows95* application that allows data from the underway files to be presented as time series plots and listed in a data grid that may be exported to other applications. The program also provides an indication of the spatial context of the data through a map of the cruise track overlaid on a coastline and bathymetric contours. The program has been tested successfully under *Windows NT 4.0*.

The content of all program windows, be it a plot, a map or a data grid may be saved onto disk or printed using any printer installed on the *Windows* system. It is designed to support one or more BODC CD-ROMs containing underway data files providing the project specific installation program has been run for each CD-ROM to be used.

The program includes full information on its use through an on-line help system, including functional descriptions of all the menu options and control buttons. However, a brief description of how to get started is included here.

When the program is launched through either the BODC entry in the Start menu, a shortcut or *Windows Explorer*, a splash screen is briefly displayed followed by the opening of the program control window. Three actions are then required to display data.

- Select the Open Project option from the File menu and choose the project appropriate to the CD-ROM currently loaded.

- Click on the Select menu to open the Selection Dialog. This may then be used to choose the cruise, time interval and up to six parameters of interest.

- Click on one or more of the three large control buttons to open the plot window, data grid or cruise track map. The icons on the buttons clearly indicate which button does what.

This is all you need to do to access the data. Control over how the data are presented and access to more advanced features such as zoom capabilities are provided through both the menus and the toolbar buttons. Consult the on-line help or simply experiment to discover what these can do.