NOAA Technical Memorandum ERL AOML-78



PROCEDURES USED AT AOML TO QUALITY CONTROL REAL TIME XBT DATA COLLECTED IN THE ATLANTIC OCEAN

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I. ABSTRACT

Quality control (QC) procedures developed and implemented at AOML for the examination of real time XBT data are presented. The steps required to QC XBT data is outlined in a "cook book" format. The methods employed are primarily subjective as many of the stages involve interactive input from the user.

II. INTRODUCTION

AOML is one of several Research Science Centers participating in a global effort to quality control oceanographic data collected from either research vessels or volunteer observing ships (VOS). AOML efforts are currently focused on XBT data collected in the Atlantic Ocean. The data being examined consists of "realtime", delayed, historical and Navy declassified modes.

The "real-time" data represents data obtained by the MEDS offices in Canada from various ships. This data has already been quality controlled by the MEDS office; nevertheless, AOML examines the data, without prejudice to the Canadian flags, and then compares its quality control flags against the Canadian flags. The delayed mode data represents both updated profiles submitted as part of the "real-time" data set and data that was not transmitted as "real-time" for 1990. The historical data represents all of the XBT data that has been archived by NODC between 1966 and 1989. The Navy declassified data is the data recently released by the Navy covering the period 1985 through 1990.

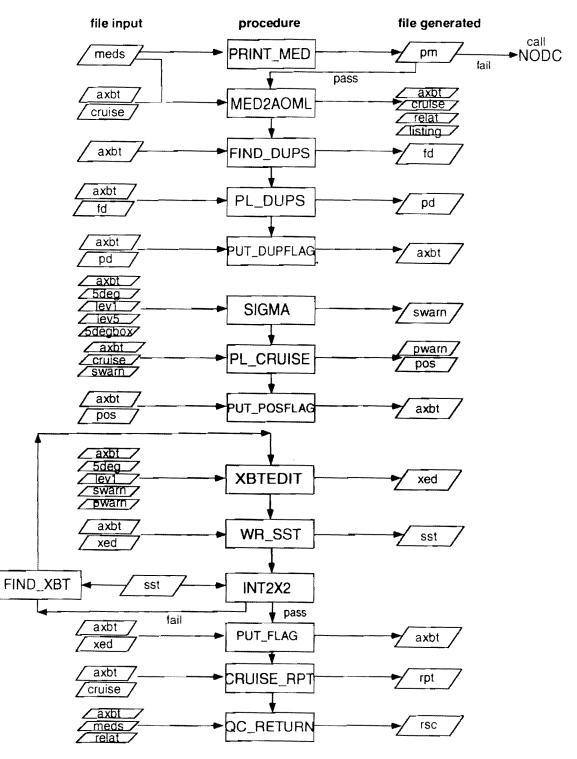
The discussion that follows gives an overview of the procedures that are used to quality control any of the XBT data sets. For exemplary purposes, the "real-time" data set is discussed. NODC first obtains a data set from the MEDS office. AOML then receives an electronic mail message from NODC indicating that a particular month of data is available. AOML then copies the MEDS data over the SPAN network. The MEDS file then rewritten into AOML's Indexed Sequential Access Method (ISAM) Database. This is a direct access "keyed" database for which XBTs are retrievable according to various keys, including: Latitude, Longitude, Time, NODC_Unique_ID_Number, NODC_Cruise_Consec_Number, MEDS_Station_Number, Ship_Radio_Call_sign.

Once the database has been updated, several programs are run to examine the XBT profiles. The quality control procedures presently employed consists of the following:

- (1) a dupilcate profile test,
- (2) a histogram test in which profiles are compared to climatological means and standard deviations to identify possible outliers,
- (3) a waterfall plot test in which profiles from a particular cruise are checked for profile to profile consistency,
- (4) a position and time test to see if profiles within a cruise are consistent,
- (5) a test in which vertical temperature sections of profiles within a cruise are plotted to insure internal consistency,
- (6) a mapping test in which monthly distributions of SST, temperature at 150m and the average temperature of the upper 400m are examined for "bulls-eyes".

In general, the AOML procedures can be characterized as more subjective than objective. There are no automatic flags established by any of these tests. Profiles that have been identified as suspicious are examined individually and flagged as appropriate. A flowchart and description of the programs used at AOML, to insure quality control of the XBT database in the Atlantic, follows.

II. AOML QUALITY CONTROL PROCEDURES



AOML XBT QUALITY CONTROL FLOWCHART

1) PRINT_MEDS

Program description:

This program is used to get a detailed listing of a MEDS format file received from NODC. Each field of every entry is listed in the output file. It counts the different types of entries so that we may compare the number with the number expected. It also does some error checking to assure that the MEDS2AOML program will be able to add the new profiles to the existing database.

Input Files :

MEDS - MEDS format file copied from NODC over the network.

Output Files :

PM - A listing file showing every field in the MEDS file from NODC.

2) MEDS2AOML

Program description:

MEDS2AOML reads an NODC MEDS format file and adds the XBT profiles to the appropriate AOML ISAM database. TESAC messages are not stored. XBTs not in AOML's defined Atlantic Region are not stored.

XBTs are stored in Indexed Sequential Access Method (ISAM) files which allow access by various keys including NODC and AOML profile numbers, time, position, or ship radio call sign.

The CRUISE file is appended to add the cruises in this new set of data.

A "relationship" (RELAT) file is written which shows the relationship between the incoming XBTs and where they are stored in the database. This relationship is important to reconstruct datasets that need to be returned (with Quality Control information) to NODC.

Input Files	:
	MEDS - MEDS format file copied from NODC over the network.
	AXBT - AOML XBT database (ISAM file).
	CRUISE - ISAM data file containing a list of cruises and profiles
	in each cruise.
Output files	:
	AXBT - AOML XBT database (ISAM file).
	CRUISE - ISAM data file containing a list of cruises and profiles in each cruise.
	RELAT - ISAM data file which contains a cross-reference between the incoming NODC designators for each XBT profile and where the XBT was stored in the database.
	 YYMM - A listing file showing every field in the MEDS file from NODC. (YYMM is the designator for the data set, usually Year and Month.)

3) FIND_DUPS

Program description:

FIND_DUPS reads the XBTs stored in Indexed Sequential Access Method (ISAM) files to find potential duplicate profiles. They are read according to the time key field. Profiles within a specified position and time space are listed in an output data file as possible duplicates.

Typically, the XBTs within plus or minus 25 hours, and plus or minus .125 degrees (centered on a quarter of a degree) in latitude of longitude are checked.

Input Files :

AXBT - AOML XBT database (ISAM file).

Output Files :

FD - ASCII file containing profile numbers of possible duplicate XBT profiles. This file will be input to the PL_DUPS program.

4) PL_DUPS

Program description:

This program is used to determine graphically if the profiles identified by the program FIND_DUPS are in fact duplicate profiles. The operator has the ability to accept or reject a profile as a duplicate.

Graphical output includes a plot of temperature vs depth and header information for all profiles identified as possible duplicates (Figures 1,2).

Input Files

2

AXBT - AOML XBT database (ISAM file).

FD - ASCII file containing profile numbers of possible duplicate XBT profiles.

Output Files :

PD - ASCII file containing profile numbers and associated profile number for which the listed profile is considered a duplicate. That is, the first profile number will be considered the actual profile and all other profiles are considered as duplicates.

5) PUT_DUPFLAG

Program description:

PUT_DUPFLAG reads a PD (ASCII) file, which contains the information about duplicate profiles. The XBT (stored in Indexed Sequential Access Method, ISAM file) is read in using its database profile number. The profile is marked as a duplicate and a pointer to the primary XBT (of which this XBT is considered a duplicate) is added and the XBT is rewritten back to the ISAM database.

Input Files

:

AXBT - AOML XBT database (ISAM file).

PD - ASCII file containing profile numbers and associated profile number for which the listed profile is considered a duplicate.
 That is, the first profile number will be considered the actual profile and all other profiles are considered as duplicates.

Output Files :

AXBT - AOML XBT database (ISAM file).

6) SIGMA

Program description:

This program compares individual profiles to statistics derived from the historical NODC database. Means and standard deviations have been estimated for those 5 degree longitude/latitude boxes with sufficient data to make these computations. The center of the 5 degree boxes begin at 97.W;37.5S and end at 17.5E;57.5N. The operator has the option of selecting which profiles to review by specifying an acceptable range (sigma tolerance) within which the real time data can fall.

Profiles can be also tested against the mean Levitus 1 degree climatology by specifying acceptable temperature tolerances around this means. This is useful in areas where there are insufficient XBT data to compute the historical means and standard deviations.

This program is typically run using a 3 sigma tolerance about the historical mean and 6 C tolerance about the Levitus 1 degree climatology. A profile is displayed if the temperature at any depth in a profile differs from the mean profile or Levitus climatology by more that the specified tolerance. The operator has the option to mark questionable profiles and save them to a "warning" file which is then used as input to other quality control programs such as PL_CRUISE and XBTEDIT.

Graphical output for each 5 degree box includes the following (Figure 3) :

- a) Mean NODC historical temperature profile (*)
- b) NODC mean temperature profile +/- 3 sigma
- c) NODC mean temperature profile +/- 5 sigma window
- d) Levitus 1 degree temperature profile
- e) Levitus 5 degree temperature profile
- f) XBT profiles that fail the tolerance tests

Input Files :

AXBT	- AOML XBT database (ISAM file).
5DEG	- Five degree historical mean temperature profiles (*).
LEV1	- Levitus one degree climatology.
LEV5	 Levitus five degree climatology.

5DEGBOX - Identifier for all profiles in a 5 degree box.

(*) Two means are available. The first is the mean calculated directly from the AOML historical XBT data base (1966-1988). The second is a mean (clean mean) which is recalculated after first discarding all profiles that are more than 2 standard deviations from the historical mean.

Output Files :

SWARN - SIGMA warning files to identify suspicious profiles.

7) PL_CRUISE

Program description:

This program examines all of the XBTs associated with a specific cruise. Profiles, as well as time and position locations, are checked for consistency with surrounding XBTs. In addition to identifying individual problem profiles, this program also provides for a useful test for quality of data received from entire VOS merchant ship tracks.

Questionable profiles identified from the SIGMA program serve as input to aid in the decision making process. All profiles identified as questionable are saved to "warning" file and later input into the XBTEDIT program. Questionable time and positions are saved to a "position" file for updating the flags in the data base.

The program can be run either an interactive or hard copy mode. Typically, hard copy output is generated for all cruises and examined. Then the program is run interactively to further examine and identify the profiles for specific cruises that are suspicious.

Graphical output includes the following (Figures 4,5,6,7) :

- a) Temperature vs depth profiles and/or geographic positions of the XBT's for any cruise.
- b) Geographic positions of the XBT's and speed plots for any cruise.
 Speed plots include : total speed, longitudinal speed and latitudinal speed vs time.
- c) Vertical temperature section plots for various types of cruise tracks.

Input Files :

	AXBT	- AOML XBT database (ISAM file).
	CRUISE	 ISAM data file containing a list of cruises and profiles in each cruise.
Output Files	SWARN :	- SIGMA warning file identifying suspicious profiles.
	PWARN POS	 PL_CRUISE warning files to identify suspicious profiles. PL_CRUISE flag file identifying a position or time field.

8) PUT_POSFLAG

Program description:

PUT_POSFLAG reads a POS (ASCII) file, which contains the information about position or time corrections for an XBT profile. This file was created by the PL_CRUISE quality control plotting program.

The XBT (stored in Indexed Sequential Access Method, ISAM file) is read in using its database profile number. The profile is updated with the corrected position and/or time and the XBT is rewritten back to the ISAM database. Input Files :

AXBT - AOML XBT database (ISAM file).

POS - ASCII file containing profile numbers and associated corrected position and/or time.

Output Files :

AXBT - AOML XBT database (ISAM file).

9) XBTEDIT

Program description:

This program interactively examines and edits any XBT profile. Suspicious profiles from previous tests are highlighted so that the operator knows what specific test a profile has failed. The historical mean climatology (5 degree box) and the Levitus climatology (1 degree box) are plotted to the screen as an additional aid in determining the quality of a profile. The operator can also request information about surrounding profiles from the cruise that containing the profile or historical data.

XBTEDIT can be run in four editing modes. The first is the initial editing stage where flags can be set for any profile that contains bad data. Data can be flagged as inconsistent (2), doubtful (3) or bad (4). One of the following 12 reasons (Bailey et al. (1994); Figures 8a-8l) is given for each flag value of 3 or 4:

- 1) BOR (Bowed Mixed Layer Reject) An unrealistic inversion near the surface.
- 2) CTR (Constant Temperature Profile Reject) An unrealistic isothermal temperature profile.
- 3) CUR (Cusping Error Reject) Unrealistic cusps in the temperature profile.
- 4) HBR (Hit Bottom Reject) An unrealistic isothermal temperature profile that is most likely caused by the probe hitting the bottom.
- 5) HFR (High Frequency Reject) An unrealistic high frequency temperature structure typically caused by electrical interference.
- 6) IPR (Insulation Penetration Reject) An unrealistic temperature profile caused by damage to the wire insulation.
- 7) LER (Leakage Reject) An unrealistic temperature profile possibly caused by cable or launcher damage.
- 8) NGR (No Good Reject) An obviously erroneous profile.
- 9) SPR (Spikes Reject) An unrealistic temperature spike in the profile.
- 10) TOR (Temperature Offset Reject) A profile inconsistent with surrounding profile.
- 11) WBR (Wire Break Reject) A large temperature charge at the bottom of a profile caused by the wire breaking.
- 12) WSR (Wire Stretch Reject) A large temperature inversion caused by wire stretch.

There is obviously considerable subjectivity between flags 2 and 3. The other editing modes allow for re-examination of previously flagged profiles, comparison of the AOML and Canadian flags and comparison of the flags generated by any 2 different operators.

Graphical options in the program give the operator full flexibility when examining a profile. These include the ability to rescale, zoom in and out of features and compare the profile with neighboring profiles from the same cruise (Figure 9).

Input Files :

AXBT	- AOML XBT database (ISAM file).
5DEG	- Five degree historical mean temperature profiles (*).
LEV1	- Levitus one degree climatology.
SWARN	- SIGMA warning file identifying suspicious profiles.
PWARN	- PL_CRUISE warning files identifying suspicious profiles.

(*) Two means are available. The first is the mean calculated directly from the AOML historical XBT data base (1966-1988). The second is a mean (clean mean) which is recalculated after first discarding all profiles that are more than 2 standard deviations from the historical mean.

Output Files :

 XED - ASCII file containing profile numbers and quality control flags associated with depth-temperature pairs in the profiles.

10) WR_SST

Program description:

:

This program generates values and associated flags for the sea surface temperature (SST), the temperature at 150m (T150), the temperature at 400m (T400), the temperature at 600m (T600) and the average temperature of the upper 400m layer (T400L) from either the AOML or Canadian database.

Input Files

AXBT - AOML XBT database (ISAM file).

XED - ASCII file containing profile numbers and quality control flags associated with depth-temperature pairs in the profiles.

Output Files :

SST - File containing values of SST, T150, T400, T600 and T400L and related XBT header information.

11) INT2X2

Program description:

This program interpolates the sea surface temperature (SST), the temperature at 150m (T150), the temperature at 400m (T400), the temperature at 600m (T600) and the average temperature of the upper 400m layer (T400L) onto a 2 degree x 2 degree grid within the region (100W-20E; 40S-60N) and contours the resulting fields (Figures 10,11,12 for example) in order to identify suspicious profiles (i.e. those producing "bulls-eyes"). The location of each data value is indicated by an x. Data values with a flag of 2 are double size. At each location a '+' indicates a positive anomaly and 'o' a negative anomaly from the Levitus 1 degree climatology. Only data values that have received a flag of acceptable (1) or inconsistent (2) are used as input for the interpolation to define additional erroneous prrofiles.

Input Files :

SST - File containing values of SST, T150,T400, T600 and T400L and related XBT header information.

12) FIND_XBT

Program description:

This program will find all XBTs that fall inside of a circle of specific radius, around a specific location. It is used to identify those XBTs that may have caused "bulls-eyes" to appear on the contours maps generated by INT2X2. Those XBTs that are identified as suspicious are re-examined by running XBTEDIT and are flagged if appropriate.

Input Files :

SST - File containing values of SST, T150, T400, T600 and T400L and related XBT header information.

13) PUT_FLAG

Program description:

PUT_FLAG reads a XED (ASCII) file, which contains the flags to be added to the database as permanent Quality Control flags.

The XBT (stored in Indexed Sequential Access Method, ISAM file) is read in using its database profile number, which is listed in the XED file. The QC flags for that profile, from the XED file, are added and the XBT is rewritten, with the added quality control flags, back to the ISAM database.

Input Files

- AXBT AOML XBT database (ISAM file).
- XED ASCII file containing profile numbers and quality control flags associated with depth-temperature pairs in the profile.

Output Files :

AXBT - AOML XBT database (ISAM file).

14) CRUISE_RPT

Program description:

This program will generate a cruise report for any cruise in the database. The report is based on a specific month and year and contains the following information :

- 1) first and last day positions,
- 2) number of profiles on each day,
- 3) number flagged on each day,
- 4) frequency distribution of profiles on each day.

This is particularily useful to identify problem VOS ships and to notify them so that problems with the "real time" data can be corrected as soon as possible.

Input Files :

AXBT - AOML XBT database (ISAM file).CRUISE - ISAM data file containing a list of cruises and profiles in each cruise.

Output Files :

RPT - Cruise report file for the year and month selected.

15) QC_RETURN

Program description:

QC_RETURN creates a file which will be used to return RSC Quality Controlled data to NODC.

QC_RETURN reads an original NODC MEDS format file looking at each XBT profile in the order of the original MEDS file.

The appropriate "relationship" (RELAT) file is read which shows the relationship between the incoming MEDS XBT and where it was stored in the AOML database. This cross-reference is used to retrieve the related XBT (stored in Indexed Sequential Access Method file) from the AOML database.

The QC flags and other appropriate QC fields are added to the original data and the MEDS file is rewritten for return to NODC.

(NODC has requested that the output of this program be changed to be an ASCII file which contains just the Quality Control recommendations from the AOML_RSC QC procedures and personnel. Therefore the output of QC_RETURN is likely to change.)

Input Files :

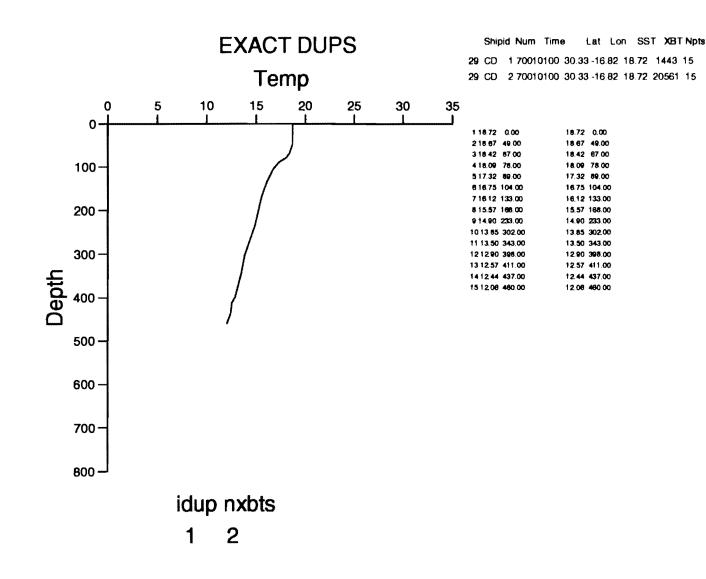
	AXBT	- AOML XBT database (ISAM file).
	MEDS	- MEDS format file copied from NODC over the network.
	RELAT	- ISAM data file which contains a cross-reference
		between the incoming NODC designators for each XBT profile and where the XBT was stored in the database.
Output Files	:	
	RSC	 MEDS formatted file containing Quality Control infor- mation to be returned to NODC.

IV. ACKNOWLEDGEMENTS

The authors wish to thank Dr. Robert L. Molinari for his contribution to the completion of this report and Rick Bailey and Gary Meyers for permission to use figures from their CSIRO report. This work was supported in part by a grant from NOAA's Long Term Ocean Observing Program.

V. <u>REFERENCES</u>

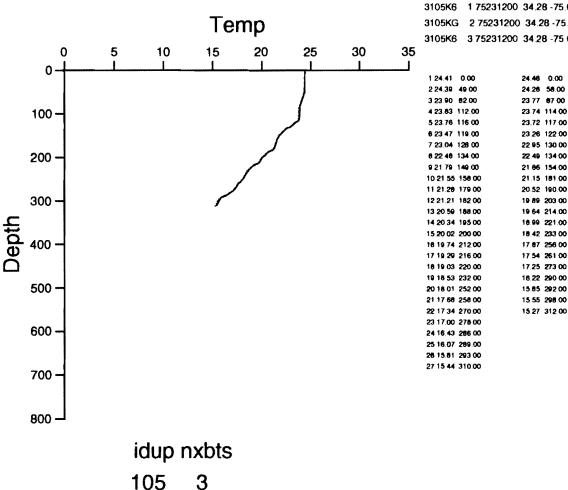
Bailey. R., A. Gronell, H. Phillips, G. Meyers, and E. Tanner (1994). CSIRO cookbook for Quality Control of Expendable Bathythermograph (XBT) Data. CSIRO Marine Laboratories Report No. 220 75 pp. In press.



(bckgmd: B-change entire C-change existing R-restore previous) (dups: S-Select I-ignore M-mark E-edit L-list N-next) Q-quit

FIGURE 1: Temperature vs depth profile of exact duplicates with header information and listing of depth and temperature values.

び



 Shipid
 Num
 Time
 Lat
 Lon
 SST
 XBT Npts

 3105K6
 1
 75231200
 34.28
 -75.67
 24.41
 8290
 27

 3105K6
 2
 75231200
 34.28
 -75.67
 24.41
 8290
 27

 3105K6
 2
 75231200
 34.28
 -75.67
 24.46
 19871
 22

 3105K6
 3
 75231200
 34.28
 -75
 67
 24.41
 21657
 27

24,41 0.00

24.39 49.00

23.90 82.00

23.83 112.00

23.76 116.00

23 47 119.00

23.04 128.00

22.46 134.00

21 79 149 00

21 55 158 00

21.28 179.00

21.21 182.00

20.59 188.00

20.34 195.00

20.02 200.00

19.74 212.00

19.29 218:00

19.03 220.00

18 53 232 00

18 01 252.00

17.68 258 00

17.34 270.00

16 43 286.00

16.07 289 00

15 81 293.00

15 44 310 00

(bckgmd: B-change entire C-change existing R-restore previous) (dups: S-Select I-ignore M-mark E-edit L-list N-next) Q-quit

FIGURE 2: Temperature vs depth profile of inexact duplicates with header information and listing of depth and temperature values.

23

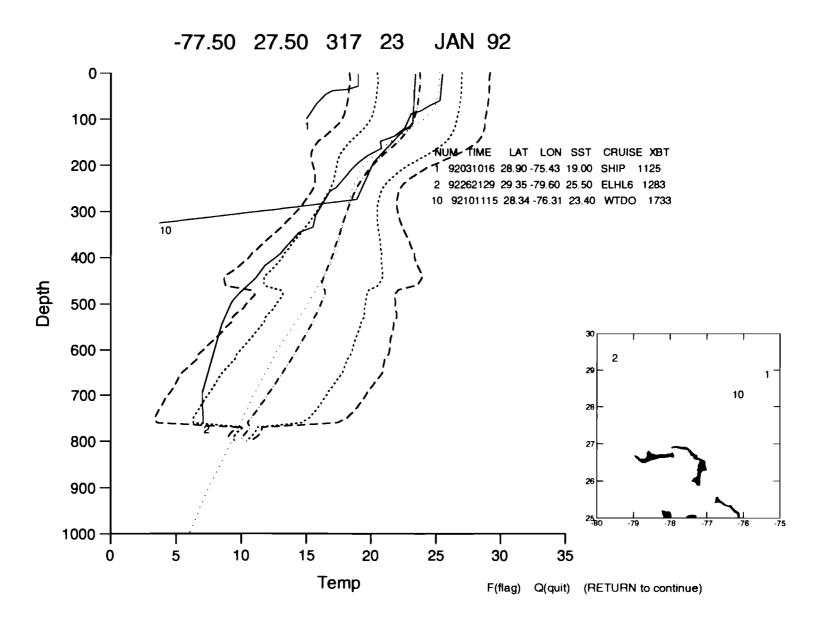


FIGURE 3 : Temperature vs depth profile that failed the Sigma tolerance test displayed with header information and map. _____ mean temperature profile +/- 5 sigma window; - - - - mean temperature profile +/- 3 sigma window; _____ . ___ . Mean NODC historical temperature profile; Levitus 5 degree temperature profile; _____ XBT profiles that fail the tolerance tests.

24

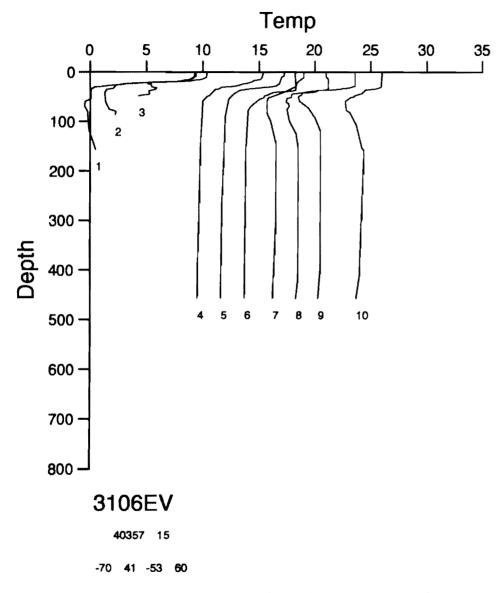


FIGURE 4: Temperature vs depth profiles of XBT's for specific cruise with header information. Each temperature profile is offset by 2 degrees from previous profile.

Num Time Lat Lon SST XBT Mon 1 67181130 53 00 -55.17 10 40 406 Aug

2 671 90535 54.20 -54.90 7 40 425 Aug

3 67191130 55 17 55 92 5.30 432 Aug 4 67191730 56 28 55 82 940 436 Aug 5 67192330 57 42 54 65 9.30 442 Aug

6 67200538 58 53 -54 82 8 20 451 Aug

9 67310535 58 00 -56 00 7 60 567 Aug 10 67311145 56 58 -56 23 8 00 577 Aug S

457 Aug

565 Aug S

7 67201130 59.75 -54.82 7 00

8 67302330 58 93 -55.62 7.00

 \mathcal{B}

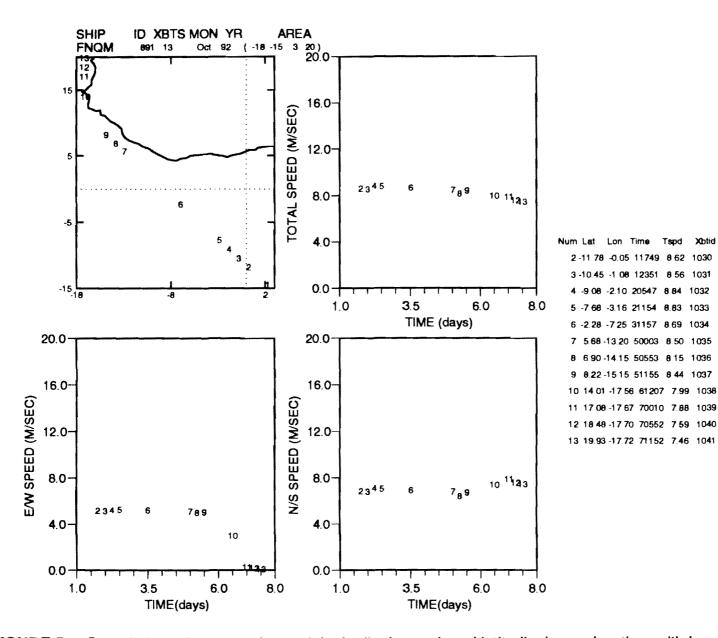


FIGURE 5: Speed plots of map, total speed, logitudinal speed, and latitudinal speed vs time with header information.

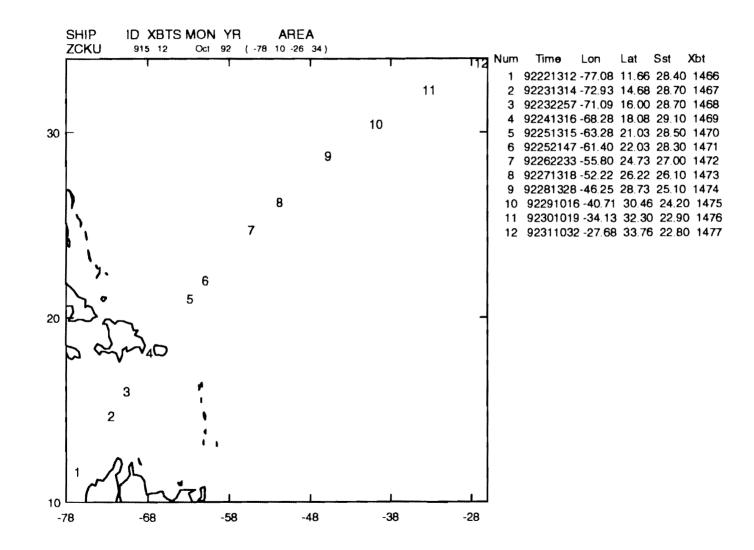


FIGURE 6: Map with header information for specific cruise.

27

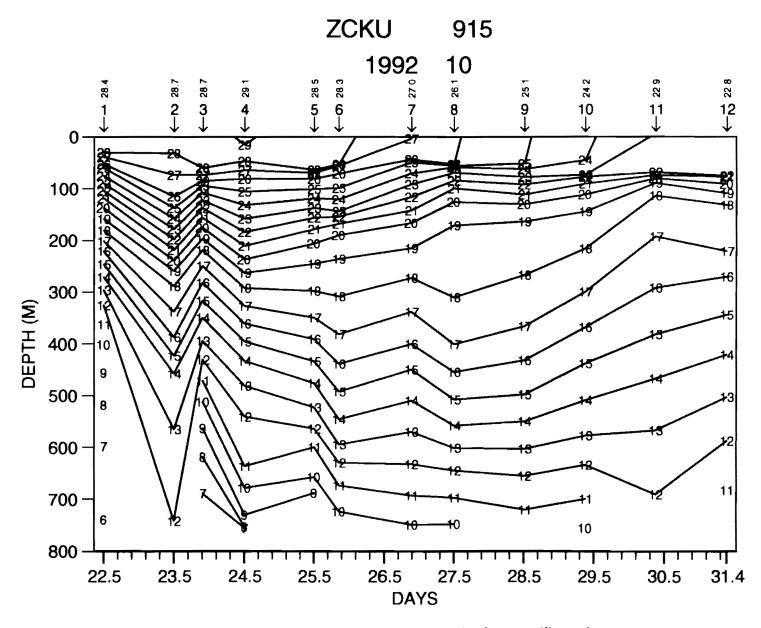


FIGURE 7: Vertical temperature section plot for specific cruise.

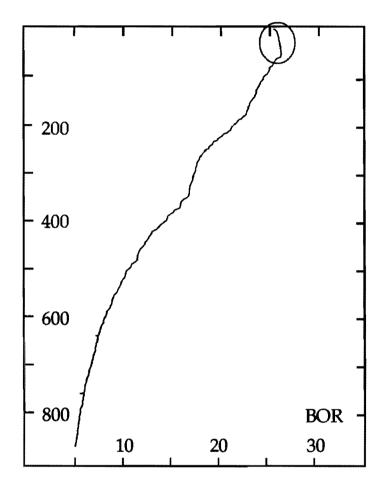


Figure 8a. Bowed Mixed Layer Reject (BOR)

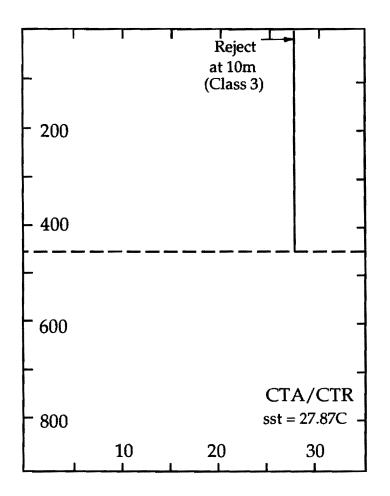


Figure 8b. Constant Temperature Profile Reject (CTR)

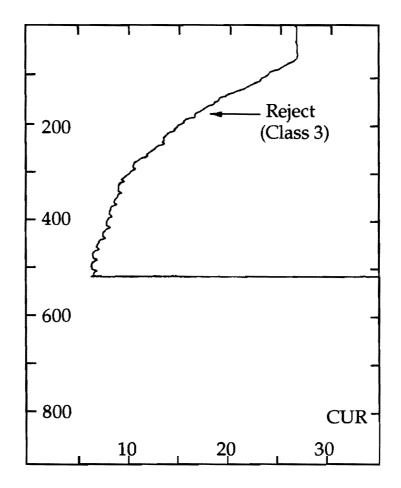


Figure 8c. Cusping Error Reject (CUR)

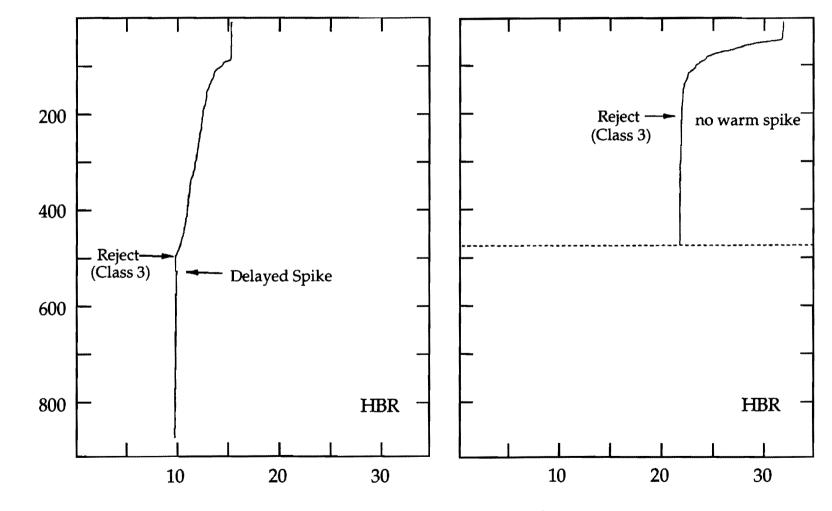


Figure 8d. Hit Bottom Reject (HBR)

32

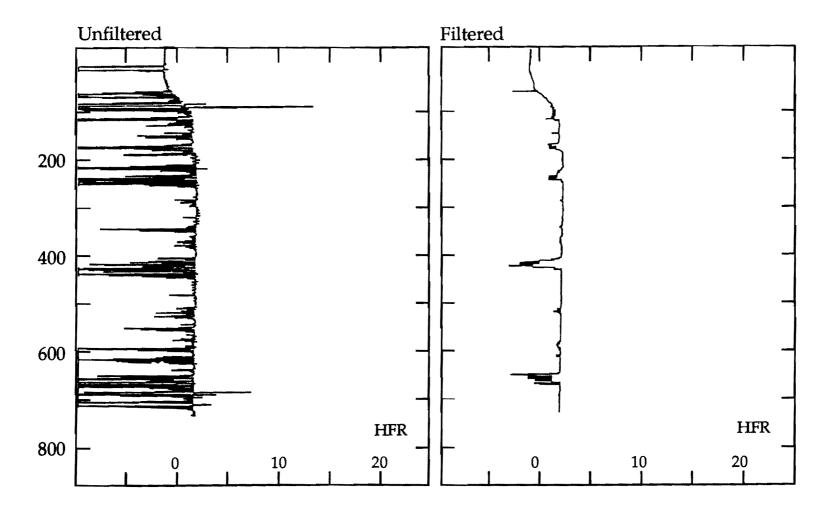


Figure 8e. High Frequency Reject (HFR)

33

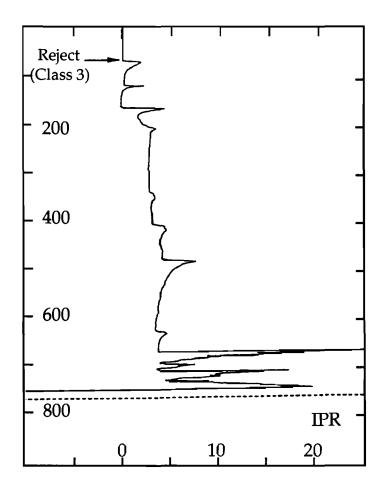


Figure 8f. Insulation Penetration Reject (IPR)

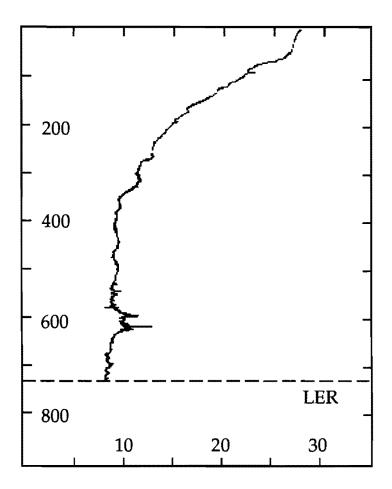


Figure 8g. Leakage Reject (LER)

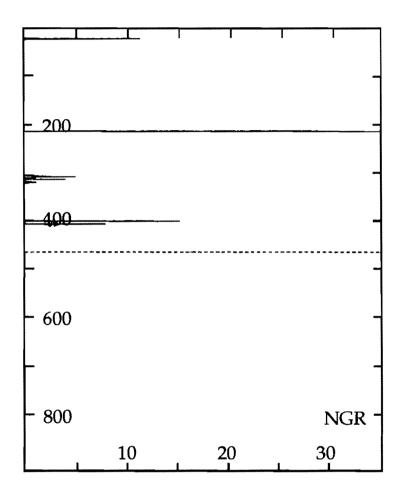


Figure 8h. No Good Reject (NGR)

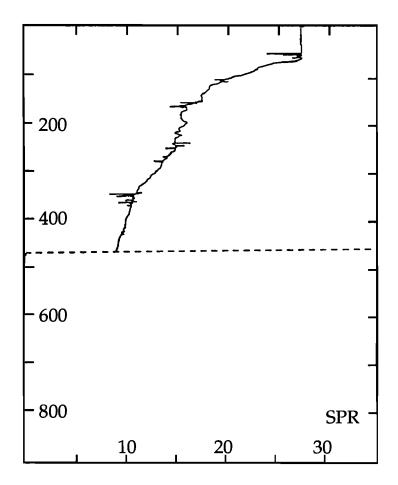


Figure 8i. Spikes Reject (SPR)

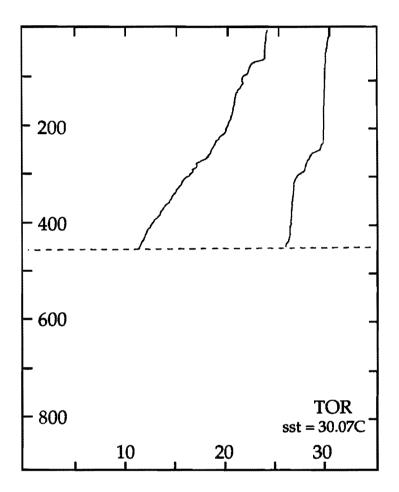


Figure 8j. Temperature Offset Reject (TOR)

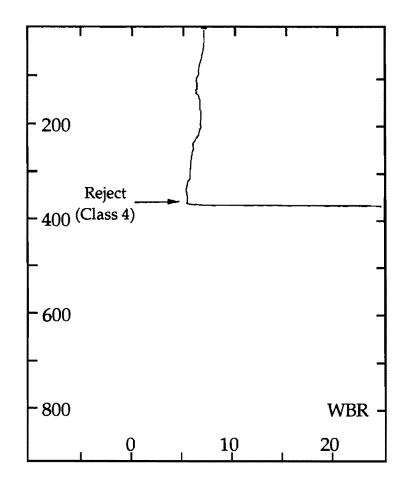


Figure 8k. Wire Break Reject from Probe Spool (WBR)

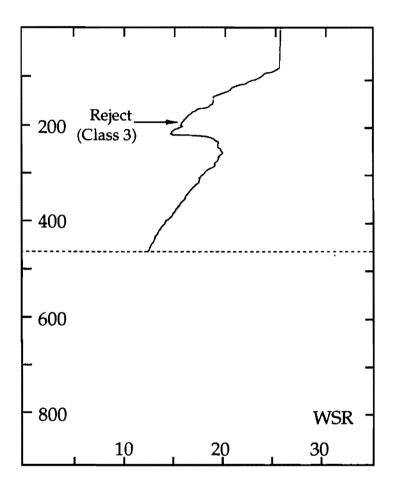
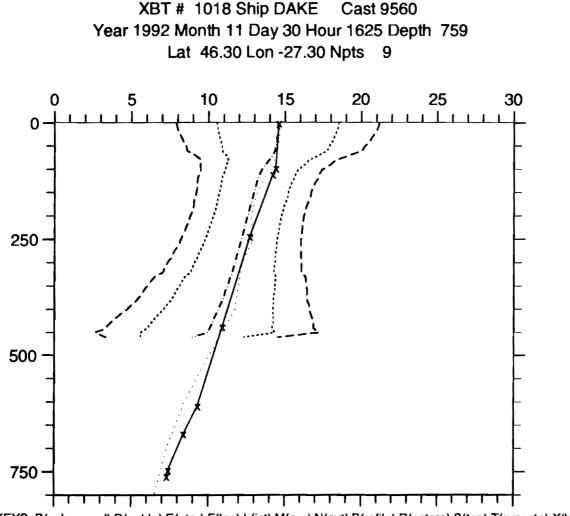


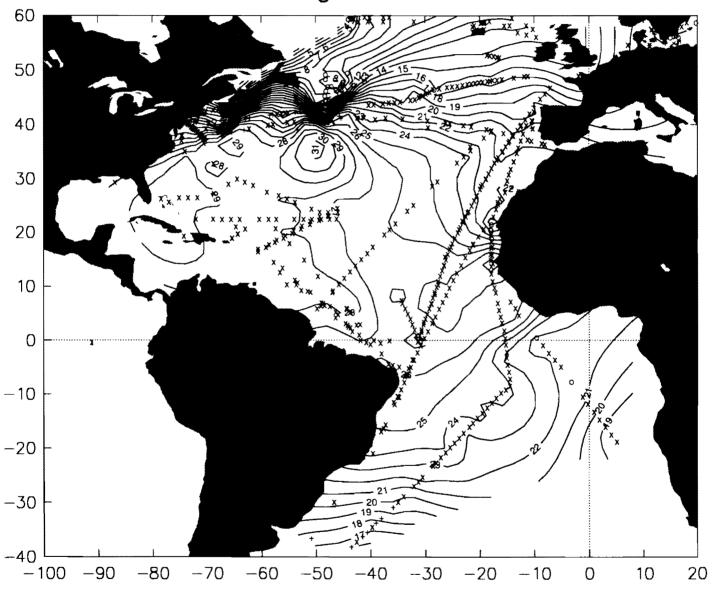
Figure 81. Wire Stretch Reject (WSR)



KEYS: B(ackground),D(ouble),E(nter),F(lag),L(ist),M(ore),N(ext),P(rofile),R(estore),S(top),T(runcate),X(bt #),Z(oom)

FIGURE 9: Temperature vs depth profile with header information. ____ mean temperature profile +/- 5 sigma window; --- mean temperature profile +/- 3 sigma window; __. Mean NODC historical temperature profile; Levitus 1 degree profile; ---x---x- XBT profile to be edited.







Sea-surface temperature contour plot.

Aug 1992-T150

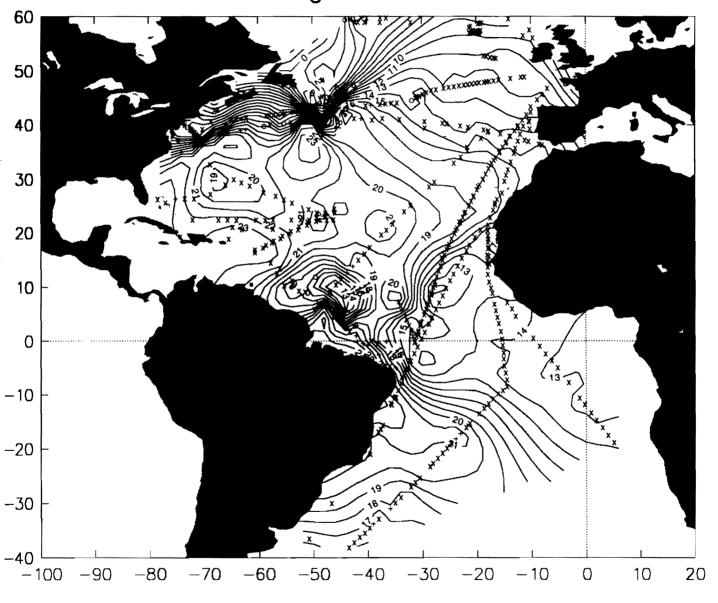


FIGURE 11 : Temperature at 150 m contour plot.

Aug 1992-T400L

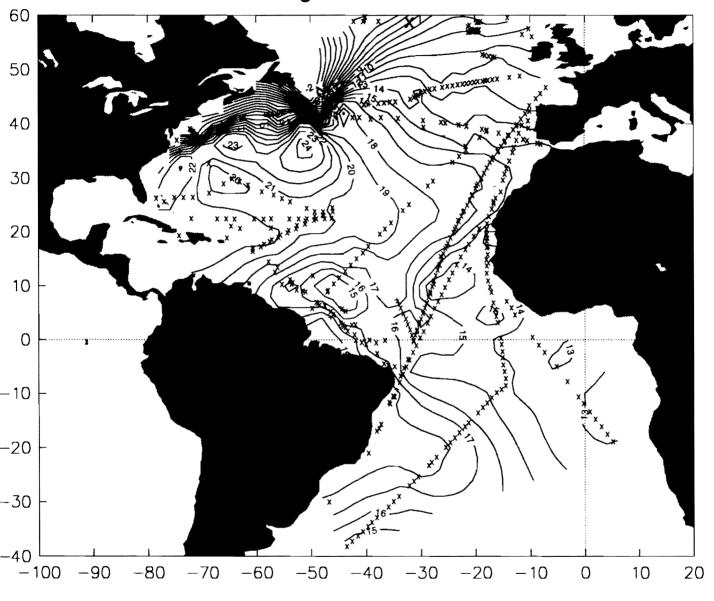


FIGURE 12: Average temperature of the upper 400 m layer contour plot.