CSCAPE 2005 David Starr Jordan CTD PROCESSING

CSCAPE 2005 CTD data files were collected using a Sea-Bird 911*plus* profiling instrument aboard the NOAA Ship David Starr Jordan (DSJ). The 911*plus* consists of the 9*plus* underwater CTD and 11*plus* V2 Deck Unit, which has high resolution sampling (24Hz) and pump-controlled conductivity and temperature flow-through sensors. Data were collected using Sea-Bird's SeaSave Win32 Version 5.34 and have been processed using Sea-Bird's SBE Data Processing SEASOFT Win32 Version 7.14e. More information regarding the SBE software and recommended data processing procedures can be found online at www.seabird.com.

Each CTD directory on the data server contains two folders named Raw and Data. CTD set-up information, pressure test results, and data collected at sea are stored in the Raw folder. All information and files used in processing are saved in the Data folder, including documentation, configuration files, calibration sheets, intermediate processing steps and final data.

Only one change in sensor use occurred on the DSJ CTD during the CSCAPE 2005 cruise: the fish/pressure sensor was swapped out for Legs 5, 6, and most of 7. The table below describes the period for which each sensor was used; no secondary sensors were used. The fish was sent to Sea-Bird and the pressure sensor was recalibrated, apparently related to inconsistencies in surface pressure readings as discussed below. The owners of the sensors were responsible for their maintenance.

	Casts	Temp	Cond	Pressure
Legs 2-4	001-055	T1448	C1165	P0311
Legs 5-7	056-103	T1448	C1165	*P0291*
Leg 7	104-107	T1448	C1165	P0311

DSJ-owned, MMTD-owned

CSCAPE 2005 DSJ CTD SENSOR CALIBRATION

SWFSC MMTD uses Sea-Bird Electronics conductivity, temperature, oxygen, and pressure sensors. Sea-Bird Electronics conductivity sensors drift with usage and time, while temperature and pressure sensors drift primarily over time. Annual calibrations of the conductivity and temperature sensors are necessary to estimate and correct for this drift during data processing. Pre and post-cruise calibration certificates for the sensors used during CSCAPE 2005 are in the \CON_Files\Calibrations folder.

Conductivity, temperature, and pressure are computed as polynomial functions of the sensor frequencies stored in the raw data file. We follow Sea-Bird recommended procedures for adjusting calibration coefficients for drift between calibrations (Sea-Bird App. Note # 31). Details can be found in the internal document "CTD Calibration Adjustments MMTD.pdf".

The Excel spreadsheet, CTDcalibrations CSCAPE 2005_DSJ.xls in the \Documentation folder, contains the pre and post-cruise conductivity, temperature and pressure sensor calibration information and allows for the calculation of the interpolated slope or offset for each sensor. It then derives slope or offset values used to correct the calibration coefficients used in both the Data Conversion and Derive modules of Sea-Bird's SBE Data Processing software. The adjusted configuration files used to process the CSCAPE 2005 DSJ data (Appendix 1) are in the \CON_Files folder.

Conductivity Sensor Correction:

The SBE 4C series conductivity sensor has a measurement range of 0.0 to 7.0 Siemens/meter (S/m), which spans the conductivity range of SWFSC MMTD's study areas. The SBE 4C sensor is rated to have an initial accuracy of 0.0003 S/m; with a resolution (at 24Hz) of 0.00004 S/m.

The conductivity sensor, C1165, was calibrated on 11 March 2004 and 31 December 2005. The difference between the iSlope values at the start and end of the cruise was less than 0.0003 and the end iSlope was less than 1.00015; consequently, no calibration adjustment was necessary for the conductivity sensor (slope = 1). The post-cruise calibration coefficients were used for processing, because the pre-cruise calibration was done more than a year before the start of the cruise.

Temperature Sensor Correction:

The SBE 3*plus* series temperature sensor has a measurement range of -5.0 to 35 °C, which spans the range of temperatures in SWFSC MMTD's study areas. The SBE 3*plus* sensor is rated to have an initial accuracy of ± 0.001 °C and a resolution (at 24 samples per second) of 0.0003 °C.

The temperature sensor, T1448, was calibrated on 2 March 2004 and 30 December 2005. The iOffset at the end of the cruise was less than 2 mdeg C; consequently, no calibration adjustment was necessary for the temperature sensor (offset = 0). The post-cruise calibration coefficients were used for processing, because the pre-cruise calibration was done more than a year before the start of the cruise.

Pressure Sensor Correction:

The SBE Paroscientific Digiquartz pressure sensor is rated to have an initial accuracy of 1.02m (i.e., 0.015% of the full scale range, which is 0 – 6800m). We do not exceed a maximum vertical depth of 1100m. Initial resolution (at 24Hz) is 0.068m (i.e., 0.001% of the full scale range).

Only one deck test was conducted on the CTD pressure sensor P0311, before removal and recalibration after cast 055, resulting in an offset of -3.878. Since the calculated iOffset from Sea-Bird calibrations was -2.960 and the pre-cruise calibration was the initial 1993 calibration, the average of the deck test offset and the iOffset, -3.374, was used in the *.con file for initial processing. However, this resulted in pressures close to or less than 0db (as low as -4.4db) at the start and end of almost all of these casts. Cast 007 was apparently recording data on deck at the end of the cast with a pressure value of -2.7db. Therefore, an offset of +1.0 was used in the *.con file for casts 001-055.

Two deck tests were conducted on the CTD pressure sensor P0291 resulting in consistent offsets of -1.605 and -1.928. Therefore, the average deck test offset of -1.766 was used in the *.con file for casts 056-103.

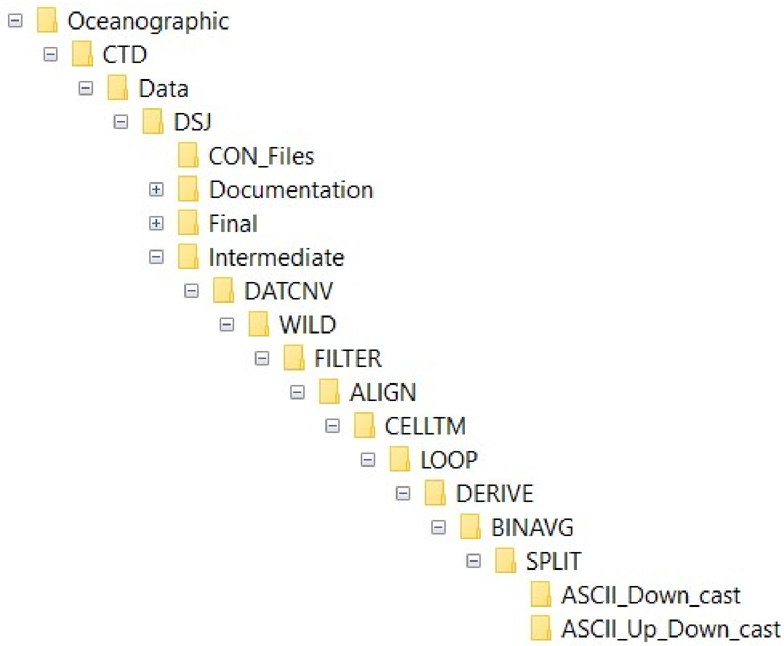
Two deck tests were conducted on the CTD pressure sensor P0311 after recalibration and reinstallation for casts 104-107. These deck tests resulted in consistent offsets of -3.895 and -3.909; these results were not consistent with the Sea-Bird calibrations from 21 October 2005 (Offset=-2.9484). Therefore, the average deck test offset of -3.902 was used in the *.con file for casts 104-107.

We use pre-cruise calibration coefficients for each sensor when available. Before running the processing modules, it is essential to ensure that the correct sensor configuration coefficients and corrections are loaded into the *.con files used by the SBE Data Processing program. Offset and slope adjustments are obtained from CTDcalibrations CSCAPE 2005_DSJ.xlsx in the \Documentation folder. Configuration files for the sensors used on the DSJ during CSCAPE 2005 are listed in Appendix 1.

CSCAPE 2005 CTD SBE MODULE PROCESSING

The SBE Data processing modules that were applied to the raw CSCAPE 2005 DSJ data are listed below. Each SBE module creates a program setup file, named *.psa. The *.psa files are located in the folder preceding their output, i.e. the ‘Derive.psa’ file is found in the ‘LOOP’ folder. Output .cnv files are kept in binary format to speed processing and reduce file sizes. The final module – ASCII Out – converts the binary data to ASCII format; if examination of the data is needed during earlier processing steps, the Translate module can be used to convert to the binary data to ASCII.

Modules are run in the following order: Data Conversion, Wild Edit, Filter, Align CTD (as needed), Cell Thermal Mass, Loop Edit, Derive, Bin Average, Split, ASCII Out. The processed data in various stages are in the \Intermediate folder:



1. **Data Conversion Module:**

Data Conversion converts raw SBE 911plus data, which are typically stored as frequencies and voltages in the *.dat file, to engineering units and stores the converted data in a *.cnv file.

The options selected for processing in Data Conversion were as follows:

> # name 0 = prDM: Pressure, Digiquartz [db]
> # name 1 = c0S/m: Conductivity [S/m]
> # name 2 = t090C: Temperature [ITS-90, deg C]
> # name 3 = flag: 0.000e+00
> # file_type = binary

Fortran program SCRDATA was used to exclude pressure values <-5.0 or >1200, temperature values <-1.0 or >33, and conductivity values <2.5 or >7.0. The program first checks the range or span of values from the primary and secondary sensors in the header file. If any span exceeds the above limits, the program writes a new file in which each bad value, and the values in the two scans preceding and the two scans succeeding the bad value are replaced with a missing value of -9.990e-29. The original file is renamed with an “x” prefix. For each edited file, the total number of scans, and for each sensor, the number of values that exceeded the limits and the number of entries replaced with a missing value are summarized in the *ScrData.dat* files in the \\Intermediate\DATCNV folder. The only data values screened were zero conductivity values in casts 007 and 096, apparently recorded on deck.

2. Wild Edit Module:

Wild Edit flags outliers in temperature, conductivity, and oxygen data so that they are not used in further processing. Wild Edit’s algorithm requires two passes through the data in blocks of *npoint* scans. The first pass computes the mean and standard deviation and temporarily flags values that differ from the mean by more than *pass1_nstd* standard deviations. The second pass recalculates the mean and standard deviation, excluding values flagged in the first pass. Scans that differ from the mean by more than *pass2_nstd* standard deviations are replaced with a bad data flag. The criteria established by *pass2_nstd* can be overridden using *pass2_mindelta*; specifically, if data are within *pass2_mindelta* of the mean, they are not flagged.

The options selected for processing in Wild Edit were as follows for all casts:

    # wildedit_pass1_nstd = 2.0
    # wildedit_pass2_nstd = 15.0
    # wildedit_pass2_mindelta = 0.000e+000
    # wildedit_npoint = 100
    # wildedit_vars = c0S/m t090C

These options are Sea-Bird defaults, except that *pass2_nstd* was changed from 20.0 to 15.0 to identify more outliers.

3. Filter Module:

The Filter module is run to reduce high-frequency noise in the pressure data, which is caused by counting jitter or other unknown sources. It is important to remove this noise before running the Loop Edit module. Loop Edit flags data that exhibit a change in the CTD velocity. Velocity is calculated using only three successive scans; consequently, noisy pressure data can result in erroneously flagged scans. Filter runs a low-pass filter on the data, which smoothes high frequency (rapidly changing) data. To produce zero phase (i.e., no time shift), the filter is first run forward through the data and then run backward through the data. Pressure data is typically filtered with a time constant equal to four times the CTD scan rate. We run a low-pass filter on the pressure data with time constant = 0.15 seconds, as recommended by Sea-Bird Electronics Inc.

The options selected for processing in Filter were as follows for all CTD casts:

    # filter_low_pass_tc_A = 0.030
    # filter_low_pass_tc_B = 0.150
    # filter_low_pass_A_vars =
    # filter_low_pass_B_vars = prDM

4. Align CTD Module:

It is essential that all variables derived from the data, such as salinity, density, and sound speed, use measurements of temperature and conductivity from same parcel of water. It is practically impossible to instantaneously measure the same parcel of water with all sensors due to the physical location of the sensors on the unit and the different time delays of the sensors. The typical time delay of conductivity relative to temperature, 0.073 seconds, is automatically corrected by the SBE 11plus Deck Unit during data collection. If spikes are observed in the processed salinity profiles, further alignment of conductivity may be necessary. The Align CTD module can be used to align the conductivity data relative to pressure.

Fortran program TRIALIGN (programmer: Paul Fiedler) was run to find the optimum alignment value for conductivity (i.e., the number of scans by which to shift conductivity relative to temperature). TRIALIGN finds the maximum temperature gradient within a 240-scan window using linear regression; TRIALIGN tests for the gradient using only the first 10,000 scans to ensure data are from the downcast and imposes the criteria that depth must change by at least 5m in the 240-scan window. Conductivity alignments are tested within the region of maximum temperature gradient because misalignment of temperature and conductivity often results in excessive salinity spikes when temperature is changing rapidly. Within the window, conductivity is shifted by -24 to +24 scans. For each shift, salinity is derived from the temperature and conductivity data in each scan and a linear regression is fit to the salinity values. The shift that results in the minimum standard deviation of the regression residuals is selected as the optimal value for that cast. Optimal values for all casts are averaged to obtain a single alignment value for the cruise (one scan is 0.042 seconds).

Inspection of the DSJ 2005 CTD profiles suggested that alignment might improve salinity profiles, although spiking was moderate. TRIALIGN gave a mean optimum advances of -0.022 sec (SE=0.0024) for conductivity sensor, C1165, (see Trialign.dat in /FILTER, which has the following columns: CTD file name, pressure (db) at the maximum temperature gradient, maximum temperature gradient (deg C/db), optimal advance (scans), and relative standard deviation of residuals). This value is equivalent to only 0.58 scans; Figure 1 illustrates that salinity spiking at extreme temperature gradients was reduced by alignment.

The options selected for processing in Align CTD were as follows:

    # alignctd_adv = c0S/m -0.022

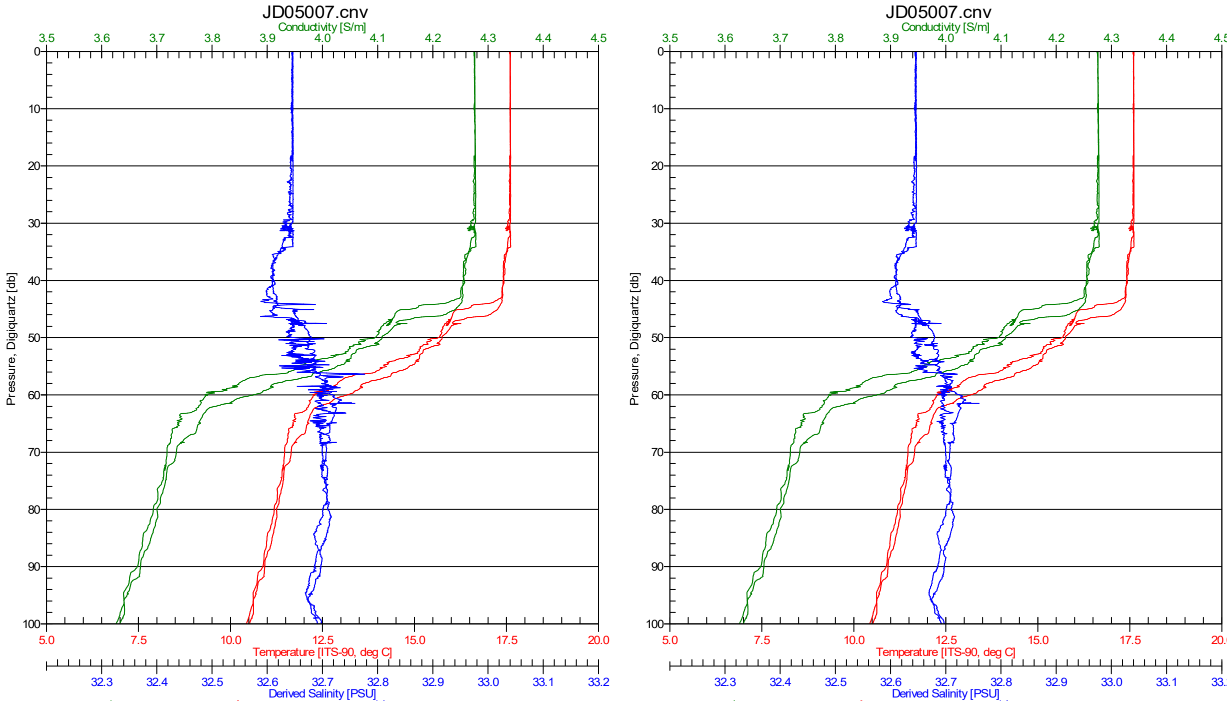


Figure 1. Surface section of CTD cast 007 before (left) and after (right) alignment. Alignment reduces salinity spikes in the thermocline.

5. Cell Thermal Mass Module:

Cell Thermal Mass uses a recursive filter to remove conductivity cell thermal mass effects from the measured conductivity. In areas with large temperature gradients, the thermal mass correction is on the order of 0.005 psu. In areas with small temperature gradients, the correction is negligible.

The following Sea-Bird Electronics Inc. recommendations for Cell Thermal Mass when processing SBE 9plus data, with TC duct, were used:

    # celltm_alpha = 0.0300, 0.0000
    # celltm_tau = 7.0000, 0.0000
    # celltm_temp_sensor_use_for_cond = primary,

6. Loop Edit Module:

Loop Edit flags data that exhibit a change in the mean CTD ascent or descent rate (e.g., pressure reversals or slowdowns). Such changes in ascent or descent rates are usually created by ship heave as the CTD unit is lowered or raised, and indicate unreliable data. Data that have been flagged are documented in the *.cnv header. In this module, we remove any scans that were flagged as bad during data collection.

The options selected for processing in Loop Edit follow the recommendations of Sea-Bird Electronics Inc. for casts in which data collection begins after the surface soak:

    # loopedit_minVelocity = 0.250

    # loopedit_surfaceSoak: do not remove
    # loopedit_excl_bad_scans = yes

Examination of pressure vs. scan count in Sea Plot showed that data collection for some casts was started before the CTD had been returned to near the surface after the 10m surface soak (i.e., data collected began either on deck or during the soak). For casts 4 and 12, the second option was changed to:

    # loopedit_surfaceSoak: minDepth = 5.0, maxDepth = 20, useDeckPress = 0

7. Derive Module:

Derive uses pressure, temperature, and conductivity from the input *.cnv file to compute the following oceanographic variables, which are routinely used in the assessment of protected species (other variables are available upon request):

- Salinity
- Density (density, sigma-theta, sigma-t, sigma-1, sigma-2, sigma-4)
- Depth (salt water, fresh water)
- Sound velocity (which can be calculated using the Chen-Millero, DelGrosso or Wilson equation)
- Average sound velocity (the harmonic mean from the surface to the current CTD depth, which is calculated on the downcast only)

The following processing options were selected in this module for all CTD casts:

    # name 3 = sal00: Salinity [PSU]
    # name 4 = sigma-é00: Density [sigma-theta, Kg/m^3]
    # name 5 = depSM: Depth [salt water, m], lat = 38
    # name 6 = svCM: Sound Velocity [Chen-Millero, m/s]
    # name 7 = avgsvCM: Average Sound Velocity [Chen-Millero, m/s], minP = 2, minS = 20

To calculate average sound velocity, the following values were used:

# minimum pressure = 2 db	[average depth of the acoustic array]
# minimum salinity = 20 psu	[recommended by Sea-Bird Electronics Inc.]
# Latitude = 38 °N	[this value is used only if NMEA latitude is not available in the header]

The profiles output by the Derive module were inspected by the Senior Oceanographer for bad data caused by sensor failure, temperature inversions, low surface salinity measurements (likely the result of rain), and spikes in salinity. Comments about each cast are in the file CSCAPE 2005 DSJ CTD Cast info.txt. Comment codes are:

A – acceptable
~A – acceptable for assessments of protected species
R – reject cast

8. Bin Average Module:

The Bin Average module averages temperature, conductivity, pressure, and derived variables in user-selected intervals; the intervals may be defined using pressure, depth, scan number, or time range. We use 1m bins, with no surface bin. In this module, we exclude scans that we flagged as bad in previous modules.

The following processing options were selected in this module for all casts:

binavg_bintype = meters
binavg_binsize = 1
binavg_excl_bad_scans = yes
binavg_skipover = 0
binavg_surface_bin = no, min = 0.000, max = 5.000, value = 0.000

9. Split Module:

Split separates the data from an input *.cnv file into upcast (pressure decreasing) and downcast (pressure increasing) *.cnv files. Downcast only files are output because they do not contain the data collected when the bottles are fired (e.g., repetitive sampling at the same pressure). Consequently, they are used to derive variables such as thermocline depth and strength.

The following options were selected in this module for all casts:

split_excl_bad_scans = no
output the downcast only (into the \Split folder). This command adds a ‘d’ at the beginning of the filenames.

10. ASCII Out Module:

ASCII Out outputs the header and/or the data from a binary data file (*.cnv). Data are written to an ASCII file (*.asc), while the header information, which lists each processing module and the variables applied, is written to a separate ASCII file (*.hdr).

This module was run twice. First, to convert the complete cast; second, to convert the downcast-only files created with the SPLIT module.

The following options were selected in this module for all casts:

Output Header and Data files
Label Column at top of the file
Column separator = space

FINAL PRODUCT

ASCII Out outputs the header and/or the data from a binary data file (*.cnv). Data are written to an ASCII file (*.asc), while the header information, which lists each processing module and the variables applied, is written to a separate ASCII file (*.hdr).

ASCII down-cast output files, containing only data recorded by the secondary sensors and no error flags, can be found in the \Final\ASCII_Down_cast folder.

The file headers have been saved separately from the final ASCII data files in both directories. The header files contain time in two separate fields: "System UpLoad Time" and "NMEA UTC (Time)". The time in the "System UpLoad Time" field is taken from the PC used to the collect the data and may not be accurate (e.g., this field may be recorded in local time, rather than Coordinated Universal Time, and may not have been adjusted for local time zone changes). The Coordinated Universal Time in the "NMEA UTC (Time)" field is taken from the GPS unit and is accurate as long as the GPS functioned properly.

The downcast profile is used to derive variables commonly used in protected species assessments, such as thermocline depth and strength. Plots of complete casts show hysteresis, or depth offsets, of 5-8 m. The error in the depth, as indicated by the offsets, are expected to occur primarily in the upcasts due to "package wake" (i.e., the "shadowing" of the sensors by the rosette and frame as the CTD is pulled up through the water column). Additionally, the upcasts include repetitive sampling of the same depth when bottles are fired to collect water samples.

In total, 107 CTD casts were conducted during CSCAPE 2005 on the David Starr Jordan. The format of the output files is shown below.

```
   PrDM      C0S/m      T090C      Sal00  Sigma-t00      DepSM       SvCM    AvgsvCM
  2.015   4.208510    17.0854    32.4871    23.5665      2.000    1510.24    1156.65
  3.023   4.208380    17.0836    32.4870    23.5668      3.000    1510.26    1511.28
  4.030   4.208562    17.0853    32.4869    23.5664      4.000    1510.28    1510.25
```

Column descriptions are as follows (only the bolded variables are included in the final downcast files):

a) PrDM = Digiquartz pressure in decibars (db)
b) C0S/m = Conductivity in Siemens per meter (S/m)
c) T090C = Temperature, in degrees Celsius (ºC), calculated using the ITS-90 standard
d) Sal00 = Salinity, in practical salinity units (psu), derived from the temperature and conductivity sensors
e) Sigma-t00 = Density [sigma-theta], in kilograms per cubic meter (kg/m^3), calculated from the temperature sensor and the derived salinity data
f) DepSM = Salt water depth in meters (m)
g) SvCM = Chen-Millero's sound velocity in meters per second (m/s)
h) AvgsvCM = Chen-Millero's average sound velocity in meters per second (m/s)

Perl program CTDPositionCheck (programmer: Dan Prosperi) was used to check the CTD cast date/times and positions recorded in the header files against the edited TSG file for the survey. The UTC times recorded in header files for casts 001-055 were changed from local time to UTC. 105 of 107 files had matching TSG records; 6 position corrections were needed.

Paul Fiedler, 17 June 2021

Appendix 1. CSCAPE 2005 DSJ Sea-Bird Data Processing Configuration Files

CSCAPE_2005 DSJ Casts 1_55.con

```
Configuration report for SBE 911plus/917plus
       CTD
-------------------------------------------

Frequency channels suppressed : 2
Voltage words suppressed      : 4
Computer interface            : RS-232C
Scans to average              : 1
NMEA position data added      : No
NMEA depth data added         : No
NMEA time added               : No
Surface PAR voltage added     : No
Scan time added               : No

1) Frequency 0, Temperature

   Serial number : 1448
   Calibrated on : 30-Dec-2005
   G             : 4.82354698e-003
   H             : 6.71702331e-004
   I             : 2.57106505e-005
   J             : 2.03596951e-006
   F0            : 1000.000
   Slope         : 1.00000000
   Offset        : 0.0000

2) Frequency 1, Conductivity

   Serial number : 1165
   Calibrated on : 31-Dec-2005
   G             : -3.97185921e+000
   H             : 5.48291816e-001
   I             : 1.67311002e-004
   J             : 2.14732040e-005
   CTcor         : 3.2500e-006
   CPcor         : -9.57000000e-008
   Slope         : 1.00000000
   Offset        : 0.00000

3) Frequency 2, Pressure, Digiquartz with TC

   Serial number : 0311
   Calibrated on : 06-17-1993
   C1            : -4.123560e+004
   C2            : 1.043267e+000
   C3            : 1.330030e-002
   D1            : 4.018400e-002
   D2            : 0.000000e+000
   T1            : 3.020637e+001
   T2            : 4.924132e-005
   T3            : 3.833950e-006
   T4            : 6.451910e-009
   T5            : 0.000000e+000
   Slope         : 1.00000000
   Offset        : 1.00000
   AD590M        : 1.167000e-002
   AD590B        : -8.165620e+000
```

CSCAPE_2005 DSJ Casts 56_103.con

```
Configuration report for SBE 911plus/917plus
       CTD
-------------------------------------------

Frequency channels suppressed : 2
Voltage words suppressed      : 4
Computer interface            : RS-232C
Scans to average              : 1
NMEA position data added      : No
NMEA depth data added         : No
NMEA time added               : No
Surface PAR voltage added     : No
Scan time added               : No

1) Frequency 0, Temperature

   Serial number : 1448
   Calibrated on : 30-Dec-2005
   G             : 4.82354698e-003
   H             : 6.71702331e-004
   I             : 2.57106505e-005
   J             : 2.03596951e-006
   F0            : 1000.000
   Slope         : 1.00000000
   Offset        : 0.0000

2) Frequency 1, Conductivity

   Serial number : 1165
   Calibrated on : 31-Dec-2005
   G             : -3.97185921e+000
   H             : 5.48291816e-001
   I             : 1.67311002e-004
   J             : 2.14732040e-005
   CTcor         : 3.2500e-006
   CPcor         : -9.57000000e-008
   Slope         : 1.00000000
   Offset        : 0.00000

3) Frequency 2, Pressure, Digiquartz with TC

   Serial number : 09P-7538-0291
   Calibrated on : 28-Jan-99
   C1            : -3.801474e+004
   C2            : 3.649520e-001
   C3            : 1.289200e-002
   D1            : 3.847600e-002
   D2            : 0.000000e+000
   T1            : 3.029981e+001
   T2            : -1.371950e-004
   T3            : 4.203520e-006
   T4            : 4.013720e-009
   T5            : 0.000000e+000
   Slope         : 0.99997000
   Offset        : -1.76600
   AD590M        : 1.146000e-002
   AD590B        : -8.308860e+000
```

CSCAPE_2005 DSJ Casts 104_107.con

```
Configuration report for SBE 911plus/917plus
       CTD
--------------------------------------------

Frequency channels suppressed : 2
Voltage words suppressed      : 4
Computer interface            : RS-232C
Scans to average              : 1
NMEA position data added      : No
NMEA depth data added         : No
NMEA time added               : No
Surface PAR voltage added     : No
Scan time added               : No

1) Frequency 0, Temperature

   Serial number : 1448
   Calibrated on : 30-Dec-2005
   G             : 4.82354698e-003
   H             : 6.71702331e-004
   I             : 2.57106505e-005
   J             : 2.03596951e-006
   F0            : 1000.000
   Slope         : 1.00000000
   Offset        : 0.0000

2) Frequency 1, Conductivity

   Serial number : 1165
   Calibrated on : 30-Dec-2005
   G             : -3.97185921e+000
   H             : 5.48291816e-001
   I             : 1.67311002e-004
   J             : 2.14732040e-005
   CTcor         : 3.2500e-006
   CPcor         : -9.57000000e-008
   Slope         : 1.00000000
   Offset        : 0.00000

3) Frequency 2, Pressure, Digiquartz with TC

   Serial number : 0311
   Calibrated on : 21-Oct-2005
   C1            : -4.123560e+004
   C2            : 1.043267e+000
   C3            : 1.330030e-002
   D1            : 4.018400e-002
   D2            : 0.000000e+000
   T1            : 3.020637e+001
   T2            : 4.924132e-005
   T3            : 3.833950e-006
   T4            : 6.451910e-009
   T5            : 0.000000e+000
   Slope         : 0.99998000
   Offset        : -3.90200
   AD590M        : 1.167000e-002
   AD590B        : -8.165620e+000
```

Appendix 2. Bottle Salinity Analyses

Bottle salinity samples were analyzed to validate CTD sensor calibration and to detect evidence of Niskin bottle leakage. Samples were collected from bottles tripped at depth and analyzed with a Guildline Portasal 8410A salinometer using standard methods (Guildline Portasal User's Manual). The results summarized below can also be found in CSCAPE 2005 DSJ Salts.xls in the \Documentation folder.

Portasal data were collected during salts runs at sea by the Autosal data collection program ASAL v2.37 (Oceanographic Data Facility, Scripps Institution of Oceanography). The raw data files, which are the files without a filename extension in each of the /Portasal_Readings subfolders within the Salts Run folders in W:\WestCoast\2005_CSCAPE\Oceanographic\Salinity \Raw\ DSJ\, were copied into a single raw data file named *salts05j.raw*.

Fortran program CR2SAL calculates salinities from the recorded conductivity ratios and bath temperatures in *salts05j.raw* using the Sea-Bird salinity algorithm. The two output files, *salts05j.sal* and *salts05j.sta*, are identical except that the sample records in the *.sta* file are truncated. Output file *salts05j.sal* lists four salinity values for each sample, calculated from the listed value and three adjusted values of the sample conductivity ratio, as discussed below.

File *salts05j.sta* was edited to list the CTD raw data file and Niskin bottle number corresponding to each sample. FORTRAN program SALTS.EXE (programmer: Fiedler) called Sea-Bird program SBEBATCH to process each raw CTD file. Specifically, the batch program creates a temporary water bottle *.ros* file from the Data Conversion module and outputs a bottle data summary *.btl* file from the Bottle Summary module. The *.ros* file contains data for each scan associated with a bottle firing, which by default are all scans within a 1.5-second period after a bottle firing confirmation is received from the water sampler. The *.btl* file contains means and standard deviations of the CTD data for each bottle. SALTS then reads the *.btl* file to find CTD salinity values corresponding to the bottle samples in *salts05j.sal*. Two files are output: *salts05j.dat* contains the CTD salinity and depth for each bottle sample and the differences between each of the four alternative bottle salinity values and the CTD salinity; *salts05j.sum* contains means and standard deviations of the differences within each salts run. Editing of *salts05j.sta* was iterative as bottle misfires and misidentifications were revealed by matching bottle and CTD salinities, as noted in the file.

Conductivity Ratio Adjustment for Bottle Salinities

When analyzing samples on the Portasal, the initial salinity standard reading should be equal to 2x the actual conductivity ratio of the standard (K_{15} on the ampule label) after correct initialization of the instrument. Referencing sample conductivity ratios to the initial standard reading may not give the best results for several reasons; for example, the initial standard reading may be erroneous (e.g., the Portasal was not sufficiently warmed up with standard water before samples are read) or the sensitivity of the Portasal may drift during the run. Adjusting the reference for sample conductivity ratios will change both the mean and the standard deviation of Bottle - CTD salinity differences if the initial and final standard readings differ. Selection of an adjustment alternative should be based on minimizing the standard deviation.

CR2SAL calculates four alternative salinity values from sample conductivity ratios that were adjusted relative to:

(0) the initial standard reading (no adjustment),
(1) the final standard reading,
(2) the average of the initial and final readings, and
(3) a standard reading interpolated between the initial and final readings.

Salinities calculated from sample conductivity ratios adjusted by method (1) resulted in Jordan CSCAPE 2005 bottle–CTD differences with the smallest means (biases) and standard deviations (RMSE) overall:

Adjustment	Mean (Bottle – CTD)	St. dev. (Bottle – CTD)
None:	+0.000488	0.013261
(1):	**-0.000105**	**0.010882**
(2):	+0.000191	0.011702
(3):	+0.000155	0.011926

Therefore, bottle salinities calculated from sample conductivity ratios adjusted by method (1) were used in subsequent analyses.

Precision of Bottle Salinity Measurements

No replicate samples were collected to test the precision of our analytical method. Guildline specifies a Portasal accuracy of ±0.003 and resolution of 0.0003 psu (although precision might not be equal to resolution). Autosal accuracies of ±0.001 are possible when special care is taken in handling the samples and when the measurements are made with room temperature maintained 1-2°C below the bath temperature (Howell, G. H., et al. (Sea-Bird). 2010, On the use of a secondary standard to improve Autosal calibration, poster presented at AGU Ocean Sciences, Portland, Oregon, USA, 22-26 February 2010).

The standard deviation of Bottle - CTD salinity differences was 0.0109 (above table, Adjustment 1). This value has been about two times the standard deviation of bottle salinity replicates when we run replicate samples, because of additional errors involved in CTD sampling and the mismatch of waters pumped through CTD sensors and sampled by Niskin bottles. The observed standard deviation of Bottle - CTD salinity differences suggests that the Portasal salinity values were not as precise (about ±0.005) as they could be, but are acceptable for our purposes.

Bottle – CTD Salinity Differences

Figure 3 shows Bottle – CTD salinity differences for all samples. Overall, the CTD salinities are very close to the bottle salinities, with scatter probably due to Portasal analytical errors as discussed above. The slight positive bias of CTD salinity during the first half of the cruise (Bottle – CTD differences less than zero) is consistent with the use of the post-cruise calibration factors after the post-cruise calibration indicated a slight decrease in sensitivity. However, when the sensors were moved to another fish for casts 056-103, the salinity bias became slightly negative.

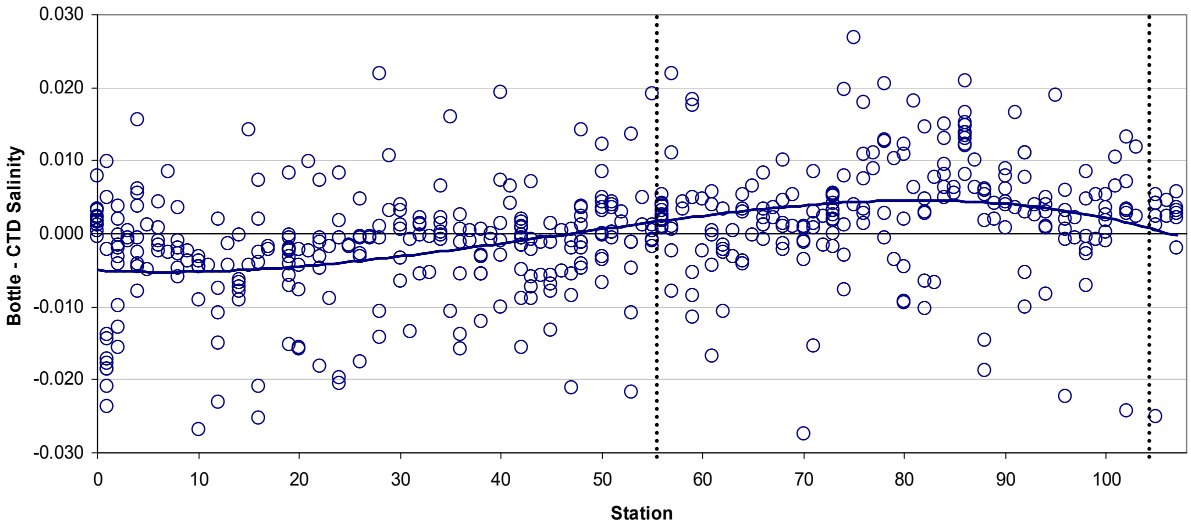


Figure 3. Bottle – CTD salinity differences for CSCAPE 2005, Jordan, using post-cruise sensor calibrations with no adjustments. Solid line is a fourth-degree polynomial fit. Dotted lines mark CTD fish changes (see page 1).

These results do not contradict the decision to use post-cruise calibration factors with no adjustment.

Test Cast Bottle vs. CTD Salinities

The following table summarizes bottle salinities and corresponding CTD salinities (mean ±sd) from the six test casts, when all 12 bottles were tripped sequentially at 700m. Although values are listed to four decimal places, the precision of the salinometer is ±0.003 and the precision of the CTD sensors is ±0.0004 psu.

	CTD Salinity	**Bottle Salinity**
Leg 1	34.3767 ±0.0006	34.3790 ±0.0019
Leg 2	34.2807 ±0.0009	34.2777 ±0.0052
Leg 3	34.2862 ±0.0005	34.2838 ±0.0053
Leg 4	34.3876 ±0.0005	34.3903 ±0.0014
Leg 5	34.2775 ±0.0006	34.2805 ±0.0024
Leg 6	34.3389 ±0.0004	34.3530 ±0.0030

The salinity of the bottle samples collected at the same depth (column labeled "Bottle" above) do not vary by any more than the precision of replicates (i.e., about ±0.005 psu) and the precision of the salinometer; consequently, the measured bottle salinity values are essentially identical.

Salinities derived from the secondary CTD sensors, after temperature and conductivity calibration adjustments, are plotted as deviations from the Portasal bottle salinities in Figure 4. The Leg 6 deviations are unusually large (see also Figure 3, cast 086).

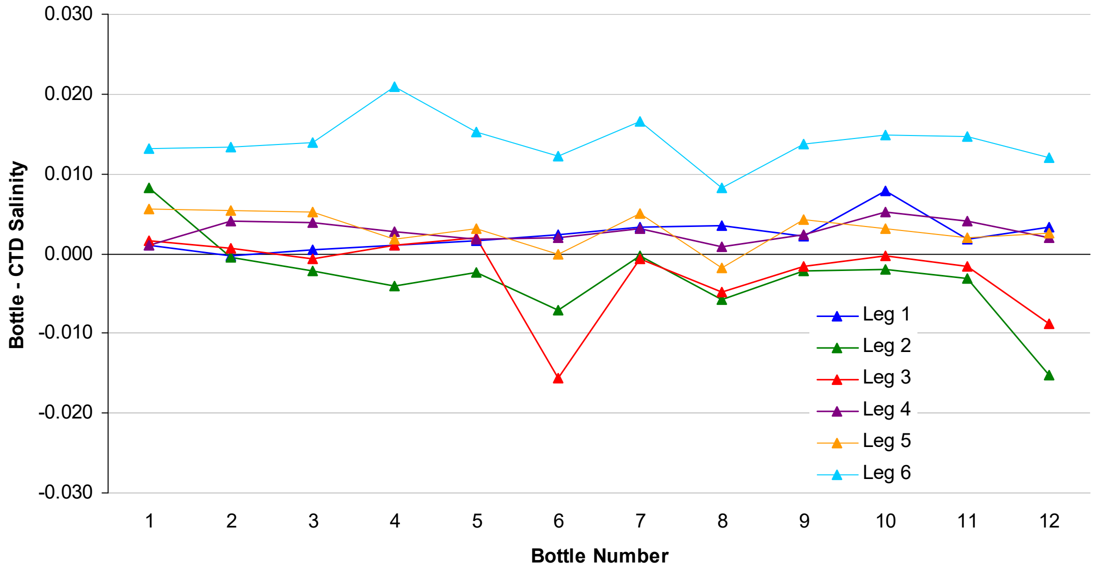


Figure 4. Bottle - CTD salinity differences for test casts on CSCAPE 2005, Jordan, Legs 1-6.

There are no bottles with consistently large negative differences that might indicate leakage of a Niskin bottle as it is brought up from depth to the surface through lower-salinity waters.