Deepwater Horizon Oil Spill (DWHOS)
Water Column Technical Working Group

NRDA CTD Processing Plan

Principal Investigator: Dr. Yong Kim, Applied Science Associates, Inc.

May 24, 2012

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Proposed Work Period:
April 1, 2012 – November 1, 2012

1. Project Description

This work plan describes the processing and validation of conductivity, temperature, and depth (CTD) data, and associated sensor (e.g., fluorescence, dissolved oxygen, turbidity) data, collected as part of the Deepwater Horizon Oil Spill (DWHOS) Natural Resource Damage Assessment (NRDA) and other deepwater sampling efforts in 2010-2011. The data to be compiled, processed, verified, and validated under this plan include those data collected during cruises conducted pursuant to various NRDA workplans developed by the NOAA NRDA Water Column Technical Working Group (TWG) as well as during other cruises where NRDA participation was requested by other members of the Trustees (e.g., cruises led by other NOAA NRDA TWGs, NOAA Response, BP or its contractors, and by third party investigators). The specific cruises that collected CTD data to be processed pursuant to this plan can be found in Attachment 1. Any additional data identified for processing will be presented as addenda to this plan to be agreed upon by the parties. The Trustees reserve the right to proceed independently and process additional data if agreement is not reached on an addendum. Dr. Yong Kim of Applied Science Associates, Inc. (ASA) will be the Project Principal Investigator, with Scott Cross of NOAA's National Oceanographic Data Center (NODC) overseeing the processing effort.

The data products resulting from this processing plan will be a compiled dataset of vertical CTD profiles (both downcast and upcast), including data from all auxiliary sensors and metadata, in electronic format (e.g., NetCDF). These files will be uploaded to the NOAA NRDA Data Content Management System for dissemination.

2. Data Handling and Prioritization Procedures

CTD data have been collected on the majority of offshore cruises for the DWH NRDA. These data have primarily been collected using widely available sensors (i.e., Sea-Bird Electronics, Inc. systems) and are therefore in a common format. In addition to the standard CTD sensors, additional (also called auxiliary) sensors were added to these units (e.g., dissolved oxygen sensors, fluorometers). All data from auxiliary sensors plugged into the Sea-Bird CTDs were recorded in the Sea-Bird data files and are available for processing as part of the CTD data. Table 1 lists the most common sensors that have been deployed as part of the NRDA CTD data collection.

Table 1. List of sensors found in NRDA CTD data.

Manufacturer	Model
Biospherical/Licor	SPAR/Surface Irradiance Sensor
Biospherical/Licor	PAR/Irradiance Sensor
Chelsea Technologies Group	Chelsea Aquatracka 3 Fluorometer
Chelsea Technologies Group	Chelsea UV AquatrackaFluorometer
Chelsea/Seatech	Transmissometer
Sea-Bird	SBE 19 Seacat Profiler CTD
Sea-Bird	SBE 19plus V2 Seacat Profiler CTD
Sea-Bird	SBE 911 Plus CTD
Sea-Bird	SBE 9 CTD
Sea-Bird	SBE 25 Sealogger CTD
Sea-Bird	SBE 43 Dissolved Oxygen Sensor
Sea-Bird	pH Sensor
Sea-Bird	SBE 50 Digital Oceanographic Pressure Sensor
Seapoint Sensors, Inc.	Seapoint Ultraviolet Fluorometer
Seapoint Sensors, Inc.	Turbidity Meter
Turner Designs	SCUFA Fluorometer
Turner Designs	C3 Fluorometer
WET Labs	WETStarFluorometer
WET Labs	ECO-FLNTU Fluorometer
WET Labs	ECO CDOM Fluorometer
WET Labs	ECO-NTU Turbidity Meter
WET Labs	C-Star Transmissometer

Data will be processed sequentially with priority going to data collected close to the time of the spill (2010) and for cruises where data are already checked for matching configuration files (see Section 3). Total processing time for all of the CTD data available on www.noaanrda.org or NODC's data repository (http://data.nodc.noaa.gov/) as of March 2012 is estimated by NODC to be approximately six (6) months. A specific prioritization scheme has not been defined.

3. Configuration File QA/QC

A preliminary review of collected CTD data indicates that a review of configuration files is in order prior to data processing. A joint workgroup consisting of representatives from both the Responsible Party (RP) and the Trustees will be tasked with reviewing each station to ensure correct configuration files are available to NODC. All configuration files will be examined to ensure that instrument serial numbers, sensor locations, and calibration coefficients match shipboard records and factory calibration sheets. All instrument serial numbers and their associated cruise will be recorded so that they can be tracked during the quality assurance and quality control (QA/QC) process. This will enable the correct configuration file to be used for processing. Additionally, if a sensor is deemed to have malfunctioned on one cruise, any subsequent deployments can be tracked to assess if the problem persisted or was resolved. Upon completion of this review, each station will have the correct configuration file (*.CON) associated with the raw data file (*.HEX) and will be available to NODC for processing.

4. CTD Data Processing Procedures

NODC has been tasked with downloading all raw, profiling CTD data from www.noaanrda.org, querying it for all sensors, processing it, applying automated, standard QA/QC measures for temperature, conductivity, density, pressure, fluorescence, dissolved oxygen, sound speed, pH, PAR, turbidity, specific volume anomaly, and oxygen saturation, and delivering a compiled data set with metadata. All Sea-Bird processing will be completed using SBE Data Processing, Version 7.21g. Details of this procedure can be found in Attachments 2 and 3.

Figure 1 and the following list of tasks provide an overview of the major steps for the processing of CTD data:

1. Initial collection and uploading of the CTD data (completed by NOAA NRDA field personnel)
2. QA/QC of configuration files by joint Trustee/RP workgroup
3. Data download (in process by NODC) – Attachment 2
4. Sea-Bird processing (to be completed by NODC) – Attachment 2
5. Conversion and automated QA/QC measures (to be completed by NODC)
    a. Quality Assurance and Control (see section below)
    b. File Conversion (Attachment 2) to NetCDF
6. Creation of metadata (to be completed by NODC, with support from NOAA NRDA) – Attachment 3)
7. Data upload to NOAA NRDA Data Content Management System (to be completed by NODC)
8. Data download by QA/QC Reviewers (to be completed by NOAA NRDA)
9. Manual QA/QC of additional sensor profiles (see dissolved oxygen, fluorometers, and remaining sensors below) (to be completed by NOAA NRDA)
10. Creation of Bin Averaged cruise-wide NetCDF (to be completed by NOAA NRDA)
11. Update of metadata to reflect QA/QC procedures (to be completed by NOAA NRDA)
12. File upload to NOAA NRDA Data Content Management System (NN-DCMS; to be completed by the NOAA NRDA)
13. Distribution of Compiled Datasets (see section below)

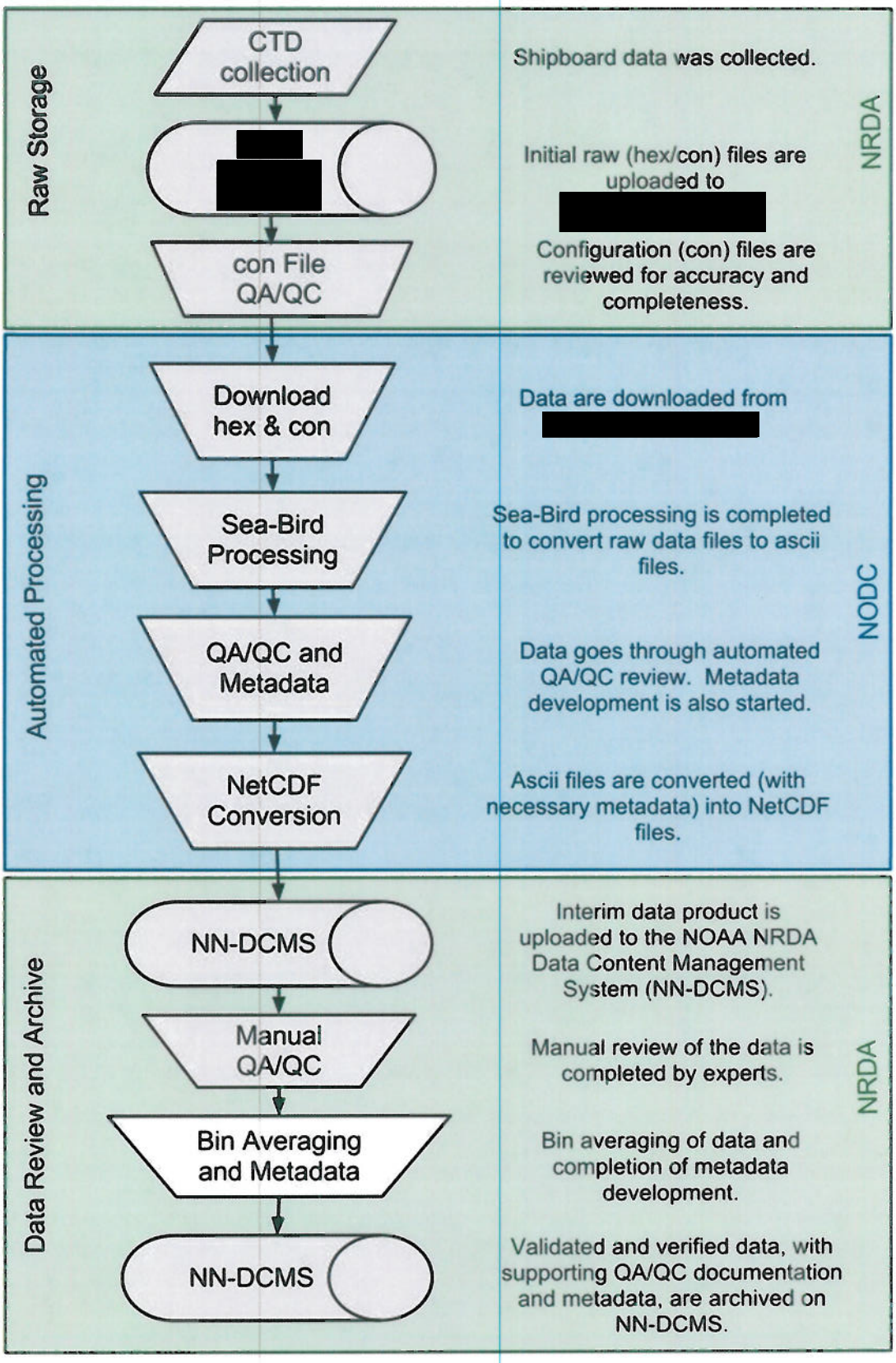

Figure 1. CTD processing steps.

5. Quality Assurance and Control Procedures

In order to verify and validate this data set, several procedures will be employed. These procedures will evaluate the accuracy, sensitivity, and precision of each sensor and the quality of every data measurement. Only one procedure (*Wild Edit*) will replace individual sensor readings for temperature, conductivity, and pressure that constitute an instrument malfunction (based on manufacturer guidelines) with an error value and these values will not be included in the bin-averaged NetCDF files. The remaining procedures will categorize (i.e., assign a Quality Flag) data as one of the following five options: unchecked, correct, inconsistent, doubtful, or erroneous.

This plan will follow the same flag designations as those proposed in the Global Temperature and Salinity Profile Program (GTSPP) Real-Time Quality Control Manual (UNESCO, 2009) developed by the Intergovernmental Oceanographic Commission[1]:

0 = no QC assigned to this element.
1 = the element appears correct.
2 = the element appears to be correct but is inconsistent with other elements.
3 = the element appears doubtful.
4 = the element appears erroneous.
6-8 = reserved for future use.

Until the data have undergone a review procedure they are assigned a '0' flag. Automated review procedures will update the flags with a '1' if it passes or '2' if data fails a test. Manual review processes will verify or update the automated flags. Elements of the original sensor data will not be altered. The reviewer will only update flags during this process and any updates, along with the reasoning behind the update, will be documented. Verified data, QA/QC flags, and QA/QC documentation will be delivered together (see Section 7). In order to ensure that erroneous measurements are not included in the Bin Average, the data will first undergo this manual QA/QC procedure prior to the production of the final, bin averaged data file. This manual review will occur after the *Derive* subroutine is performed when the data is fully processed but not yet bin averaged. The processes for the automated and manual reviews are described below.

Automated Data Review Procedures

The first step during the automated data review is to run *Wild Edit*, a Sea-Bird processing routine. This will find impossible readings from temperature, conductivity and pressure sensors and overwrite these impossible values with an error value which will be flagged as 'inconsistent' (see Attachment 2 and the paragraphs below for a description of the exclusion criteria). The Quality Flag values will then be changed to 'erroneous' during the manual review so as to not include these data in the final bin-average. *Wild Edit* criteria have been selected based upon Sea-Bird recommendations for these sensors. These criteria are designed so that any data flagged for exclusion by *Wild Edit* are excluded based on impossibility and not on marginal sensor performance.

[1] http://www.iode.org/components/com_oe/oe.php?task=download&id=1405&version=1.0&lang=1&format=1

Following the completion of the Sea-Bird processing, the data will be run through an additional automated review process. This process will assign a flag to all elements of the following sensors for all CTD casts. Values for the Global Impossible Parameter (GTSPP) tests are based on normal ranges observed in open ocean environments and instrument ranges for fluorometers.

For **temperature and salinity**, this step is based on several algorithms in the GTSPP. The following checks are conducted on the temperature and salinity profiles (following the GTSPP procedures and nomenclature):

1. Spike
2. Top and Bottom Spike
3. Gradient
4. Density Inversion
5. Levitus Monthly Climatology

Values that fail these tests will be flagged as 'inconsistent'.

For **dissolved oxygen (DO)**, an impossible parameter value check for ranges outside of > 0 and </= 8 mL/L is performed. Values outside of this range will constitute a fail and will be flagged as 'inconsistent' for all DO variables.

For **fluorometers (FL)**, an impossible parameter range check for values for each fluorescence sensor will be performed. Values outside of the fluorometers-specific allowable range (see Table 2 for sensor-specific allowable ranges) will constitute a fail and will be flagged as 'inconsistent'.

For **pH**, an impossible parameter range check for values > 8 and < 8.7 is performed. Values outside of this range will constitute a fail and will be flagged as 'inconsistent'.

For **transmissometers**, an impossible parameter value check for beam attenuation ranges outside of >0 and <15 m^{-1} is performed. Values outside of this range will constitute a fail and will be flagged as 'inconsistent'.

For **turbidity sensors**, an impossible parameter value check for ranges outside of >0 and <10 turbidity unit is performed. Values outside of this range will constitute a fail and will be flagged as 'inconsistent'.

For **PAR** and **SPAR sensors**, an impossible parameter value check for ranges outside of >0 and <3000 $\mu E/(m^2*s)$ is performed. Values outside of this range will constitute a fail and will be flagged as 'inconsistent'.

All **remaining sensors** (e.g. altimeter) are not reviewed as part of the automated procedure and will be flagged as 'unchecked'.

Table 2. Allow ranges for the different fluorometers deployed.

Fluorometer Model Name	Allowable Range	Units
Chelsea UV Aquatracka	-1 to 11	ug/L Carbazole
Seapoint Ultraviolet Fluorometer	0 to 5	ppb
Turner SCUFA Fluorometer	0 to 600	RFU
Turner CYCLOPS-7 Fluorometer	-5 to 100	ppb
WET Labs WETStar Fluorometer	-5 to 74	ug/L
WET Labs ECO-NTU Turbidity Sensor	-5 to 10	NTU
WET Labs ECO-AFL/FL Fluorometer	-5 to 30	ug/L
WET Labs ECO CDOM Fluorometer	-5 to 100	ppb QSD

Instrument Evaluation and Manual Review of Data

All sensor data will also be evaluated by one of the NOAA Water Column TWG QA/QC reviewers. Reviewers will have experience in physical oceanography and knowledge of open ocean data sets. Lauren Decker, Matthew Grennan, Yong Kim (ASA), or someone under their purview, will perform the QA/QC reviews of the sensor data sets. All data will be subjected to the same, impartial review for completeness, consistency, and reasonableness. The reviewer will determine if any portion of the data should be flagged differently than the flags produced by the automated processes. For example, if the reviewer agrees that an element flagged as a '2' by the automated QA/QC process is indeed erroneous, that flag will be changed to a '4'. If the reviewer does not agree with this, but does not have sufficient evidence to change the flag to a '1', then the flag will remain unchanged. If the reviewer disagrees that the element is inconsistent, and has sufficient reason to change the flag to a '1', then he or she will do so. All flag adjustments and the reasons for adjusting these flags will be tracked and documented, which will be provided along with the dataset as part of the QA/QC package (see Section 7).

In the first step of the review, all file collections will be reviewed to ensure that all expected files are present (see Attachment 2 for a list of files), and that all files have been processed completely and accurately. This will be assessed using the Header (*.HDR) file generated during the *ASCII Out* Sea-Bird processing step. A reviewer will also evaluate whether or not all settings were correct within the Sea-Bird routines, and will compare the *.HDR file to the configuration file used during processing to ensure that all sensor serial numbers and voltage locations match between the two files. Then, the reviewer will check the single-station NetCDF file to make sure that for all sensors that have undergone automated checks, those variables have been populated with a value other than "0" (no QC assigned to this element). This check will be performed on all variables to ensure that the Quality Flags associated with the physical measurements have been carried over to the derived variables. The final step of this initial review will be to view a plot of the station locations to ensure that the spatial and temporal range of the data is reasonable. If the data fail any of these checks, appropriate measures will be taken to ensure that the file is re-processed correctly.

In the second step of the review, a reviewer will determine whether each sensor performed to the accuracy and sensitivity prescribed by the manufacturer. This will be evaluated by assessing each sensor's documentation, as created by the manufacturer during construction and calibration of the instrument. If a sensor is found to have been outside the industry standard ranges during

any data collection or at its post-use calibration, all instances where that sensor was used will be flagged as 'inconsistent'. If evidence of a clear point of failure can be identified during the use of the sensor, the 'inconsistent' flags on the data collected prior to that point may be switched to 'correct' and the flags on the data after that point may be switched to 'erroneous'. As with all other cases where flags are changed, the reasoning will be documented.

As part of this second step, a reviewer will also determine whether the precision for each sensor was consistent during individual deployments. The behavior of all sensors will be evaluated to determine how consistently they behaved during an entire cast. If a profile, or portion thereof, contains abnormalities the data in question will be flagged as 'inconsistent' or 'erroneous' depending on the magnitude of the deviation. This review encompasses an assessment of the casts on the whole to determine if there are artifacts present in the data, an evaluation of all 'inconsistent' flags generated by the automated processes, and a check for reasonableness against expected environmental conditions within the Gulf of Mexico.

Within this review of sensor precision, the upper portion of the water column will be examined, and all data comprising the "surface soak" will be flagged as "erroneous". The "surface soak" data will be defined as all data collected prior to the instrument beginning its descent through the water column. The "surface soak" will end at the minimum pressure reading measured after the maximum soak depth has been reached. If an adequate surface soak was not performed, data will be closely examined to ensure that the instrument was functioning correctly. If it appears that this is not the case, then all affected data will be flagged as 'inconsistent'. Surface fluorometer data will also be reviewed for effects of sun glint that may not have been flagged within the automated range checks. If it is believed that sun glint is causing unreasonably high readings in near-surface waters, but not high enough to have been flagged within the automated QA/QC process, then those data will be flagged as 'erroneous'. Any full-scale readings flagged as 'inconsistent' by the automated process will be updated to 'erroneous' so as to eliminate these readings from subsequent averaging. Any profiles showing signs of hysteresis will be flagged as 'inconsistent', with hysteresis being provided as the reasoning for the Quality Flag update. If a reviewer chooses to change a Quality Flag, he or she will provide the exact depth of the flag being changed, as well as the reasoning behind his or her decision to change it. Some data may not fit within the definition of the Quality Flags defined in this plan. In this event, a Flag value within the range 6-8 will be defined and assigned to the data. This value, along with its definition, will be presented as an addendum to this plan. The metadata files and associated QA/QC documentation will also be updated to reflect the new addition.

All data will be subjected to the same review criteria, and all checks will be documented within a rubric. If this rubric needs to be modified prior to the complete validation of the data, all data validated previously will be reevaluated to determine if the Quality Flags need to be updated. All reviewer decisions will be documented within a database, from which a report will be generated describing the QA/QC status as well as all Quality Flag updates and their associated descriptions. This process and associated information will be conducted and provided for 100% of the CTD and sensor deployments from all cruises listed in Attachment 1.

At the end of the manual review, the data will be considered verified and validated. The data will include the Quality Flags and will not eliminate any of the 'erroneous' or 'inconsistent' data.

The reasoning behind the flags generated by the automated and manual review processes will be documented and distributed with the validated data sets. Because there will be many users of this data set with varying parameters, goals, and other data to which these data will be compared, and because it is not feasible to mark data only as 'usable' or 'erroneous', the data set will remain whole. Therefore, it is the responsibility of the end user to review the Quality Flags prior to utilizing the data set.

6. Bin-Averaging of Verified and Validated Dataset

In an effort to efficiently generate the final, bin-averaged dataset, the NOAA Water Column TWG QA/QC reviewers will be tasked with bin-averaging all data following their final review. Data will be averaged over 1 meter depth intervals utilizing MATLAB® due to a number of restrictions within the Sea-Bird software. Data will be averaged based upon their associated Quality Flag value. All data with a Quality Flag value of '4' will not be included within the average. The Quality Flag value will carry over to the bin-averaged data. After the data has been bin-averaged, the NOAA Water Column TWG QA/QC reviewers will generate a cruise-wide NetCDF dimensioned by Depth and Station ID and update the associated metadata to reflect the QA/QC process.

7. Distribution of Compiled Datasets

NODC will coordinate with the NOAA NRDA Data Management Team to upload data to the NOAA NRDA Content Management System which will serve as a repository of information. Data for each cruise will be uploaded in a uniform folder structure, where the main folder will be named based on the vessel initials and cruise number as designated by the Water Column TWG and Data Management Team. Additionally, the NOAA NRDA QA/QC Reviewers will upload (i) a cruise-wide, bin-averaged, verified, and validated NetCDF file, (ii) a series of verified and validated single-station NetCDFs, and (iii) all the QA/QC documentation associated with those NetCDFs.A brief description of what will be found within the main, cruise-wide folder can be found in Table 3.

Table 3.Description of folder structure to be delivered by NODC and QA/QC Reviewers.

Folder Name	Description
0-Data	Contains any relevant cruise documentation, along with all raw data.
1-Data	Contains all intermediary files, along with a NetCDF of each individual cast.
1-Data_QA/QC	Contains all individual NetCDFs from 1-Data that have been updated based on the manual QA/QC procedures.
About	Contains an XML of all relevant metadata for the cruise and all associated QA/QC documentation.
Bin Averaged	Contains the two (downcast and upcast) cruise-wide NetCDF files.

Data sets will be made available when data for an entire cruise have been verified and validated. The data and supporting information, including all electronic files generated as part of this plan (e.g., intermediate datasets uploaded by NODC and the QA/QC reviewers) will be made available to the parties of this agreement by means appropriate to the data type as determined by the NOAA NRDA Data Management Team. NOAA and the Louisiana Oil Spill Coordinator's Office (LOSCO) on behalf of the State of Louisiana and BP (or Cardno ENTRIX on behalf of BP) will be alerted when these data become available for download.

In the interest of maintaining one consistent data set for use by all parties, only the verified and validated data set made available by the NOAA NRDA Data Management Team shall be considered the consensus data set. In order to ensure reliability of the consensus data and full review by the parties, no party shall publish consensus data until 14 days after such data have been made available to the parties. Any questions raised on the consensus data set shall be handled consistent with the procedures in Section 7.2 of the Deepwater Horizon NRDA Analytical Quality Assurance Plan.

- The trustees and BP shall each designate an individual responsible for raising questions, if any, on the consensus data set.
- If questions are raised, the two designated individuals will meet to determine the source of the difference and resolve.
- The questions raised and their resolution shall be distributed to all parties.
- No changes to the consensus data set will be made if the differences are considered immaterial by both designated individuals, acting on behalf of the parties.
- If the parties agree that changes to the dataset should be made, the dataset will be updated in accordance with the resolution and reposted with a notation that the dataset has been revised.
- If the designated individuals do not agree on how to resolve the difference concerning the consensus data set, the designated individuals shall request assistance from the Assessment Managers for the trustees and BP.

8. Retention of Materials

All information will be retained and maintained during all review steps in the process, stored in secure locations under trustee control, and will be made available to all parties should a need for such supplemental information be identified.

All materials associated with the collection or analysis of samples under these protocols or pursuant to any approved work plan, including any remains of samples and including remains of extracts created during or remaining after analytical testing, must be preserved and disposed of in accordance with the preservation and disposal requirements set forth in Pretrial Orders ("PTOs") # 1, # 30, #35, # 37, #39 and #43 and any other applicable Court Orders governing tangible items that are or may be issued in MDL No. 2179 IN RE: Oil Spill by the Oil Rig "DEEPWATER HORIZON" (E.D. LA 2010). Destructive analytical testing of oil, dispersant or sediment samples may only be conducted in accordance with PTO # 37, paragraph 11, and PTO # 39, paragraph 11. Circumstances and procedures governing preservation and disposal of sample materials by the trustees must be set forth in a written protocol that is approved by the state or federal agency whose employees or contractors are in possession or control of such materials and must comply with the provisions of PTOs # 1, # 30, # 35, 37, #39 and #43.

9. Budget

The Parties acknowledge that this budget is an estimate, and that actual costs may prove to be higher due to a number of potential factors. The costs indicated in Budget Chart # 1 below and any additional reasonable costs within the scope of this workplan that may arise shall be reimbursed by BP upon receipt of written invoices submitted by the Trustees. The Trustees will make a good faith effort to notify BP in advance of any such increased costs. It is anticipated that the work will require approximately 8 months to complete.

Budget Chart #1. NOAA labor costs.

NODC Processing	**$150,000**
QA/QC Review	**$85,000**
TOTAL	**$235,000**

10. Attachments

Attachment 1. CTD Data Inventory
Attachment 2. CTD Data Processing Standard Operating Procedures
Attachment 3. Metadata Creation and Template

Deepwater Horizon Oil Spill (DWHOS)
Water Column Technical Working Group

NRDA CTD Processing Plan

Principal Investigator: Dr. Yong Kim, ASA

Plan Date: May 24, 2012

Approvals

Approval of this sample processing plan is for the purposes of obtaining data for the Natural Resource Damage Assessment. Parties each reserve its right to produce its own independent interpretation and analysis of any data collected pursuant to this plan.

	Printed Name	Signature	Date
BP Approval	Joyce Mileu	Joyce Mileu	6/1/12
Federal Trustee Approval	[illegible]	[signature]	[illegible]
Louisiana Approval	KAROLIEN DEBUSSCHER	FOR ROLAND GUIDRY	6/19/12