RELATIVE STATUS INDICATOR

Development and Evolution of a Relative Measure of Condition for Assessing the Status of Water Quality and Biological Parameters Tracked in the US/EPA Chesapeake Bay Program Long Term Monitoring Programs

FINAL REPORT

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Under contract to The Interstate Commission for the Potomac River Basin

September 2009





ICPRB Report 09-4

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Acknowledgements

Most of the thinking behind the relative status measure was done by Drs. Alden and Perry. Dr. Ray Alden left Old Dominion University in 1997. Dr. Elgin Perry continued to lead the work to its current state in conjunction with other Bay Program partner analysts. He remains an independent consultant to the Chesapeake Bay Program. Contact: 2000 Kings Landing Rd, Huntingtown, MD 20639, 410-535-2949, eperry@chesapeake.net. Thanks also go to Mike Lane at Old Dominion for his interest in the status method along the way and for taking the time to review and comment on this document. Funding for this report was provided by the US EPA Chesapeake Bay Program grant #CB97339103.

Introduction

In the Chesapeake Bay region, "Save the Bay" is a bumper-sticker call to action laden with explicit and implicit meaning. That the Bay needs saving means the Bay is threatened, it is already changed in some undesirable way or is on the brink of it, and that the threatened state differs in various respects from our notion of an unthreatened, healthy Bay. It implies that direct and/or indirect actions undertaken by the sticker-viewing public can ward off the threat, and the viewer can infer that there are ideas out there about what those Bay-saving actions are, their beneficial effects, and a vision of what a saved Chesapeake Bay would look like.

The USEPA Chesapeake Bay Program arose from such a call to action. Under the broad umbrella of its federal, state and local partnerships, the Bay Program has led efforts to define quantitatively and qualitatively the conditions implied by the bumper sticker. The initial work in the late 1970s and early 1980s was to gather available quantitative data about the Chesapeake Bay environment, to characterize how it was THEN, at some point in the past, and how it was NOW. The work included hypotheses on the causes of change and proposals for their reversal. Since then, nutrient and sediment reduction goals have been set; various restoration goals, habitat requirements and water quality criteria have been established to define desirable endpoints; and management actions have been implemented to reduce pollutants, to conserve and protect resources. A long term monitoring program was established in 1984 to provide ongoing information about water quality and certain biological groups that are sensitive to water quality changes that could serve as early indicators of improvement or degradation.

The Chesapeake Bay Program is now 25 years old, and along the way we've asked, in simple bumper-sticker terms: How's the Bay doing? Are we making progress? The answer to the deceptively simple questions aren't simple, and a number of tools have been developed to grapple with the complexity of the assessments as well as the mixed results likely to be found in such assessments. Consequently, we have suites of environmental indicators including, among others, indices of biological integrity, goal and criteria attainment assessments, trend tests and status measures to help us articulate, illustrate and contextualize how the Bay and its plant and animal inhabitants are doing-how they're coming along.

This paper focuses on the development and application of a relative status measure in the Chesapeake Bay Program (CBP): the basis of its methodology and lessons learned from its use in assessing the condition of water quality and biological parameters tracked in the CBP long term monitoring programs. This status measure has been in use and in the grey literature of the Bay Program analysts for over a decade, but has not been formally published previously.

Relative versus reference status

The term status in the general sense is the condition of something, its relative position within a range of conditions. In the context of water quality, for example, status is a measure of current condition compared to some benchmark or point of reference. If the reference condition is defined, e.g., if the characteristics of 'healthy' water quality were precisely known, then a status assessment could determine if current water quality characteristics met, failed or were borderline with respect to those 'healthy' reference characteristics. Regulatory standards, restoration goals and habitat criteria are other examples of reference points against which *reference status* assessments can be made.

In fact, in the Chesapeake Bay and its tributaries, precisely defined reference levels are not available for many water quality and biological parameters, due in large part to the high temporal and spatial variability inherent in estuaries where land-based fresh water inputs intersect with salt water from the ocean, the dynamic nature of estuarine biological processes, and also to the paucity of "pristine", unaltered habitats in the estuary to serve as exemplary reference sites. In this circumstance, a measure of *relative status* can be a fallback. A relative status assessment determines where a parameter value lies within a range of observed values. Usually, but not always, one end of the spectrum is believed to be more desirable than the other and is reflected in the qualitative assessment terminology. For example, a relative status assessment could determine if current nutrient concentrations at a site were among the 'best' (with lower concentrations) or 'worst' (with higher concentrations) of all assessed locations or somewhere in between. Here, 'best' may or may not be equivalent to healthy or desirable and 'worst' may or may not be unhealthy or undesirable. We know only where the site condition lies within the range of observed conditions.

The CBP measure of relative status

Early version

One of the charges of the group overseeing the CBP Water Quality and Biological Monitoring Program--then called the CBP Monitoring Subcommittee--was to communicate to management and the public the state of the Bay and tributaries and progress toward their restoration. In the mid 1990s, failing reference points for many of the monitored parameters, the Subcommittee's Data Analysis Work group (DAWG) found that it needed a measure of relative status in its assessment toolbox. Two work group members, Dr. Ray Alden, a statistician at Old Dominion University, and independent consultant statistician Dr. Elgin Perry proposed such a measure in their white paper "Presenting Measurements of Status" (1997, Appendix 1). As the title implies, the proposal includes both a detailed statistical assessment methodology and a protocol for presenting results that would be easily understood, applicable across different monitored groups, and would convey comparable qualitative interpretation of the results across groups. The assessment methodology would be structured so that positive results represent improvements and negative results represent degradation. Other objectives and desirable characteristics of the status measure are also offered in the paper.

The authors modified the first draft of the methodology and presentation protocol in response to input from other work group members and issued a revised version in time for the method to be exercised in status assessment analyses supporting the 1997 State of the Bay and Re-Evaluation reports.

In brief, this assessment methodology

- defined a 'current' assessment period: the most recent 3-years for which there are data;
- defined a benchmark or reference period: 1985 through 1996;
- defined 'habitats' within which comparisons are made based on salinity and depth and which are applicable basin-wide;
- defined the most appropriate statistic to be analyzed for status: i.e., the median value for physical and chemical parameters and the geometric mean value for biological parameters. These values are computed for each station or segment within month over the assessment and benchmark periods in order to balance unequal sampling effort at different times of year. The monthly values are then assembled to form the assessment and benchmark datasets;
- defined a linear scoring scale from 0 to 100, with 0 representing extreme, undesirable values and 100 representing extreme desirable values. The scale endpoints are the parameter's 5th and 95th percentile values in the benchmark dataset within the salinity and depth category and these are assigned respectively to the undesirable or desirable ends depending on whether low or high values are desirable for the parameter. The 5th and 95th percentiles are used instead of the minimum and maximum values to lessen distortion from outliers. The median or geometric mean assessment values are scored by proportionally adjusting the values for representation on the 0-100 scale: e.g., where low values are undesirable: score = [(value pct05)/(pct95–pct05)] * 100; and where high values are undesirable: score = [(value—pct95)/(pct05-pct95)]*100.
- defined the status indicator value for water quality as the median of the medianbased scaled scores in the 3-year assessment period; and for biological data, as the arithmetic mean of the geometric mean-based scores in the 3-year assessment period;
- translated the 0-100 numeric scale to a qualitative status measure by dividing the scale into thirds such that if the indicator value fell in the upper third, the status was "good", "fair" if in the middle third and "poor" if in the lower third.;

• included a discussion of the influence on the status results of different censoring strategies for below-detection level (bdl) values and put forward the protocol that bdl-values be censored at one-half the laboratory method detection limit (MDL) in place at the time of sample collection. This is in contrast to censoring at the 'worst' MDL in place during the assessment and benchmark periods, as is done for CBP trend analyses.

Complaints, Experiments, Changes

The methodology was revisited over the next several years in light of the status results for the 1997 reports. That exercise had revealed a number of unsatisfactory aspects to what later would become known as the 'linear scoring' method:

- The benchmark period, 1985-1996, was essentially the full period of record at that time and included the 1994-1996 three-year assessment period; that is, the benchmark dataset included the test dataset. If this practice were to continue, then if an assessment period were particularly bad, the less favorable score would be mediated by the fact that the relevant endpoint, pct95 or pct05, would also likely change in the same direction. The user community for this product also asked that the benchmark period be made constant so that status could be compared from year to year.
- The final scoring categories--upper, middle and lower thirds—were labeled as "good", "fair" and "poor" in order to help convey the scores' meaning in terms of environmental condition or health. However, there was no scientific basis for the association; the categories were relative to the range of data in the benchmark dataset, not to an empirically desirable endpoint. That disconnect was sometimes disquietingly apparent.
- Indeed, it was observed that for many parameters--specifically for parameters with an asymmetric distribution--the distribution of scores among the "good", "fair", "poor" categories was uneven, tending to have more "fair" scores than seemed right. The expectation for the relative status measure was that the scores would be more evenly distributed among the categories.
- The collective results for individual stations compared to results for the segment sometimes didn't make sense. This seemed best explained by the fact that for many parameters the variances of space and time are not equal. That is, stations have only temporal variance, while segments have both temporal and spatial variance.

A small "ad hoc" team of DAWG members led by Dr. Perry was formed to resolve the issues. The group chose the 6-year period 1985-1990 as the new benchmark period because it was early in the monitoring program, long enough to include a wide range of climatic conditions (e.g., wet/dry years) and short enough to exclude later years in which

improvements, if any, from management actions would begin to be reflected in the data. The choice was made recognizing that as time between the benchmark and assessment periods increases, the status measure becomes more like a measure of trend. This problem would have to be revisited sometime in the future.

To solve the asymmetric distribution problem, some research was done to determine the best transformation for each parameter that would be symmetric and reasonably approximate some standard statistical distribution. A log transformation produces symmetry for most water quality parameters, and both the normal and logistic distributions approximated the distribution of the transformed data as determined by the probability plot correlation coefficient. The log-logistic was chosen because it is easier to compute the cumulative distribution function (CDF) of the logistic distribution than for the normal.

In the revised method, data in both benchmark and assessment datasets are log transformed. A logistic CDF based on the mean and variance of the parameter in the benchmark dataset grouped by depth and salinity category is used to perform a probability integral transform on all parameter values in the benchmark and 3-year assessment datasets similarly identified by depth and salinity category. Under the assumption that the logistic distribution is a reasonable model for the log-transformed data, the probability integral-transformed data in the interval (0,1) follow a uniform distribution. The median of this 3-year assessment dataset is the status indicator for the assessment period. For purposes of the status score, the indicator score is scaled to between 0-100. The scale is divided into thirds and assigned to good-fair-poor categories as before. This version would be known as the 'CDF scoring method'. Dr. Perry likened the procedure of scoring data using the logistic CDF to the classroom procedure of "grading on a curve" often prayed for by high school and college students. In this case, the "curve" is set by the mean and variance of the benchmark dataset whereas in classroom applications, the "curve" is set by the mean and variance of test scores for the class.

Trials using this CDF method revealed that the majority of scores still fell in the middle of the range. Dr. Perry suggested two features of the new method that might be to blame, both having to do with the way variance is computed for the benchmark dataset. One feature is that the variance used to define the CDF is the variance of individual observations in the benchmark data. The status indicator is a median of a 3-year period. A 3-year median should exhibit less variance than individual observations, thus the 3year median should be, on average, closer to the center than the individual observations. It follows that by being closer to the center, the median would fall in the middle category more often. The second feature which should inflate the frequency of status indicators falling in the middle category relates to seasonal variance. The variance computed for the benchmark data and used in the above equation includes a seasonal component that will make the CDF broader than one that represents the variation of seasonally adjusted status indicators and result in over-representation of status scores in the middle category. To adjust for seasonal variance, one could compute the variance for the benchmark dataset with the seasonal trend removed using Analysis of Variance with a seasonal term. The mean squared error from this ANOVA will estimate variance in the benchmark data with season removed. This adjustment was ultimately not implemented. Instead, it was decided to reduce the effects of seasonal variance somewhat by making status assessments on the seasons most relevant to each parameter (e.g., summer months for bottom dissolved oxygen, March-October for surface chlorophyll), not necessarily on the full annual period as had been done previously.

To improve the distribution of the 3-year medians across status categories, i.e., to adjust for 3-year medians inherently having less variance than the individual observations, an adjustment factor was applied to the variance of the individual observations. It is known that if the original data follow a log-logistic distribution, then data transformed as described above will follow a uniform distribution on the interval (0, 1) (Roussas, 1973). It is also known that the median of n observations taken from a uniform distribution will follow a Beta(m,m) distribution where m=(n+1)/2 (Roussas, 1973). Thus, the medians of the scored data follow a Beta(m,m) distribution. The distribution of 3-year medians from the benchmark dataset can be partitioned into thirds according to the 66.7 and 33.3 percentiles of this Beta distribution to create the good-fair-poor status categories.

With this modification, the method now produced status assessments spread more evenly across categories, but with the side-effect of variable cut points for the status categories-something not easily explained to managers and the public. Using percentiles of the Beta distribution as the cut points automatically adjusts for differences in sample size (since m=(n+1)/2). This has the beneficial effect of evening the status results among categories, but sample size can and does vary systematically and randomly within the Program, resulting in different cut points, i.e., different definitions of what constitutes good-fair-poor between assessment groups. It was further found that in most cases serial dependence of the raw data resulted in the population of 3-year medians having greater variance than expected if the distribution were Beta(m,m). To adjust for this, the variance of the Beta density was increased by a function of the ratio of among-station variance to within-station variance.

This is where the evolution of the CBP's relative status measure stopped. The CDF version with these last modifications adjusting for the effect of sample size and serial correlation were incorporated into the relative status measure computer code (Appendix 2) distributed to Bay Program analysts. While the results became more internally consistent and comprehensible with these methodological improvements, managers and communicators remained frustrated by the fact that the relative status endpoints are obtained from benchmark data and are not grounded in absolute values indicating health or degradation. As restoration goals and habitat and water quality criteria were developed within the Program, support for this indicator was discontinued in favor of those reference-based measures. Relative status assessments may still be part of the suite of regular reports to management, but they no longer play a major role in communicating with the public. However, it has been and continues to be a useful tool in exploratory

analyses where little is known about the endpoints. Some applications are discussed in the section below.

Abandoning this assessment approach was short-sighted in this author's opinion. Dr. Perry states that there is no reason why the mathematical machinery developed for this method cannot be reframed as a *reference* status indicator by specifying the desired mean and variance for a reference population and scoring the recently observed (test) data against this reference standard rather than against an existing benchmark dataset. The challenge remains, of course, to determine or formulate the desired mean and variance of the reference population, but scoring/assessing a habitat relative to optimal distribution criteria seems philosophically and scientifically superior to scoring on pass/fail or distance-from single-point criteria, which is the path the Bay Program chose to take.

Applications of the relative status measure

Although other status measures have supplanted "relative status" as the direct measure of condition, the methodology has been used in conjunction with other information to explore and develop first-cut discriminatory categories for reference points:

In the late 1990's, the Data Analysis Workgroup was working on Environmental Indicators for total nitrogen and total phosphorus, both of which consisted of a plot of concentration over time with an overlay of the trend line. They wanted to include a reference line to indicate what a "healthy" or desirable endpoint concentration would be. It was recognized that no single concentration could serve for all tidal waters of the Chesapeake basin nor for all times of year, but healthy restoration levels of nitrogen and phosphorus had not yet been defined for the various salinity zones and seasons. This author was asked to research recent and historical nutrient data from the Chesapeake to come up with empirically derived "healthy" concentrations, which then could be used in conjunction with experimental data in the literature as basis for the reference lines.

The resulting analysis was documented in a report to DAWG (Olson, 2002). The approach was first to identify instances of best overall water quality in the long term data record based on relative status scores of a suite of parameters, then characterize the nutrient concentrations in these best instances and evaluate them as reference concentrations. The author believed that a single-parameter approach would not necessarily yield "healthy" concentrations. In the eutrophic Chesapeake environment, reducing nutrient loading is the general objective, but lowest concentrations are not necessarily the same as optimum and low concentrations of a nutrient can occur in both healthy and unhealthy environments for various reasons. Instead, the author chose to use the CDF-based relative status assessment of multiple parameters to define and identify instances of healthy water quality and to use these data to derive the reference concentrations.

Four parameters were used in the analysis: total nitrogen (TN), total phosphorus (TP), chlorophyll_a (CHLA) and suspended sediments (TSS). The long term data record (1950-1999) constituted the test data and these were partitioned by parameter, decade,

season, salinity zone and depth layer (in the end, the analysis included only surface data). Individual parameter values within these groups were scored between 0 and 100 according to the relative status method using the 1985-1990 period for the benchmark dataset. The median scores within group were assessed as "good", "fair", or "poor" using as status category cut points, the 66.7 and 33.3 percentiles of the Beta distribution of the corresponding group in the benchmark dataset

Each decade/season/salinity zone was then evaluated to determine if it could represent "healthy" nutrient and sediment levels. The qualifying rules were arbitrary: none of the four parameters could have a "poor" assessment; only one parameter could have a "fair" assessment, one or more parameters had to be "good". If less than the full suite of four parameters was available, as often occurred in the pre-1984 years, there was no penalty. Then, to obtain the reference statistics for each individual parameter, the 'healthy' data pool was further restricted by including only the data in which the status of the parameter of interest was 'good.' Finally, from these "best of the best" data, the mean, median, 10th and 90th percentiles were computed for each group, with the median serving as the default proposal for the reference concentration.

The resulting reference concentrations were then compared to good-healthy concentrations proposed by others. When the TN and TP reference concentrations from the relative status method were compared to levels derived from nutrient limitation experiments, it appeared that the relative status reference concentrations for all salinity zones and seasons were, with one exception, near but still lower than the experimentally derived levels. The relative status reference concentrations for CHLA and TSS were considerably lower than maximum concentrations established as CBP restoration requirements for healthy SAV habitats. As of the date of this publication, no further action was taken by DAWG to formalize these or other proposals for the nutrient reference levels. Work on chlorophyll and sediment reference levels continued on a different track as part of the effort to develop biologically based water quality criteria for Chesapeake Bay, which focused on chlorophyll, dissolved oxygen and water clarity.

A project to characterize phytoplankton reference communities in Chesapeake Bay (Buchanan et al., 2005) used the relative status method (in conjunction with Classification and Regression Tree (CART) analysis (Breiman et al., 1984)) to assist in classifying samples from impaired and unimpaired phytoplankton habitats. Three parameters were used in the habitat water quality assessments: concentrations of dissolved inorganic nitrogen (DIN) and orthophosphate (PO4), and Secchi depth, a measure of water clarity. The assessment classifications were: Worst, Poor, Better and Best. Separate assessments were made for different season-salinity zone groupings. The authors used the relative status method to define classification cutoff points, i.e., to determine the classification criteria for Worst, Poor, Better and Best classes for Secchi depth and for Worst nutrient classes. The Best, Better/Poor criteria for the nutrient classes were not based on relative status scores, but on nutrient concentrations shown to limit phytoplankton growth in bioassay experiments. Based on the Worst-Poor-Better-Best classification results of the three water quality parameters, six different classifications were ultimately defined that combined the three status assessments: 1) Worst light--both nutrients in excess; 2) Poor and Worst light--both nutrients in excess (including class 1); 3) poor light--mixed nutrient levels including limiting, 4) better light--excess or mixed nutrient levels, 5) better light--limiting nutrient levels (including class 6) and 6) best light--limiting nutrient levels. Once these categories were defined, the long term phytoplankton data record was subjected to a binning process, in which each phytoplankton sample was assigned to one of the 6 categories based on the classifications of the nutrient and water clarity parameters measured at the time of sample collection. The data were then grouped by category, season and salinity zone and the phytoplankton community characteristics of each group analyzed.

The authors determined that the classification and binning processes were successful in identifying distinct phytoplankton habitat categories in Chesapeake Bay, and that these habitats yielded phytoplankton communities that were quantitatively and qualitatively different from one another when multiple parameters are viewed as a whole. The habitats with deeper light penetration and limiting or mixed nutrient concentrations yielded phytoplankton communities with more desirable characteristics (such as consistently low chlorophyll a and pheophytin concentrations, among others), thus the communities from these habitats were chosen as the desirable or least-impaired phytoplankton communities; less desirable communities came from habitats with low light penetration and higher nutrients. Lacouture et al (2006) expanded on this work, using the reference communities to develop a Phytoplankton Index of Biotic Integrity (P-IBI) for Chesapeake Bay and its tributaries. The index is a management tool to assess phytoplankton community status relative to habitat quality. In a validation exercise, the P-IBI correctly classified 70.0-84.4% of the impaired and least-impaired samples in the calibration dataset.

The Buchanan et al. (2005) paper includes a discussion of the validity of the light classification criteria derived using the Relative Status Method. The authors believe analyses of some of the phytoplankton community parameters support the light classification criteria. Elsewhere, it has been shown that the range of chlorophyll a concentrations as well as chlorophyll cell content (CHL:C) values decrease with increasing Secchi depth to a point, then level off. In the analyses conducted for this paper, the Secchi depths where these relationships leveled off corresponded approximately to the Secchi depth classification criteria from the relative status method. This is a reminder that the Relative Status Methodology can be very useful as a first cut approach and that subsequent insights along the way can possibly provide feedback validation or refinement of the initial results or be, in themselves, a better basis for different reference points. The "relative" approach is at least a good way to get started.

Supplemental information about the relative status measure is available in several appendices:

- Appendix 1 is the initial paper by Ray Alden and Elgin Perry, "Presenting Measurements of Status".
- Appendix 2 contains a SAS[®] computer program that computes relative status using the Cumulative Distribution Function (CDF) methodology, including the last improvements.
- Appendix 3 contains an exchange between Dr. Perry and Mike Lane, a statistician at Old Dominion University and member of DAWG on the subject of the CDF method. It includes a brief step-by-step description of the method and schematic of the assessment process.
- Appendix 4 is an excerpt from a DAWG methods document, "Assumptions and Procedures for Calculating Water Quality Status and Trends in Tidal Waters of the Chesapeake Bay and its Tributaries A cumulative history" which describes data preparation and method implementation for Bay Program partner analysts.

Note: The Monitoring Subcommittee was supplanted by the Monitoring and Analysis Subcommittee (MASC) in November 2001; the Data Analysis Work Group (DAWG) was supplanted by the Tidal Monitoring and Analysis Work Group (TMAW).

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Appendix 1

Presenting Measurements of Status

Prepared for the Chesapeake Bay Program Data Analysis Workgroup

> by R. W. Alden III and E. Perry

1. PURPOSE

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Information on a wide variety of environmental indicators is collected by different components of the Chesapeake Bay monitoring program. Measured environmental indicators range from concentrations of chemicals dissolved in Bay waters, to numbers and kinds of organisms such as submerged aquatic vegetation, phytoplankton, zooplankton, and benthos living in Bay waters or at on the Bay bottom. Different units of measurement are used for different environmental indicators. Environmental indicators are measured at temporal and spatial scales which are appropriate for each indicator. This information is collected by researchers at many different organizations in several political jurisdictions under the umbrella of the Chesapeake Bay Program.

Presenting the information collected by these diverse programs in a form useful to State and Federal Agencies and the public is not an easy task. Results from the different programs should be coherent and comparable. Positive results should be presented as improvements and negative results as declines in Bay water quality and living resources, although scientific tradition would rather present changes with no subjective preference or value judgement.

The guidelines presented here are a step toward achieving this goal. Desirable characteristics of an evaluation and presentation protocol are presented in Section 2. The guidelines are presented in Section 3, and they are discussed and briefly evaluated in Section 4.

These guidelines are a step in a process which commenced at a *Bioindicators Synthesis Workshop* on held October 24-25, 1996. At the workshop, most investigators used similar graphical tools (e.g. maps with "benchmark gradient scales" and "pointers" to indicate current conditions along the scales), but the methods by which the data were scaled from "poor" to "good" varied dramatically. It was decided that a common protocol should be developed, so that the 1997 Nutrient Strategy Re-evaluation effort will have continuity in status presentations and among-indicator comparisions. The authors acknowledge the contributions of workshop participants and Data Analysis Work Group members for aiding in development of the ideas presented here.

2. DESIRED CHARACTERISTICS

Desired characteristics for a status presentation protocol include:

- Indicate status relative to similar areas throughout the Bay,
- Clearly define data used to calculate the benchmark gradient scale and the position of the status condition "pointer",
- The scale should be quantitative, monotonic, (preferably, linear), relatively

simple to calculate, easily understood, and with endpoints that represent the extreme ranges of "poor" and "good" relative conditions of environmental quality. The scale should illustrate absolute as well as relative differences. It should also be relatively robust to the potential effects introduced by extreme outliers and amenable to application for metrics (both multivariate and univariate) of very different initial scales (e.g. IBI scores versus chemical concentrations versus mesozooplankton food availability index values, etc.).

• Allow presentation of threshold values (goals, reference values, criteria, etc) to provide context and perspective.

3. GUIDELINES

3.1 General. These guidelines provide a means to present monitoring data for many different environmental indicators and from different habitats on a 0-100 scale. In addition to the 0-100 score, the scale permits simultaneous display of measured values and accepted "good/bad" thresholds. A value judgement is explicit in the scale because 0 and 100 represent the undesirable and desirable extremes of observed conditions, respectively (Fig. 1).

In order to apply these guidelines to an environmental indicator variable, it is necessary to identify habitats, adjust for seasonality, establish scale endpoints, and then apply the scale to observed measurements and reference values. Each of these steps is described below.

3.2 Habitats. Data are assembled and comparisions are performed separately by habitat. The objective is to compare indicator variable values from similar habitats throughout the Bay. This applies equally to test and benchmark data. For example, tidal freshwater areas of the Potomac River would be compared with tidal freshwater areas of the Patuxent River rather than oligohaline, mesohaline or polyhaline areas of the Potomac River. For many indicator variables, observed and expected values vary by habitat and, therefore, "good" and "bad" endpoints will vary in a similar manner. Benchmark data are used to establish scale endpoints (see below).

For most indicator variables, habitat is defined by salinity regime. Salinity regimes are defined using the Chesapeake Bay Program segmentation scheme, and confirmed or adjusted station by station by comparing the long-term surface and bottom salinity record to regimes defined by the Venice System (Symposium 1958). Additional habitat variables are defined for some indicators. For example, polyhaline benthic communities are different in mud and sand bottoms and habitats are defined accordingly.

3.3 Seasonality: The benchmark data from each station should be averaged on a monthly basis to ensure that an unbalanced design does not bias the data for certain seasons (e.g. monthly water quality collections during the winter versus twice a month during the rest of the year would heavily weight warmer month measurements if this step was omitted). Certain

metrics are only meaningful for specific seasons (e.g. bottom dissolved oxygen for summer months, SAV criteria for growing seasons, food availability index during spawning seasons, etc.). For continuity, the experts assessing each metric in the different political jurisdictions should reach a consensus before finalizing which specific seasons are incorporated into Baywide benchmark data sets.

3.4 Data Reduction: Stations will be characterized by their median or geometric mean values for environmental indicators. To characterize stations, multiple indicator variable measurements should be converted to a single value. The median is appropriate for most physical and chemical indicator variables while the geometric mean is appropriate for most biological variables. The median or geometric mean should be calculated for the appropriate seasonal or annual time period.

3.5 Scale Endpoints: Scale endpoints will be identified from a benchmark data set.

3.5.1 Benchmark Timeframe: Data from 1985 to 1994 will be assembled to create the benchmark scale. This period was selected because it was the first ten year period with measurements for almost all environmental indicator variables. The first 10 years of data collected Bay-wide for the environmental indicator (parameter/metric/index) are assembled to create the benchmark scale. If the status of a metric is to be directly compared to that of another indicator for any given region, the first common 10 years of data should be considered (e.g. if phytoplankton was first collected in 1985, but zooplankton monitoring for the salinity regime was not begun until 1986, then, for continuity, the investigative team synthesizing the "status" report should consider the 1986-1996 data set for both types of data). If less than a ten year time series is available for any given data set, all of the data will be used, and the report footnoted to indicate limitation and non-congruence of these benchmark data.

3.5.2 Pre-defined Endpoints: Good and poor endpoints are inherently defined for some variables, and no further scaling effort is necessary. For example, Indices of Biotic Integrity (IBI) scores are based on scaling variables on a 1-3-5 scale with 1 and 5 representing the endpoints of the data set.

3.5.3 No Pre-defined Endpoints: Many other indicator variables do not have pre-defined endpoints. Therefore, the endpoints must be defined.

Good and Poor end-points are defined for each environmental indicator variable as follows:

- (A) <u>Assemble a Benchmark Data Set of Station Medians</u>: The annual (or annual seasonal) medians or geometric means for each station are calculated and assembled into a "benchmark data set" for each habitat.
- (B) <u>Identify Endpoints:</u> The 5th percentile and the 95th percentile values of the benchmark data are the endpoints of the scale.

(C) Identify Polarity: The investigator will determine which ends of the scale represents the "good" and which end the "poor" extreme. Polarity depends on the nature of the environmental indicator variable (parameter/metric/index) being assessed. For example, the 5th percentile for bottom dissolved oxygen concentrations would be considered "poor", while the 5th percentile for nutrients would be considered "good." Best professional judgement should be used in assessing whether these centile values represent meaningful endpoints and polarity assignment should be by consensus of Baywide and outside experts and supported by information from status reports.

3.6.1 Applying the Scale: For any value "X" to be displayed on the benchmark gradient scale, the generic scaling formula is as follows:

 $X^* = \frac{(X - "poor" endpoint)}{("good" endpoint - "poor" endpoint)} x 100$

where X^* is a scaled value ranging from 0 ("poor") to 100 ("good"). If the values happen to fall below 0 or above 100, they are set to the appropriate extreme value. If values beyond the endpoints are a frequent occurrence, the endpoints should re-evaluated. The following describes how to calculate scaled data for the two possible types of data sets.

3.6.2 Low values are "poor": If Low Values (e.g. 5th percentile) represent "poor" conditions (e.g. secchi readings, dissolved oxygen concentrations, mesozooplankton food availability index values, etc), the general equation is as follows:

$$X^* = ((X - 5^{th} \text{ percentile})/(95^{th} \text{ percentile} - 5^{th} \text{ percentile})) \times 100.$$

Operationally, the data would be processed as follows:

- (1) Subtract the 5th percentile value from all values to be located on the benchmark gradient scale.
- (2) Divide the resulting values by the range between the endpoints (95th percentile 5th percentile) and multiply by 100, so that the scale is now expressed as a percentage scale: 0 = poorest conditions generally observed Bay-wide for the type of habitat; and 100 = best conditions generally observed Bay-wide for the type of habitat.

Example: The 10-year, Bay-wide benchmark summer bottom dissolved oxygen data (medians of June to September monthly averages for each station for each year) for the tidal fresh water regime has a 5^{th} percentile value of 2.47 mg/l and a 95^{th} percentile of 8.41 mg/l. Any value X^{*} to be displayed on the benchmark gradient scale would be calculated by the following equation:

$$X^* = ((X - 2.47 \text{ mg/l})/(8.41 \text{ mg/l} - 2.47 \text{ mg/l})) \times 100.$$

Using this formula, the median oxygen concentration at station TF3.3 of 6.89 mg/l would be scaled as

$$100 \ge (6.89 - 2.47) / (8.41 - 2.47) = 74.$$

Note present both origina and univer scale shown	Benchmarks (10 year) 95th percentile = 8. 5th percentile = 2. D.O. goal = 5. Scaling Calculatio	.41 Median = 6.89 .47 .00 n: $x^* = \frac{(6.89 - 2.47)}{(6.89 - 2.47)} \times 100$		that, in ations, the l scale the sal 0-100 can be , as well
as, bench such D.O. (Figur	Poor	$\begin{array}{c} \text{DO Goal} \\ \hline \\ \text{5.0} \end{array} \\ \begin{array}{c} \text{(8.41 - 2.47)} \\ \text{(8.41 - 2.47)} \\ \text{(8.41 - 2.47)} \\ \hline \\ \ \\ \text{(8.41 - 2.47)} \\ \hline \\ \ \\ \ \\ \ \ \ \ \ \ \ \ \ \ \ \ \$	Good 100 	other marks as the goals e 1).

Figure 1. Example presentation of status for bottom dissolved oxygen at Station TF3.3 in the

Rappahannock River, Virginia. Benchmarks for this example were calculated using only data collected from the Departmental of Environmental Quality's tributary monitoring stations.

3.6.3 High values are "poor": If High Values (e.g. 95th percentile) represent "**poor**" conditions (e.g. nutrient concentrations, chlorophyll concentrations, TSS concentrations, etc) the general equation is as follows:

$$X^* = ((X - 95^{th} \text{ percentile})/(5^{th} \text{ percentile} - 95^{th} \text{ percentile})) \times 100.$$

Operationally, the data would be processed as follows:

- (1) Take the difference between the 95th percentile and all values to be located on the benchmark gradient scale (in most cases, this value should be negative).
- (2) Divide the resulting values by the range between the endpoints $(5^{th} \text{ percentile} 95^{th} \text{ percentile}; this value should be negative, so in most cases the resulting quotient should be positive) and multiply by 100, so that the scale is now expressed as a percentage scale: <math>0 = \text{ poorest conditions generally observed Baywide for the type of habitat; and 100 = best conditions generally observed Baywide for the type of habitat.$

Example: The 10-year, Bay-wide benchmark median data for chlorophyll concentrations during the growing season in the oligohaline regime has a 5th percentile value of 10.0 μ g/l and a 95th percentile of 90.0 μ g/l. Any value X^{*} to be displayed on the benchmark gradient scale would be calculated by the following equation:

 $X^* = ((X - 90.0\mu g/l)/(10.0\mu g/l - 90.0\mu g/l)) \times 100.$

3.6.4 Below Detection Limits: When values in the status data set are "below detection limits" (BDL), all such values are be set to a value of $\frac{1}{2}$ of the detection limits. In general, this convention does not affect estimates of the position of the status pointer unless more than 50% of the 3-year data set (see Section 3.7) are BDL. However, calculation of the benchmark gradient scales are affected (due to the calculation of the 5th percentile), so this convention is important for the initial calculations of the scales. A detailed assessment of this issue is presented in the Appendix.

3.6.4 Segments Containing Sites that Shift Between Salinity Regimes: Since both the calculation of the benchmark gradient scales and the status pointer are specific for a given salinity regime, those segments containing sites that shift from one salinity regime to another

over the time require special conventions:

(1) For water quality data:

- (a) Salinity data from each sample in the long-term data sets are used to identify the appropriate salinity category of each observation prior to calculation of the benchmark scale for each salinity regime, according to the methods described previously.
- (b) Salinity data from each sample in the status data set are used to categorize the observation into its appropriate salinity regime, so that it can be compared to the appropriate benchmark scale in calculating its X* value on the 0-100 benchmark scale. The position of the status pointer is determined by calculating the median of all X* values from the segment. For presentation purposes, the overall salinity regime of the segment is identified as being the long-term salinity regime determined in the revised CBP Segmentation Scheme. If separate status assessments are to be done for surface and bottom layers, this process would be based upon the salinities of the surface and bottom samples.

(2) For Living Resource Data:

- (a) Salinity data from each sample in the long-term data sets are used to identify the appropriate salinity category of each observation prior to calculation of the universal benchmark scales by salinity regime. These salinity-specific categories are used to determine the appropriate IBI thresholds, for biotic communities for which IBI systems have been developed, or for calculating the universal benchmark scales by centiles for each salinity regime, as described previously and in 3.6.4.(2)(b).
- (b) Salinity data from each sample in the status data set are used to categorize each observation into its appropriate salinity regime, so that it can be compared to the appropriate benchmark scale. For biological data with fully developed IBI systems, the average IBI score for each sample is calculated by comparing its values for the various IBI metrics to the reference thresholds for the appropriate salinity regime. The IBI scores for all samples collected in the segment during the status period are averaged (arithmetic mean) to determine the position of the status pointer on the benchmark scale.

For biological data without an IBI system, it was decided by consensus of investigators that status pointer locations should be based upon 3-year geometric means rather than the medians used for water quality. Thus, the calculation of status requires a slightly different approach:

- Transform all data by logarithmic transform first (either log(x) or log(x+c), where x is data and c is constant).
- (2) Set the salinity specific scaling parameters for the universal scale by finding 5th and 95th centiles by salinity zone for the log metric.
- (3) Scale each log transformed datum against the appropriate salinity zone scaling parameters based on the sample specific salinity.
- (4) Take a arithmetic average of the resultant scaled data by segment for location of the status pointer on the benchmark scale.

3.7 Current Status: The status data set for any indicator/region combination should be assembled from the most recent three years of data, unless there is justification to the contrary. Deviations, and their justification, should be indicated in the status presentation.

3.8 Supplementary Information: A separate scale graphic will be prepared for each habitat and the status of every geographic region in that habitat for which data are available will be represented by a pointer representing its scaled median. Other reference values which may be scaled in a similar manner and placed upon the benchmark gradient scale to provide context include:

- a) Threshold values, goals, criteria, etc.
- b) Median values for the "starting conditions", such as the 1985-1986 median.
- c) Measures of uncertainty confidence limits around the median produced from the three-year centiles or calculated by other means (e.g. "Bootstrap" simulations).
- d) Subdivisions of the scale based upon "best professional judgement" interpretation of ecologically significant breakpoints in the raw benchmark median data set (e.g. values separating "good" from "fair"; or "stressed" from "poor"; etc.). Such breakpoints could be delineated initially by certain centile ranges in the benchmark median data set, but these values should be evaluated by experts for ecological relevance/significance, and, if necessary, redefined (see below, discussion of concerns with centiles).

4. DISCUSSION

4.1 Needs Met. The proposed protocol has all the desired characteristics:

- Provides a summary of the status of a metric/region combination relative to all other similar habitats elsewhere in the Bay for which data are available. Since the scaling method is absolute, apparent contradictions such as an improving trend that results in decreased relative condition will be avoided. The system facilitates presentation of data throughout the Bay, and neatly compares different environmental indicators in a single area of the Bay.
- The definitions for a 10-year "benchmark data set" and a 3-year "status data set" were provided by a consensus of investigators at the *Bioindicators Synthesis Workshop*. Although the time frame should be consistent throughout all status evaluations the specifics can be changed by consensus (e.g. by the Data Analysis Workgroup).
- The status scale is monotonic and based upon a percentage scale (a concept that most people understand) that ranges from 0 ("poor") to 100 ("good") regardless of the initial scale of the metric being assessed. Furthermore, the scaling functions (two variations of a simple mathematical relationship) can be readily programed on the computer or used in hand calculations. If discussion is enhanced by relating a metric to the original units, the original units can (and should) be presented on graphical axes by a second set of labels.
- The use of medians or geometric means, both in the benchmark and in the status data sets tends to reduce the effects of extreme outliers (as compared to the use of arithmetic means).
- The scaling process can be applied to a variety of reference values to indicate the significance of the status condition.

4.2 Improvements: The proposed process builds on previous efforts and has a number of specific advantages over previous presentation methods. Synopses and brief contrasts follow:

• Use of Centiles to Directly Scale Benchmark Conditions: Centiles provide equal divisions of the benchmark data sets into subdivisions (e.g. quartiles or 20-percentiles). Unfortunately, the distribution of most environmental data sets are such that the final scale usually deviates dramatically from a linear relation to the original data. Thus, a modest change along the scale near the middle of the benchmark gradient may represent a very small change in conditions, as measured by the original units, but a similar change near the extremes of the gradient may represent quite large absolute changes (a situation exacerbated by skewed distributions typically found for environmental data sets). Most people viewing what appears to be a linear presentation would not appreciate the nonlinear nature of the scale, particularly if they attempt directly to compare the status of regions with "pointers" (medians) located in different positions along the gradient; or they watch changes in status along the gradient scale slow dramatically from year to year as the ends of the gradient are approached. The proposed approach presents a more directly linear relationship: when median values are separated by any given amount in original units of measurement, the status pointers are separated by a proportional amount along the scale (relative to the "poor" and "good" endpoints); and when the median of a metric/region changes from one reporting period to the next, the pointer moves along the scale in a proportionate manner, regardless of where it happens to be on the scale.

The investigators using centiles in the past to provide the status scale have taken two slightly different approaches:

Use Bay-wide Status Data Sets as Benchmark: By using the most recent three year data sets from similar habitats throughout the Bay to develop the Benchmark scale, the status of any given region is presented relative to all others. On the surface, this may appear advantageous, since it provides investigators and managers with a feel for the relative condition of a region compared to all other similar habitats in the Bay. However, the consistent use of only the most recent 3-years of data provides a "moving target" that should not have specific endpoints of environmental quality assigned (i.e. there will always be a bottom centile and a top centile, regardless of absolute conditions, so the use of classifications such as "poor" or "good" become meaningless). In addition, the use of only the most recent three years may not provide a broad enough range of conditions to build an adequate benchmark data set (e.g. the most recent three years may not have incorporated a truly "good" set of conditions due to natural factors such as weather; or a habitat type may not have a truly "poor" endpoint if it is improving Bay-wide). The proposed approach uses a 10-year data set in an attempt to incorporate a range of environmental conditions from "poor" to "good".

If investigators wish to continue with the centile approach, it is easily superimposed on the scale proposed here by adding tic marks at the desired centiles along the scale. This presentation will have the added advantage that the reader will become aware of non-linearities such as will result if the 0-20 centile interval is larger than the 40-60 centile interval. The reader may also assess each datum for proximity to the centile boundaries.

■ Use of the 1985-1986 Data Base as the Benchmark: By consistently

using the baseline years of 1985 and 1986 to construct the benchmark data set, investigators develop a constant scale onto which relative status positions can be located (i.e. the "moving target" aspect of the previous approach is avoided). Unfortunately, the potentially limited range of conditions found during the first two years of the Chesapeake Bay Program may provide a misleading status scale (e.g. all environmental conditions in any given habitat type may have been of relatively lower quality than they are today, so the "poor" to "good" scale may actually be from "poor" to "less poor, but not really good"). Again, the proposed scaling approach not only uses a constant benchmark data set to avoid producing the "moving target" scale, but it incorporates a data set of sufficient size to ensure that both "poor" and "good" endpoints are incorporated.

- <u>Use of Trends to Determine Relative Status</u>: Some of the investigators examined trend analyses to determine whether the status of a metric/region had significantly improved or degraded relative to the status during previous reporting period. This sort of approach tends to confuse the audience as to the differences between status and long-term trends and does not provide a scale for relative comparisons (e.g. comparisons relative to the benchmark conditions; comparisons between regions; comparisons to thresholds, goals or criteria, etc.). The proposed approach does provide a meaningful scale upon which the status and reference points (including, if desired, status of the metric/region at the time of the previous report) can be located.
- Use of Thresholds or Criteria to Determine Status: Some investigators use the attainment/nonattainment of a threshold, criterion, or goal as the indicator of status. While this provides a simple visual summary (which probably should be included in any status report), it does not indicate "how bad is bad" or "how good is good" relative to the threshold/criterion/goal or to similar habitats throughout the Bay. The proposed scaling approach addresses this issue, and would, therefore, provide more quantitative, complementary information to the status presentation.

Reference:

Symposium on the Classification of Brackish Waters. 1958. The Venice System for the classification of marine waters according to salinity. *Oikos* 9(2):311-312.

APPENDIX

Calculation of Status for Water Quality Data Sets That Include Data Below Detection Limits

The Issue:

To create a baywide benchmark data set for status calculations, it is necessary to address the treatment of values below the analytical limit of detection (BDLs). Detection limits have changed over the period of the Monitoring Program. The sensitivity of sample analysis has improved over time, thus detection limits in the earlier years are generally higher than in more recent years. Also, at any given time, there are differences in the detection limits between labs and, consequently, between states. In past analyses, which generally focused on status and trends at individual stations or stations sampled and analyzed by the same agency, all BDLs within the period of analysis were set to the "worst case", i.e., to the highest detection limit within the period of analysis. However, when the entire data record for all Monitoring Program participants are pooled--as they are for calculation of baywide benchmarks-- applying the worst case detection limit across the board results in large percentages of censored data, reducing the range of the summary statistics and forfeiting the information gains of the improved laboratory procedures.

Proposed Solutions:

- First, the data set could be censored to the worst case detection limit value if the percentage of censored data was not high enough (less than 50%) to skew calculation of the median, which is a principal metric in determining status.
- Second, the BDLs could be used as currently represented in the database. (As labcensored data, BDLs are set to the value of the detection limit in use by the lab at the time of sample analysis).
- A proposal to drop earlier data to improve (lower) the worst case detection limits was explored, but found unsatisfactory due to the large amount (more than one or two years) of information that would be lost.

The Analysis:

To determine how much of the data would be censored by using the worst case detection limit, a simple counting analysis was conducted on the entire 1985-1995 data set, including both Maryland and Virginia mainstem and tributary stations (Table 1). In general, for most of the parameters of interest (TKNW, TKNF, DOC, TOC, SI, NO₂, TP, TSS) the method of censoring

the data to the worst case detection limit does not impact the calculation of the status benchmark data set. However, for NO_{23} , NH_4 , PO_4 and TDP there is a much larger, unacceptable impact on the calculation of status, and by censoring the data to the worst case detection limit much of the information will be lost.

The Decision:

The worst case detection limit method will censor more of the data for NO_{23} , NH_4 , PO_4 and TDP than is acceptable for the purpose of calculating status baywide. For these parameters, the labcensored database values should be used for analysis of status. For the remaining parameters, censoring at the worst case detection limit is acceptable, but for the sake of consistency across the analyses, the lab-censored data from the database should be used to calculate status for these parameters as well.

The Method For Creating a Benchmark Data Set:

The source data for each parameter will be the data as provided by the laboratories and available in the database. BDLs (any lab-censored data) should first be divided in half and then included in the benchmark data set. When a parameter is a calculated variable (e.g. $DIN = NO_{23} + NH_4$), the individual components (i.e. NO_{23} and/or NH_4) that are detection limited should be divided in half *before* the variable is calculated.

Table 1. Detection-limited data in the 1985-1995 data sets, shown as the total number of reported measurements in each category (n) and as a percentage of total (%). The category "Additional data censored to worst case" includes the number and percentage of data that are not detection-limited due to sample analysis but that would be censored under the worst case detection limit method. Totals of both categories are given as "All data below worst case".

Parameter		All Mary	All Maryland Data		All Virginia Data		TOTALS	
		n	%	n	%	n	%	
NO ₂₃	Total data set	41552		24837		66389		
	BDLs in lab-censored data	2388	6	5118	21	7506	11	
	Additional data censored to worst case	10183	25	7166	29	17349	28	
	All data below worst case	12577	30	12284	49	24861	37	
NH	Total data set	41380		26278		676658	i	
	BDLs in lab-censored data	3520	9	8615	33	12135	18	
	Additional data censored to worst case	17439	42	9284	35	26723	39	
	All data below worst case	20959	51	17899	68	28858	57	
PO₄	Total data set	41287		26923		68210		
	BDLs in lab-censored data	4431	11	7311	27	11742	17	
	Additional data censored to worst case	20700	50	8784	33	29484	43	
	All data below worst case	25131	61	16095	60	41226	60	
TDP	Total data set	32311		23816		56127	1	
	BDLs in lab-censored data	3254	10	2936	12	6190	11	
	Additional data censored to worst case	8387	26	7076	30	15463	28	
	All data below worst case	11641	36	10012	42	21653	39	
TKNW	Total data set	22514		16151		38665		
	BDLs in lab-censored data	57	0	50	0	107	0	
	Additional data censored to worst case	324	1	433	3	757	2	
	All data below worst case	381	2	483	3	864	2	
TKNF	Total data set	21969		2184		24153		
	BDLs in lab-censored data	251	1	4	0	255	1	
	Additional data censored to worst case	1543	7	49	2	1592	7	
	All data below worst case	1794	8	53	2	1847	8	

Parameter		All Maryl	All Maryland Data		All Virginia Data		TOTALS	
		n	%	n	%	n	%	
TOC	Total data set	41110		0		41110		
	BDLs in lab-censored data	42	0			42	0	
	Additional data censored to worst case	429	1			429	1	
	All data below worst case	471	1			471	1	
DOC	Total data set	38458		0		34458		
	BDLs in lab-censored data	86	0			86	0	
	Additional data censored to worst case	162	0			162	0	
	All data below worst case	248	1			248	1	
NO2	Total data set	41246		27051		68297		
	BDLs in lab-censored data	1143	3	3411	13	4554	7	
	Additional data censored to worst case	7117	17	5239	19	12356	18	
	All data below worst case	8260	20	8650	32	16910	25	
ТР	Total data set	41049		26236		67285		
	BDLs in lab-censored data	269	1	57	0	326	0	
	Additional data censored to worst case	3635	9	3104	12	6739	10	
	All data below worst case	3904	10	3161	12	7085	11	
SI	Total data set	41421		23592		65013		
	BDLs in lab-censored data	1468	4	1514	6	2982	5	
	Additional data censored to worst case	2085	5	3526	15	5611	9	
	All data below worst case	3553	9	5040	21	8593	13	
TSS	Total data sct	45038		23195		68233		
	BDLs in lab-censored data	1020	2	732	3	1752	3	
	Additional data censored to worst case	7768	17	2143	9	9911	15	
	All data below worst case	8788	20	2875	12	11663	17	

.

Appendix 2

SAS Language Computer Program (STATMAC.SAS) to Compute Relative Status Indicator

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statmac(4) .SAS A macro to compute status based on logit centiles of the benchmark data set. programmer: Elgin S. Perry, Ph. D. date: 4/99 Modified by Marcia Olson, 5/99, and again 6/2000 to provide status reports for stations and segments. Note: her modifications are NOT to the fundamental method of determinng Relative Status. 2000 Kings Landing Rd. address: Huntingtown, Md. 20639 (410) 535-2949 voice phone: fax/modem: (410)257-2937 (by arrangement on voice line) email: EPERRY@chesapeake.net

Documentation --

The user must supply a benchmark data set and a monitoring data set. The macro assumes that both SEGMENT and STATION identifiers are in both data sets, and the user must indicate whether status is to be scored by segment or by station. The user must indicate the period within that monitoring data set for which status is to be evaluated, a variable defining salinity zone, a depth zone variable, which can be any set of categories, a parameter to evaluate (name must be the same in benchmark and monitoring data), "GOOD" or "BAD" depending on whether high values of the parameter are rated as good or bad, a filename for an external results file, and the units of the untransformed parameter. If no external file is to be created a dummy name should be entered. The variable for defining salinity zone can be based on fixed station or segment zones or sample salinity. It must be defined by the user in both the monitoring and the benchmark data before calling this macro, and the variable name for salinity zone must be the same in both data sets. There could be an option for using the salinity zone implied in the segment name if other salinity designation is not available.

The macro assumes that benchmark and status data sets are similarly summarized prior to input. As written, the macro assumes that data are summarized by station year month and depth-zone, and median calculations are made with all data pooled by segment or station and depth-zone without further summarization. If individual sample values are included in the data sets, then the additional step to calculate median values by month (to improve the seasonal balance of the data) needs to be added to the code, before the median score is calculated.

On completion, the macro can produce several kinds of output:

- a print file for data checking with the values of intermediate variables, cut points and status, and the distribution within status categories,
- 2) a formatted formal results table with a limited number of variables and status, and
- 3) a comma-delimited ascii file of results.

The user may select any or all them by adding or removing the asterisk preceding the macro call.

STATSTAT - is a final data set that has a record for each station or segment with the variables: SEGMENT, STATION (if selected), &layvar N, MEDVALU CUT1, CUT2, MEDSCORE, STATUS.

MEDVALU - is the median value of the original, untransformed parameter

```
MEDSCORE - is the median score for the status period
            - is the 1/3 centile=poor-fair cutpoint if a high score for
   CUT1
             param is good, or fair-good, if a high score is bad.
   CUT2
            - is the 2/3 centile=fair-good cutpoint if a high score for
             param is good, or poor-fair, if a high score is bad.
   STATUS
          - is the status rating
Arguments for the macro STATUS
        (segsta, bmdata, mondata, statper, salvar, layvar, param, gob, filenam).
   &segsta is either SEGMENT or STATION, Upper Case sensitive
   &bmdata is the input benchmark data set
   &mondata is the monitoring data set
   &statper is a boolean expression that defines the status period
            eg ('01jan96'd <= date <= '31dec98')</pre>
   &salvar is the variable name for salinity regimes
   &layvar is the variable name for layers
   &param is the parameter being evaluated
           is a variable that indicates whether high values of the
   &gob
           parameter are Good Or Bad. Enter good or bad.
   &filenam is the name of an output text file.
          is the units of measure of the original parameter, for example
   &unit.
            ug/L for CHLA, mg/L for TN, and m for Secchi depth.
Search for "Edit" to find the lines of code which require User input.
End of documentation ;
                        */
options CENTER linesize = 78 pagesize = 55 replace ;
option symbolgen MPRINT;
    *Option to Print out raw information for internal use;
%MACRO PRNTRAW (data);
 PROC SORT DATA=&data OUT=PRNT; BY descending &layvar;
 PROC FREQ DATA=PRNT; by descending &layvar;
   TITLE "Distribution of categories for &param by &bycat and layer";
   TITLE2 "Assessment period &statper, Season = &seas";
   TABLES STATUS;
   RUN:
    * PROC PRINT DATA=&data;
    * TITLE "Statistics for &param by &bycat" ;
    * VAR SEGMENT &bycat &layvar N B AN F MEDSCORE CUT1 CUT2 STATUS;
%MEND;
%MACRO STAT; ** A submacro of the macro STEP1;
    * find median score by segment or station, depending on choice;
 PROC SORT DATA=SCORE;
   BY sortord &bycat &layvar;
 PROC means DATA=SCORE NOPRINT;
   BY sortord &bycat &layvar;
   ID SEGMENT;
   VAR LCDF;
   OUTPUT OUT=STATSTAT MEDIAN = MEDSCORE N = N;
 RUN;
 DATA STATSTAT; SET STATSTAT;
        BY sortord &bycat &layvar;
        IF N=0 THEN DELETE;
     * compute F-statistic for segments or stations to measure dependence
 within station;
 PROC SORT DATA=BENCHMARK; BY &layvar;
```

```
PROC GLM OUTSTAT = FSTAT DATA=BENCHMARK NOPRINT;
   BY &layvar;
   CLASS &salvar &bycat;
   MODEL LCDF = &salvar &bycat(&salvar);
     *proc print;
 RUN;
     * subset to station F-statistic and compute exponent to use in adjusting
   sample size as a function of F;
 DATA FSTAT (KEEP = &layvar f b);
   SET FSTAT;
   PUT "&bycat(&salvar.)";
   AGGROUP="&bycat";
   IF SOURCE = "&bycat(&SALVAR.)" AND TYPE = 'SS1';
   IF \overline{A}GGROUP = 'SEGMENT' THEN b = 0.01 + 0.001*f;
   ELSE IF AGGROUP='STATION' THEN b = 0.02 + 0.003 * f;
  RUN;
     *PROC PRINT DATA=FSTAT;
     *TITLE "&param";
       * Compute 33% confidence intervals for medians by station/segment;
   PROC SORT DATA=STATSTAT; BY &layvar;
   DATA STATSTAT;
   MERGE STATSTAT (IN=A) FSTAT;
   BY &layvar;
   IF A;
   M = (N+1)/2;
   AN = N / (N - ((N-1)/F^{**B}));
   IF F < 1.5 THEN AN = N;
   AM = (AN + 1)/2;
   MEDVAR = 1/(4*(AN+2));
   C1 = 1/3;
   C2 = 2/3;
   CUT1 = BETAINV(C1, AM, AM);
   CUT2 = BETAINV(C2,AM,AM);
   %IF (&gob=&good) %then %do;
     IF MEDSCORE < CUT1 THEN STATUS = '1POOR';
     IF CUT1 <= MEDSCORE < CUT2 THEN STATUS = '2FAIR';
                               THEN STATUS = '3GOOD';
     IF CUT2 <= MEDSCORE
   %END;
    %IF (&gob=&bad) %THEN %DO;
     IF MEDSCORE < CUT1 THEN STATUS = '1GOOD';
     IF CUT1 <= MEDSCORE < CUT2 THEN STATUS = '2FAIR';
     IF CUT2 <= MEDSCORE
                              THEN STATUS = '3POOR';
   %END;
 PROC SORT; BY SORTORD &bycat DESCENDING &layvar;
 RUN;
%MEND; /* of STAT macro; */
%MACRO STEP1(bmdata,mondata); ** A submacro of macro STATUS;
 %LET GOB = %UPCASE(&gob);
 %LET SALVAR = %UPCASE(&salvar);
 %LET GOOD = GOOD;
 %LET BAD = BAD;
 PROC SORT DATA=&mondata OUT=STATUS;
    BY &salvar &layvar;
   * get mean and variance for each salinity zone x depth stratum;
 PROC SORT DATA=&bmdata;
```

```
BY &salvar &layvar;
PROC MEANS NOPRINT MEAN VAR DATA=&bmdata;
  BY &salvar &layvar;
  VAR &param;
  OUTPUT OUT=MNVAR MEAN(&param) = MNPARM VAR(&param) = VARPARM;
RUN;
DATA BENCHMARK;
  MERGE &bmdata MNVAR;
  BY &salvar &layvar;
  IF &param NE .;
  BETA = SQRT (VARPARM*3/(3.1415*3.1415));
  LCDF = 1/(1+EXP(-(&param-MNPARM)/BETA));
   * merge mnvar with status data and compute scores;
DATA SCORE;
  MERGE STATUS MNVAR;
  BY &salvar &layvar;
  IF &param NE .;
  BETA = SQRT (VARPARM*3/(3.1415*3.1415));
  LCDF = 1/(1+EXP(-(&param-MNPARM)/BETA));
RUN;
%STAT;
%MEND; /* of STEP1 macro ; */
%MACRO FILTER ;
SEGMENT=SEGMNT98;
IF &param. GT . ;
IF SEASON="&seas";
PARNAME="&param";
IF PARNAME='SECCHI' AND &param LT 0.001 THEN DELETE;
IF PARNAME='DO' AND LAYER='S' THEN DELETE; ;
IF SEASON=:'SAV' AND LAYER='B' THEN DELETE;
IF PARNAME='CHLA' THEN &param=&param + 0.05;
&param
          = log(&param);
AGGROUP = "&bycat";
%MEND;
%MACRO STATUS(bycat,bmdata,mondata,statper,seas,salvar,layvar,param,
             gob,filenam,unit);
   *Baseline data set;
DATA benchmark;
LENGTH PARNAME $8;
SET IN.&bmdata
     (KEEP=SORTORD SEGMNT98 STATION &layvar &param YEAR MONTH SEASON &salvar);
       IF SEGMNT98='ELIMH' THEN DO;
            SEGMNT98='ELIPH';
            SORTORD=77;
            &SALVAR='PH';
       END;
       %FILTER;
RUN;
     *Current data to be assessed;
DATA mondata;
LENGTH PARNAME $8;
SET IN.&mondata
     (KEEP=SORTORD SEGMNT98 STATION &layvar &param YEAR MONTH SEASON SALREGIM);
       &SALVAR=SALREGIM;
```

```
IF &statper;
      MEDVALU=&param;
      %FILTER;
 RUN;
    *Call the main macro;
  %STEP1(benchmark,mondata);
    *Calculate the median of the original parameter;
 PROC SORT DATA=mondata OUT=MEDFILE;
        BY SORTORD &bycat descending &layvar YEAR MONTH;
    *this step is unnecessary, but harmless, if data are already aggregated
 to station/layer monthly means;
 PROC MEANS NOPRINT DATA=MEDFILE;
        BY SORTORD &bycat descending &layvar YEAR MONTH;
        ID SEASON SEGMENT AGGROUP PARNAME &salvar;
        VAR MEDVALU;
        OUTPUT OUT=MEDFILE MEDIAN=MEDVALU;
 RUN:
 PROC MEANS NOPRINT;
        BY SORTORD &bycat descending &layvar;
        ID SEASON SEGMENT AGGROUP PARNAME &salvar;
        VAR MEDVALU;
        OUTPUT OUT=MEDFILE MEDIAN=MEDVALU;
 RUN;
 *Merge the median parameter value with the status statistics;
 PROC SORT DATA=STATSTAT; BY SORTORD &bycat descending &layvar;
 DATA STATSTAT;
        MERGE STATSTAT (IN=A) MEDFILE;
        BY SORTORD & bycat descending & layvar;
                IF A;
 RUN;
 *Preparing for printing out data;
 PROC SORT DATA=STATSTAT; BY &salvar;
 PROC SORT; BY SORTORD & bycat descending & layvar;
 %PRNTRAW(statstat); *Prints raw data;
%MEND;
    /* EDIT the macro call statements with these arguments:
 (bycat, bmdata, mondata, statper, salvar, layvar, param, qob, filenam, unit).
 Note that values for bycat and layvar are case sensitive - need to be
 upper case; */
%MACRO SEGORSTA (bycat, segsta);
       /\,\star\, These statements tell where to put the spreadsheet (.csv) and
          printable output files (.lis) and the statmac4.log file; */
FILENAME NEWDAT
"\\nas\Users\molson\alpha\home\work\status\&yr\&tmpdir\ST&outfile._&segsta..csv";
FILENAME NEWLIS
"\\nas\Users\molson\alpha\home\work\status\&yr\&tmpdir\ST&outfile. &segsta..lis";
FILENAME LOGOUT
"\\nas\Users\molson\alpha\home\work\status\&yr\&tmpdir\statmac4.log";
PROC PRINTTO NEW LOG=LOGOUT PRINT=NEWLIS;
RUN;
```

```
DATA _NULL_;
               /* Star this out if not invoking the MAKEFILE macro for the
                   web-format, spreadsheet file, below; */
FILE NEWDAT;
PUT
"*&bycat,STRTY,ENDY, PARAM, SEASON, LAYER, DATATYPE, STATUSTYPE, VALUE, SCORE,
STATUS, VERSION, CALC-AG, SOURCE" ;
RUN;
        /* TN ; */
%status (&bycat,BNCHSEAS,&dtfile,&strtyr <= YEAR <= &endyr,ANNUAL,&segsta.regim,</pre>
       LAYER, TN, BAD, TNSEANN, mg/L);
 %MEND;
%MACRO PERFILE (dtfile,yr,strtyr,endyr,tmpdir,outfile,calcag,colag);
     %SEGORSTA (SEGMENT, seg);
      PROC PRINTTO;
      RUN;
      %SEGORSTA (STATION, sta);
      PROC PRINTTO;
      RUN;
      QUIT;
%MEND;
      /* Program execution starts here ; */
```

LIBNAME IN '\\nas\Users\molson\alpha\home\work\status';

%perfile (BAS0204,04,2002,2004,BAY,0204BAY,CBPO,MD-VA);

Appendix 3

An exchange on the subject of the CDF scoring method, including a schematic of the status assessment method The following is an exchange between Mike F. Lane, Old Dominion University, and Dr. Elgin S. Perry about the Relative Status methodology. [Date Unknown]

MFL: If the LCDF is essentially a frequency distribution, why couldn't the test data set (data set for which status is to be determined) be compared to a cumulative frequency distribution curve (as opposed to a function) plotted from the benchmark data?

ESP: In theory, scoring the test data against the empirical distribution function of the benchmark data is a possibility and it is one that I have considered. However, the computational aspect of this seems fairly complicated and difficult to program. That is if your test datum that you are scoring falls between two observations in the benchmark data, you would have to somehow interpolate to get the corresponding score. Should this interpolation simply be linear point to point or some kind of smooth of the plotted distribution? To me it seemed simpler to fit a distribution so that scores could be computed from an algebraic expression. Don't let my choice for simplicity discourage you from pursuing this more nonparametric alternative.

MFL: Is it because the distribution function is a continuous function as opposed to a frequency distribution curve developed from discrete intervals? We assume that the distribution function provides an estimate of what the 33rd and 67th percentiles would be (for a given salinity regime/parameter combination), whether or not they are present in the benchmark data set. Is this the case?

ESP: Yes, basically that's it.

MFL: Another issue which is not entirely clear is whether or not the test median value is transformed to a Beta value or whether or not the benchmark Beta values are back transformed to concentrations for the cutoff comparisons. Can you tell which is correct?

ESP: The theory roughly goes like this: The first step is to identify the distribution of the raw data. I have universally assumed log-normal. Note that for some parameters, e.g. DO, Secchi and temperature, this is not a good assumption. The second step is to transform the data through its distribution function onto a (0, 1) scale. This step is called the Probability Integral Transform and is discussed in most Math-Stat books. If the identified distribution is correct (or close to it) then the Probability Integral Transformed data follow a Uniform (0, 1) distribution. The median of n observations taken from a uniform distribution follows a Beta distribution with parameters (m, m) where m = (n+1)/2 and n is the number of observations. We then use the percentage points of the appropriate Beta distribution to get the 1/3's that form the categories for the median score.

MFL: Finally, do you know if there are any citable references that describe the relative status determination process?

ESP: I don't know if there is a reference that chains these theorems together like this. That may be my own creation, but I've not researched this enough to know. The individual theorems are all in:

Roussas, George G. (1973), <u>A First Course in Mathematical Statistics</u>. Addison-Wesley, Reading, Mass.

MFL: Our current explanation of the process is provided below. Is it accurate? Also take a look at the figure below and let us know if it accurate as well.

"Relative status scores are determined by comparing median values of the segment, parameter and time period of interest against values derived from a benchmark data set consisting of the first ten years of water quality data in Chesapeake Bay. A logistic cumulative frequency distribution curve was developed for each parameter within each of four salinity regimes: tidal freshwater, oligohaline, mesohaline and polyhaline using data from the benchmark data set. The logistic cumulative frequency distribution curve was used to generate a *Uniform* probability density distribution which ranged from 0 to 1 such that higher values in the distribution represented poorer or less desirable water quality conditions. Transformed median values from the test data are distributed according to a *Beta distribution and* were assigned a score based on their location along the Beta density distribution. If high values of a parameter are considered to be indicative of poor water quality (nutrients, chlorophyll a, and suspended solids) then median values with a corresponding Beta value greater than the 67th percentile of the Beta density distribution (approximately) are classified as poor. Median values less than the 33rd percentile (approximately) are classified as good and all values between these two cutoffs are considered fair. If high values of a parameter are considered to be indicative of good water quality (Secchi depth) then median values with a corresponding Beta value less than the 33th percentile (approximately) are classified as poor. Median values greater than the 67th percentile (approximately) are classified as good and all values between these two cutoffs are considered fair. See the figure below for what we believe is the status determination process." [ESP edits in Italics and underlined]

ESP: The above is pretty close - here is my [version]:

"The status of each station is determined by comparison to a benchmark data set comprised of all data for the years 1985-1990 collected by both Virginia and Maryland programs.

Each station is rated as poor, fair, or good relative to the benchmark data. For each salinity zone the ratings are obtained by the following steps:

1) For each parameter in the benchmark data set, a transformation is chosen that yields a distribution that is symmetric and reasonably well approximated by the logistic cumulative distribution function (CDF). In most cases, the logarithm transformation is satisfactory.

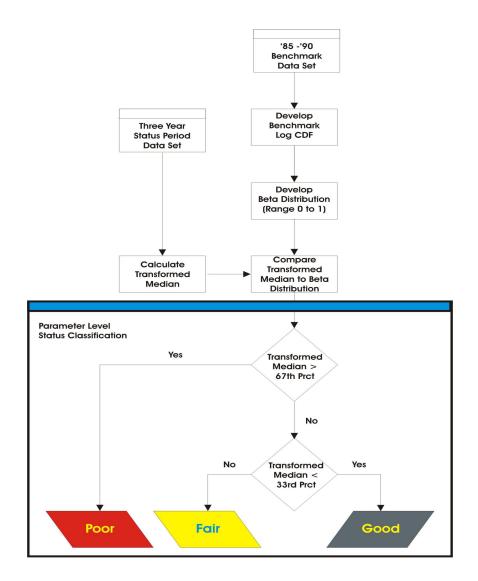
2) A logistic CDF based on the mean and variance of each parameter of the benchmark data set is used to perform a probability integral transform on all data in the most recent 3-year period. This results in data in the interval (0, 1) which follows a uniform distribution (Roussas, 1973).

3) The 3-year median of this 0-1 data is computed as an indicator of status in the current 3-year period. The median of n observations taken from a uniform distribution follows a Beta distribution with parameters (m, m) where m = (n+1)/2 and n is the number of observations (Roussas, 1973).

4) Based on the Beta density, the distribution of 3-year medians from the benchmark data is divided into thirds. If the median of the current 3- year period is in the upper third (where upper is chosen as the end of the distribution that is ecologically desirable), then the status rating is "good", a median in the middle third is rated "fair", and a median in the lower third is rated "poor"."

In most cases, serial dependence of the raw data resulted in greater than expected variance in the Beta density of the medians. To adjust for this, the variance of the Beta density is increased by a function of the ratio of among-station variance to within-station variance.

ESP: I think [the figure below] works.



Appendix 4

Excerpt from

Assumptions and Procedures for Calculating Water Quality Status and Trends In Tidal Waters of the Chesapeake Bay and its Tributaries

A cumulative history

Prepared for the Tidal Monitoring and Analysis Workgroup (previously the Data Analysis Workgroup) Chesapeake Bay Program by Elizabeth Ebersole, MD/DNR Mike Lane, VA/Old Dominion University Marcia Olson, NOAA Chesapeake Bay Office

Elgin Perry, Statistical Consultant Bill Romano, MD/DNR

Updated January 2002

Introduction

The Chesapeake Bay Monitoring Program Analysis Methods were compiled at the direction of the Tidal Monitoring Analysis Work Group (TMAW, formerly the Data Analysis Work Group–DAWG) of the Monitoring Subcommittee. This document summarizes the data analysis methods used by the Monitoring Program investigators to determine status (current condition) and trends (overall increases or decreases over time). This document also describes the adjustments made over time and as necessitated by the individual peculiarities associated with analyzing water quality, living resource or benthic data.

<u>Status</u>

Status is a measure of current condition compared to some benchmark. For some water quality and living resource parameters, reference levels such as restoration target levels or goals have been established and the current condition of an area can be assessed with respect to that level. Status assessment determines if current levels "meet," "fail," or are "borderline" with respect to the target level. Because reference levels are not available for many parameters and because there is some interest in how areas compare to others of similar type, efforts to develop a relative measure of status have been ongoing. Relative status compares recent data for a specific parameter at a particular station or segment to all stations and segments of the same salinity regime in a benchmark dataset. Based on this comparison, the station or segment is given a ranking of "good", "fair" or "poor" for the parameter in question. For most measures of status in the TMAW analyses, using either reference or relative benchmarks, "recent" or "current" data are those collected during the most recent three years.

Reference status – The number of water quality parameters and living resources that have specific goals, target levels, or regulatory criteria is limited, but growing. Methods of assessing status with respect to these levels are different, depending both on the parameter and how the reference level is defined. For example, habitat requirements for submerged aquatic vegetation (SAV) have been determined, and acceptable levels of five parameters critical to SAV growth (light, DIN, DIP, chlorophyll, and suspended solids) established for the various salinity zones during the SAV growing season. The requirements apply only to surface waters. Initially, status was assessed by comparing the 3-year seasonal median values to the requirement value. For example, the requirement for suspended solids is met if seasonal median concentrations are at or below 15/mg/L. More recently, a more rigorous approach has been used in order to give statistical confidence to the assessment. The Wilcoxon Signed Rank Test uses the individual monthly values to determine if the location is significantly (p<0.05) above or below the requirement level or not significantly different (borderline).

Goals for dissolved oxygen (DO) have also been established. These apply to spring spawning and summer seasons and set target levels specific to above- and below-pycnocline waters. The goals and methods for assessing attainment are described in (ref). However, new DO criteria and compliance measures currently being developed as part of the TMDL (Total Minimum Daily Load) process will no doubt supercede thoe habitat restoration goals. **Relative status** - The first version of the relative status method was developed and implemented for the 1997 Re-evaluation effort (Alden and Perry, 1997). Briefly, data from all stations, basin-wide, for the period 1985-1996 were assembled and each datum categorized as tidal fresh, oligo-, meso- or polyhaline, depending on the salinity associated with the data record. For each station and (if relevant) depth layer, separately, the data were averaged by month within year. Then, the data within each salinity regime were pooled and the 5th and 95th percentiles calculated. The 5th and 95th percentiles were empirical endpoints representing the extremes of "good" and "bad" within each salinity regime as observed over the history of the Monitoring Program. This constituted the benchmark data set.

To assess current condition, each datum from the most recent three years was scored relative to these benchmarks: Each datum was categorized according to its associated salinity and scored as a percentage (between 1 and 100) of the distance between the benchmark endpoints for that salinity regime. A composite score for the station or segment was obtained by finding the median monthly score over the three-year period.

The method was simple to implement, it resulted in a score between 0 and 100 which could then be equated to a categorical qualitative assessment, and it could be applied broadly to both water quality and living resource parameters. In retrospect, however, the method did not work exactly as anticipated. One of the underlying assumptions of this relative characterization is that the basin wide distribution of measurements for any particular parameter can be partitioned generally into thirds, each third equating to a status of "good", "fair" and "poor". As implemented, however, that method yielded unequal distributions, i.e., in some cases the method resulted in too many areas characterized as "good" when they were clearly unsatisfactory and vice versa.

For the 1998, 1999 and year 2000 status updates, a modified version of the method was used. The modifications are several:

- The benchmark period and benchmark data set are reduced from the entire period of record and include only the first six full years of data: data collected between January 1985 and December 1990. Additionally, both the benchmark and status data are log transformed prior to analysis. (Note, that for water quality parameters, the log and square root transformations are about equal in effecting a normal distribution of the data, and more effective than an inverse transformation or using untransformed data. This may not be the case for other parameters.)
- The benchmark and current status data (from the most recent three years), grouped as before by station or segment, depth layer and salinity zone, are partitioned using a beta cumulative distribution function and the status data set is scored using the logistic probability integral transform.
- The score is then adjusted based on sample size to account for interdependence of observations. The lack of independence in observations at a site tends to result in too many observations in the ends of the distribution, i.e., too many in the good and poor categories, too few in the midrange. The adjustment effects a more equal distribution of scores in the benchmark data set. In the status data set, however, the scores may have quite a different distribution, since the two data sets are independent of one another. For example, if improvements in a parameter were substantial and widespread, then a larger proportion of

recent data would be "fair" or "good" relative to the benchmark period and a smaller proportion would be "poor."

References

Alden, R. W. III, and E. S. Perry 1997. *Presenting Measurements of Status*. A "white paper" written for and presented to the Chesapeake Bay Program Data Analysis Workgroup; 15 pp.

Maryland and Virginia Mainstem and Tidal Tributaries

A Little History

Over the years of the Monitoring Program, analytical methods have changed or been modified. Some of the changes have been due to changes in parameters and laboratory techniques, others have been due to new statistical techniques and/or new thinking; still other changes have followed because of technological advances in data management and communications. In the wake of such change, comparability and consistency issues have been and will continue to be challenges to the workgroup.

Historically, responsibility for water quality status and trend analyses was divided among the primary Monitoring Program partners, albeit under the auspices and guidance of the analytical workgroup. Maryland state staff or grantees performed the analyses for Maryland tidal tributaries; Virginia commonwealth staff or grantees performed the analyses for Virginia tidal tributaries; and USEPA Bay Program staff performed the analyses for the mainstem Bay. Although analyses were performed by different entities, the same methods, conceptually, were used and modified as necessary to conform to the individual sampling programs. With the advent of the CIMS data base and universal access to data through the web, it was thought that cost efficiencies and consistency could be gained by centralizing the analyses. In year 2000, preliminary data preparation was performed by the separate partners, but the status and trend analyses (covering data through 1999) for the Bay and tributaries were all done by Bay Program staff. Although benefits were derived from that exercise, the responsibility for review and interpretation of the results still resided, rightly, with the separate partners, and the back and forth of data sets and results proved cumbersome and time-consuming. In 2001, Maryland staff performed the analyses for the Maryland tributaries and Bay Program staff performed the analyses for the mainstem and Virginia tributaries. Both groups used the same computer programs for all aspects of analysis and reporting.

Note: in the following sections, terms such as "1997 update" refer to analyses of data records that have been updated with data collected in the year named, e.g., 1997. The analyses were actually performed and the results reported in the following year.

Parameters

The core parameters for which status and trend analyses are conducted each year are listed below.

Four nutrient parameters:

- total nitrogen (TN);
- dissolved inorganic nitrogen (DIN);
- total phosphorus (TP); and
- dissolved inorganic phosphorus (DIP).

Eight additional parameters:

- total suspended solids (TSS);
- active chlorophyll a (CHLA), as a response indicator of nutrient enrichment and habitat quality;
- bottom dissolved oxygen (DO), as a response indicator of nutrient enrichment and habitat quality;
- Secchi depth (SECCHI), as a measure of water clarity;
- "percent light at the leaf (PLL)," a calculated estimate of light reaching submerged aquatic vegetation (SAV) at various depths. PLL is derived from the measurements of DIN, DIP and TSS. For this update, PLL at 0.5 m and at 1m were analyzed.
- KD, a measure of light penetration; and
- salinity and
- water temperature.

Similar analyses for additional parameters may be available as well: e.g., particulate phosphorus (PP), nitrite/nitrate (NO23), ammonia (NH4), silicate (SI) and carbon compounds (e.g. PC); also nutrient ratios, such as TN:TP and DIN:DIP.

Flow-adjusted trend analyses have been conducted only on the four nutrient parameters TN, DIN, TP, and DIP, and on TSS, CHLA and bottom DO. The most recent flow-adjusted trends for water quality are for the 1985-1998 period. The flow-adjustment methodology is currently under review.

Spatial and Temporal Scales

Water samples for laboratory analysis of nutrients, chlorophyll and suspended solids are collected at surface and bottom and at 1 m above and 1 m below the pycnocline, if one exists. For status and trend analyses, where both surface and above-pycnocline samples are collected, measurements are averaged, resulting in one value for the surface-mixed layer. Likewise, where both bottom and below-pycnocline samples are collected, measurements are averaged, resulting in one value for the surface-mixed layer. Likewise, where both bottom and below-pycnocline samples are collected, measurements are averaged, resulting in one value for the bottom-mixed layer. Trend analyses are done separately for surface-mixed and bottom-mixed layers. In the Virginia tributaries, chlorophyll is measured only at the surface and in some regions, the number of missing values for other parameters preclude analysis of bottom measurements.

[Note: in 1997 and 1998, status assessments for surface chlorophyll used only surface measurements, even when above-pycnocline measurements were available. Chlorophyll is measured only in surface waters in the Virginia tributaries, and this was intended to equalize data handling among segments. In subsequent years, it was decided to use all available data and treat as indicated above.]

Water temperature, salinity and dissolved oxygen are measured *in-situ* at 1- to 2-m intervals through the water column. In the case of dissolved oxygen, only bottom concentrations are analyzed for status and trends. For salinity and water temperature, only surface and bottom measurements are analyzed for trends; status is not evaluated for these two parameters.

Annual routine status and trend analyses are conducted using water quality data collected from the Chesapeake Bay mainstem and tidal tributaries from January 1985 (or from the beginning date if the program began later) through December of the most recent year. The core seasonal analyses include:

- the *annual* season or calendar year (months 1-12);
- the *SAV growing season* (months 4-10 in tidal fresh, oligohaline and mesohaline regions, and months 3-5 and 9-11 in polyhaline regions);
- *spring* (months 3-5 in polyhaline regions and 4-6 in other salinity zones); and
- *summer*, which is defined differently for different parameters. For dissolved oxygen, summer includes months 6-9; for chlorophyll a, summer includes months 7-9. For most parameters, analyses are done for all season definitions.

The flow-adjusted data are analyzed for trend only over the annual season (months 1-12). Flow-adjusted data are not assessed for status.

For a regional picture of status and trends, stations are aggregated for analysis into segments. Prior to 1997, by-segment analyses used the original CBP segmentation scheme. The segmentation was modified for the1997 Reevaluation Effort to reflect more closely the salinity conditions of the evaluation period, i.e., 1985 and subsequent years. Status and trend analyses for the 1997 update used this station aggregation. In 1998, the segmentation scheme was further modified slightly. This scheme is the basis for 1998 to present by-segment analyses. Documentation of the chronology and definition of the several schemes (Olson, 2000) is available on line in the TMAW Source Library.

Status Calculations

As described in the introduction (page 1)

Trend Analysis and Flow-Adjusting Procedures

As described in the introduction (page 1), with the following additional details.

Flow adjustment in the mainstem Bay – The mainstem Bay receives discharges from large and small tributaries up and down its length and it is difficult to remove the effects of flow for main Bay stations in the same way as done for the tributary stations. At the request of the data analysis workgroup, Ray Alden and colleagues developed a flow-adjustment for the main Bay in time for the 1997 trend update. Like the flow adjustment procedure for the tributaries, this method is also currently under review. The flow-adjusted analysis was not performed for the 2000 update.

The "adjustment" for the mainstem is, in fact, segment-specific regression models that include a flow factor as well as various pre-selected month, depth, salinity and/or water temperature factors, if they added significantly to the model fit. The input value for daily flow is the sum of the daily flows of the major tributaries discharging to the Bay at or north of the segment being analyzed. Similar to the procedure applied in the tributaries, the procedure finds the best predictive flow variable among several and removes the variance associated with flow and

associated variables by subtracting the least squares prediction from the observed response. Copies of these programs are archived online in the TMAW Source Library.

Decision Rules for Reporting Trends With Observations Below Detection Limit - In the CBP water quality monitoring database, parameters whose levels are below the detection limit of the analytical method are assigned the value of the detection limit. Over the history of the Monitoring Program, many of the laboratory analytical techniques have changed or improved and lowered their limit of detection. An artifact of this advance is that the lower values of the BDL measurements later in the data record may be falsely detected as a downward trend. To avoid this, water quality values are censored to the highest detection limit of the analysis period as part of the data handling prior to analysis. Censoring is based on the detection-limit history of each station for the individual station analyses. For segment analyses, however, where stations within a single segment are monitored by different organizations and have different detection limits, the censoring level is the highest detection limit of the stations in the segment. After censoring, all censored data are set to one-half the detection limit value.

Data sets having large numbers of values below detection limit (BDLs) may create statistical problems for trend analyses. The Seasonal Kendall test for trend, and similar sign tests such as the Van Belle and Hughes test, adjust variance estimates upward for ties in magnitude. Since BDL values in the raw data set produce such ties, trend analyses of data sets with high percentages of BDLs will be based upon greater variances than those without BDLs, all else being equal. Thus, the power of the trend analyses for the data sets with BDLs will be reduced compared to those without detection limit censoring.

There is an additional wrinkle to flow-adjusted data. When a data set with BDL values is flowadjusted by the procedures previously described, many ties in magnitude disappear, since each datum is adjusted based upon the flow measurement from the day of collection. As a result, the trend analyses conducted after flow adjustment will, in all probability, have fewer ties in magnitude, lower variances and an artificial increase in power compared to the trend analysis based upon the observed data. This increase in power is an artifact of the flow adjusting process and is not based on changes in the magnitude of trends that are due to flow.

The DAWG guidelines for reporting Seasonal Kendall trend test results, with respect to BDLs, have changed over the years. For the 1985-1997, -1998 and –1999 updates, the following rules applied:

- If a significant trend result is obtained and more than 5% of the data are below the worst case detection limit, then report the direction of trend, but not the magnitude (percent change).
- If more than 20% of the data is censored, then report neither the direction nor magnitude of trend.
- If results are significant only for flow adjusted data and more than 5% of which are BDL, confirm the results through the use of a Tobit analysis procedure (Tobin,1958). Tobit analysis is a regression-based procedure that is designed to handle left censoring such as occurs with lower detection limits.

For the 1985-2000 trend updates, DAWG adopted different decision rules:

- If the percentage of BDL observations is 15 or less, report the Seasonal Kendall trend test p-value and direction as well as the Sen Slope estimator of the magnitude of the trend (e.g., 35 %).
- If the percentage of BDL observations is greater than 15 and less than or equal to 35, report the Seasonal Kendall trend test p-value and direction, but do not report the Sen Slope estimator of trend magnitude.
- If the percentage of BDL observations is greater than 35 and less than or equal to 50 and the Seasonal Kendall trend test p-value indicates a significant trend, report the Seasonal Kendall trend test p-value and direction, but do not report the Sen Slope estimator of trend magnitude.
- If the percentage of BDL observations is greater than 35 and less than or equal to 50 and the Seasonal Kendall trend test p-value does not indicate a significant trend, report nothing, noting that there are too many observations below the detection limit to determine the presence or absence of trend.
- If the percentage of BDL observations is greater than 50, report nothing, noting that too many observations were below the detection limit to determine the presence or absence of trend.

Rationale - The rationale for these rules is based on findings demonstrated by simulation analysis for the Seasonal Kendall test and Sen slope estimator (Alden, Perry and Lane, 2000) and is briefly summarized here: 1) The false positive rate of the Seasonal Kendall test does not seem to be affected by the level of censoring of the data; 2) The power of the Seasonal Kendall test begins noticeably to decline when censoring exceeds 35 %; 3) The Sen slope estimator begins noticeably to exhibit bias when censoring exceeds 15%. At levels of censoring of 15% or less, both the Seasonal Kendall test results and the Sen slope estimator are reliable and should be reported. At levels of censoring greater than 15%, the Sen slope estimator should not be reported because it becomes biased. The Seasonal Kendall test retains a robust type I error rate and a flat power response up to 35% censoring and thus should be reported up to that level. If the Seasonal Kendall test produces a significant result when the level of censoring exceeds 35%, one may infer that this result is obtained in spite of the loss of power and therefore is a valid result and should be reported. If the Seasonal Kendall procedure fails to produce a significant result when censoring is in the 35% to 50% interval, this failure may have resulted from a loss of power and should be reported as a non-significant result, which carries the implication that the trend is below the level that we have power to detect with an uncensored data set. While the Seasonal Kendall procedure continues to exhibit the nominal type I error rate for levels of censoring that are greater than 50%, and thus significant results for these high levels of censoring might be judged reliable, the risk that the uncensored data are unduly influenced by a large scale stochastic event (e.g. drought, hurricane, etc.) becomes large and these results should not be reported.

Determining percent BDL – This aspect of the analytical methodology seemed selfevident at first and was not formally discussed or delineated in detail. The several reporting entities used the same censoring procedure for each datum (i.e., setting values lower than the highest theoretical detection limit to one-half the detection limit value), but otherwise each "did their own thing." For the 1998 and 1999 updates, the workgroup defined a more detailed procedure. It was modified somewhat for the 2000 update. • Flag and censor each value below the highest detection limit over the trend period.

For parameters that are *directly measured* during the whole time period, the detection limit is simply the highest measured detection limit used for that parameter over the time period. For example, the highest detection limit for orthophosphate (PO4) at stations in Maryland minor tributaries between 1985 and the present is 0.01 mg/L. This was the detection limit at the analytical laboratory from 1985 to May 31, 1986.

For *calculated parameters*, i.e., parameters derived by addition or subtraction from directly measured parameters, the theoretical detection limit is the sum of the detection limits of the constituent parameters. The highest theoretical detection limit, then, is the highest of such sums over the trend period. For example, total nitrogen (TN) is obtained from TKNW+NO23 and/or from PN + TDN, depending on which constituents are measured. Both methods have been used over the history of most stations in the Monitoring Program. For example, at mainstem Bay stations, TN was obtained by the first method from the beginning until October 1987, and by the second thereafter. At a station in the lower Bay sampled, say, by VIMS, the highest detection limits for TKNW and NO23 at any given time in those years sum to 0.11 mg/L; the highest for PN+TDN is 0.10. Thus, the data are censored to one half of the higher of the two methods, to 0.11/2 mg/L.

• Censor monthly mean values. The Seasonal Kendall trend test is performed on monthly mean values for separate depth layers of various definition, e.g., surface, surface-mixed, lower-mixed, and bottom layers. In the first version of the procedure, the monthly value for each layer was considered BDL if the number of censored (flagged) measurements was >= 50% of the individual sample values. For example, 2 sampling events at a deep water station in July yields 4 total values in the mean for the surface-mixed layer: 1 sample each from surface and above-pycnocline layers, times 2 events. If 2 or more of those 4 values are BDL, then the monthly value was considered BDL in this version.

This decision rule was modified in the 2000 update. Since the BDL issue is actually an issue of "ties" between months in the Seasonal Kendall test, the possibility of a tie due to censoring is eliminated if any one of the values in the monthly mean is *not* BDL. Thus, in the modified version, a monthly mean value is flagged as BDL only if all of the values in the mean are BDL.

• Compute BDL percentage based on station/segment-layer-season group. The trends are calculated either by segment or by station for a given layer for various defined seasonal groupings. The percent BDL for a parameter is the number of BDL monthly mean values divided by the total number of monthly mean values in the station/segment-layer-season group of values for that parameter. The results, with respect to BDLs, are reported or suppressed based on the decision rules given above.

Reporting Rules for Non-homogeneous Trend Results - The procedure by van Belle and Hughes (1984) is used to test for homogeneity of trend among months to see if the trend is consistent across months within seasons and across stations within segments. Homogeneity within seasons is tested and considered significant at $p \le 0.01$. If trends among months within

seasons for a given station are not homogeneous, then the analyst reviews the data and uses professional judgment to determine if the overall annual trend is considered valid and can be reported with confidence. The default rule is to report the trend. If the analyst finds reason for no confidence, then "no trend" is reported.

Related Information

For details on water quality field sampling or laboratory analysis methods in Maryland, see <u>http://www.dnr.state.md.us/bay/tribstrat/status_trends methods.html</u> or contact Elizabeth L. Ebersole, Tidewater Ecosystem Assessment, Maryland Department of Natural Resources, 580 Taylor Avenue, Annapolis, MD 21401, <u>bebersole@dnr.state.md.us</u>. In Virginia, contact F. A. Hoffman, VA Dept. of Environmental Quality, P.O. Box 10009, Richmond, VA 23240, <u>fahoffman@deq.state.va.us</u>.

References

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