Philadelphia PWD Water Department

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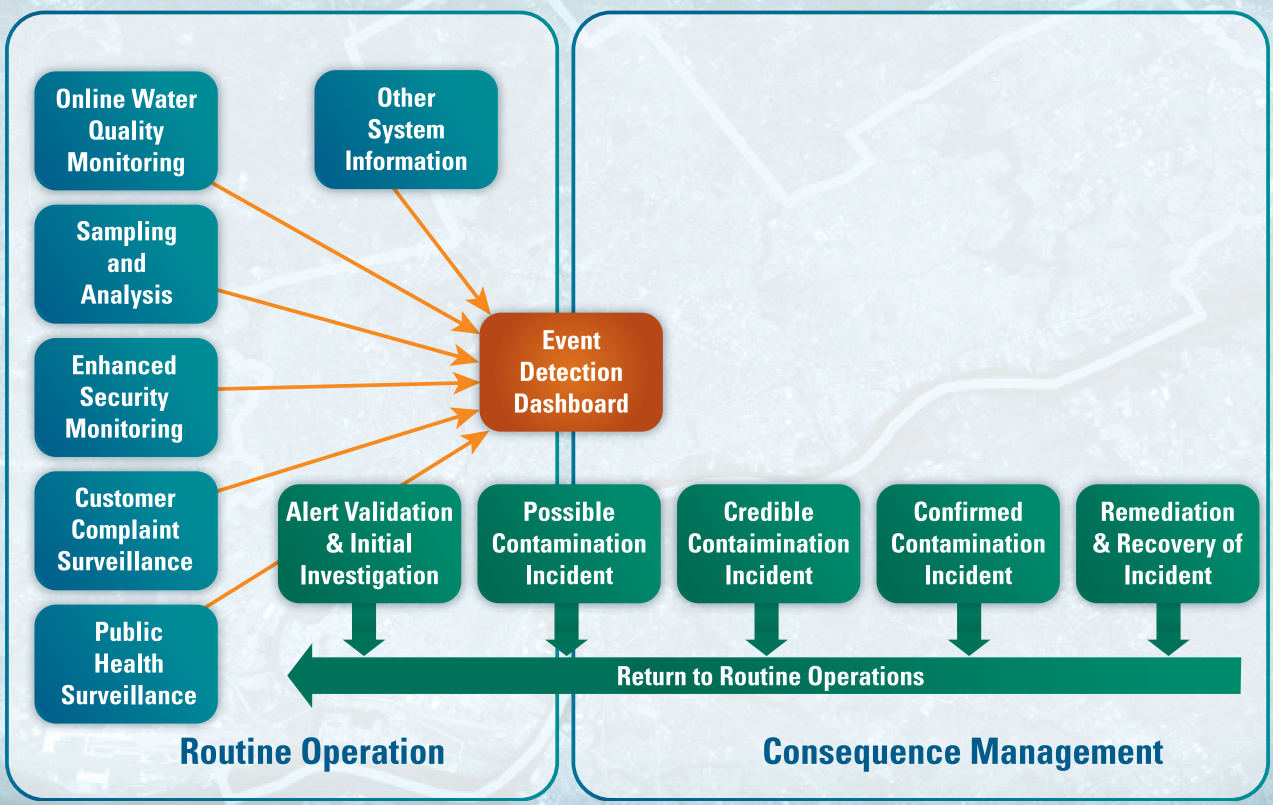
Philadelphia Water Department
Contamination Warning System Demonstration Pilot Project:

Development of Control Limits for Baseline Water Quality Monitoring



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This paper can also be downloaded from www.ch2mhill.com/iws.

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Abstract

The Philadelphia Water Department (PWD) developed a comprehensive contamination warning system (CWS) for its drinking water system under a Water Security (WS) initiative grant of the U.S. Environmental Protection Agency (EPA). One of the sampling and analysis (S&A) component objectives is to provide and characterize water quality data for specific contaminants and contaminant classes under normal operating conditions. The data are obtained as part of baseline monitoring through sample collection in the distribution system and sample analysis, or mining historical data. These data are then used to develop a baseline water quality profile. Control limits are established limits against which sample concentrations are compared to identify abnormal concentrations. This paper provides a stepwise approach that was used by PWD to analyze and interpret the baseline data to establish control limits for use in identifying abnormal water quality.

Project Background

PWD developed a comprehensive CWS for its drinking water system under a WS initiative grant. The WS initiative is a program developed by the EPA in partnership with drinking water utilities and other key stakeholders in response to Homeland Security Presidential Directive 9. The WS initiative involves designing, deploying, and evaluating a model CWS for drinking water security. A CWS is a systematic approach to the collection of information from various sources, including monitoring and surveillance programs, to detect contamination events in drinking water early enough to reduce public health and economic consequences. The WS initiative goal is to develop water security CWS guidance that can be applied to drinking water utilities nationwide.

The project has six major components:

1. Online water quality monitoring
2. Sampling and analysis
3. Enhanced security monitoring
4. Consumer complaint surveillance
5. Public health surveillance
6. Consequence management

One objective of the S&A component is to provide and characterize water quality data for specific contaminants and contaminant classes under normal operating conditions. The data are obtained through sample collection in the distribution system and sample analysis, or mining historical data. These data are then used to develop a baseline water quality profile. This data collection effort is referred to as baseline monitoring. The EPA defines baseline monitoring, in the context of a CWS, as an S&A activity of specified duration with the object of establishing EPA priority contaminant and contaminant class occurrence (contaminants, levels, and frequency of detection) and method performance (precision, recovery, and interferences) in utility system water samples. Baseline monitoring is a key component of the S&A activities with the objective of defining analytical method performance, determining background or "baseline" levels of targeted and non-targeted contaminants, and interpreting the baseline data in a manner that supports threat evaluation during the CWS process of event response.

CH2M HILL served as the project contractor and supported PWD in development of its CWS. CH2M HILL supported PWD in the design and implementation of the baseline and maintenance monitoring programs, analysis of water quality data, and establishment of control limits.

Description of PWD and Routine Water Quality Monitoring

PWD is a municipal utility providing integrated water, wastewater, and stormwater services to the greater Philadelphia region. PWD delivers reliable and safe drinking water to more than 1.6 million people in Philadelphia and its suburbs. Source water is obtained from the Delaware and Schuylkill rivers.

PWD maintains 84 drinking water sampling stations for routine water quality monitoring and regulatory compliance purposes. The monitoring sites include PWD facilities and various other sites (such as police and fire stations) spread throughout the distribution system. PWD also conducts optimized corrosion control sampling at 13 locations throughout the distribution system and at the entry points to the distribution system to comply with Pennsylvania Department of Environmental Protection permit requirements under EPA's Lead and Copper Rule. The 13 locations throughout the distribution system are sampled quarterly. Entry points to the distribution system are sampled weekly. Each parameter has a designated monitoring schedule that may require daily, weekly, monthly, quarterly, or annual analysis at the Bureau of Laboratory Services. PWD routinely analyzes for general water quality, metals, and biologicals. Volatile and semivolatile organic compounds are collected and analyzed quarterly.

Control Limit Types

Control limits are established limits used to evaluate sample concentrations to identify abnormal results. Abnormal concentrations could indicate a potential contamination incident. If a contamination incident is confirmed, then control limits can also help to establish the spatial extent of contamination and determine a target endpoint after remediation to demonstrate a return to normal conditions.

Several potential limits could be selected as control limits to identify abnormal concentrations, such as the following:

- **Reporting Limits –** Reporting limits can be used as control limits for parameters that are never or infrequently detected at very low concentrations. A general practice may be to consider any detected concentration that is greater than the reporting limit for any of these parameters as an abnormal result.
- **Regulatory Limits –** Under the Safe Drinking Water Act, maximum contaminant levels (MCLs) are developed to establish a contaminant concentration that would result in noncompliance conditions. MCLs ensure that drinking water does not pose short- or long-term health risks. These regulatory limits may be used for parameters that have MCLs (or secondary MCLs) to identify abnormal results.
- **System Operational Limits –** PWD maintains system operational triggers (0 and 1), which the laboratory analysts use to identify abnormal results at the time the measurement is made. Level 0 triggers are limits that require the analyst to notify the laboratory supervisor by a telephone or e-mail message. Level 1 triggers are limits that require the analyst to notify the laboratory supervisor immediately and by direct contact. These may be used as control limits for parameters that show little variation in source water and throughout the distribution system.
- **Statistically Derived Limits –** Statistically-derived upper-bound limits may be developed and used as control limits for parameters that have a high frequency of detection, do not already have predetermined limits, and show significant seasonal, spatial, or source water variation.

Establishing Control Limits

For this project, control limits were established using the following steps:

1. Define the individual analytes to be included in the baseline database.
2. Develop the water quality baseline database and summarize the data structure.
3. Calculate analyte-specific summary statistics.
4. Evaluate the applicability of pre-existing limits, such as MCLs or facility operational limits, for use as control limits.
5. Statistically determine the effect of variables such as source water, distribution blends of treated water, and seasonal water quality changes.

6. Statistically develop analyte- and variable-specific control limits (upper/lower bound limits) that define a departure from normal baseline conditions but minimize false negatives and positives.
7. Develop user-friendly outputs in graphical or tabular formats to share with high-level managers when water quality results depart from the baseline, indicating possible water contamination.

The following provides detailed information on how the baseline data were analyzed and control limits were statistically generated.

Baseline Data and Statistical Analyses

The individual analytes of interest were defined and the water quality baseline database was developed. Five years of data, including data collected during the baseline period and historical data, were compiled and stored in a Microsoft Access database. The data structure was summarized and analyte-specific summary statistics were calculated to understand parameter occurrence and baseline concentrations. All data were pooled and basic statistics generated, including number of samples, number of detects, frequency of detection, as well as detected parameters minimum, maximum, standard deviation, and coefficient of variation.

Three primary factors that could affect analyte concentrations and are commonly representative of baseline conditions include source water and distribution blends of treated water, seasonal conditions affecting analyte levels throughout the year, and spatial differences occurring in different locations within the distribution system. Because PWD obtains water from two rivers known to differ in levels of individual inorganic, indicator, and metal concentrations, the evaluation of source water differences was completed to identify the analytes that differ significantly between source waters and require source-specific control limits.

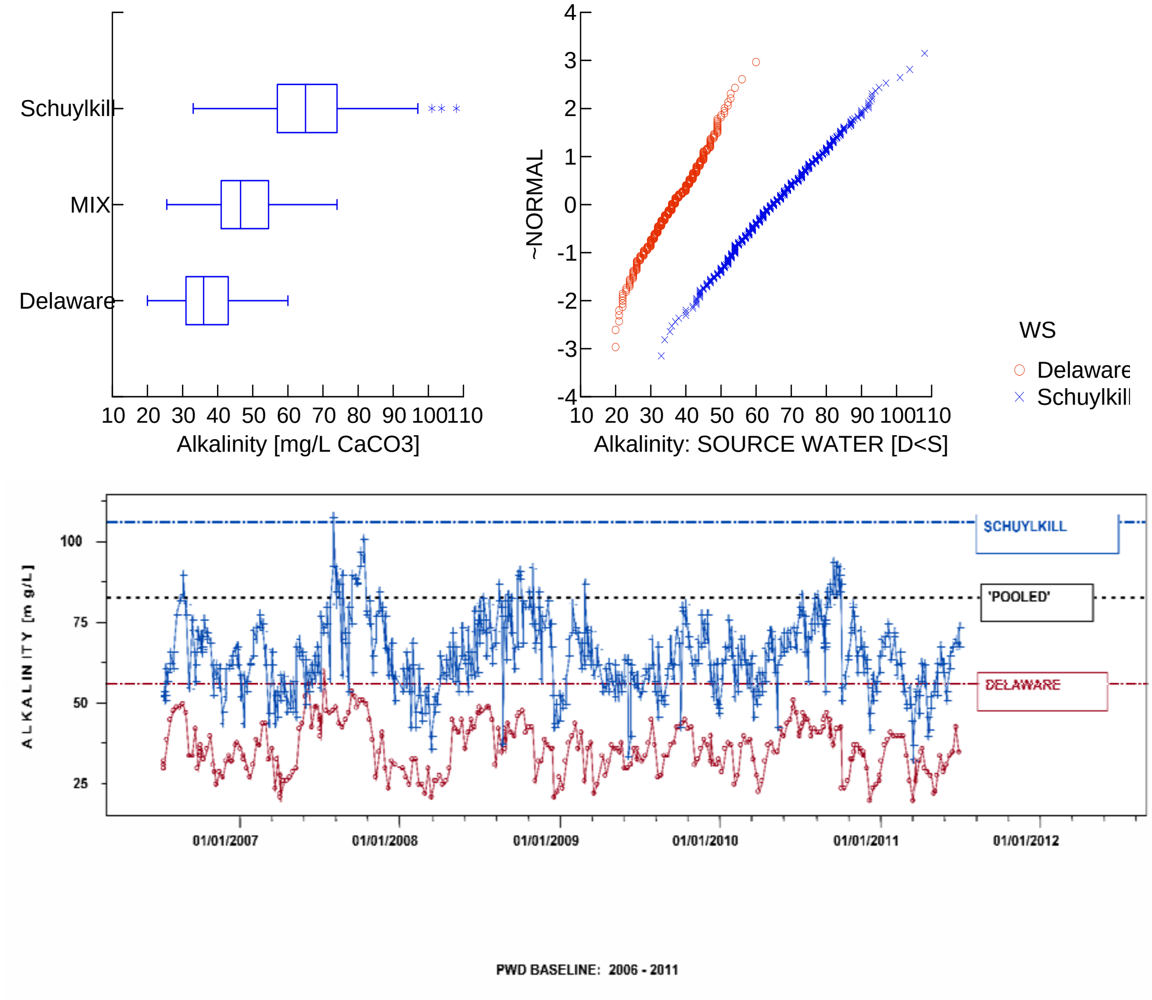
These factors can visually be evaluated using box plots, probability plots and time series plots. Example graphics are provided in Figure 1. Treated water from the Schuylkill River has a greater hardness, conductivity, and alkalinity than the treated water from the Delaware River. The upper left display compares the distributions of alkalinity for the Schuylkill and Delaware sources and for a blend using a box and whisker plot. As expected, “mixed” source locations lie midway between the higher Schuylkill levels and lower Delaware source water levels. The upper right panel includes probability plots of the data, limited to the two “pure” source water locations. The lower panel compares upper bounds based upon the pooled data [black broken horizontal line] versus the Schuylkill [blue] and Delaware [red]. These graphics show that applying a pooled limit would be overly conservative for Schuylkill levels and insufficiently conservative for Delaware levels.

Generating Statistically Derived Limits

Reporting limits, regulatory limits, and system operational limits should be evaluated for each analyte to identify the pre-established limits that are available. If a pre-established limit is unavailable or a pre-established limit is not representative of water quality concentrations, then the development of a statistically derived limit should be completed.

Statistically derived upper-bound estimates (upper tolerance limits [UTL] and upper prediction limits [UPL]) can be used as control limits. For this project, UTLs and UPLs were developed for selected inorganic and indicator parameters, and total metals. These analytes were selected because they were frequently detected, did not have pre-established limits, and/or have shown significant variation in the source water. The upper bound estimates were developed using source water-specific locations or pooled locations based on the results of the source water statistical analysis. The following provides the methods PWD used to statistically derive control limits.

FIGURE 1
Example of Data Analysis Graphical Displays



Methods

Source water-specific UTL and UPL control limits were calculated to demonstrate the differences between the potential upper bound statistics. Both UTL and UPL estimates require specification of two characteristics: the coverage, or the proportion of the distribution being considered as the upper bound of interest, and the confidence, or the relative uncertainty about that estimate of a specific upper proportion of the baseline observations.

Confidence and coverage are the only characteristics required to calculate a UTL. For example, a UTL with 99 percent coverage and 95 percent confidence is an estimate of the 99th percentile of the distribution with an upper 95 percent confidence interval around the 95th percentile, meaning that if the UTL were calculated 100 times, it would encompass the population estimate 95 percent of the time. However, as noted in EPA's *Unified Guidance for Groundwater Statistics,* successive application of a UTL over many datasets results in an inflation of the average coverage of the UTL over successive comparisons. That is, multiple applications of a 99th percentile UTL to multiple datasets (or sequential observations) can, when the successive comparisons are accounted for, be expected to identify an exceedance of successively lower percentiles, representing a relaxation of the calculated 99th percentile UTL. For example, a single application would be expected to result in rejection of 1 percent of the population, whereas 5 applications of the same limit to the same population would be expected to result in rejection of about 5 percent of the same population.

To address the uncontrolled inflation that occurs in multiple applications of UTLs, UPLs were proposed as alternative upper bounds. Calculation of a UPL requires, in addition to the coverage and confidence characteristics sufficient for calculation of the UTL, specification of both the number of values to which the UPL is to be compared and the actual value that will be compared. For example, a 95|95 UPL (designating 95th percentile coverage with 95 percent confidence) may be calculated for five future values. Further, different limits may be calculated to establish the upper bound expected from any of the individual five future observations or, alternatively, the upper bound, which would be expected to contain the average of the five future observations.

For the PWD CWS project, two upper bound estimators were selected to generate upper bound control limits on selected analytes. The 99th UTL with 95 percent confidence and the 99th UPL with 95 percent confidence for 25 subsequent observations were determined to be most appropriate and selected as the estimators. Upper bound baseline control limits were developed using EPA's ProUCL statistical software on data collected between 2006 through 2011 for the selected analytes.

Steps in the statistical calculation process are (1) identification and examination of potential outliers in available data, (2) evaluation of potential trends, (3) examination of underlying theoretical distributions, and (4) distribution fitting, each of which is briefly summarized below:

- **Outliers –** Potential outliers were identified using the Rosner test, which is based upon normal distribution parameter estimates. Outliers identified by the Rosner test were excluded in UTL and UPL calculations.
- **Trends –** The potential existence of increasing or decreasing trends in observations used in UTL and UPL calculations could adversely affect results. If temporal changes are occurring over the period of record, available data cannot be considered representative of steady-state baseline conditions. Potential trends were examined visually through the use of time series plots for the periods of record. Explicit testing for trend, by application of the Mann-Kendall test, was applied only if visual inspection suggested the need.
- **Distribution Testing –** ProUCL test observations against three theoretical distributions included the normal, lognormal, and gamma distributions. Goodness-of-fit testing applied included the Shapiro-Wilks or Anderson-Darling tests. Results that verified the observed values and do or do not exhibit the theoretical distribution were used to select the appropriate distribution model for the calculation of the UTL and UPL estimates.
- **Assumed Distribution –** Distribution equations (assuming goodness-of-fit test results indicate adherence to the theoretical distribution) were prioritized to select (in decreasing order) normal, gamma, and nonparametric estimates. Lognormal estimates were preferentially not used, given unsatisfactorily unstable upper bound estimates that occur, particularly with small sample sizes.

Selected Control Limits

All control limit types for a given parameter were evaluated by calculating the frequency at which the detectable concentrations were greater than or less than the associated limit. The most appropriate control limit was then selected based on the parameter's frequency of detection, behavior in the distribution system and source water, the availability and representativeness of predetermined and statistically derived limits, and the ability of the control limit to identify abnormal water quality without increasing the number of false positives.

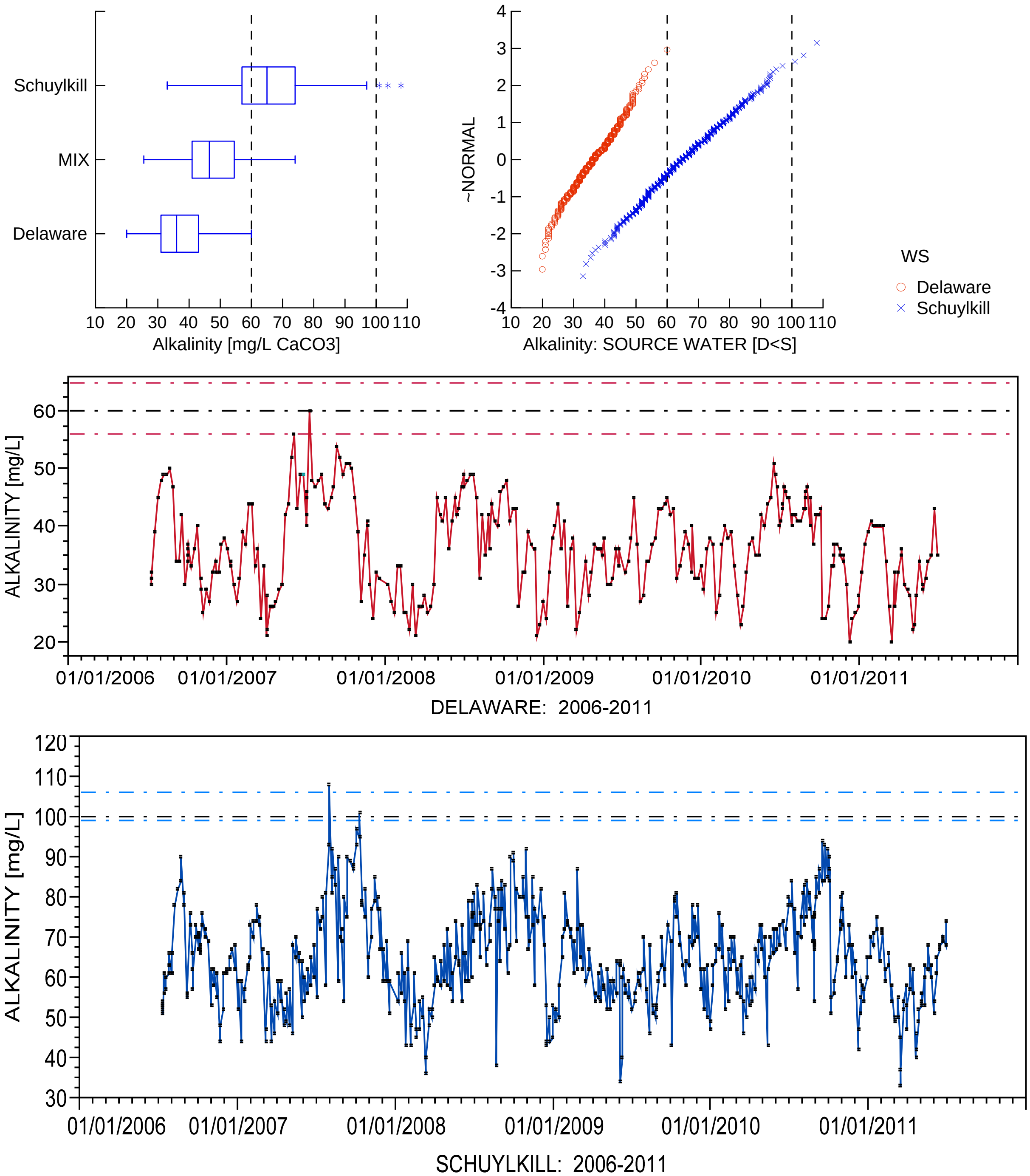
Reporting limits were selected for VOCs, SVOCs, herbicides, pesticides, and PCBs. In general, VOCs, SVOCs, pesticides, PCBs, and herbicides were never or infrequently detected at very low concentrations. Given this behavior, any detected concentration that is greater than the reporting limit could be considered an abnormal result.

Regulatory limits were selected for metals, biologicals, and radiologicals. MCLs (SMCLs) have been developed for metals and radiologicals. Either a fraction (i.e., half) of or the total MCL concentration was selected because it would provide an adequate limit to identify an abnormal result while ensuring that drinking water does not pose a short- or long-term health risk to the public. The regulatory limits for total coliform, *E. coli,* and heterotrophic plate count were selected as control limits.

System operational limits were selected for fluoride, pH, and total chlorine residual because they are controlled by the water treatment schemes and showed little variation in source water and throughout the distribution system.

Statistically derived limits were selected for alkalinity, conductivity, hardness, nitrate-N, sulfate, total organic carbon (TOC), and sodium because they had a high frequency of detection; significant seasonal, spatial, or source water variation; and did not have predetermined limits. When a difference in the upper bound estimators occurred, a final control limit was selected to account for both estimators. For example, the UTL and UPL for Delaware River alkalinity were calculated to be 56 and 65 mg/L $CaCO_3$, respectively. The selected control limit was 60 mg/L $CaCO_3$. Figure 2 presents quick reference graphical displays of alkalinity in the Delaware and Schuylkill rivers that had statistically derived control limits (both UTLs and UPLs).

FIGURE 2
Example Data Analysis Graphical Displays with Control Limits



Data Management

All finalized laboratory results and relevant quality assurance/quality control (QA/QC) data should be stored in a Laboratory Information Management System. At PWD, all laboratory results are stored in the Bureau of Laboratory Services' Laboratory Information Management System (Microsoft SQL Server 6.5). PWD will implement a new system in the near future that includes software to improve data entry and reporting capabilities, enhance information management, and accommodate important metadata related to QA/QC and analytical methods.

All selected control limits are readily available to laboratory analysts to compare against analytical results to identify abnormal results at the time the measurement is made. PWD will continue to use its system operational categories of Level 1 and Level 0 that determine the urgency and type of communication required with the laboratory supervisor. These control limits will be used in response to contamination indicators by other CWS components, including Online Water Quality Monitoring and Consumer Complaint Surveillance, as part of the credibility determination and the consequence management response, remediation, and recovery actions.

The pre-existing control limits (i.e., reporting limits, regulatory limits and system operational limits) will continue to be used. The statistically generated control limits will be periodically reviewed and evaluated to identify the correct system operational category that should be applied. Control limits will be re-evaluated and updated either on a systematic (i.e., every 2 to 3 years) or on an as-needed (changes in source water or treatment goals) basis.

Recommendations and Conclusions

Public water utilities track water quality through routine water quality monitoring programs to ensure high-quality drinking water is provided to the public, monitor system performance, and to satisfy regulatory compliance requirements. These data can be used to evaluate water quality and determine when an analytical result is "normal" or "abnormal." It is impractical to prescribe one pre-established control limit or statistical application to every parameter. This stepwise approach can be used to analyze and interpret the baseline data to establish control limits for use in identifying abnormal water quality. Understanding a system with respect to different contaminants and water quality parameters can help to apply the best control limits, whether defined by regulations, the system's operational goals, or statistics.

Abbreviations and Acronyms

$CaCO_3$	Calcium carbonate
CWS	Contamination Warning System
EPA	United States Environmental Protection Agency
MCL	Maximum contaminant level
mg/L	Milligram per liter
PCB	Polychlorinated biphenyl
PWD	Philadelphia Water Department
QA/QC	Quality assurance/quality control
S&A	Sampling and Analysis
SMCL	Secondary maximum contaminant level
SVOC	Semi-volatile organic compound
TOC	Total organic carbon
UTL	Upper tolerance limits
UPL	Upper prediction limits
VOC	Volatile organic compound
WS	Water Security

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