NATIONAL WATER QUALITY LABORATORY
NEWSLETTER
U.S. DEPARTMENT OF THE INTERIOR U.S. GEOLOGICAL SURVEY
Volume 7 Number 1 January 1999

Analytical services to be provided throughout move to new Lab

As most of you probably know, a new laboratory is being built for the National Water Quality Laboratory (NWQL). The move to the new Laboratory is scheduled to begin about March 1 and to continue for 6 to 8 weeks. The timing of the move is fortunate because sample flow is generally low in March and April. Later in the summer, sample flow increases, and consequently increased turnaround times are normal.

During the move, the NWQL intends to continue providing full services with minimal disruption to analytical work. Minimal disruption means keeping the sample turnaround time within normal production schedules. One approach to preparing for the move will be the elimination of existing backlogs before the move begins. However, because of move logistics, backlogs may increase but this should not be substantial. At the worst, analyses for samples submitted during the move should be completed by the end of the summer, but hopefully sooner.

Nearing Completion - Construction of the new building for the National Water Quality Laboratory is on schedule for occupancy to begin in March at the Denver Federal Center. This view of the north wing looking east was taken at the end of November.

To help us out, we do request that you minimize the number of samples sent to NWQL during March and April. If the time of sampling is not critical, we request that you collect those samples before or after those months. All samples received at the NWQL shortly before the move will have to be transported to the new Laboratory, and there is the risk of loss or damage to those samples. Therefore, if your sampling schedule allows, please send samples after we are in the new Laboratory. If your project commitments require sampling during the time of the move, be assured that your samples will be received and analyzed within the holding-time requirements. We are asking you to consider changing sampling plans only if you have flexibility and it will not interfere with project commitments.

Again, please consider our schedule for moving to the new Lab when planning your project work this spring. We are doing everything we can to avoid disruption of service to the U.S. Geological Survey. However, we are not so naïve as to believe that moving $10-million worth of instruments and property and nearly 200 employees will not be without unforeseen problems.

We will provide additional updates as information becomes available. Please visit our homepage at http://wwwnwql.cr.usgs.gov/USGS and select Laboratory Relocation for updated information on the new facility.

- Bob Williams, Chief, NWQL

New Lab taking shape

Construction of the new National Water Quality Laboratory at the Denver Federal Center has advanced rapidly in the past few months. Fume hoods have been installed in the south wing, along with wall cabinets and service ledges. Lighting is installed and connected for use. Air-handling units were turned on in early December. Progress in the north wing lags behind the south wing by about a month.

The main lobby is taking shape and finishing touches are being applied in some areas. The carpet is scheduled to be installed in late January. Furniture has been ordered with a tentative shipping date of January 22 and installation beginning February 1. Roads and parking lots are paved, grass has been seeded, and trees were planted last month.

The move-management company BTG completed its first pass through the old Laboratory and was fine-tuning the data base to track all equipment and furniture. NWQL personnel and BTG are developing strategies for the move to determine the most efficient process and transfer schedule from the old site to the new facility. A smooth move is planned, but glitches can be expected once the actual relocation gets underway.

Bailey's, an Allied Van Lines contractor with a government-wide contract through the General Services Administration, has submitted a cost proposal. The company reportedly has an extensive background in laboratory moves and is expected to provide the required expertise to carry out the transfer.

- Pat Timme

Emerging contaminants targeted by scientists for method development

Twenty U.S. Geological Survey (USGS) scientists met September 16-18 in Estes Park, Colorado, to confer on emerging challenges to environmental quality. The group had three objectives: (1) to develop a list of emerging contaminants for methods development and field reconnaissance; (2) to coordinate resources and methods-development activities; and (3) to identify a network of collaborators with access to samples from susceptible environments.

Topics of discussion included human and agricultural pharmaceuticals, industrial chemicals, pesticides and metabolites, and mixtures of these contaminants in natural or waste water. The group agreed to a plan of action that included establishing lines of communication and information exchange among its members and other interested USGS scientists, inventorying the chemical use of emerging contaminants, enlisting scientists with opportunities to collect samples from suspected sources of emerging environmental contaminants, conducting reconnaissance studies, and coordinating group activities with human and environmental health agencies.

Attendees at the Estes Park meeting are the initial members of a working group that would be available as a technical resource for management decisions. The emerging environmental contaminants working group will meet next in conjunction with the Toxic Substances Hydrology National Technical Meeting, March 8-12, 1999, in Charleston, South Carolina. A poster session on emerging contaminants research will be a feature of that meeting.

Participants at Estes Park included Larry Barber, National Research Program (NRP), Boulder, Colo.; Mark Burkhardt, NWQL; Herb Buxton, Toxic Substances Hydrology Program, West Trenton, N.J.; Bob Eganhouse, NRP, Reston; Bill Foreman, Ed Furlong, and Bob Green, NWQL; Fran Hostettler, NRP, Menlo Park; Dana Kolpin, Iowa District; Kathy Kuivila, California District; Steve Larson, Minnesota District; Tom Leiker, NWQL; Mike Majewski, California District; Mike Meyer, South Carolina District; Carl Orazio, Columbia Environmental Research Center; Pat Phillips, New York District; Colleen Rostad, NRP, Denver; Mark Sandstrom, NWQL; Mike Thurman (meeting coordinator), Kansas District; and Steve Zaugg, NWQL.

If you would like more information or to be included in the E-mail distribution for this topic, contact Mike Thurman, Herb Buxton, or Bob Green.

- Bob Green

Commercial Laboratory Information Management System selected

The search for a commercial Laboratory Information Management System (LIMS) culminated on November 12 with a contract award to LIMS, USA. The product selected is known as StarLIMS. Jan Coffelt is the contracting officer and Linda Pratt is the contracting officer's representative.

The final selection was made by a multidisciplinary technical evaluation team consisting of Melanie Clark (Wyoming District) and Richard Coupe (Mississippi District), and Ted Struzeski, Steve Smith, Tom Bushly, and Sandy Turner from the NWQL under the leadership of Steve Glodt. Glodt was involved with the project from the beginning-he documented the specifications, solicited requests for bid, and issued the final contract award.

A LIMS manages the workflow of a sample through the laboratory from receipt of sample to archiving the sample. The StarLIMS is built around a Relational Data Base Management System and will work with Ingres software. StarLIMS has a multitiered architecture that treats business rules, programs, and data as separate tiers. This process allows the system to be customized. StarLIMS has a World Wide Web (WWW) interface to allow entry of requests and query of status of jobs. Other features include the following: produces barcode labels for received bottles, automatically interfaces with instruments, and provides quality-control features such as charting, summarizing, tracking, and reporting.

The system supports laboratory practices conforming to the International Organization for Standardization (ISO) and United States' Good Laboratory Practices (GLP) recommendations for audit trailing, security, data integrity, archiving, and quality control. The StarLIMS is expected to be operational in August 1999. More information can be found about StarLIMS on the WWW at http://www.starlims.com/ .

- Sandy Turner

New titles in print

Garbarino, J.R., and Struzeski, T.M., 1998, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory-Determination of elements in whole-water digests using inductively coupled plasma-optical emission spectrometry and inductively coupled plasma-mass spectrometry: U.S. Geological Survey Open-File Report 98-165, 101 p.

Kociolek, J.P., Spaulding, S.A., and Kingston, J.C., 1998, Valve morphology and systematic position of *Navicula walkeri* (Bacillariophyceae), a diatom endemic to Oregon and California (USA): Nova Hedwigia, v. 67, nos. 1 and 2, August 1998, p. 235-245.

Preparing for the millenium

How well is the National Water Quality Laboratory prepared for the new millenium? This was the question that Charlie Merk, the U.S. Geological Survey's Y2K coordinator, asked the NWQL senior staff in the fall.

Merk presented various potential problems with software, computer hardware, and especially with instruments that have embedded technology chips. After the presentation, Linda Pratt, Chief of Laboratory Operations, appointed John Crisci and Sandy Turner as NWQL Y2K coordinators to assess Laboratory compliance with Y2K issues.

The first step in the assessment was to itemize the equipment and prepare a list of the steps that must be performed to test the instruments. Representative instruments for each analysis were chosen and laboratory personnel evaluated the impact on the system. They were also asked to prepare several scenarios for correcting any problem that was found.

Sample Inspection - Ann Watterson examines polypropylene vials with 2.0 milliliters of Ultrex 7.6N nitric acid. The new polypropylene vials are also being shipped with 1.0 milliliter of 4.5N sulfuric acid. Ann is a chemist in the Water Quality Management Program at the National Water Quality Laboratory. She has been working in U.S. Geological Survey analytical laboratories for 31 years.

Chris Lindley performed one of the early tests on the gas chromatograph/mass spectrometer line of instruments. There were errors and the vendor was contacted for a solution. These systems were purchased between 5 and 10 years ago. In the intervening years, the vendor has switched from Unix controllers to NT controllers. The vendor provides limited support and has no plans to make these systems Y2K compliant. As an added complication, the present instruments will not operate with the NT controller.

Ted Struzeski, NWQL chemist, worked on the inductively coupled plasma/mass spectrometer instruments. When he advanced the date beyond the year 2000, the instrument "froze." Struzeski later duplicated the test and then made some changes to force the instrument into action. He thought he had found a solution, however, the following morning, the entire analytical line was corrupted and had to have software reloaded. With further research, Struzeski found that the Y2K problem can be corrected with new software and new controllers.

The first assessment of the NWQL instruments was submitted to Merk. Subsequently, the NWQL was granted $970,000 for compliance. In November, Bill Pfancuff of the U.S. Department of the Interior visited the Laboratory for a tour and assessment. He encouraged the NWQL to consider its operation "Mission Critical" and asked for further assessment to ensure that all areas of operation have been covered and that adequate contingency plans are in place. The NWQL is working with Merk to ensure that it will provide defensible data well into the next millenium.

- Sandy Turner

New methods replace hydride generation atomic absorption for As, Se, and Sb

The National Water Quality Laboratory replaced hydride generation atomic absorption methods for the analysis of arsenic, selenium, and antimony with graphite furnace atomic absorption methods last October 1. The changes are outlined in NWQL Technical Memoranda 98.11 and 98.12.[1] The Open-File Report documenting the new method for arsenic and selenium is in press.[2] Lab codes,[3] bottle type,[3] and prices[4] are available in the NWQL on-line catalog.

All antimony samples, including filtered and whole-water recoverable (WWR), will be analyzed using U.S. Environmental Protection Agency (USEPA 200.9) methodology. Filtered antimony samples will be analyzed using the FA bottle type. A bottle type of ERA (sample designations and bottle types are defined in the on-line Catalog) is still required for WWR antimony. Method-reporting levels (MRLs) for antimony remain at 1 µg/L (microgram per liter). The analytical range has expanded from 1-20 to 1-25 µg/L.

Arsenic and selenium samples are now being analyzed simultaneously using graphite furnace-atomic absorption spectrometry. This change has improved laboratory efficiency by reducing personnel requirements from 1.8 to less than 1 full-time equivalent analyst. In addition, the laboratory has reduced the amount of waste from about 280 to 1 liter per month. NWQL customers will also see a price reduction because of the laboratory's increased efficiency.

The RAH sample type is no longer needed for either arsenic or selenium analysis. Filtered samples use the FA bottle type, and WWR samples will use the existing in-bottle digestion procedure with the RA bottle type. The MRLs for arsenic and selenium remain at 1 µg/L. The analytical range has been expanded to 50µg/L, decreasing the number of dilutions required. Lab codes and test identification (ID) numbers for the parameters are listed in the following table.

Parameter	Lab code	Test ID
Arsenic, filtered	2160	1000C
Arsenic, WWR	2162	1002E
Arsenic, bottom material	2316	1003D
Antimony, filtered	2319	1065B
Antimony, WWR	2320	1067C
Selenium, filtered	2161	11458
Selenium, WWR	2163	1147D
Selenium, bottom material	2317	11469

1NWQL Technical Memoranda are available on the Web at http://wwwnwql.cr.usgs.gov/Public/nwql_memo.html

2Jones, S.R., and Garbarino, J.R., in press, Methods of analysis by the U.S. Geological Survey National Water Quality Laboratory-Determination of arsenic and selenium in water and sediment by graphite furnace-atomic absorption spectrometry: U.S. Geological Survey Open-File Report 98-639.

3Access the NWQL Catalog Web site at http://wwwnwql.cr.usgs.gov/USGS/Catalog/CatIntro.html

4Access the NWQL price list at http://wwwnwql.cr.usgs.gov/USGS/pricelist_main.html

- Glenda Brown

An analogy for

Chemical analysis and data interpretation

The NWQL is planning to provide long-term method detection levels (LT-MDLs) and nondetection values (NDVs) for many of its methods. These values provide the data user with NWQL's best estimate of the concentration ranges that are quantitative (above the nondetection value), semiquantitative (between the nondetection value and the detection level), and not quantitative (below the detection level). The following analogy illustrates how different data users might approach reporting levels and nondetections.

A famous cookie company produces one million cookies a day and is concerned about cookie pilfering by its elf employees. They hire a cookie detective to search the worker elves as they leave. The cookie detective thought about the task of detecting pilfered cookies.

The cookie detective knew he could reliably count and identify a quantity as small as one cookie if he found it. Ah, but finding just one pilfered cookie was a problem. The detective knew that he couldn't reliably identify every elf that was absconding with just one cookie. A cookie or two could be stashed in an inside pocket or concealed in some other way. How many cookies would an elf have to take to be caught most of the time? After testing various cookie-stashing methods, he concluded that it would be fairly difficult to stash a dozen cookies and walk out without detection. A dozen cookies, then, was the minimum number of cookies that he could routinely and reliably find. Now, what if an elf was found with crumbs or parts of cookies? Well, the elves make cookies all day and everyone knows that "cookies crumble," so a few crumbs should be expected. Parts of cookies, therefore, wouldn't count as evidence of theft.

The detective summarized the search method for management and elves as follows:

Finding at least one whole cookie was evidence of a theft.

Any elf who tried to pilfer 12 or more cookies would almost surely be caught.

Elves who pilfered 1 to 11 cookies would sometimes be caught and sometimes get away with it.

Cookies eaten by elves on the job don't count. That is biodegradation.

Crumbs don't count. That is a blank contamination problem.

More concisely, LT-MDL = 1 cookie and NDV = 12 cookies.

(The mathematical relation between the LT-MDL and the NDV is different in this case from what the Laboratory is proposing, but NWQL is basing its definition on a different statistical probability than the cookie detective.)

Next, the cookie detective set about detecting cookie theft by elves. He carefully measured and honestly reported the data to cookie company management and to the elf union. He was shocked to find that the use of his data depended on the perspective and personal agenda of who was interpreting the data. Here is what he found.

- **1:** Company management wants to find out how much money is being lost to cookie-pilfering elves. So, the management elf in charge of loss estimation adds up all of the sure detections of cookie theft and considers that sum to be the minimum loss. But he knows that the cookie detective doesn't catch all of the pilfering elves. He assumes that every elf who wasn't caught (nondetections) had actually pilfered 11 cookies (<NDV) and gotten away with it. He further assumed that all of the elves caught stealing just a few cookies (low-level detections) had really stashed 11 cookies, but all of them hadn't been found. (Those elves are clever rascals.) Then he adds these with the losses from thefts of 12 or more cookies to arrive at the maximum cookie loss. He reports the potential range of cookie loss to the chief elf. The chief elf is shocked that the elves could be stealing so many cookies.

- **2:** The cookie business hasn't been so good lately and the company needs to renegotiate the contract with its worker elves. The management elf in charge of the negotiation wants to justify that the worker elves need to make some hefty concessions. He thought about using the high estimate of cookie theft that the chief elf had shown him, but he thought that the estimate was biased too high. After all, not every elf stole 11 cookies all the time. So, he assumed that every elf who wasn't caught (nondetections) had actually pilfered six cookies (half the NDV) and added that result to all of the other thefts. That number was probably high, too, because some of the employees took nothing and very few probably took 11. So the average was probably much less than six, but it was an estimate and he wanted a bargaining chip. He presents the theft loss to the elf union and says they had better compromise.

- **3:** The elves' union representative doesn't like the way cookie management counted theft. He wants to assume that every elf who wasn't caught stealing was innocent. But, he knows that occasionally a cookie is pilfered and he doesn't want to sound as biased as that lousy company negotiator. To show his good faith, he is willing to assume that every nondetection could be counted as 0.5 cookie (half the LT-MDL). He reasons that, sure, a few elves pilfer a cookie now and then, but the problem is small and if the company paid the elves a decent salary, they wouldn't have to steal cookies to feed the hungry little elves at home. He realizes that this assumption is probably biased low, but he doesn't want to admit that cookie pilfering by elves is a problem. He also wants a bargaining chip (also called a chocolate chip by the wily elves). He presents his theft estimate and requests binding arbitration.

- **4:** An individual elf has been watching the manipulation of data by the company and her union and she is offended. She has never stolen a single cookie in her life-not even when they were making double chocolate chip. Yet everyone seems to have assumed that she pilfered cookies. She doesn't care if they assume 0.5 or 1 or 6 or 11. Her pilfering was zero. She is sick and tired of everyone not realizing what a terrific employee she is. She feels wrongly accused and is considering filing suit for defamation of character. Character is important to elves.

- **5:** The company is going to lay off elves. It decided that pilfering elves would be the first to go. A particular elf had never pilfered cookies, but making cookies wasn't lucrative and his twin elflets' 4th birthday was coming up and he didn't have a present. So, one day he pilfered two cookies-one for each of the twins. He wasn't very good at pilfering and got caught. He was fired. He thought this wasn't fair. This was his first offense and it was only two cookies. The elf who worked next to him pilfered six cookies every day and smuggled them out in a cleverly concealed cookie pouch under his elf hat. That guy never gets caught. The fired elf complains to the company, but it reasons that someone who was caught with even one cookie must have pilfered more than someone who hasn't been caught. The elf decides to talk with the union representative.

All of the aforementioned cases mimic actual practices with real water-quality data. The problem with cookie detection and analytical chemistry is that detection is not perfect-there is a gray area, a range that is semiquantitative. The problem can be minimized by improving detection ability, but neither cookie detectors nor NWQL can achieve detection capability that quantitates zero. The NWQL is proposing to use LT-MDLs and NDVs together to communicate ranges of certainty and uncertainty of measurements. That data will be used by someone.

Data interpretation will always be an issue. Users can bias results either by ignorance or by design. Unfortunately, few tools exist to help users interpret data and calculate statistics for a mixture of semiquantitative, nonquantitative, and quantitative data.

Data interpretation can be improved as follows:

- Use the best available laboratory methods to maximize quantitative data;
- Educate data users because they need to know the pitfalls of interpreting the data;
- Data users must be honest about what they know and what they don't know and think about how they intend to use the data; and, finally,
- Explore new approaches and develop new methods for handling the data.
- Bernadine Bonn, Hydrologist. Oregon District Office

Newsletter Staff

Jon Raese, Editor

The National Water Quality Laboratory Newsletter, is published quarterly by the National Water Quality Laboratory, U.S. Geological Survey, Box 25046, MS-407, Denver Federal Center, Denver, CO 80225-0046. For copies, call Jack Raese (303) 236-3464.