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Williams accepts NAWQA job

Robert S. (Bob) Williams, Jr., Chief of the National Water Quality Laboratory, has accepted a job as Assistant Chief for Operations with the National Water-Quality Assessment Program (NAWQA). Williams said that he will be working as an assistant to Tim Miller, NAWQA Chief. Effective starting date was October 1.

His new duties include principal NAWQA contact with the National Water Quality Laboratory, where he served as Lab Chief for the past 2 years. Williams will also serve on the NAWQA Leadership Team. Merle Shockey, Assistant Chief, will serve temporarily as Acting Chief while a vacancy announcement is issued for a permanent replacement. Shockey's telephone number is 303-236-3501 or he can be contacted by E-mail (mshockey@usgs.gov).

Focazio replaces Low

Mike Focazio has joined the Office of Water Quality for a 4-year term appointment to oversee the National Park Service Program. The program was formerly coordinated by Walton Low in the National Water-Quality Assessment Program.

StarLIMS prepared for orbit; data base to shine in New Year following test, validation phases

The National Water Quality Laboratory has purchased a commercial off-the-shelf Laboratory Information Management System (LIMS). The new system was purchased from LIMS USA, and the product being placed on-line is StarLIMS, version 7.0. The NWQL has been working with the vendor to customize the product to meet the Laboratory's diverse needs. StarLIMS was selected primarily because of the design flexibility that it offers. The StarLIMS product has a three-tiered design that consists of the data-base tier, the business rules tier, and the StarLIMS tier. The data-base tier contains the data and the Relational Database Management System (RDBMS). Oracle was chosen as the RDBMS for the Laboratory. The last layer contains the base StarLIMS executable software. The middle layer - the business rules layer - makes NWQL customization possible. The NWQL can add, change, or modify any of the business rules without impacting the other two layers. Also, the vendor can provide updates to the software without changing NWQL business rules.

A prototype of the data base was delivered in mid-August and NWQL personnel have been working with LIMS USA to validate the developed business rules and to test system applications. Over the next several months, the NWQL will parallel test the present LIMS system with the new StarLIMS and then conduct complete end-to-end testing. Plans call for placing the new system on-line soon after the New Year. The NWQL will be working closely with the Water Quality Users Group (Phoenix) to validate any part of the system that might impact District users. Tests will be set up with several District offices.



Kim Pirkey



Charles (Chip) G. Groat (left), USGS Director, toured the National Water Quality Laboratory June 29 as part of a continuing effort to become familiar with Survey sites. Gary Cottrell (right), NWQL chemist, who organized the tour, explains the operation of the sample log-in area. Others shown are Tom Maloney, chief, NWQL Quality Management Program and Dennis Markovchick, NWQL physical science technician.

Program chiefs named

Merle Shockey, assistant chief of NWQL, has announced selections for the Inorganic and Organic Chemistry Program chiefs. Linda Pratt was named chief of the Inorganic Chemistry Program, and Mark Burkhardt was appointed to fill the chief's position in the Organic Chemistry Program. Both appointments became effective April 11.

Pratt has been at the Lab for 17 years. She was first hired as a student in 1982 and worked in the Metals Unit. She worked her way up to supervisor of the Low-Ionic Strength Unit. In 1992, she was appointed chief of Laboratory Operations; 3 years later, the Computer Services Unit was added to Pratt's management responsibilities. Burkhardt has been a chemist and project chief in the Methods Research and Development Program since 1992. He served a year-long stint as acting chief, Organic Chemistry Program, in 1994. Burkhardt has worked in commercial environmental laboratories as a chemist and as a manager. He received his Ph.D. in analytical chemistry in 1989. Primary research interests include liquid chromatography coupled to mass spectrometry and the implementation of custom methods.

Mark Burkhardt (right), chief, NWQL Organic Chemistry Program, explains the operation of a mass spectrometer to Charles G. Groat (center), USGS Director, during a tour of the semivolatile analysis lab June 29. A mass spectrometer is used to determine pesticides. Seated in the foreground are Leslie Kanagy and Chris Lindley, chemists.



Balancing act required to keep metrological instruments calibrated

The National Water Quality Laboratory's analytical balances were moved with minimal interruption from the former NWQL facility on Ward Road to the new Laboratory on the Denver Federal Center. The balances were moved in three stages to minimize interruption in analytical operations. Several balances were shared between analytical units during the move so that some instruments would be operational at both locations simultaneously.

The Laboratory's analytical balances are calibrated, operated, and maintained within certain specifications. Analyst, balance representative, supervisor, balance coordinator, and balance contract specifications are set forth in a Standard Operating Procedure (SOP). All analytical balances are required to have a logbook. Balance logbooks contain periodic weight verifications, calibration checks, and maintenance records. The balance logbooks provide the documentation required for auditing purposes.

The NWQL balance service representatives calibrate, maintain, and certify that NWQL analytical balances are compliant with SOPs and operate within manufacturer's and national specifications. Manufacturer's specifications include maintenance of balance calibration, linearity, repeatability, and off-center loading. National specifications include the use of weight sets that are certified by the Colorado Bureau of Weights and Measures and are traceable to the National Institute of Standards and Technology.

Direct comments or requests for additional information to Beth Kellogg, NWQL balance coordinator (ekellogg@usgs.gov; 303/236-3477).



Beth Kellogg

Lab certified Y2K compliant after rigorous tests

Y2K compliance requires rigorous testing and documentation of all computer hardware and software, as well as for systems with embedded chips. Most of the instruments at the NWQL rely on embedded chips and proprietary applications programs. Although testing is best performed in a stable environment, this process was complicated at the NWQL by the move in March to the new laboratory and the replacement of many systems.

Moreover, there are about five personal computers (PCs) circulating between the Computer Services Unit (CSU) workshop for repair and the Production Program at any one time. Repaired PCs must be re-certified before they are returned to production.

The first step to certification was to inventory all equipment, including model numbers, operating systems, application software, and proprietary vendor software. The inventory also had to include versions of each software package plus any patches applied.

Vendors were contacted to determine known compliance and known patches. The compliance of the facility and network also had to be documented.

Analysts were required to document the compliance of their systems through vendor certification or by testing their systems with specified rollover dates. The first series of tests showed some surprising Y2K vulnerabilities. New systems, software, and patches were obtained, and systems were tested again. In addition, the analysts worked up contingency plans in case the system failed. Most instruments have PCs as instrument controllers; these PCs had to be tested independently and in conjunction with the instrument. There were over 300 PCs that had to be individually tested by using special software from NSTL, Inc. Diagnostics were run and the operating system was upgraded to be compliant. Application software had to be upgraded, and specified patches had to be applied. There were times that the application of an upgrade or a patch caused the whole system to die, which resulted in a steady stream of PCs entering the CSU workshop for repair.

Computer systems in CSU also had to be tested. The Distributed Information System was helpful in verifying the Data Generals and the general-purpose software. The laboratory-based software, however, had to be independently tested and verified. Systems were taken offline for end-to-end laboratory testing on two afternoons this past summer. This effort added to the workload because it was CSU's busiest time of the year.

The General Services Administration certified that the Laboratory was compliant, and the USGS Office of Program Support certified the network. The NWQL was certified compliant in August after collecting two file drawers of documentation! LANDesk software, meanwhile, was obtained to help with the upgrades on PCs and to maintain an inventory of software on each PC. Y2K work is still continuing. Vendor compliance must be checked regularly to ensure that a system is not removed from compliance lists. In addition, the NWQL is working with USGS Headquarters to develop plans for "Day One" on January 1st. Customers should be confident that the Laboratory will be operating and providing correct data the first week of the new millennia.

 Sandy Turner



Rachel Griffiths (standing on the right), of Thru-Put Systems, Inc., provided training recently for Organic Chemistry Program personnel in the operation of Target© chromatographic data-processing software. The Organic Chemistry Program is implementing the use of Target© software to standardize the processing of all chromatographic information for about 30 analysts who produce data for more than 30 lab schedules. This new package will reduce the number of data-reduction software platforms from three to one, and thereby streamline and improve cross-training, analyst flexibility, documentation, and software support.

USGS open house a hit with school children Visitors discover "Science for a Changing World"

Nearly 3,000 children looked at more than 100 interactive exhibits and experiments August 27 at the Denver Federal Center and the USGS National Earthquake Information Center in Golden, Colo. Hundreds of adults attended the same exhibits put on by 500 current and former employees along with other volunteers August 28.

As part of the Survey's 120th anniversary, the National Water Quality Laboratory provided tours and demonstrations for about 900 students and visitors August 27. Gary Cottrell and Dennis Markovchick helped to organize the lab tours.

Tom Casadevall, USGS Deputy Director, said "The public knows we make maps and register earthquakes, but the other things we do seem to be invisible." As the nation's largest water, earth, and biological science and civilian mapping agency, the USGS works in cooperation with more than 2,000 organizations across the country to provide reliable, impartial, scientific information to resource



LeJuan Ray explains colorimetric analysis for students during the USGS open house.

managers, planners, and other customers. This information is gathered in every State by USGS scientists to minimize the loss of life and property from natural disasters, to contribute to the conservation and the sound economic and physical development of the nation's natural resources, and to enhance the quality of life by monitoring water, biological, energy, and mineral resources.



Dick Hadley (retired, USGS) explains how sediments can be used to explore water quality. He presented a slide program at NWQL as part of the USGS open house.



Pat Alex (right), waits to meet her group from Bell Middle School as they arrive for tours, interactive exhibits, and experiments at the National Water Quality Laboratory during the USGS open house August 27 at the Denver Federal Center.



Biological Unit staffers Scott Grotheer (with cap) and Dan Pickard (right, background) collected live aquatic insects for the children to study at the USGS open house.



Kathy Lindblom demonstrates the polymerization process by making silly putty.



Mary Olson (right) discusses gas chromatography/mass spectrometry with a group of middle school students during NWQL tour at the USGS open house.



Three young guests explore inductively coupled plasma technology with Carl Harris (background) who makes a point during lab tours at the USGS open house.



Students learned about an Internet Web site where real-time streamflow data are available. Rick Crowfoot (standing behind table) explains the exhibit.



Chris Kanagy explains how organic compounds are extracted from water samples and then concentrated prior to analysis.

Surrogate terbuthylazine removed from schedules 2001, 2010, 1379

The triazine terbuthylazine has been used as a surrogate in NWQL schedules 2001, 2010, and 1379. It was selected as a surrogate because we believed that it would not be found in the United States (an assumption found to be untrue). More recently, results of the analysis of terbuthylazine provided by the manufacturer showed small amounts (less than 1percent) of simazine and atrazine. Unfortunately, these "impurities" - similar compounds that probably resulted from synthesis of the terbuthylazine - are compounds in each of the methods. For these reasons, terbuthylazine has been removed from the schedules, effective July 1999. The isotopically labeled compounds alpha-HCH-d6 and diazinon-d10 remain as surrogates.

Significant concentrations of terbuthylazine may be present in environmental water samples, and, therefore, it will be considered a selected method compound, with the reporting units changed from "percent recovery" to " $\mu\text{g/L}$ " (microgram per liter). The National Water Information System parameter code used to reflect this change is 04022. Detections will be qualified using the E (estimated value) code until a method validation study is completed.

The NWQL has prepared new field surrogate mixtures for schedules 2001/2010, which do not contain terbuthylazine (they still contain diazinon-d10 and alpha-HCH-d6). Surrogate mixtures containing terbuthylazine will no longer be provided. Note that detections of terbuthylazine from older surrogate lots, if used, will be reported as a concentration. For example, what would have been recovery at 109 percent will now become $0.109 \mu\text{g/L}$ (assuming 1,000-milliliter sample size). However, the result will be qualified with an E (estimated) code: E0.109.

A memorandum titled "Surrogate Terbuthylazine Removal from Methods 2001/2010 and 1379" was posted June 30 to usgs.nawqa and usgs.water.quality news groups. More information about the removal of this surrogate from the schedules can be found there, as well as the schedule 2001/2010 page available to USGS employees at <http://wwwnwql.cr.usgs.gov/USGS/WWW2001/2001qc.html>.



Standley presents seminar on molecular tracers

Dr. Laurel Standley, chemist at the Stroud Water Research Center, Avondale, Penn., reported to NWQL that sources of organic matter in ground and surface water are a growing concern to the drinking-water industry. Standley said the presence of organic matter in drinking water might promote regrowth of pathogenic microorganisms in distribution systems. She said the microorganisms could be transformed into toxic byproducts during disinfection.



Dr. Laurel Standley (left), Stroud Water Research Center, Avondale, Penn., spoke on "Molecular Tracers of Organic Matter Sources to Drinking-Water Supplies," at a Lab seminar August 3. Bob Green, chief, NWQL Methods Research and Development Program, discusses issues with the speaker.

Water-quality specialists to meet in California

The Office of Water Quality and the Regional Water-Quality Specialists are winding up plans for the 5th National Water-Quality Specialists Meeting, November 30 through December 3, in Costa Mesa, California. Primary objective of the meeting is information and technology transfer within the U.S. Geological Survey. Topics include new technology, data-base and data-analysis operations, emerging contaminants, and regulatory issues. The meeting will combine plenary sessions with concurrent workshops. NWQL participants include Bill Foreman (long-term method detection levels) and Ed Furlong (contaminants of emerging environmental concern), research chemists in the Methods Research and Development Program. Information regarding the conference is available on the Web at <http://water.usgs.gov/usgs/owq/specialistmtg/index.html>.



Diane Stephens

Vasquez retires

I would like to thank everyone for the nice cards, send-off lunch, fantastic gift certificate, and best wishes extended to me as I go off into another phase of my life. It has been a pleasure working at the NWQL despite the tough year. In a short time, Y2K and StarLIMS implementation will be behind you and this lab will become the first class one-of-a-kind organization it was destined to be.



Juan Vasquez,
Nutrients Unit Chief

Earth Science Week

Earth Science Week will be celebrated October 10-16. This annual event was started last year by the American Geological Institute to highlight the vital role that geosciences play in society's stewardship of the environment. "Earth Science Week provides an opportunity for the U.S. Geological Survey to increase public awareness of the exceptional job we do by integrating hydrology, geology, biological science, and mapping for the public good," said Charles G. Groat, USGS Director, in a recent message to employees.



Dr. Pamela Greenlaw, Department of Energy Environmental Measurements Lab, New York, addressed NWQL staff on the subject of "Data Validation" at a seminar August 3.

Method detection levels discussed in new report

The USGS Office of Water Quality has published the following report: Childress, C.J.O., Foreman, W.T., Connor, B.F., and Maloney, T.J., 1999, New reporting procedures based on long-term method detection levels and some considerations for interpretations of water-quality data provided by the U.S. Geological Survey National Water Quality Laboratory: U.S. Geological Survey Open-File Report 99-193, 19 p.

Newsletter Staff

Jon Raese, Editor
Stacy Steyer, Production Assistant

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