Water Quality and Resource Management Issues

WORKSHOP REPORT

Facilitated By:
National Water Research Institute

in cooperation with:
Lawrence Livermore National Laboratory
University of California

January 28-30, 2003

Wente Vineyards
Livermore, California

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FOREWORD

In 1992, the National Water Research Institute (NWRI) searched for a means that would bring together water professionals from varying disciplines, viewpoints, and responsibilities and enable that group to reach consensus regarding a significant question. William Gaither, Ph.D., then Executive Director of the Weston Institute, Chester, Pennsylvania, recommended a group process known as the Nominal Group Technique (NGT), which was developed in the 1960s by Andre L. Delbecq, Ph.D., from the University of Santa Clara (California), and his colleagues, Andrew W. Van de Ven and David H. Gustafson, both from the University of Wisconsin.

The NGT is a robust and rigorous process, and its protocol provides a controlled environment that allows every voice to be heard regardless of perspective. The ability of the workshop participants to focus on a single question allows for the maximum use of time and energy during the intensive 2 days where no single individual can provide an adequate response. The participants attending were invited because of their expertise and credibility in their respective fields.

The original NGT comprised 3 elements: issue identification, consolidation, and prioritization. However, in collaboration with Dr. Gaither, NWRI modified the Delbecq method by adding a fourth component that provides for working groups to further refine the prioritized consolidated issues into a more meaningful report that includes strategies to reach positive outcomes or actions to resolve the identified barriers, impediments, issues, or problems.

This document reports the results of the NGT workshop that NWRI conducted on behalf of the Lawrence Livermore National Laboratory (LLNL) to assist in building a research strategy by linking the skills and talents of the staff at LLNL from a variety of water-related science and engineering disciplines. The focus of the workshop was the question: ***What priority research issues need to be addressed to enable LLNL to make a unique contribution to national and international water quality and resource management needs?***

This document comprises 2 parts: Part 1 (Working Group Reports) presents a more detailed version of the top 10 issues that were prioritized from the 18 consolidated issues generated during the NGT portion of the workshop. Participants were assigned to one of the 10 working groups. Each group was asked to digest and synthesize all of the individual issues that were consolidated under their priority issue. The Power Point slides that were used by the working groups to enhance their presentations are found in Appendix D.

Part 2 (NGT Workshop) reports the results of the issue identification and consensus-building elements of the workshop. The participants identified 80 research issues that were consolidated into 18 overarching themes. The fact that the participants were able to identify 80 issues demonstrated the significance of the workshop question from their individual perspectives for the need to create a strategically integrated organization to engage in water science and engineering research opportunities.

This document reports the results of the creative efforts of all those who participated in the 2-day event with as little editing, as needed, to ensure the integrity of the participants' contributions.

The success of the NGT is in no small part due to the support provided by and collaboration between the NWRI and LLNL staff. Special thanks are extended to the Workshop editors Patricia Linsky and Gina Melin; Word Processing Coordinator Tammy Russo; Word Processors Cheryl Kuks, Holly Barnes, and Paula Foerschler; Photographer Maureen Rausch; Graphics Coordinator Barbara Close and her assistant Jane Wimborough, who did a masterful job of keeping the flow of ideas and issues in front of all the participants.

Special thanks go to Brian Brady, who so masterfully served as the Workshop Secretary and kept track of the issues to ensure their clarity. Thanks also is extended to Dana Christensen, Deputy Associate Director of the Energy and Environment Directorate, and Dave Rice, Group Leader of the Environmental Chemistry and Biology Group, for giving NWRI the opportunity to assist LLNL in their endeavors to advance research excellence in water science and technology.

Ronald B. Linsky
Executive Director
National Water Research Institute

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PARTICIPANTS

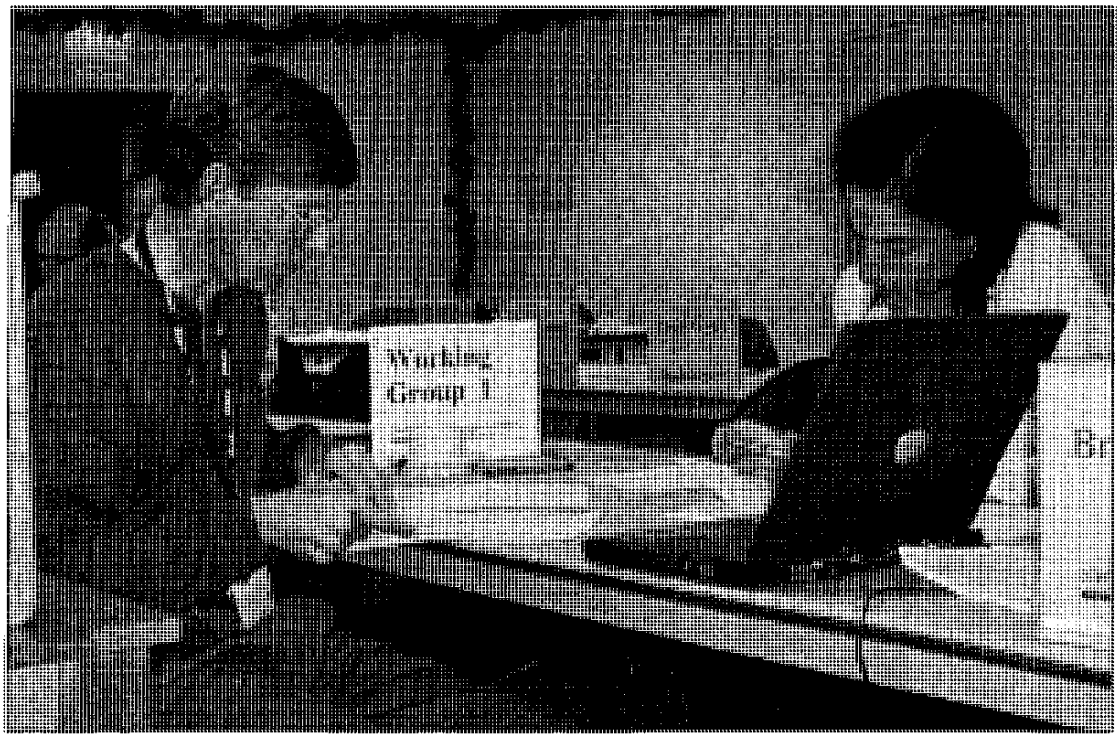
Top Row (Standing): Dave Rice, Brendan Dooher, Walter McNab, William Boucier, Harry Beller, Dana, Christensen, Steve Grey, Alan Lamont, David Layton, Kevin O'Brien, Greg Mack, Jean Moran, Jeff Stewert, Ron Linsky (Facilitator) Brad Esser, Brian Brady (Secretary)

Middle Row (Seated): Peg Folta, Nina Rosenberg, Joanne Horn, Robin Newmark, Betsy Cantwell, Jessie Coty, Jill Watz, Gina Melin (Editor), Tammy Russo (Workshop Coordinator), Barbara Close (Graphics), Patricia Linsky, (Editor), Jane Wimborough (Graphics Assistant)

Bottom Row: Bill Hoppes, Bryan Hudson, Dick Woodward, Daniel Barsky, Cheryl Kuks (Word Processor), Paula Foerschler (Word Processor), and Holly Barnes (Word Processor)

PART 1

WORKING GROUP REPORTS


Working
Group 1

PRIORITY 1

Value Water

WORKING GROUP MEMBERS:

Bourcier and Coty, in collaboration with Stewart

Research Issue Description:

The success of water research and development (R&D) projects demands an understanding of the value of water. This requires integrating attributes of complex systems, including impacts of climate change, natural and man-made storage and conveyance systems, changing land use, multiple quality demands, water-material interactions, technology integration, as well as others.

This model for determining the value of water will direct the types of R&D activities that will help to ensure water quality and supply. Water value modeling provides a basis for multiple R&D efforts. These include:

- Understanding the economic contribution of adding new water to the system.
- Selecting infrastructure investments.
- Optimizing water allocation for environmental uses.
- Determining appropriate water technologies and energy system structures.
- Determining the value of remediation efforts.

Importance:

- Key to eventually meeting the world's water needs in the most economic way.
- Non-optimal investments in water research, development, and deployment wastes society's resources.
- Avoid investments into remediation efforts that are not effective or economic in providing new water supplies.

- Better identify the types of water technologies that should be used and help identify how the energy system should be structured to efficiently accommodate water management.

- Provide an understanding of the different values of water for different users (i.e., water value not only based on cost, but also services and/or other values).

How Do You Propose Meeting or Complying with This Research Issue?

- Implement an action plan that identifies a key sponsor.

- Include potential sponsors on the advisory board for model enhancements.

- Conduct semi-annual CALVIN training seminars for state and Federal agencies, universities, and international and national non-governmental organizations (NGOs). This has been started by the University of California, Davis (UC Davis) and would be expanded to include LLNL.

- Review other water optimization models.

- Extend existing water economics models and develop additional models. These include the CALVIN optimization and CALSIM models in conjunction with CALFED published goals. This will be done with CALFED staff.

- Use the enhanced models to evaluate the value of proposed water R&D projects.

- Use a Water Resources Integration and Assessment team (i.e., that includes key agencies and NGOs) to assess each project proposal for its applicability, usefulness, transferability, and economic viability.

- Establish a web-based interface for sponsors to run "simple" scenarios on LLNL servers. Complex model runs would be run by LLNL staff.

- Allow universities to use models for classes and research via the web.

Water value modeling provides a basis for the following projects:

- Develop a water resources research integration and assessment program that will assess proposed water resource technologies and tools to provide guidance that ensures applicability, usefulness, and transferability. This assessment team should also include an advisory board comprising representatives and stakeholders of key agencies.

- Consider the benefits of the wholesale abandonment of aquifer remediation efforts in lieu of allocating resources directly into wellhead treatment and institutional controls.

- Create a National Center to organize, integrate, develop, and apply science-based systems to manage supply, storage, distribution, quality, and use.

Exit Plan:

- Add potential sponsors and key NGOs to the Model Requirements Committee to ensure that model upgrades will create a need by potential sponsors.

- Consistently conduct training workshops nationwide for funding agencies, universities, and NGOs. This will help foster current and future reliance on our model.

Key Additional Tasks:

- Incorporate basic research evaluations into this proposal.

- Incorporate marketing of these capabilities, including workshops, demonstrations, and others (Note: Ensure these are given in the language of clients, rather than modeling lingo.).

- Participate in the annual LLNL Water Research Workshop and Training.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

- Alan Lamont, Decision Scientist, LLNL

- Jeffrey Stewart, Economist, LLNL

- Yiming Yao, Optimization, LLNL

- Professor Jay Lund, Water Resources Engineer, UC Davis

- Professor Richard Howitt, Agricultural Economist, UC Davis

- UC Davis Grad Student/Post Doc

- LLNL Researchers

- CALFED

- U.S. Department of the Interior, Bureau of Reclamation (USBR)

- California Department of Water Resources

- U.S. Army Corps of Engineers (COE)
- Key NGOs
- World Bank
- United Nations Development Programme

Budget:

- Couple CALSIM with CALVIN model; develop statistical techniques to reduce data requirements and enhance usefulness in data-poor environments. (Months 1-18)
- Add a non-linear optimization solver to CALVIN for modeling of water quality and more complex scenarios. (Months 19-36)
- 2 FTEs plus $100K for UC Davis.

Deliverables and Goals:

- Model runs demonstrating integration of CALVIN and CALSIM. Have state line item funding set up for continued support of CALVIN. (Years 1-2)
- Obtain federal funding from agencies represented on the advisory board for applied research. (Year 3)

Comments:

"This vision for the value issue is too small. Let's start by seeing what policy bodies in the U.S. address this issue. Do the CALVIN project, as proposed, but spend some marketing money getting people on NSF panels, speaker committees, etc. Look for early high-value external partners." – ***Betsy Cantwell***

"Get an action in place to assure ourselves that someone wants improved CALVIN with optimization. Make certain we are optimizing around parameters of interest to other users. Get an action focused on 'sponsor's problem'." – ***Dana Christensen***

"Didn't see all seven 'ideas' in the report. Non-linear modeling expertise exists in (ASC-suggest a consultation). The board to steer/recommend seems to be made up of too narrow an audience. Unclear what the purpose of the board is? (Yes/No on project?) Directions? Large overlap with priority group 8). – ***Peg Folta***

"How do you incorporate non-economic value factors (e.g., environmental integrity/biodiversity; things like energy production, which has a value but may be central to other critical processes). Fix-up the review board function to clarify intent." – ***Joanne Horn***

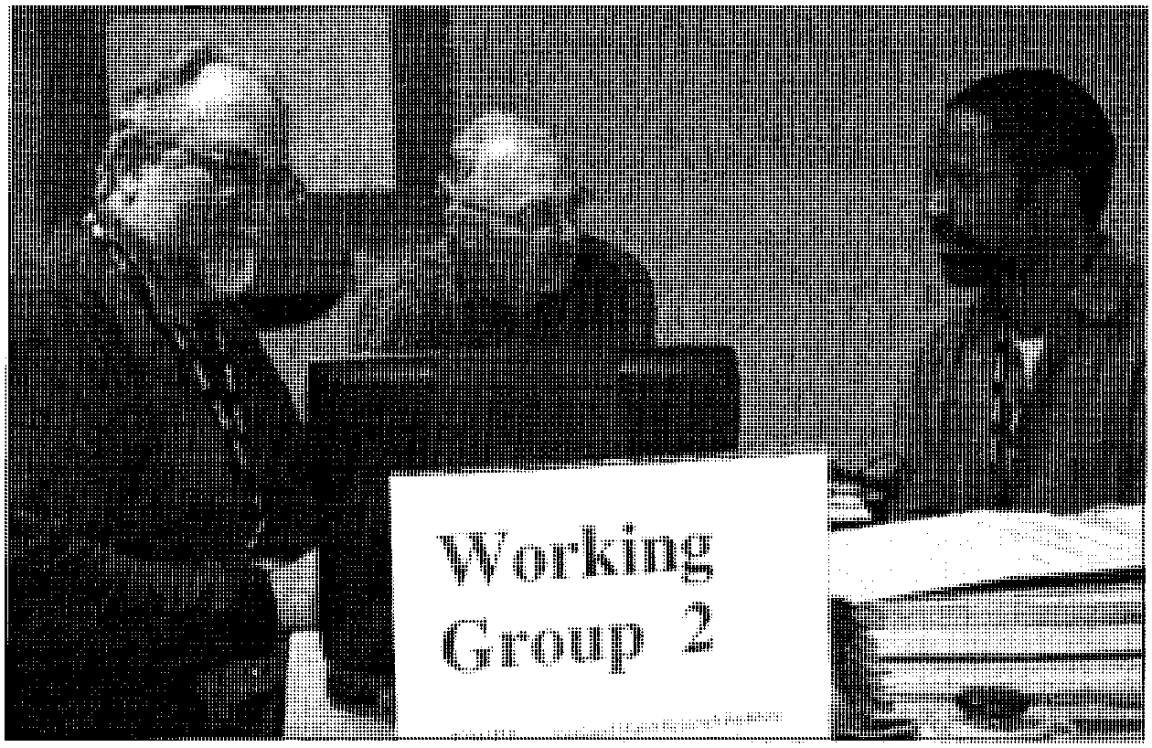
"The proposed 'value' models represent a beginning, but they seriously lack 'real' quantitation. So, the first issue is to explore the range of valuation estimates. It will take significant work to establish the ability of the proposed models to actually calculate the value of water. How will this project demonstrate its reliability and accuracy?" – ***Bryant Hudson***

"Utterly brilliant. Comments from the crowd indicate a need for better discussion of who would use model; what they would use it for; and what value it would provide." – ***Alan Lamont***

"I'm not sure this should be Priority #1 research, as stated. It is an important thing to be kept in mind but does not have an exit plan or identified funder. There are other groups (GOs and NGOs) who are further along in this area. Some of the original ideas proposed under this area were not included." – ***Jean Moran***

"Having an advisory committee to assess the impact or value of proposed R&D projects is a good idea. The composition of such a committee must include perspectives from multiple facets of the water world, and thus must include people familiar with multiple stakeholders, if not actually be those stakeholders. While the proposed enhancements to CALVIN seem useful, and its application may be significant in California, I had hoped this working group would make some effort to address the more fundamental, yet diverse, issues regarding the value of water – not just to CALFED or California, but from other perspectives. (We talked about industry, for example.)" – ***Robin Newmark***

"In establishing the value of water, examine and incorporate, as appropriate, approaches to valuation that others have used. For example, the Wisconsin models." – ***Dick Woodward***


Working
Group 2

PRIORITY 2

LLNL Water Resources Simulator: A Coupled, Scalable, Data-Driven System to Optimize Water Management Solutions

WORKING GROUP MEMBERS:

Layton, Rice, and Stewart

Research Issue Description:

Water management in the 21st century will deal increasingly with issues involving both hydrologic and biogeochemical processes. Accordingly, if LLNL is to play a role in developing robust solutions for various kinds of water management challenges (e.g., water banking, remediation, well siting, nitrate contamination, salinity management, etc.) in different geohydrologic settings, then a simulation system must be developed that can deal with complex, coupled processes. In addition, simulation of distributed geohydrologic and geochemical processes requires spatial and temporal information on the system being addressed. Hence, the cost-effective acquisition and analysis of relevant data are essential parts of developing realistic and valid simulations of a given system.

There are two key components to this challenge. The first is the identification and acquisition of relevant data, and the other is the processing of that data to provide the necessary model input parameters and associated revisions from calibration exercises. Existing data can come from well data (e.g., logs, pump tests, tracers, and isotopic composition of water), historic hydrologic and climatic data, and remote sensing information (e.g., land uses, InSAR, etc.). The analytical software for processing data will directly support the LLNL modeling system used to simulate geohydrologic/biogeochemical processes.

Importance:

Decisions regarding the development and operation of sustainable water systems (for supply and quality) will be one of the single most important challenges facing the global water management community. Failure to develop and apply models that can simulate complex hydrologic (coupled surface and subsurface flows) and biogeochemical processes will inhibit the implementation of scientifically defensible solutions for site-specific hydrologic and water-use conditions.

Methodology and Schedule:

The LLNL Water Resources Simulator will consist of four principal components:

- Dynamic Data Warehouse, a data warehouse where applicable information on a given site is stored.

- Data Processing and Analysis Rule Sets, a data processing system for preparing inputs to the core water resources simulation system.

- Water Resources Simulator, a hierarchical set of scalable, coupled hydrologic-biogeochemical models.

- User Friendly Interface, a user interface consisting of visualization tools to aid in the interpretation of hydrologic simulations.

Development and implementation of the system should begin with specification of design criteria, preparation of a conceptual model that incorporates the design, and then a determination of how to implement the conceptual by modifying existing computer models and/or creating new ones. Important design criteria include:

Dynamic Data Warehouse

- Facilitates geospatial data sets (e.g., land uses, geology, etc.) and manipulation.

- Capable of data mining from web sources and other distributed data sources.

- Incorporates remote sensing data.

- Can include data from existing sources (e.g., groundwater ambient monitoring and assessment [GAMA], Georeferenced Integrated Environmental Management Systems [GIEMS], etc.).

Data Processing and Analysis Rule Sets

- Seamlessly connects data processing algorithms to data warehouse.

- Capable of performing parameter inversions on multiple geohydrologic and geochemical parameters.

- Incorporates geostatistical techniques for handling sparse data.

- Includes data fusion tools to process data from the warehouse.

- Provides seamless preparation of inputs to the water resources simulation system.

- Capable of processing data on variable spatial and time scales.

- Significantly cuts the costs and time of model data preparation compared with existing techniques.

- Takes advantage of tera-scale computing at LLNL.

Water Resources Simulator

- Designed to handle a broad variety of water resources processes and issues:
  - coupled surface and subsurface water flow
  - coupled water and biogeochemical processes (e.g. salt build up, nitrate transport, and fate)
  - runoff from agricultural and urban lands to surface water
  - spatial distribution of water use
  - artificial recharges using streams, infiltration ponds, aquifer-storage recovery wells, etc.
  - land subsidence
  - contaminant transport and transformation
  - surface water dynamics, including ecological processes as a module

- Takes advantage of tera-scale computing at LLNL.

User Friendly Interface

- Enables efficient problems setup.

- Permits "options gaming" by water policy decision makers.

- Allows clients to see how they may use the system.

Implementing Team:

The research team would consist of a group of LLNL scientists who have a strong background in the simulation of geohydrologic systems, including water movement in saturated/unsaturated flow regimes and associated biogeochemical processes. Other staff are needed who have expertise in geostatistical techniques, Geospatial Information Systems (GIS) software and applications, database design and supporting software, data fusion, inversion methods, etc. Finally, software engineers are required to develop and implement the visualization tools, connectivity of data and models, and user interfaces. The LLNL staff would be complemented by researchers from the University of California.

Proposed Budget:

- Dynamic Data Warehouse: 1.5 FTEs/yr ($300K)

- Data Analysis and Processing Rule Set: 3 FTEs/yr ($600K)

- Water Resources Simulator: 3 FTEs/yr ($600K)

- User Friendly Interface: 0.5 FTEs/yr ($100K)

Comments:

"Nice vision; might need a bit more involvement from external sources who do this type of thing for other appropriate areas (like businesses - e.g., Siebel, Oracle)." – ***Betsy Cantwell***

"Simulate water supply, quality, and security. Scope: California only? Nation, Global? Major change. Design: s/w h/w needs more thought. Design, you aren't there yet. If ever thinking of licensing, s/w, h/w (system) design will be a huge issue – do it right the first time. Please involve comp. Early. I'm ready, willing, and able; we can leverage immensely from the National Atmospheric Release Advisory Center (NARAC)." – ***Peg Folta***

"Probably should add MODFLOW (visual) to the Resources Simulator. Try to map computationally intense models into smaller (lower resolution) models that could run on PC and still retain 80 to 90 percent of the content. Priority 1 is a subset of Priority 2? – ***Bryant Hodson***

"CALSIM has developed a 'complete' water modeling environment. It includes data files for the structure of a water system, data, model solver, software to reduce, analyze, and display results. Developing this system to be compatible with CALSIM would make it much more accessible to Illinois State and get us more closely involved with the State's work." –***Alan Lamont***

"Early in the presentation, I heard references to this priority research area being similar to ARAC. Apparently Hal Graboske coined a team to encapsulate this area called 'WARAC'." – ***Greg Mack***

"How will you attract and gain sponsorship? When? (In project.) I'm worried about the 'if you build it, they will come' mentality). Addressing the data access/mining issue is good. For each application, however, we may need to build a separate model with case-specific data streams. Marketing and multiple sponsorship in specific regions will aid in our success. Ultimately, we need to find a sponsor who will pay for both the capability and the service." – ***Robin Newmark***

"Looks like a great package – one that would include many of the lab's strengths in water. Unless LLNL gets in on the ground floor of AB 599 efforts, the state of California will be paying someone else to do the IT work. Supercomputing effort is unique to LLNL but requires a customer with deep pockets. Comments on scaling down a high density model need to be part of the plan." –***Jean Moran***

"Add regional climate runs to the modeling tool set." –***Jeff Stewart***

PRIORITY 3

Water Infrastructure Security

WORKING GROUP MEMBERS:

Christensen, Rosenberg, and Watz

Research Issue Description:

Water security is linked to energy security, and both are intimately linked to national security. This applies both nationally and internationally.

On the national side, this initially involves vulnerability assessment of key water and energy infrastructure (e.g., water utilities, reservoirs, dams, power plants, aqueducts, canals, distribution systems). Addressing these vulnerabilities then involves developing technologies that contribute to building redundant systems, hardening systems, and establishing monitoring systems (advanced sensors/detectors/signaling systems). This also involves emergency response planning and preparedness as well as recovery.

On the international side, many of these same concepts apply in the first world. In the developing world, water security first involves meeting the more basic demands for clean water and energy. Regional security in many important parts of the world requires addressing conflict over shared water resources (e.g., Nile, Jordan, Aral Sea, Tigris-Euphrates) and energy infrastructures. Addressing the security of these water/energy systems will lead to improved international stability.

Importance:

- Ensures adequate and reliable water and energy supplies for national needs.
- Reduces the probability that water and energy conflicts/problems will lead to regional instabilities in areas of the world of strategic importance to the U.S.

How Do You Propose Meeting or Complying with This Research Issue?

The responsibility for protecting the domestic water sector currently rests with the U.S. Environmental Protection Agency (USEPA). We will build on existing relationships with the two key organizations at USEPA for water security (Water Protection Task Force at headquarters and Homeland Security Research and Development Center in Cincinnati). LLNL currently has a good relationship with both organizations, including an existing (WFO) contract with the Water Protection Task Force. We have been invited to participate in R&D stakeholders meeting with

USEPA; have had several meetings with key persons; and are planning a visit of key persons to LLNL this spring. We plan to continue our dialogue with USEPA about their R&D needs and continue to respond to proposal requests. We will also continue to build on existing relationships with individual major water utilities in California and consortia of water utilities (e.g., BASIC, American Water Works Association Research Foundation [AWWARF]) and other federal agencies with an interest in water (e.g., USBR, COE). We need to also build relationships with the high-level decision makers at USEPA to establish a leadership position. We need to identify Congressional committees that influence the related funding decisions. We need to explore other possible customers with water security concerns (e.g., U.S. Department of Defense [USDOD]).

Key water sector security needs are:

- Integrating vulnerability analyses across agencies and across the nation.
- Establishing early warning systems.
- Preparing for analytical responses to suspected intentional contamination events.
- Understanding fate and transport of contaminants within distributions systems (e.g., reaction with chlorine, ozone).
- Continuously improving on threat assessments.

Key LLNL "calling cards" include:

- Well-established and formal systems to protect sensitive information.
- Access to and ability to properly and securely handle classified materials.
- A national security culture/experience with respect to threats.
- A reputation and recognized expertise in high-tech sensors and detectors (e.g., BASIS, HANNAH).
- Experience with handling significant quantities of hazardous and dangerous materials, especially including nuclear-biological-chemical materials.

Applying these capabilities to the problems surrounding water and water infrastructure is a key step for LLNL.

LLNL needs to prepare white papers and marketing plans to take advantage of the opportunities in this area.

The organizations with interest in the international aspects of water security include the Department of State, USDOD, and U.S. Department of Energy (USDOE), but the money

available for these activities is very limited and difficult to obtain. We have existing relationships and several very small projects in this area. Possible actions to consider include:

- Strategizing post-Iraq war opportunities for regional recovery in the Gulf.

- Following-up on international activities regarding the development of tools to address transboundary aquifer problems.

- Further exploring reducing the cost and energy intensity of water treatment technology as a means of increasing access to clean water in the developing world and, therefore, promoting greater stability.

Another key focus for LLNL's water-related activities in the international area is China. LLNL will continue to engage China. LLNL has memorandum of understanding with Beijing University to work on water purification technology and is planning to host a visit by the Chair of the Environmental Engineering Department in 2003. LLNL will also continue to participate in the interagency group planning for the 2008 Olympics in China.

Energy is critical to water systems. Energy is derived from water (e.g., hydropower). Water is consumed in energy production (e.g., cooling towers, processing). Moreover, energy (electricity) is critical to treating and distributing water (especially in California). Interdependencies between energy and water systems are not well characterized and needs to be better assessed for the purposes of preparedness planning.

The responsibility for Critical Infrastructure Protection for the energy sector is moving from the USDOE Office of Energy Assurance (OEA) to the Department of Health Services (DHS) on March 1, 2003. LLNL is participating in an OEA's DOE-wide symposium on key lab technologies in support of protecting U.S. energy infrastructure.

What do we have to offer with respect to energy security?

- We have experience with vulnerability assessments in the energy sector under the VRAP program, and we are currently trying to expand the analysis to include more sophisticated LLNL decision and risk analysis capabilities.

- We are recognized as a major player in cyber security, which underpins the critical assets of the energy sector, such as SCADA and electricity markets/operations systems.

- We are recognized for physical protection capabilities (e.g., ARGUS, JCATS, smart camera) and emergency response capabilities (e.g., NARAC).

- We have experience and are recognized for sensors systems for intrusion detection.

- In order to protect the future electric grid from potential threat, an entirely new paradigm for systems control is required. Additionally, there has been a request by the Federal Energy Regulatory Commission [FERC] to develop a national electric grid monitoring system for

future markets, which could be developed into a dual-role system for real-time grid monitoring and control for security. Redesigning of a national electric grid control system is a massive, long-term undertaking requiring new mathematical, engineering, and computational approaches. LLNL has capabilities in the areas of supercomputing, control systems, signal processing, and visualization tools for large-scale dynamic system monitoring and assessment and system science. These capabilities, coupled with partners with expertise in power systems dynamics such as Carnegie-Mellon University (CMU), Electric Power Research Institute (EPRI), various International Organization for Standardization (ISO), and key industry partners (e.g., General Electric [GE], ABB, Honeywell), provide a team capable of meeting the mid- and long-term research needs in this critical area.

Near-term actions include:

- Identifying the new decision makers in DHS, particularly the Office of Information and Critical Infrastructure Protection.

- Expanding the VRAP program to include better analysis tools.

- Developing a white paper to evaluate interdependencies between the energy and water sectors (DHS/USEPA?) and threat protection/response options.

- Evaluating types of tools developed in the cyber security program that can be applied to energy sectors. Proposing new or augmented tool development for control and protection schemes.

- Developing and submiting a white paper between LLNL, CMU, and EPRI (possibly RAND) to DHS for a comprehensive research program in the next generation electric grid modeling and control (i.e., software and hardware).

Who are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue:

Water security team members at LLNL include: Nina Rosenberg, Betsy Cantwell, Brendan Dooher, Dick Woodward, John Reynolds, Alan Burnham, and others. External organizations include: USEPA, DHS, USBR, AWWARF, water utilities (Metropolitan Water District of California, San Francisco Public Utilities Commission and others), BASIC, Edgewood, AMWA and the first responder community.

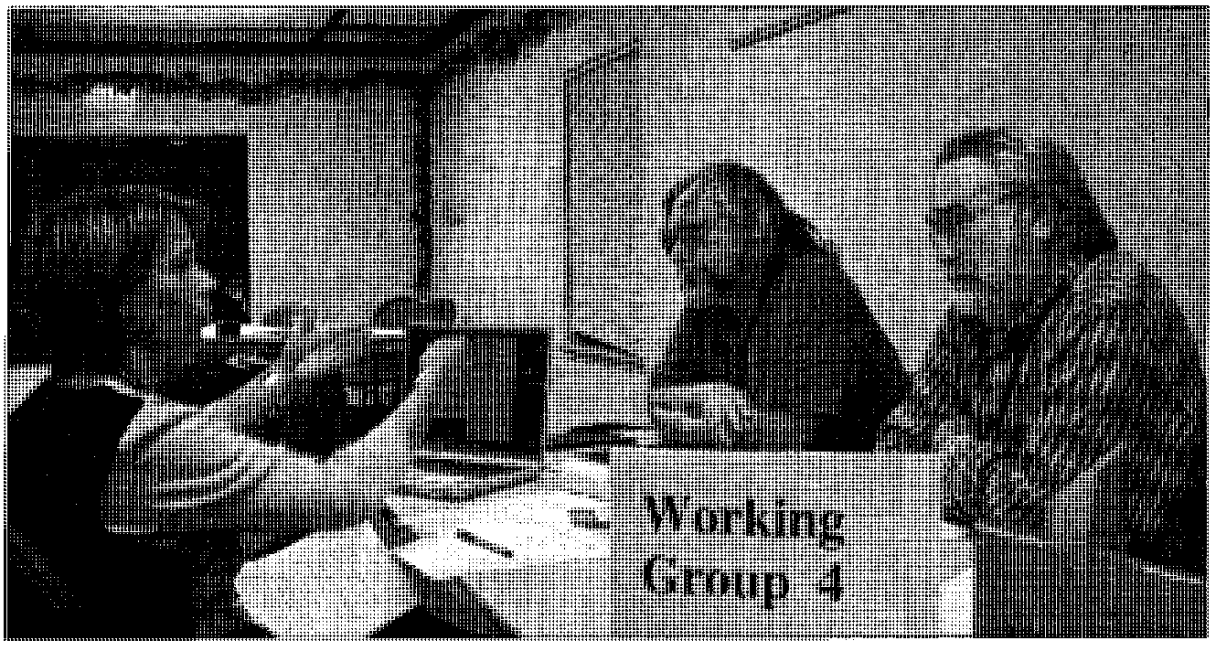
Energy security team members at LLNL include: Jill Watz, Ed Jones, Craig Schultz, Steve Azevedo, Tom Edmunds, Brian Lopez, Jean Savy, Greg Davis, and others. External organizations include: CMU, EPRI, RAND, FERC, CAISO, USDOE, CEC, DHS, U.S. Army Corps of Engineers, and USDOD.

Comments:

"A real opportunity exists for community involvement – should talk soon to Susan Houghton (runs Public Affairs) about the value to LLNL of doing this. Also, I think LLNL needs a multi-directorate steering committee for water security. No more than four people!" – ***Betsy Cantwell***

"How about incident intervention/mitigation – you spoke about detection, but shouldn't we address response?" – ***Joanne Horn***

"Seem to have a good feel for the landscape (technical, needs, and players), as well as action plans for building in this area. Multiple potential sponsors – this will require investment to pursue them." – ***Robin Newmark***


Working
Group 4

PRIORITY 4

Assess and Predict the Impact on Water Quality of Choices in Land Use and Management Practices

WORKING GROUP MEMBERS:

Hoppes, Newmark, and Woodward, in collaboration with Esser

Research Issue Description:

We will develop a capability that includes coupled model systems that encompass the range of atmospheric/surface/groundwater interactions that control water quality. Temporal and spatial scales need to reflect realistic cases. Key components include:

- Atmospheric precipitation driving models coupled through the surface.
- Groundwater flow models.
- Particle-based transport modeling.
- Reactive transport models, with appropriate biogeochemistry; need to address fluxes resulting from specific land uses (parameterization will be important).
  - natural ecological sources
  - urban/industrial runoff
  - agricultural runoff
  - point and nonpoint source discharges

Scenarios must be able to simulate outcomes from different management practices, at the appropriate time scales. These include choices in water use and discharge restrictions specific to each land use. These models must be field-testable using a suite of groundwater tracers and age dating techniques, coupled with groundwater flow models. Examples of management practices are:

- Irrigation methodologies, volumes, locations, and timing for a specific basin and/or crop.
- Land conversion practices for habitat restoration.
- Choice of water conveyance: speed and volume.

- Flood management practices.

Importance:

Managers do not currently have the science-based tools necessary to guide policy decisions in land use planning and choices in management practices. What is needed is a robust means to correlate changes in groundwater quality and quantity with changes in land use, agricultural operation management practices, and water management practices (including artificial recharge). While individual portions of the problems can be addressed by specific models (i.e., groundwater flow or water allocation models), an integrated suite of tools must be used to assess the impact of such decisions on overall water quality and quantity. A multi-faceted approach is needed.

Factors affecting water quality and quantity in California include the following:

- Regulatory limits (which tend to decrease over time [e.g., arsenic]).
- Use of groundwater basins to store and manage surface water supplies (conjunctive use).
- Intrusion of poor quality groundwater, saltwater, or brine as a result of excessive pumping.
- Salinization of aquifers resulting from surface irrigation by imported surface water.
- Recharge using reclaimed water (e.g., Orange County, California).
- Nonpoint source pollution (e.g., nitrate).
- Water supply.
- Changes in surface water elevation due to groundwater drawdown, often accompanied by surface subsidence.

How Do You Propose Meeting or Complying with This Research Issue?

- Build coupled model systems (described above).
- Validate the process through demonstration in historic case analyses in which management decisions can be tested through a combined experimental/simulation analysis in partnership with water resource agencies and agricultural interests.

An integrated approach would:

- use groundwater tracing (with noble gas tracers and tritium-helium ages)
- determine the true groundwater ages (with groundwater models strongly coupled to apparent groundwater age)

- develop and demonstrate source tracers (with isotope and trace inorganic and organic geochemistry)
- develop and run forward simulation scenarios
- analyze and compare results

Examples from Santa Clara Valley, California:

- Assessing the impact of a nitrate management plan: In the Santa Clara Valley, California, changes in agricultural practices, in terms of timing and application of fertilizers and irrigation, were due to guidance by the agricultural extension service. A historic case analysis would document the changes in agricultural practices and map the distribution of nitrate and other key constituents in groundwater. Age dating, coupled with groundwater flow modeling, can provide insight into the changes in fluid contaminant load during the period the nitrate management plan has been in place.

- Land use evolution: Over the past 50 years, dramatic land use changes have occurred, from agricultural use (orchards) to suburban settings. Nitrate concentrations in young groundwater are expected to be markedly reduced. A historic case analysis combining field sampling and forward simulation may provide an important predictive validation.

The Santa Clara Valley Water District is interested in working with LLNL on these issues.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

Interdisciplinary team, including members from the **technical community** (e.g., hydrogeology, atmospheric and surface water modeling, computations, geochemistry, ecology, economics, information management specialist, land use specialist) and the **user communities** (e.g., State Water Resources Board, water managers [e.g., Santa Clara Valley Water District], University of California, Davis, Alameda County Flood Control and Water Conservation District, water suppliers, U.S. Department of Agriculture [USDA], Agricultural Extension Service, land planning agencies, and NGOs, such as the Sierra Club and Friends of the River).

***Budget Estimate*:**

Technical components, such as model evolution, field survey design, and performance and analysis, as well as substantial interactions, problem definition, data collection, and exchange. ($4 million over 3 years)

Who Is the Sponsor and What Is Our Product?

- Water resource agencies.
- Case studies.

Issues discussed: How to package our results. Can we do optimization?

Does not include: economics and water allocation models

Comments:

"Many models exist and are being developed outside of LLNL. Current LLNL efforts in this arena need to enhance extant water models rather than provide redundant models. Additionally, need to make an effort to provide interim products to stakeholders and work in an ongoing basis with stakeholders to: (1) build an interest in LLNL model efforts during the ongoing development process and (2) integrate their values and needs in the model development. Our models run the risk of irrelevancy in applied, on-the-ground projects if we have developed the model in a manner that has not been actively engaged and collaborated with clients and key stakeholders/users from the beginning and throughout the modeling process." – ***Jessie Coty***

"Should not include urban land use and reclamation? As cities sprawl, their collective contribution to land use is necessary. If NO_3 is a big problem, should include biogeochemistry as this is (primarily?) a microbially mitigated process." – ***Joanne Horn***

"The water resources simulation system mentioned under Working Group 2 could serve as the underlying analytical framework for evaluating the impacts of land use change on water supply and quality." – ***David Layton***

"Good presentation. Since other institutions have models, we need to 'sell' better science. We could also sell our expertise to agencies looking for peer review over low-budget research plans. Can this be done in the timeframe of most sponsors?" – ***Jeff Stewart***

"The National Research Council (NRC) Water Science Technology Board acknowledged in a recent Water Science and Technology Research agenda report the many new/emerging models for evaluating the effects of land use on water resources. LLNL's work plan should evaluate the state of potentially completing models to determine the appropriate 'value added' and to complement LLNL's work. Consider the Economic Development agencies in states and Economic Development offices in federal agencies (such as the USDA and USDOI) as clients." – ***Jill Watz***

PRIORITY 5

Cost-Effective Sensor and Communication Systems for Detection in Raw Water Media and Analysis of the Result

WORKING GROUP MEMBERS:

Cantwell and Dooher, in collaboration with Folta, Hoppes, Horn, O'Brien, and Rosenberg

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Research Issue Description:

There is an urgent need for rapid chemical, biological, and physical assessments of environmental water quality and properties, particularly in regard to public health and perception of water safety. These areas of research should include four separate solution paths, developed in parallel with the communications networking systems:

- Chemistry sensors.
- Biosensors.
- Ultra-low velocity sensors.
- Radio and memory systems.

Increased use of recycled water contributes to the risk (perceived or real) of exposure to pathogens (e.g., bacteria, viruses, endrocine disrupters, or other chemicals) that survive the wastewater treatment process or are released from industrial or farm processes. Present methodologies for analysis of chemical and biological agents in water, and the physical properties of groundwater and surface water systems, are time- and labor-intensive, expensive, and especially for the biochem detection systems, have low efficiencies in natural waters. Filter-based systems designed to remove biological contaminants from water do not provide for the adequate recovery and integrity of pathogens for subsequent analysis and are unsuitable for monitoring applications due to clogging. A comprehensive approach is needed that addresses all aspects of the sample collection, processing, and detection process in real-water matrices (at relevant volumes) to provide highly reliable data in a rapid time frame.

Water resource professionals also must make time-sensitive management decisions concerning water resources and water in distribution systems. These decisions must be based on water information that cannot, at present, be delivered quickly. Our current analytical capabilities often cannot answer questions such as what was released, how much, where, and when the

release may have originated, and if it still may be occurring in a cost-effective manner with adequate spatial and temporal resolution in order to take informed actions. Challenges facing us include:

- Development of detectors that are free from the benchtop and can be deployed in the field and operated by a trained technician, remotely or in a wireless environment. These should work reliably in the field in such places as:
  - sewage
  - seawater
  - brackish water
  - stormwater
  - other places (where it is difficult to get sensors to work, but where managers need information about water quality in real-time and of high quality)

- Development of sensor and detector technologies that provide real-time or near real-time measurement and analytical capabilities for water quality, water level, and water flow rates. Such sensors should be capable of storing and periodically tying into the internet using wireless standards and public protocols, or be capable in critical situations with giving an autonomous continuous stream of information.

Needs also include early warning systems (e.g., sensors, communication, etc.) in water distribution systems, field kits for first responders to an event, sampling and analysis for rapid contaminant identification, and better understanding of the fate and transport of contaminants in a water supply system (including reactions with chlorine). Any technology developed should be dual-use, protecting against both intentional and non-intentional contamination.

Development of flow sensors for riverine systems and water-level sensors for water wells should be fairly pedestrian. What is difficult is the development of durable velocity sensors for the extremely low velocity flow rates that occur in wells. Yet such sensors would give direct knowledge that now must be estimated based on uncertain hydraulic conductivity measurements, usually produced through expensive tests. Direct velocity sensors exist, but they are bulky and high maintenance. Efforts must be made to change this.

Finally, major engineering and communication system challenges exist in producing a high-fidelity, commercializable versions of the above sensors and systems for transmitting this data in real or near real-time conditions. No one has done it yet, primarily because most efforts have been scattered and under-funded. In addition, it must be stressed that significant challenges must be faced in order to build teams to develop these types of monitors. Multidisciplinary teams must be unified and work together side-by-side. Usually, these types of projects require significant resource allocations to get to successful field trials.

Importance:

An understanding of the dynamics of groundwater and surface-water systems calls for more than quarterly data tracking. There is the additional issue of increased awareness of the vulnerability of

our drinking-water supplies, and the need for pre-symptomatic action in the event of a biothreat attack against water resources or water systems. As water distributors need to make costly and timely decisions based on accurate information concerning whether to divert a water supply from public consumption, real time and near-real time data collection and assessment are critical. Such data collection should consist of, at least:

- Well water levels in order to track contaminant movement from point-source releases in order to understand the dynamics of nearby public, private, agricultural, and industrial extraction wells.

- Development of reliable, low-cost methods to measure groundwater movement (as opposed to estimating groundwater velocities); stream and river flow rates are necessary to understanding the system's dynamics.

- Chemical sensors capable of accuracy levels of at least hundreds of parts per billion (with capabilities in the parts to tens of parts per billion for critical areas) and report at least on a day-to-day basis, or send instantaneous alerts if there is a detection.

- Development of real-time field portable or *in situ* sensors that differentiate human fecal coliform from other sources in seawater samples (admittedly, a challenge).

- Real-time identification of pathogen contamination in water.

- Biosampling downstream from ultrafiltration with a detection of log reduction of 6 and lower.

- A system for rapid and quantitative separation and concentration of biological materials from nonbiological materials.

- Sample preparation steps that preserve the integrity of the biological materials collected.

LLNL is a world-recognized leader in detection methodologies for pathogens in air. This technology development can be leveraged, though water has its own unique set of interferences for detection methodologies and engineering complexities when dealing with large volume samples. However, the detection and quantification of biological agents is only part of the solution, as the real concern is whether the agents are viable and/or infective.

Manpower is often the greatest cost in assessing contaminants and monitoring drinking water sources, so developing cost-effective, energy-efficient sensor systems would allow better monitoring and understanding of water quality and water systems.

Other important uses are tied to management of acute occurrences, such as deciding whether to close beaches due to fecal coliform outbreaks. Contaminant-free water is extremely important in developing countries, and even in first-world countries, chlorine treatment is not always effective. In addition to human health per se, distribution system monitoring is also a homeland security and military/defense issue.

The need is huge and will only become more pressing as water resources are compromised due to use pressures. We will not only need to understand the various constituents, but also need to attempt to identify the source and understand mitigation problems. These sensors should act as sentries for deliberate, as well as non-deliberate, contaminants and their movement and would be invaluable for not only contaminant sites, but for drinking-water wells and riverine systems.

For biological sensors, computational methods have been highly successful in developing candidate DNA signatures. These signatures are the basis of probes that uniquely identify pathogens and are recognized as the "gold standard" for the Centers for Disease Control (CDC). The process has been successfully deployed to detect airborne pathogens. Modification of this system to support the detection of water pathogens would leverage successful, well funded, more mature work.

How Do You Propose Meeting or Complying with This Research Issue?

It is important to leverage off proven LLNL capabilities in biodetection, microtechnology, water monitoring systems, genomics, assay development, and communication systems for large sensor networks. As an example, preliminary research on Microelectromechanical Systems (MEMS)-based dielectrophoresis (DEP) systems, as a means of selectively concentrating biological material from raw water, is already underway in the Center for Microtechnology at LLNL. Concentration by DEP is dependent on a dipole moment induced in each particle in a non-uniform electric field. A key advantage to DEP is that body forces can be exerted on biological particles without occluding channels, thus mitigating clogging, the biggest impediment to continuous monitoring. The forces can be applied using alternating current fields up to megahertz frequencies, allowing for the collection of bacterial cells at an electrode surface with a subsequent release of cells when the electric field is removed.

These types of sensors have been shown previously to be able to effectively separate DNA molecules in solution. Another advantage of DEP is that there can be some capture selectivity depending on the frequency of excitation. This technology may provide the front-end to a continuous autonomous pathogen detection instrument for water monitoring.

Other combination techniques (e.g., DEP coupled with ion exchange technology) need to be explored to better capture these moieties.

The key is to develop a ollection system (perhaps DEP) and an analysis system. Partnering potential may include:

- Industry (a real option here if field test opportunities of mutual interest can be defined).

- UC campuses are pushing the envelope with "motes" – miniaturized data acquisition and transmission systems based on a new, low-power, low-memory wireless sensor networks that communicate seamlessly with each other and use "bucket brigade" methods to pass on information.

- State agencies, such as the State Water Resources Control Board (SWRCB) that spends up to $200 million/year to reimburse data collection and analysis at underground storage tank (UST) sites.

- Oil companies that spend up to $400 million/year.

- A local water agency, such as Zone 7.

Phase I

- Explore the ability of this real-time system on a prototype level (low flow rates).

- Increase sensitivity through coating of electrodes.

Phase II

- Pilot-scale unit testing; unit designed to operate at 20 gallons per day.

- Couple with existing processes.

Phase III

- Demonstration phase at specific water plants or in other field studies.

- Develop matching funds from industry.

Need to involve:

- Original equipment manufacturers (OEMs) for membrane and filter manufacturing.

- USEPA, water utilities, emergency response community, the California Office of Emergency Management, and the State of California Department of Health Services (DHS).

- Robin Miles, Alan Burnham, Kevin Ness, Paul Daley, Paula McCready, Bill Colston, Betsy Cantwell, Kevin O'Brien, Staci Kane, Steve Azevedo, Nina Rosenberg, Tom Slezak, and Pat Fitch.

- Other personnel in the LLNL Center for Microtechnology, the Biology and Biotechnology Program, and Nonproliferation, Arms Control, and International Security (NAI).

Propose a Budget to Assess the Problem:

The following table illustrates cost estimates to solve the major issues (with timelines). The timeline is the soonest that it would be feasible to solve the problem; it could conceivably be much longer.

Problem Solution	Cost to Solve	Minimum Time to Solve
Biosensor	$1.5-$2 M	3-4 years to integrated instruments
Chemsensor	$800 K - $1 M	2-3 years to integrated instruments
Low-Flow Velocity Sensor	$500 K	1-2 years
Sensor Communication Systems and Networking	$2 - $4 M	4-5 years (intense)

Sponsors in years 1-3 may include initial Laboratory Directed Research and Development (LDRD) funding, AWWARF, Janet Jensen, Defense Advanced Research Projects Agency (DARPA), and DHS.

Sponsors in years 3-5 may include USEPA, AWWARF, Industry Partners, DOD, DHS, and state agencies, such as the SWRCB.

Comments:

"Not clear on how it is determined; once sensors are developed, what is the optimal configuration of deployed sensors to achieve end use (both in terms of truly capturing adequate quantity and quality of data, as well as economic efficiency in the deployment)? A multidisciplinary team may need to include staff capable of taking sensor from development to achieving on-the-ground efficacy and efficiency. This is critical to ensure that a key technology is truly used in applied settings and the resource realities of users." – ***Jessie Coty***

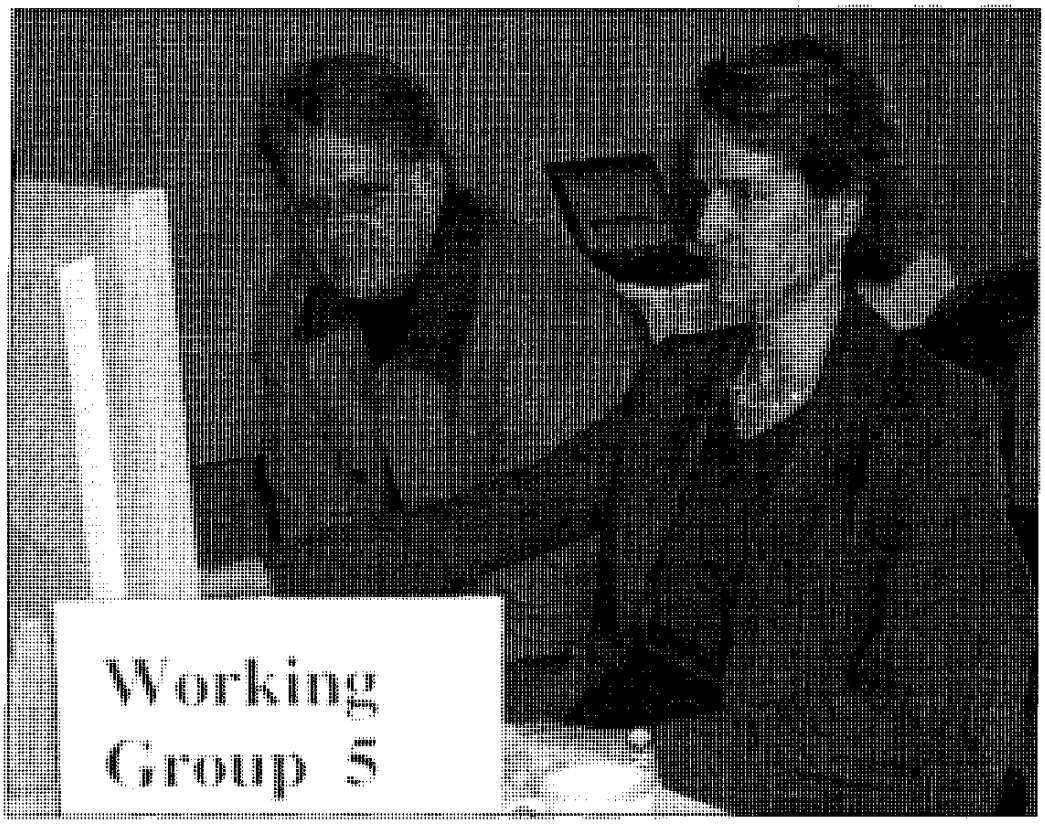
"Groundwater is really not the best target for this work. Water treatment plants and water distribution systems are the high payoff targets. Wellborne water velocity measurements are so unrelated to bulk groundwater flow that these measurements are not valuable" – ***Bryant Hudson***

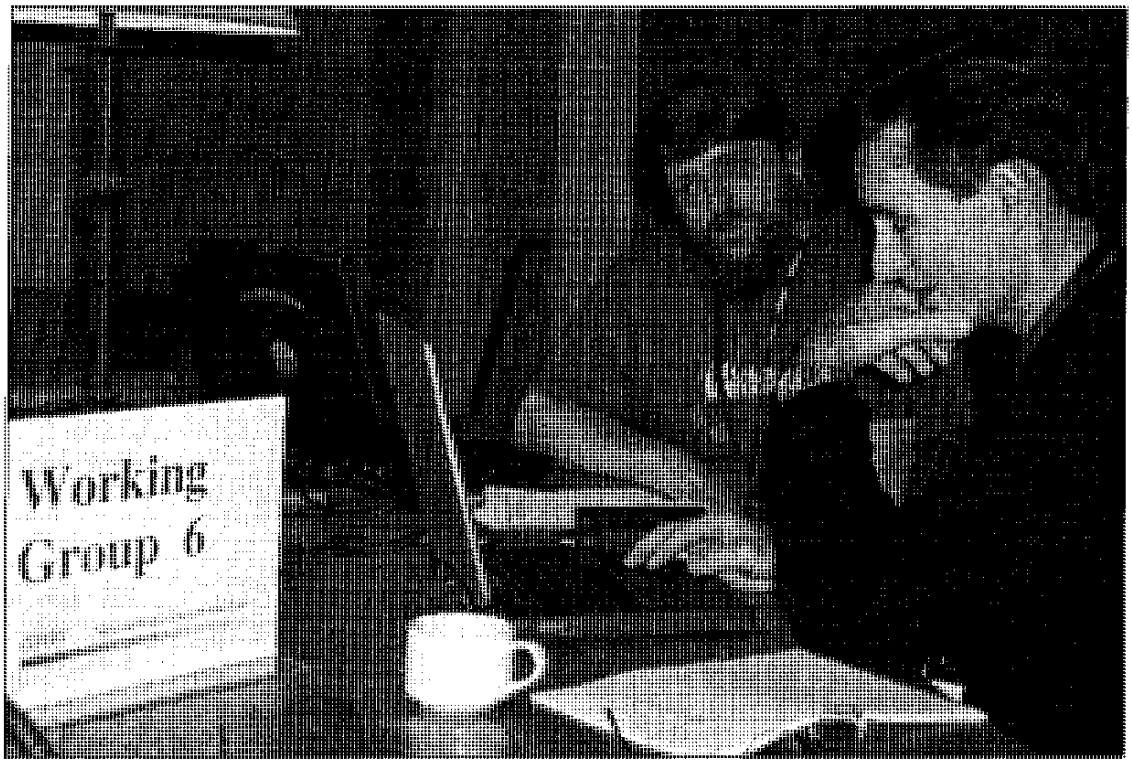
"Sensor communication will need to utilize existing or future technologies based on industrial standards. Will imaging capabilities be included as part of this priority research area? Should it? Sensors can be powered by materials and technologies developed at LLNL: Advanced Li-Ion batteries; super capacitors; fuel cells; bulk and thin-film thermoelectric." – ***Greg Mack***

"Excellent perspective on an action plan and what it will take to deliver." – ***Robin Newmark***

"Even if a testing matrix is used to evaluate the environmental impacts of a fuel's life cycle, how do we determine whether those impacts are acceptable or not? What criteria are used to determine unacceptable impacts – or impacts that are very difficult to mitigate?" – ***David Layton***

"Many of the details – lab studies, key chemical parameters, etc. – are written for aqueous systems only. Corollary details for air quality, transformation issues should also be added." – ***Susan Powers***




Working
Group 6

PRIORITY 6

Brine Use and Management Technologies for Gas and Oil Production, Power Plants, and Wastewater Recycling Operations

WORKING GROUP MEMBERS:

Hudson and O'Brien

Research Issue Description:

An important class of water clean-up technologies range from RO to electodialysis reversal (EDR) to ion exchange. Most systems are a combination of separation processes, e.g. ultrafiltration (UF) coupled with RO. In all these processes, there are waste streams (brine) generated. Reduction of brine volume can only be achieved through a systems approach. This needs to be achieved in a cost-effective manner. The more *efficient* the separation process, the *less* brine volume generated (although same mass of dissolved materials).

In many situations, brine handling is the major economic driving factor. Many projects in the Central Valley of California were cancelled because of this factor alone. It is important that we not exchange one non-usable resource for another (i.e., create non-reusable contaminants that will need to be handled).

Importance:

This was listed as the *most important* issue from an industrial perspective at the recent American Membrane Technology Association Conference.

Brine generated from gas, oil, and coal bed methane production could have one or more of these components:

- Naturally occurring radioactive materials (NORM), such as ^{226}Ra, ^{238}U. These contaminants could be a special challenge.
- Toxic elements, such as arsenic, chromium, and selenium.
- Toxic naturally occurring organic compounds (e.g., benzene).
- Bulk of effluents: sodium, calcium, magnesium, chloride, and carbonate.

- Some produced waters have total dissolved solids (TDS) ~ 1000; therefore, nearly usable as produced. Thus the water content makes these "brines" especially valuable.

- USDOE funding is available to examine this issue.

Brine generated from power plants comes from the "polishing" of feed water for use in boiler/steam system and could have one or more of these components:

- The quality of water supplied *into* the boilers will be *more stringent* than potable standards.

- Bulk of effluent would be sodium, calcium, magnesium, chloride, and carbonate. (NOTE: Expect more similar levels of sodium, calcium and magnesium).

- Since the starting water is relatively good, high efficiency in the "polishing" treatment can be especially effective at reducing the volume of the brine effluent.

- Identified as one of the major issues for the Power Plant industry at a recent USDOE Combustion Science Meeting held in Salt Fork, Ohio, August 2002.

- Funding available through USDOE to approach this issue.

Brine generated from wastewater recycling facilities could have one or more of these components:

- Bulk of effluents would be sodium, calcium, magnesium, chloride, and carbonate.

- Expect several hundred parts per million (ppm) of a vast array of different organic compounds, some of which will be toxic.

- Potentially, some pathogens could be present.

How Do You Propose Meeting or Complying with This Research Issue?

One of the key goals of the research would include both methods to facilitate disposal or recover a resource:

- Increase percentage recovery beyond the 90-95% achieved by current RO systems. Examine tradeoffs from an economic viewpoint.

- If brine is transported, then volume reduction directly relates to *energy* and *infrastructure* costs.

- Methods to economically separate radionuclides and toxic transition metals need to be developed. Work done by Coleman, Environmental Protection Department (EPD), and

Reynolds, Chemistry & Materials Science (CMS), using functionalized aerogels mixed with granular activated charcoal, show promise.

- Explore the use of the bulk constituents to produce a higher value added material, e.g., building materials (equivalents of concrete blocks and dry wall). This generates *revenue* and reduces disposal costs. Need to examine properties of final end products produced with these recycled materials.

- Explore the concentrations of valuable metals present in the brine, such as cobalt and vanadium. These may represent economically valuable ores, which are already in solution.

- Expect that a *systems approach* will be required (i.e., linking power plants, building materials plants, water treatment facilities, etc.). Need to leverage handling equipment, which is already in place.

- Economic analysis will be specific to a specific geographical areas and specific brine compositions (e.g., how close to oil field, power plant, waste facility, etc.).

- Key will be to select appropriate targets *upfront,* then work closely with stakeholders to show success. This would serve as a model for future interactions at additional sites.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

- Needed within the team:
  - Membrane scientist
  - Chemical Engineer
  - Chemist
  - Modeler for economic analysis
  - Molecular modeler
  - Personnel familiar with policy issues
  - Civil Engineering
  - Geoscientist
  - Engineering Firm(s)
  - Power Plant Facility for demonstration testing (Northern Arizona perhaps)
  - Waste Water facility (Southern California water recycling project)
  - Boiler Original Equipment Manufacturers (OEMs)
  - Chevron/Texaco (Coal Bed Methane, Power River Basin)

- Effort is *highly leveraged off existing industrial contacts.*

Budget:

(FTEs and $)

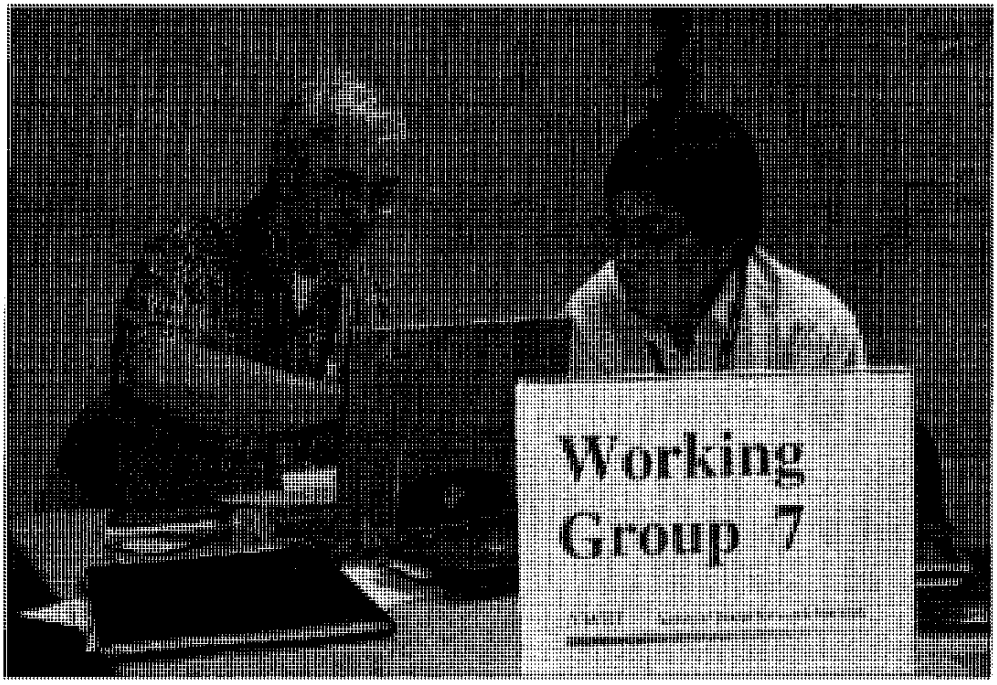
	Year 1	Year 2	Year 3	Total
FTEs	6	8	9	23
Total Cost (thousands)	$1,500	$2,000	$2,500	$6,000

Comments:

"Add the California Energy Commission as an interested funding agency. They are currently funding geothermal brine treatment technology development at LLNL and have a vested interest in brines associated with fossil fuel extraction in California." – ***Bill Bourcier***

"Action plan looks good. Make sure all of our internal people are 'on the same page' because the marketing efforts for this project dictate the same clear message from everyone." – ***Betsy Cantwell***

"We could focus on brines being transported by existing brine drain lines in California." – ***Alan Lamont***



PRIORITY 7

Innovative Approaches to the Characterization, Management, and Treatment of Nitrate Contamination in Groundwater

WORKING GROUP MEMBERS:

Esser and Grey

Research Issue Description:

New technical approaches are needed to manage pervasive nitrate contamination in groundwater. The problem is multifaceted and will benefit from a multidisciplinary approach. Issues include:

- Characterizing the source, history, and extent of current contamination.
- Quantifying nitrogen transport and biogeochemistry in the vadose and saturated zones. (i.e., aquifer assimilative capacity).
- Understanding the economic consequences of different management/treatment approaches.
- Developing science-based approaches to source mitigation and treatment.
- Demonstrating the impact of different water management plans on groundwater quality.

LLNL has the analytical capabilities, expertise, and experience in building teams to solve large problems to make significant progress in each of these areas. Specific contributions include development of the following tools and applications:

- Tools:
  - aquifer assimilative capacity: denitrification
  - source attribution and co-contaminant characterization
  - age-coupled groundwater modeling
- Applications:
  - nitrate management assessment
  - groundwater basin assessment
- Management:
  - optimization of management options.

Importance:

The presence of high levels of nitrate in ground and surface water had adverse effects on human health and ecosystems. In California, nitrate contamination of groundwater consistently accounts for the highest number of exceedences of drinking-water standards of any single contaminant in public drinking supply wells. In ecosystem research, the largest and most poorly understood of all issues related to coastal eutrophication is the fate of nitrogen in aquifers. We do not understand the current extent of problem, the response of aquifers to different levels of nitrogen loading on the basin-scale, or the most cost-effective way of dealing with the problem. The SWRCB recognizes these issues and has asked LLNL's help in dealing with them.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has expertise in the following:

- Tracing groundwater (with ^{3}H- ^{3}H age-dating and noble-gas tracers).
- Characterizing contaminant sources and geochemistries (with inorganic mass spectrometry and trace organic analytical chemistry).
- Using molecular biology probes to understand biogeochemical processes in the subsurface.
- Modeling groundwater flow and the reactive transport of contaminants.
- Managing and visualizing large data sets.
- Optimizing the management of complex systems.

With respect to nitrogen biogeochemistry, we have developed membrane inlet mass spectrometry to allow for a fast, sensitive, and precise determination of the ultimate product of denitrification — nitrogen gas — and demonstrate the existence of autotrophic denitrification at a local field site. These techniques and capabilities should be integrated into a larger research effort to provide the science necessary to manage nitrate contamination at the field to basin-scale. If funded the research will produce the following products:

- A tool kit for assessing *aquifer assimilative capacity.*
- A tool kit for determining *nitrate source.*
- A new and more *robust modeling approach* to constraining groundwater flow.
- A robust method for *assessing the impact of land use* and management on nitrate in groundwater.

- An approach to *assessing the current state of nitrate contamination* in State of California groundwater.

- A tool for optimizing management and treatment of nitrate-contaminated groundwater in the State of California.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

- LLNL:
  - CMS: Esser, Hudson, Moran
  - EE: Carle, Bourcier
  - EPD: Bellar, Kane, McNab, Demir, Dooher
  - Engineering: Lamont, Stewart

- Collaborators:
  - Santa Clara Valley Water District
  - Alameda County, Zone 7
  - UC-Davis Agricultural Extension: Thomas Harter
  - U of Arizona: Brenda Erkwurzel

Plan and Budget:

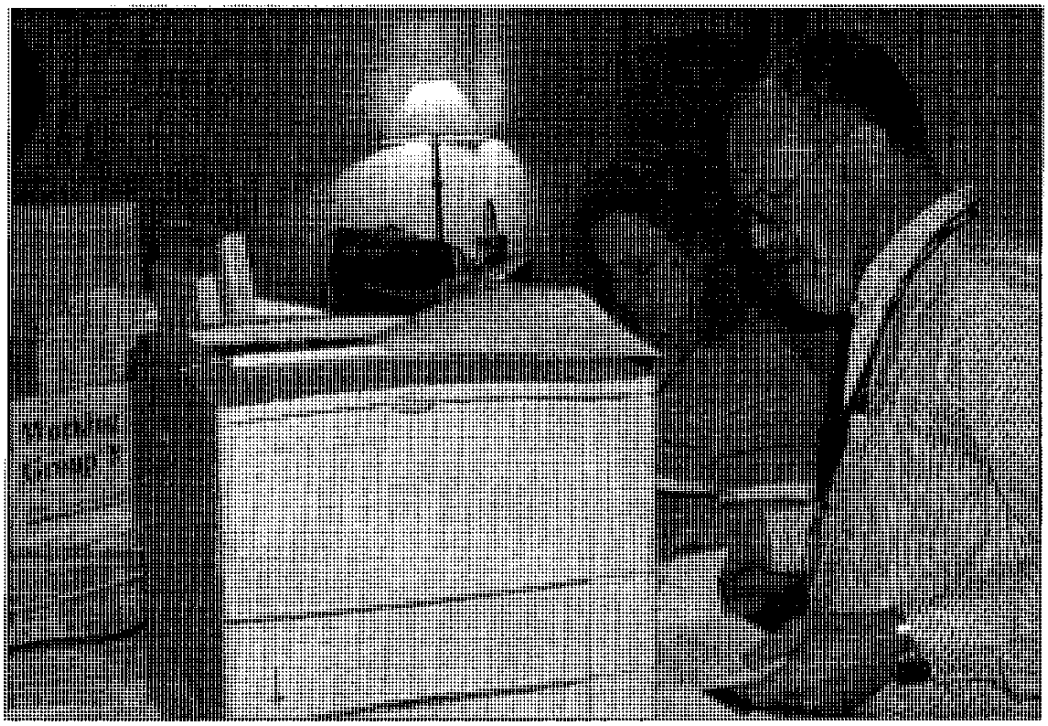
- Stategic plan:
  - Develop new tools (LLNL funding)
  - Use existing tools to collaborate with water districts & universities on field studies (LLNL and matching funds/resources)
  - Approach State Board for role in basin assessment
    - Leverage GAMA and inclusion of "ages" in AB599 plan
  - Market tools through an LLNL water organization

- Budget:
  - 2-4 FTEs/year

Comments:

"Should be a top priority to fund now." – ***Betsy Cantwell***

"Good active approach that can help create a market niche; good connection and possible funding. However, LLNL remains in a service role. Long-term strategy? CAMS model?" – ***Robin Newmark***



PRIORITY 8

Impact of Climate Change on Water Management and Infrastructure

WORKING GROUP MEMBERS:

Folta and Lamont

Research Issue Description:

Current California water management decisions are based on average climate conditions over the past decades. These assumptions can be catastrophic if climate conditions were to change leading to changes in overall averages and the patterns of precipitation.

This research effort will evaluate the changes in water management strategies and infrastructure in California that may result from future climate changes. For example, we can expect under some climate change scenarios that there may be more precipitation, a smaller snowpack, and greater wintertime runoff. The existing water storage infrastructure and management patterns generally are not well adapted to these conditions. The fact that a large amount of the runoff may occur during a few months in the winter implies that we may need to use substantial amounts of storage from season to season in order to provide reliable water supplies for agricultural and urban uses throughout the year. It is likely that most of the new storage will be subsurface, resulting in large-scale cycling of the groundwater reservoirs.

This research will use a series of models and analyses to evaluate these effects. We will first evaluate the potential changes in water availability over the years based on climate modeling, and then find optimal water management strategies to maximize the value of the delivered water. Since these strategies may rely heavily on groundwater storage, we will evaluate the impacts that these strategies may have on groundwater aquifers. As a secondary investigation, we will also explore the role that better long-range water forecast might have in improving our water management strategies. These efforts are outlined below.

Climate Modeling

The basic challenge of this research effort is to predict the nature and magnitude of climate change/variability impacts on water supply and demand in California and elsewhere in the country. In order to address this challenge, predictions of temperature, precipitation, and hydrologic responses to climate change and variability in major watersheds will be developed using a suite of models, including high resolution global and regional climate models and a watershed-scale hydrological model. Initial efforts will simulate present climate/hydrologic conditions (matching statistical and spatial climate/hydrologic attributes of selected regions) and

then predict future climate change/variability impacts for different scenarios of greenhouse gas emissions.

Water Management Strategies

We can expect that climate change will cause changes in precipitation, patterns of precipitation and runoff, and soil moisture. In California and elsewhere, the water storage infrastructure and patterns of water use have been developed to meet the requirements of the existing climate. As the climate changes, we will need to develop different management strategies, infrastructures, and patterns of use.

The impacts of climate change depend on how we respond. We cannot understand the long-term economic impact of climate change unless we first understand how to best manage the water under the new regime. From that, we can draw conclusions about the actual impacts of climate change.

This research will first identify optimal management and infrastructure responses to climate change in California. It will then evaluate the overall impact of climate change.

Use of Large-Scale Aquifer Storage/Recovery to Address Storage Needs

Impacts of climate change to California's water distribution system may include changes in the spatial distribution of rainfall and a reduction in the storage capacity offered by snowpack in the Sierras. Taking into account population growth, the need for significant additional storage capacity is obvious. Economic and environmental considerations may preclude significant new surface-water storage capacity, while the direct recharge of aquifers through recharge and infiltration may also be problematic for a variety of reasons; therefore, aquifer storage through injection may offer a practical means of establishing new, large reservoirs of water. Key issues, however, will need to be addressed:

- Where will we find the most economical sources of recharge water in a climate-altered California?

- What are the issues associated with long-term management of recharged aquifers and recharged well fields (e.g., aquifer geochemistry and well clogging)?

Value of Long-Term Water Forecasts in Managing Water Resources

The optimal water management strategies include allocations of water between years when water is plentiful and water is scarce. When we run water management optimization models, we assume that the water availability is known for each year. This provides an estimate of the very best that we can do through water management. This, of course, is not completely realistic. Water managers do not know the availability for future years and, thus, must hedge their strategies, which leads to less than maximum performance. Better water forecasts would help them reach the optimal level of performance.

The questions are:

- How important is accurate forecasting? It might be that the existing forecasts give us enough information to nearly achieve the maximum value.

- How good must the forecasts be? How accurate?

- What must be forecast? For example, the exact precipitation is probably not important; it may only be important to forecast the onset or end of droughts.

The result of this research will be recommendations for future research in climate modeling to improve multi-year forecasting.

Current users and sponsors include East Bay Municipal Water District, the California State Department of Water Resources, Scripps Institute of Oceanography and USDOE Office of Science. Potential users include the USBR, and COE.

Importance:

The impacts of climate change in California could be severe, and preparations to effectively deal with the changes will be needed. This research will help us understand the magnitude and nature of the impacts and what will be required to address them. Possible management strategies may include new technologies. This research will provide us with some guidance about the role of those technologies and help identify the characteristics of the technologies that need to be developed. New infrastructure will undoubtedly need to be developed. These may include water storage facilities, pumping facilities, and new water conveyances. This research will indicate what sort will be needed, their capacities, and locations.

The costs of water could be expected to change significantly. This could strongly affect the patterns and viability of agriculture in California. Through this research, we can develop an understanding of the types of changes that might occur.

There is significant concern about the impact of large-scale aquifer storage/recovery. This will inject large amounts of water into existing aquifers having a chemistry and temperature different from the existing waters. There is concern that this could cause chemical changes in the water, affecting its quality and affecting aquifer capacities. This research will allow us to anticipate such problems and design strategies or locate storage facilities so as to avoid them.

Developing better forecasting methods might assist us in meeting these challenges. The results of this research will give us a better understanding of the extent to which improved forecasting could help and identify the particular aspects of forecasts that should be improved.

How Do You Propose Meeting or Complying with This Research Issue?

This research will be developed through a series of models and analyses as follows:

The Climate Modeling Group is developing a high-resolution global and regional climate model that can resolve regions within California. This will provide details on precipitation, temperatures, and the size of the Sierra snowpack. This modeling, combined with watershed hydrological models will provide us with the basic water inflows to the California system over a series of modeled years.

The water inflows will provide the basic input needed for the water management models. We anticipate using the CALVIN model developed at UC Davis and currently running at LLNL. This model takes the monthly water inflows as its basic input. It also includes extensive data on the value of water for agricultural and urban uses. CALVIN is an optimizing model that finds the optimal set of water allocations over a model horizon (e.g., several decades) to maximize the total value of the water. These results tell us the amounts of water directed to each location and used in California each month; the amounts directed to storage; and amounts withdrawn from storage. It also provides the value of additional water supplies at each location each month and the value of increasing the capacities of each element of the water management infrastructure.

Understanding the values of additional waters will provide an estimate of the economic feasibility of various proposed water treatment technologies since their costs can be compared to the value of the water they produce. The values of increasing the infrastructure capacity can similarly be used to evaluate the economic viability of new infrastructure.

Water quality will affect the value of water and can be expected to partly determine water management policies in the future. The existing CALVIN model does not model water quality nor take it into account in valuing water. Incorporating water quality will require converting CALVIN to a non-linear form and applying a new solution algorithm. New models of the value of water, as a function of water quality, will also be developed.

The optimal water management plan will include the use of aquifer storage/discharge. This will provide an estimate of the frequency, magnitude, and location of aquifer cycling. This information will be needed to evaluate the impact of such cycling on the aquifers. We will evaluate these impacts by leveraging LLNL strengths in geochemical reactive transport modeling, along with applying coupled groundwater-surface water modeling (i.e., calibrated to groundwater age data collected under the GAMA study) to identify recharge strategies (e.g., infiltration versus injection) on a basin-scale across the state.

To address the value of long-term water forecasts, we will adapt the water management models to first understand the way that uncertainty about future conditions affects current water management decisions and the long-term value of those decisions. We can then evaluate the impact of reducing the uncertainty and identify the most important aspects of uncertainty to address. Then, working with the Climate Modeling Group, we can identify ways that these uncertainties might be reduced. We recognize that some uncertainties will be harder to address than others. Developing a research plan will require a balancing between the value of reducing

an uncertainty and the feasibility of reducing that uncertainty. This will identify a course of research that has a high probability of leading to an effective forecasting capability.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

Developing this research will require the following groups and possible personnel:

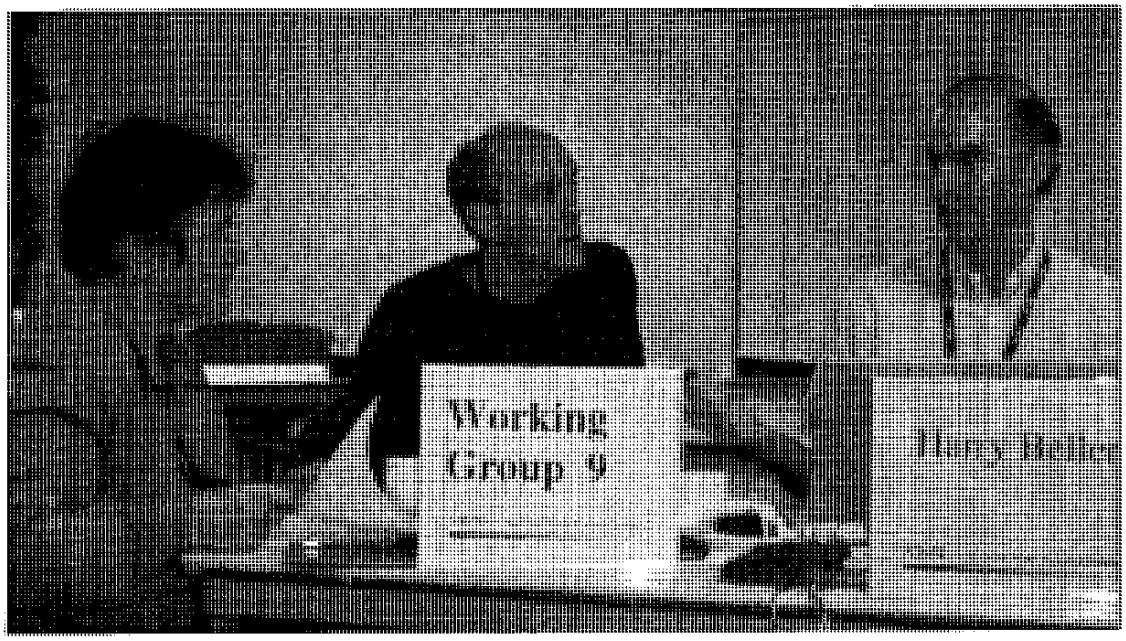
- Climate Modeling Group: Phil Duffy
- Computations: Pete Eltgroth, Carol Woodward
- Engineering: Alan Lamont, Jeff Stewart, Yiming Yao
- Energy and Environment: Bill Boucier, Bill Glassley
- Environmental Protection Department: Walt McNab

Required Effort:

Approximately six FTEs. Two FTEs are currently covered by LDRD.

Comments:

"In addition to using CALVIN to evaluate the impacts of climate change on water management, other models, such as CALSIM, should be used to study management responses given current operating practices and infrastructure." – ***David Layton***


Working
Group 9

PRIORITY 9

Advanced Assessment of Biogeochemical Processes Involved in Intrinsic and Engineered Aquifer Remediation

WORKING GROUP MEMBERS:

Beller, Barsky, and Horn in collaboration with Esser

Research Issue Description:

Microbially mediated processes exert significant control over the cycling and fate of organic and inorganic contaminants in aquifer systems. Understanding of the fundamental processes underlying biogeochemical cycling of contaminants is critical for prediction of chemical behavior under intrinsic conditions (e.g., for natural attenuation) and for designing engineered in situ remediation processes. This project addresses inorganic contaminants (e.g., nitrate and uranium) and a gasoline-related organic compound (e.g., methyl tert butyl ether, or MTBE); these have been chosen as representative compounds that are either priority contaminants in California or in the USDOE complex. As described below, the project goals vary somewhat depending on the contaminant being addressed but will focus on integrating a fundamental understanding of biogeochemical cycling with field measurements that will provide evidence of those processes. For all contaminants, integration of empirical measurements with reactive transport modeling will be included to address the role of abiotic processes on contaminant behavior (e.g., advection, dispersion, geochemical reactions, such as precipitation and complexation).

Gasoline-related organic compound

Groundwater contaminated with organic pollutants is a worldwide problem that effectively reduces the amount of potable water available. In the U.S., over 400,000 leaking underground storage tanks have been confirmed, and many of these affect underlying groundwater. Intrinsic bioremediation (or natural attenuation) by indigenous bacteria has been promoted as the most cost-effective approach to groundwater restoration, but the science underlying the application of this approach is less than rigorous at many sites. Even when intrinsic biodegradation is well documented, a particularly intractable aspect has been the estimation of in situ biodegradation rates, which must be distinguished from the effects of dilution and dispersion. Rigorous biogeochemical methods are needed to definitively demonstrate whether biodegradation is occurring at a given site and if so, at what rate.

Nitrate

Nitrate contamination is a very significant groundwater quality problem that is effectively rendering large volumes of water nonpotable in California and in many other agriculturally intensive areas of the U.S. Basin-scale models that incorporate nitrate transport and fate will be developed at LLNL to assist the state in optimizing water management strategies. Such models will require quantitative input for an important nitrate sink, namely, denitrification. Denitrification is a natural, bacterially mediated process that converts nitrate to harmless nitrogen gas; thus, denitrification is an intrinsic bioremediation process that defines the assimilative capacity of an aquifer for nitrate. Quantifying *in situ* denitrification requires a combination of highly specialized kinds of data that are not conventionally accessible.

Uranium

The USDOE is currently responsible for remediating 1.7 trillion gallons of contaminated groundwater and 40 million cubic meters of contaminated soil at its facilities. More than 60% of USDOE facilities are estimated to have groundwater contaminated with metals or radionuclides, such as uranium.

Oxidation state is a major control on the solubility and mobility of many metals and radionuclides in groundwater. In particular, uranium is highly insoluble in its (IV) oxidation state and is soluble in its (VI) oxidation state. Thus, microbially mediated reduction of uranium is being considered as a groundwater cleanup approach that would immobilize uranium *in situ*. This remediation approach is of great interest to USDOE, which, in FY2002, awarded tens of millions of dollars to several projects addressing metal/radionuclide reduction under the Genomes to Life program. Despite recent funding efforts, the biogeochemical cycling of uranium is not well understood.

Importance:

Gasoline-Related Organic Compound

If documented in a scientifically credible manner, intrinsic biodegradation can lead to highly cost-effective and productive restoration and management of groundwater. However, if inaccurate claims of intrinsic bioremediation (including overestimates of degradation rates) are accepted by regulators, this will either delay the necessary engineered cleanup or represent a risk to those who may be exposed to the contamination.

Nitrate

Nitrate contamination of California drinking water supplies is pervasive–about 10% of California public drinking water supply wells produce water that exceeds the regulatory drinking water limit, and a much larger fraction produce water that approaches the limit. Nitrate concentration exceeding the drinking water standard was the most common reason for shutting down 8,000 public drinking water wells statewide. As the population of California increases by 50% over the

next 20 years, water resources will be in critically short supply. Thus, careful management of water resources will be required to minimize the volume compromised by nitrate contamination. Accurate assessment of denitrification in aquifers is a key component of models being developed for management.

Uranium

Considering the serious attention that USDOE has paid to *in situ* reductive immobilization and the need for this restoration strategy to be effective for thousands of years, it is essential to have a high degree of understanding of the complexities of biogeochemical redox cycling of metals and radionuclides. In particular, the potential for re-oxidation needs to be better understood.

Approach:

Gasoline-related organic compound

An interdisciplinary approach is required, involving emerging techniques in analytical chemistry, molecular biology, biogeochemistry, hydrogeology, and reactive transport modeling. The approach would involve:

- Identification and *in situ* detection in groundwater of signature metabolites associated with specific contaminants.
- Identification and *in situ* detection of genes (and mRNA transcripts) associated with the degradation of specific compounds.
- Compound-specific isotope ratio mass spectrometry of parent compounds and metabolites *in situ.*
- Age-dating of groundwater.
- Ractive transport modeling of specific contaminants in the subsurface that incorporates these and other data.

Implementation of this project would require some or all the following, depending on the study compound chosen:

- Biochemical elucidation of key metabolites in degradation pathways and highly sensitive and selective mass spectrometric methods for metabolite detection in groundwater, such as isotope dilution liquid chromatography-tandem mass spectrometry.
- Elucidation of genes that encode key degradation enzymes (e.g., based on comparative genomic studies for degrading bacteria) and highly sensitive and selective methods for detection of target nucleic acids in groundwater.
- Purchase of the appropriate instrumentation for compound-specific isotope ratio mass spectrometry, which is not currently available at LLNL.

Nitrate

Kinetic parameters for *in situ* denitrification need to be developed for integration into reactive transport models. These parameters will be quantified by using a combination of area-specific data and kinetic constants, including:

- Quantification of denitrifier populations and activities based on detection of diagnostic genes and associated mRNA.
- Measurement of excess nitrogen gas in groundwater.
- Measurement of stable isotope ratios of nitrogen and oxygen in dissolved nitrate.
- Laboratory studies of denitrification kinetics of representative aquifer bacteria.
- Estimates of groundwater age using isotope hydrology.

These data will allow for multiple, independent assessments of *in situ* denitrification rates.

Uranium

Many aspects of this topic require much more intensive study, including in particular, an understanding of the following:

- The physiology and biochemistry of aquifer bacterial communities that can oxidize, as well as reduce uranium.
- How environmental conditions control expression of genes involved in respiration.
- How heterogeneous conditions across a colonized surface effect both reaction rates and their products.
- How bacteria can respire using insoluble mineral phases that cannot be transported into the cell.

Using high resolution analytical chemistry techniques, we can investigate these surfacial interactions between bacterial biofilm components, the mineral surface they colonize, and the surrounding bulk solution. We will utilize existing and new and unique LLNL facilities with capabilities to determine surfacial reactions and their products on very small scales. In particular, a high-resolution, multi-collector Secondary Ion Mass Spectrometer (NanoSIMS) may enable us to document isotopic fractionation signatures of uranium that provide evidence of microbial oxidation/reduction. In situ, real-time analysis may be accomplished by employing, for example, emplacement of micron-size beads coated with various indicators within biofilms. Most current experimental work in this field focuses on the continuum scale and does not capture the pore-scale spatial, morphological, and chemical heterogeneity inherent in natural and most engineered systems of interest. Similarly, conceptual and numerical models based on continuum scale observations give little insight into causal mechanisms and are not useful for predictive modeling. Therefore, data collected in experiments exploring pore-scale interactions will be incorporated into a pore-scale reactive model that will be accurately scaleable to the continuum

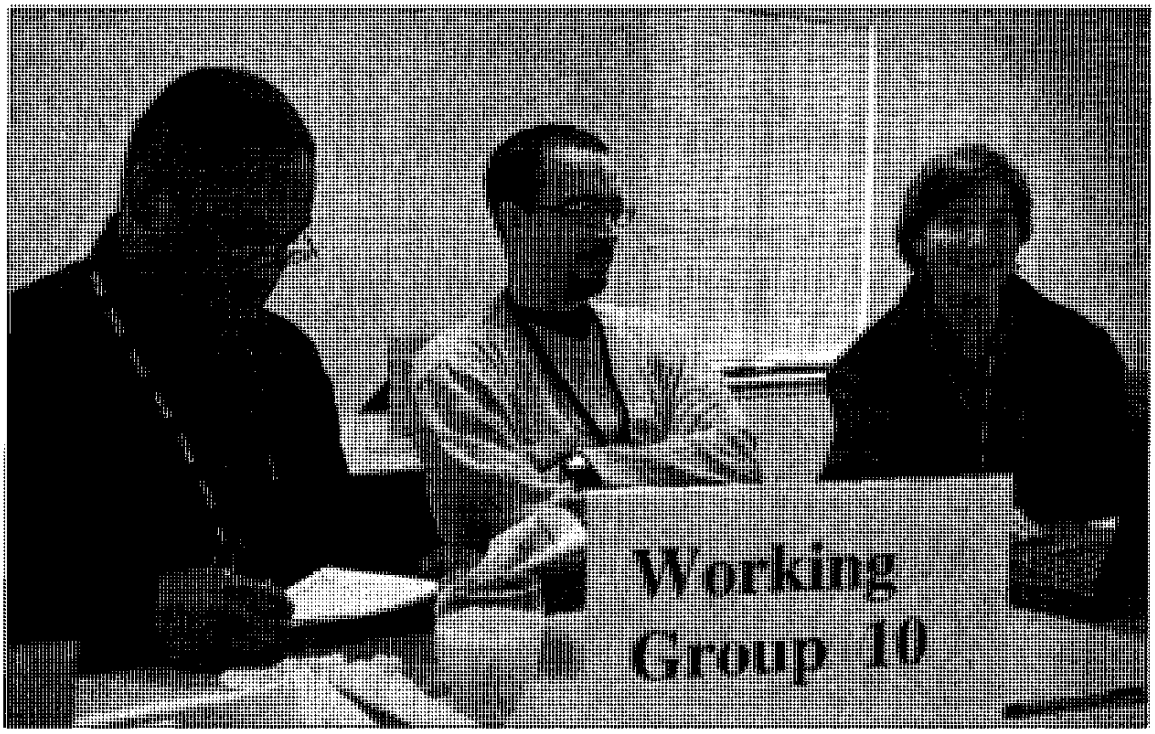
level. Scaled models can be tested in larger-scale experimental systems to evaluate their accuracy.

Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

H. Beller, S. Kane, J. Horn, D. Barsky, B. Hudson, W. Bourcier, B. Esser, I. Hutchins, B. Viani, C. Steefel, W. McNab, and one or more postdoctoral researchers specializing in geobiology (for the uranium work).

Budget:

Purchase of a continuous-flow isotope ratio mass spectrometer for analysis of degradation kinetics of organic compounds. (6FTEs for 3-years)


Working
Group 10

PRIORITY 10

Assess Artificial Recharge, Groundwater Banking, and Conjunctive Use with LLNL's Advanced Analytical and Modeling Capabilities

WORKING GROUP MEMBERS:

Mack, McNab, and Moran

Research Issue Description:

Apply advanced analytical and modeling techniques to questions of artificial recharge, water banking, and conjunctive use on a basin or sub-basin scale:

- What is the nature of the groundwater and recharge water – quantity and quality?
- What is the relationship between the recharge water and the basin hydrogeology?
- What are the key biogeochemical processes that affect the fate of chemical constituents in the recharge water?

Importance:

- Lack of viable surface water storage.
- Impending increased demand in urban areas and desire to increase groundwater proportion.
- Water agencies, permitters, regulators need to know what will happen when groundwater banking is undertaken?

How Do You Propose Meeting or Complying with This Research Issue?

Nature of Groundwater and Recharge Water – Action Items:

- Set up liaison with water agency /stakeholders.

- Data integration and information management.
  - assimilate and use existing data
  - construct GIS database

Hydrogeology – Action Items:

- Use isotopically enriched noble gas tracers for determination of near-field flow.

- Use GAMA ages for determining basin-scale flow field.

- Calibrate integrated groundwater-surface water flow model (IGSM) to tracer and age data.

Water Quality Changes – Action Items:

- Construct reactive transport model coupling a IGSM with solute transport and geochemical speciation (e.g., PHREEQC) components.
  - flow & transport
  - aqueous and surface complexation, mineral precipitation/dissolution, ion exchange, redox
  - reaction kinetics (PHREEQC uses a flexible scripting language)
  - specific IGSM capabilities (surface water, land subsidence, etc.)

- Assimilate existing pertinent kinetic data for transformations involving chemicals of concern.

- Conduct targeted research to fill data gaps.
  - N isotopes/excess N for denitrification studies
  - signature metabolites of specific contaminants

Workplan:

- Conduct pilot project with Santa Clara Valley Water District (SCVWD).
  - jointly funded
  - tailored to specific technical concerns of the SCVWD
  - run model scenarios
    - water balances
    - track recharged water
    - chemical evolution of groundwater under recharge
    - land subsidence issues
  - calculate value of additional storage capacity
  - enlist DWR/ DHS/ RWQCB/ SWRCB as advocates

- Market full-service program to other agencies/basins.
  - Sacramento Area Metropolitan Water Agencies (SAMWA)
  - Northern California counties
  - Central Valley irrigation districts
  - high growth urban areas

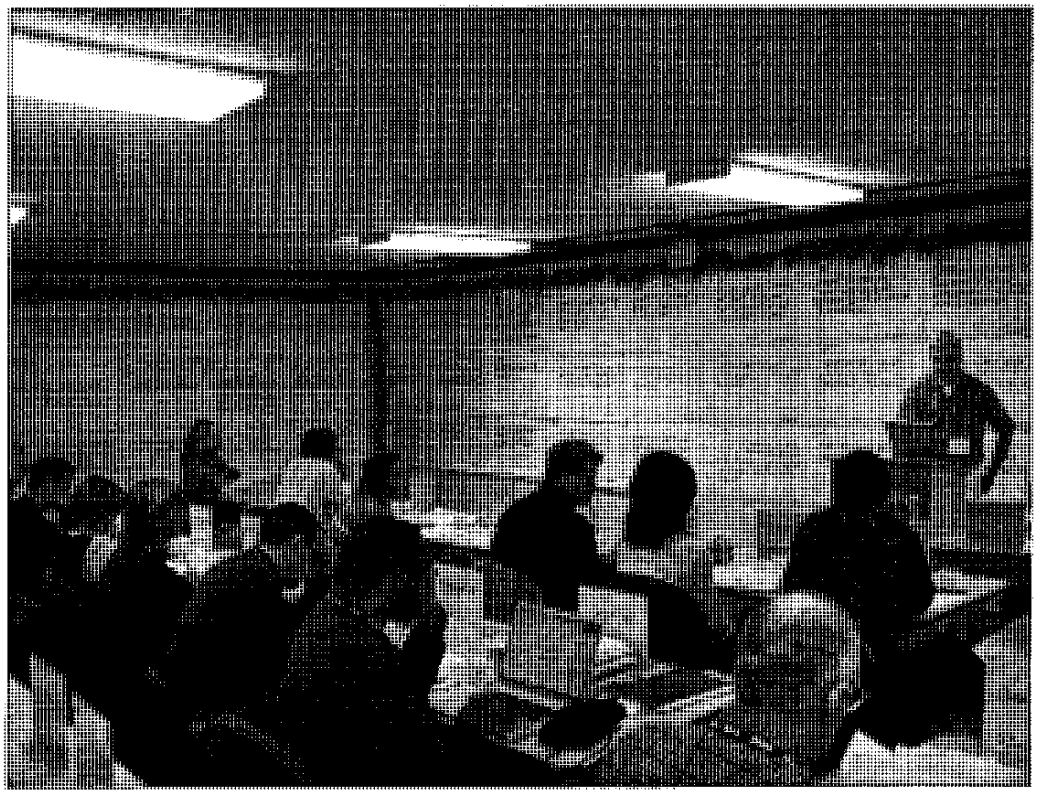
Who Are the Individuals Best Able to Address, Illuminate, Refine, and Focus This Research Issue?

- Hydrogeology and water chemistry: Jean Moran, Bryant Hudson, Brad Esser, Harry Beller, Staci Kane

- Modeling: Walt McNab, Andy Tompson, Steve Carle, Carl Steefel

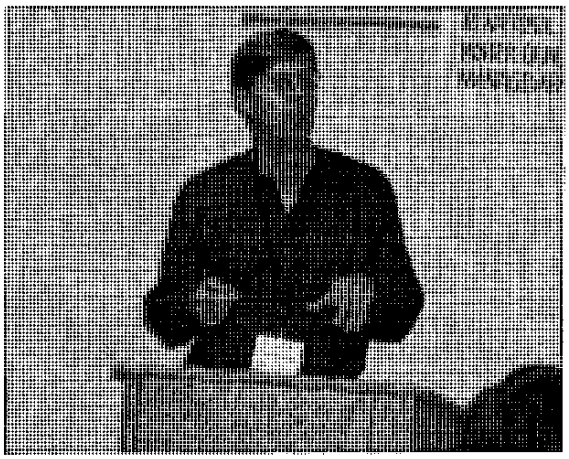
Budget

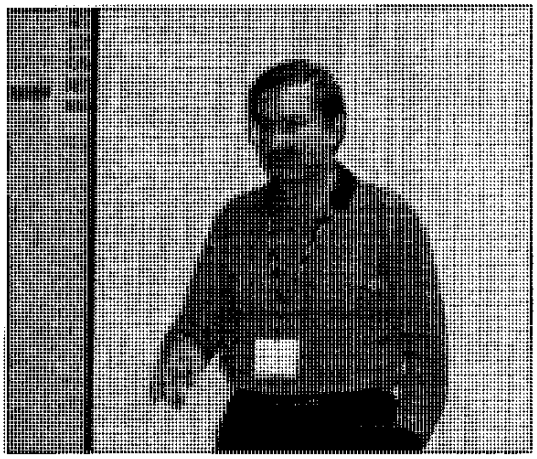
- 3 FTEs over 3 years (1 from SCVWD)



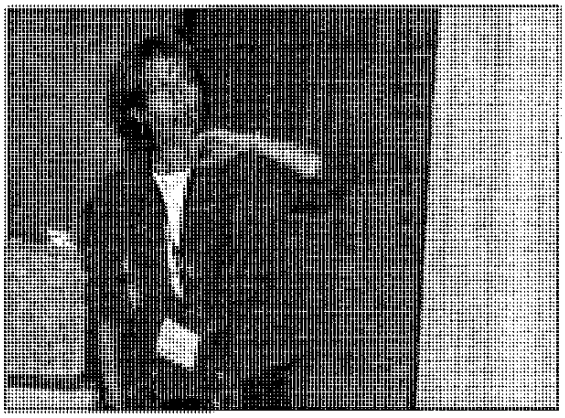
PART 2

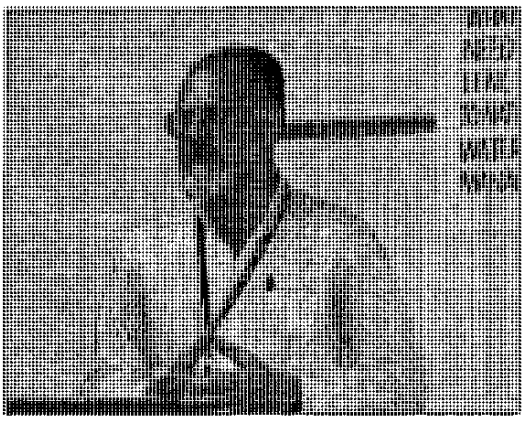
NGT WORKSHOP






Walter McNab





PRIORITY 1

What Is the True Value of Water?

Originators:

Bourcier on behalf of himself, Christensen, Coty, Folta, Lamont, McNab, Newmark, Stewart, and Woodward

The following issues were consolidated under the above title:

Title: **What Is the True Value of Water?**

Originator: Bourcier

Research Issue Description:

Develop a method for determining the true cost of water in various uses at different points of use. Current water costs do not reflect the true value or real cost of water.

Importance:

In order to evaluate directions for possible research areas in water quality and resource management, we need to be able to identify problem areas that are most significant. A water value analysis helps determine the best direction for research.

How Do You Propose Meeting or Complying with This Research Issue?

Create a team of economists, system modelers, and technical people to develop a detailed model of rate costs.

Title: **Determine the Best Water for Human Use**

Originator: Bourcier

Research Issue Description:

With time, water supplies will more and more be a product of treatment technologies. Should these technologies be tuned to produce water that is optimum for human (or animal) health? Is there a composition of water that is most healthy (or tasty) for human consumption?

Importance:

Important for human health.

How Do You Propose Meeting or Complying with This Research Issue?

- Develop a statistical analysis of correlation between human health and water quality.
- Build a mechanistic understanding of water mineral content or human physiology.

Title: **A Sound Basis for Major Infrastructure Investments**

Originator: Christensen

Research Issue Description:

Major infrastructure investments are made to provide water resource for 50-plus years. Water supply, demand, and quality vary on much shorter time scales. Sound investments must take into account the varying supply and demand algorithms. This requires the integration of knowledge of complex systems involving climate change, natural and man-made storage and conveyance systems, changing land use, changing quality demands, water-material interactions, and anticipating the aging of existing systems.

Importance:

- Traditional water supplies do not meet demands.
- Investments are being made to overcome shortfalls (storage, conveyance, and purification systems).
- Most discussion addresses relatively short-term issues, and knowledge of long-term change is not taken into account.
- Investments are costly.

How Do You Propose Meeting or Complying with This Research Issue?

- Create a National Center to organize, integrate, develop, and apply science-based systems to manage supply, storage distribution quality, and use.
- Integrate our forecasting capabilities in climate change with surface and subsurface hydrology, with knowledge of aging effects of existing systems and advanced purification systems.
- Build scenarios around changing demand.

Title: **Water Resources Research, Integration, and Assessment Programs**

Originator: Coty

Research Issue Description:

Develop a water resources research integration and assessment program that assesses proposed water resource technologies and tools to provide guidance that ensures applicability, usefulness, and transferability.

An analogy to this proposed program is the example of a patent office. A patent office performs "market research" and provides guidance such that scientists modify their research so it may be patented. This water integration and assessment program would provide guidance on modifying and enhancing research to better ensure applicability and usefulness.

Importance:

- Enhance the interdisciplinary and integrated nature of water resources research and technologies at LLNL to fill gaps in water research arena.
- Maximize the potential for usefulness, applicability, and use of technology and research for intended water resource issues by stakeholders/clients.
- Bridge chasms between science and values by incorporating these in projects upfront.
- Carry out market research that guides how a problem is framed and addressed.
- Maximize the potential that better science will actually be used in the real world rather than have the science remain irrelevant to the issue resolution or decision-making.

How Do You Propose Meeting or Complying with This Research Issue?

- Form a committee within a Water Center or focus area at LLNL that develops this assessment program.
- Form an advisory board that includes multiple disciplines as well as external members from key agencies, NGOs, etc.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Economics of Water Management Strategies**

Originator: Lamont

Research Issue Description:

As water supplies become scarce, much of the need for water can be alleviated through better management. This includes allocating water to more valuable uses and between years when water is either scarce or plentiful. Accomplishing this will require greater use of storage strategies, such as conjunctive use. We need to understand the value of new infrastructure and water treatment technologies to accomplish this management. This is key to understanding the actual value of water at different locations and times.

The value of water, and the value of new infrastructure, depends on the water management strategy that is used. Consequently, in studying water management strategies, it is essential to first identify optimal strategies. Based on these strategies, we can more clearly understand the economic contribution of adding new water to the system, adding infrastructure, and changing the amounts of water allocated for environmental uses.

Importance:

This is key to eventually meeting the world's water needs in the most economic way. It is also needed to properly evaluate the value of new water technologies, water treatment, and the need for new infrastructure.

How Do You Propose Meeting or Complying with This Research Issue?

An optimization model of water management will find the allocations that maximize the total value of water. Once this is done, the results of such analyses can tell us the value of new infrastructure and additional water supplies.

Extend existing water economics models and develop additional models. These include the CALVIN optimization model of the California water system and the CALSIM model.

This will include the evaluation of water applied to agriculture and its use in urban areas. These steps have been done in the case of California to a large extent. These estimates can be refined. In addition, the effects of water quality on economic value of water can be included.

Title: **Economic Interaction of Water Management and Energy Systems**

Originator: Lamont

Research Issue Description:

Water management requires energy. We use energy to pump and move water. New water treatment technologies will require very large amounts of energy. The cost of energy is a major cost in their operation; however, the cost of energy is not constant over the day or over seasons. The cost of energy at any given time depends on the total demands on the energy system and the types of generators used in the energy system.

The patterns of energy cost affect the operating strategies for water technologies. Typically, we would try to run the water treatment technologies during hours when energy costs are low; however, this reduces the total utilization (duty cycle), which in turn affects that total amount of capital that must be invested to obtain a given water output rate, thus affecting the capital costs of the water system. This may lead to different trade-offs between the capital and operating costs of treatment technologies. At the same time, adding significant amounts of water treatment technologies to the energy system will result in a restructuring of the energy generation system to economically deal with the changed demand systems.

We can study the interaction of the structure of the energy generation system as well as the types of water treatment (and management) technologies and the patterns of their use. If these are optimized together, their total cost will be reduced.

Importance:

By understanding the economic interaction between these two systems, we can better identify the types of water technologies that should be used and help identify how the energy system should be structured to efficiently accommodate water management.

How Do You Propose Meeting or Complying with This Research Issue?

We can use existing LLNL modeling systems (META•Net) to investigate the optimal structure of a water management-energy supply system. This would provide us with guidance about the preferable tradeoffs between capital and operating costs and help us identify the most cost-effective water treatment technologies. It will help us understand how we should organize the energy supply system as we increase water treatment and management.

Title: **Cost-Benefit Analysis of Aquifer Remediation for Public Health Goals Versus Freeing Additional Water by Universal Wellhead Treatment**

Originator: McNab

Research Issue Description:

The goal of any water resources management strategy, whether implied or stated explicitly, is to make additional water resources available for use. In contrast, the goal of aquifer remediation efforts (e.g., pump-and-treat, *in situ* remediation, monitored natural attenuation) is to be protective of public health by striving to reduce contaminant concentrations below applicable toxicity thresholds. From a certain perspective, this public health-oriented approach does not efficiently provide for additional water resources because it is characterized by a high cost associated with remediation but yields no new water, as aquifers remain contaminated in most cases even though the overall mass of contamination may be reduced. Therefore, it is worth considering the benefit of the wholesale abandonment of aquifer remediation efforts in lieu of allocating resources directly into wellhead treatment and institutional controls. An analysis of this approach, using California as an example, should consider:

1. The overall geographic distribution of contaminated groundwater across the state, including basins or sub-basins that are presently deemed unusable as a result of contamination. Predictions of the long-term spread of contaminants on basin-wide scales in the absence of aquifer remediation would need to be addressed through modeling.

2. An analysis of the lumped costs associated with state-wide groundwater remediation efforts.

3. An analysis of the lumped costs associated with the widespread implementation of applicable wellhead treatment technologies and the imposition of institutional controls.

Importance:

This issue is of enormous importance, considering the costs associated with groundwater cleanup efforts. The overall quantity of new water that would be made available is probably unknown at this time. It is worth noting that such a study would likely be very politically charged and polarizing.

How Do You Propose Meeting or Complying with This Research Issue?

The aforementioned Item #1 is largely being addressed at LLNL through the Groundwater Ambient Monitoring and Assessment (GAMA) and Geotracker projects; basin-scale groundwater modeling would be needed to assess future contamination impacts. Approaches for the economic analyses associated with Items #2 and #3 need to be developed.

Title: **Center for Environmental Consequences**

Originator: Newmark

Research Issue Description:

Develop coupled atmospheric/surface/groundwater models that account for the migration and fate of containment releases at different temporal and spatial scales. Factors include:

- Source term.
- Transport (forward).
- Fate (reactive bio-geo-chemistry.)
- Uncertainty (in a Bayesian context, so data-driven collections can be utilized and improved).
- Health and environment risk.
- Data integration and assessment.
- Consequences of recovery alternatives.
- Implications for societal impact.

Importance:

- Preparation for strategic planning, emergency response, and recovery.

- Dual use:
  - Homeland/national security: emergency response to and recovery from an accidental or intentional release (i.e., radioactive dispersal device [RDD] at a Sacramento park at the confluence of two rivers).
  - Environmental/civilian: accidental release response (i.e., railroad car spill). Help assess response to regulatory requirements (i.e., non-point source contributions).

How Do You Propose Meeting or Complying with This Research Issue?

Establish a Center for Environmental Consequences at LLNL, using existing capabilities (fundamental understanding, codes, experimental validation) and filling gaps.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.

- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.

PRIORITY 2

Regional Scale, Data-Driven Water Supply/Demand/Quality Forecasting and Optimization Models

Originators:

Rice on behalf of himself, Cantwell, Coty, Dooher, Folta, Layton, Stewart and Woodward

The following issues were consolidated under the above title:

Title: **Regional Scale Data-Driven Water Supply/Demand/Quality Forecasting and Optimization Models**

Originator: Rice

Research Issue Description:

Integrated, coupled atmospheric, hydraulic, biogeochemical models on a regional scale represent significant computational and information system challenges worthy of a national multidisciplinary laboratory.

Importance:

Development of a coupled, integrated modeling system will support water allocation and infrastructure investments to address future climate changes and to meet increasing water needs for the twenty-first century.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL should partner with the State of California to use GAMA, Geotracker data, and other data centers to use California water problems to develop model system functionality. Start with existing California water management codes and reimplement and integrate, and then add solute transport to them.

Title: **Center for Water Information Management or Water Information Management Program for the Environment (WIMPE)**

Originator: Cantwell

Research Issue Description:

- Data acquisition and management across diverse sensor systems, storage devices, and software interfaces.
- Data mining and information fusion across information sources for every aspect of water from sources to delivery at a use-point to waste stream processing and reuse.
- Delivery of the right information at the right time to the right people.

Importance:

Unintegrated information about different segments of our water world is the source of significant conflict in water management.

How Do You Propose Meeting or Complying with This Research Issue?

Use LLNL's capabilities in water management tools, like Geotracker, data mining, management of data from large-scale modeling, and web-based information systems for defense applications.

Title: **Develop a Tool Box for Total Maximum Daily Loads (TMDLs) Management Tools**

Originator: Coty

Research Issue Description:

Develop a TMDL technology and management system toolbox composed of integrated, yet multiple and separable, capabilities that fit user needs across the nation that includes:

- Coupled and unique (yet critical) water quality models (e.g., surface to groundwater; atmospheric to surface water; estuary).

- An allocation model.

- An economic analysis tool to assess alternative best management practices (BMPs) for the efficacy and efficiency of resource use (i.e., couple water quality model with economic model).

- A framework for decision making with uncertainty and incomplete knowledge.

Importance:

- It is burdensome (resource intensive) to mitigate nonpoint source pollution.

- It is resource intensive, contentious, and a slow process.

- There is a national need for tools that enhance resource-limited use and capabilities to quantify water quality issues; make difficult allocation decisions; understand uncertainty in analyses; and develop the best implementation plan to mitigate contamination.

- Forty-thousand TMDLs need to be addressed and within a contained timeframe.

How Do You Propose Meeting or Complying with This Research Issue?

Develop a program within the water resources research area that is multidisciplinary and uses a teamwork framework to develop integrated tools, including:

- Water models.

- Economic and decision science (allocation) models.

- Assessment tools for valuing of water quality for various uses.

- Geospatical Information System (GIS) tools and interfaces.

- Decision-making tools to deal with uncertainty and risk.

- Work with multiple agencies and stakeholders in partnership to build the toolbox.

Title: **Cooperative Water Collection and Data Assessment in Groundwater and Surface Water Systems**

Originator: Dooher

Research Issue Description:

The internet has made it possible to quickly share large amounts of information and ideas in ways that have not been heretofore possible. Additionally, database development and storage capacity has developed to the point where huge modeling efforts can be easily stored and the results displayed over the internet. The next obvious step is to incorporate the efforts of various researchers and consulting groups so that the diverse skills and knowledge of each group can be shared and built off of, and to use group efforts to attack and solve the issues in hydrology and geochemistry associated with our huge and poorly understood aquifer and riverine systems.

Importance:

There are many different research groups that are actively collecting data of multiple types for use in their own research issues. Other researchers may have need of such data, but have no way to access it, or may have information of their own that the first research group may need and be unaware of. Additionally, there are thousands of detailed groundwater and surface water modeling and data collection efforts that are occurring and reoccurring at the small scale, then are later abandoned when the project is completed, only to be redone later by other research or consulting groups. This duplication of effort increases research and assessment costs that could be better spent on either additional data gathering or modeling efforts.

The assessment and modeling of groundwater and surface water systems is not like the effort put into designing a new engineering product. In the earth sciences, we truly should be standing on the shoulders of others. Projects, when finished, should and could be added to the tapestry of knowledge as a whole.

LLNL should take the lead in acting as a clearing house, creating iterative models and knowledge bases that build upon each other. Because the real world is so huge, and because there are so many different projects, giving researchers, consultants, and regulators a clearing house of modeling and data information over the internet, with qualifications as to the estimated veracity of the modeling and measured data, would increase the accuracy and decrease the time needed to understand these systems.

Components should be built into the system so that it is "living," as opposed to static, with a collaboration of different ideas resulting in a product that more closely resembles what actually occurs in the real world. The result of such efforts would be available through the internet, leading to an increase in public trust in the resultant data collection and modeling efforts.

How Do You Propose Meeting or Complying with This Research Issue?

Information management and computation groups within the lab would, of course, have to work together, but an application of Bayesian statistics to combine these diverse models of varying quality would also be necessary. Numerical modelers would have to develop ways to integrate detailed assessments of uncertain quality into larger, less detailed fabrics. The final result would be iterative, concentrating on areas that are of great interest to many, and directing resources to areas where there has not been enough efforts taking place. Multiple groups within the lab can attack this problem, with university collaboration becoming the first step towards this communal model.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Scalable Simulation System for Coupled Surface and Subsurface Hydrology and Biogeochemical Dynamics**

Originator: Layton

Research Issue Description:

Water management in the 21st century will deal increasingly with issues involving both hydrologic and biogeochemical processes. Accordingly, if LLNL is to play a role in developing robust solutions for various kinds of water management challenges (e.g., water banking, remediation, well siting, salinity management, etc.) in different geohydrologic settings, then a simulation system must be developed that can deal with coupled processes.

Importance:

Decisions regarding the development and operation of sustainable water systems (for supply and quality) will be one of the single most important challenges facing the global water management community in the 21st century. Failure to develop and apply models that can simulate complex hydrologic (coupled surface and subsurface flows) and biogeochemical processes will inhibit the implementation of scientifically defensible solutions for site-specific hydrologic and water use conditions.

How Do You Propose Meeting or Complying with This Research Issue?

A team of LLNL modelers would develop a conceptual model of the relevant processes that need to be simulated and, then based on that conceptualization, a strategy would be followed of either modifying an existing model or creating a new one that can achieve the desired simulation criteria.

Title: **Decision Support Tool for Managing Saline Groundwaters**

Originator: Layton

Research Issue Description:

The salinization of groundwater basins is a growing worldwide problem. If unchecked, entire aquifers can become unusable for irrigation or domestic uses. Salt management requires a balanced approach of operational decisions, as well as water treatment. In order to implement integrated, cost-effective approaches for preventing and/or remediating groundwater salinization, a decision support tool is needed that:

- Explicitly addresses salt accumulation processes based on land uses, as well as the subsurface flow and transport of salts.
- Includes a suite of salt control alternatives with supporting cost data.
- Optimizes the routine for comparing sets of alternatives.

Importance:

Salt accumulation in groundwater due to surface irrigation of arid lands is an age-old problem, but one that is becoming more important to deal with as reliance on groundwater supplies increases. Large urban and agricultural areas relying on aquifers undergoing salinization could face significantly increased costs of water unless timely decisions are made regarding salt management.

How Do You Propose Meeting or Complying with This Research Issue?

The development of the salt management decision tool could easily build on a new LLNL hydrologic/biogeochemical model that includes salt accumulation processes. Team members would include staff familiar with decision analytic methodologies (Lamont/Stewart), groundwater modelers (Tompson, McNab, etc.), geochemists, and engineers.

Title: **Identify Data Rules for the Application of Decision Representative Conceptual Model Spatial Scales**

Originator: Rice

Research Issue Description:

Data analysis and modeling rules need to be developed so that the spatial scales associated with sparse hydrogeologic data can be explicitly considered and applied during regional modeling.

Importance:

Data may be appropriate for decision making at one hydrogeologic scale, but not applicable at another scale. The development of data spatial scale rules will allow the application of data fusion techniques to integrate sparse data at appropriate spatial scales. This would also allow models that can flux into different or adjacent scale domains. This type of uncertainty needs to be represented if data driven hydrogeologic modeling is to take place on large spatial scales (e.g., State of California).

How Do You Propose Meeting or Complying with This Research Issue?

The LLNL Environmental Protection Department has experience creating the data interpolation rules to model hydrogeologic settings (plume history analysis [PLUHA] approach). This approach needs to be applied to the issue of spatial scales.

Title: **Systems Modeling of Water Resources and Water Technology**

Originator: Stewart

Research Issue Description:

A model that measures the value of water, proposed technologies, and research plans will improve the efficient allocation of research and development programs.

Importance:

Many research plans are proposed that have little or no influence with decision makers.

How Do You Propose Meeting or Complying with This Research Issue?

- Work with regulators (USEPA, etc.) and policy makers to develop and maintain a transportable water optimization tool.
- Partner with water technologists, geochemists, hydrologists at LLNL, and other professionals outside LLNL.

Title: **Use the Proposed Livermore Information Library and Analysis Capability for Water Research and Analysis**

Originator: Stewart

Research Issue Description:

Demonstrate large-scale computations and data integration capability for unique insight.

Importance:

Few can do it. LLNL can gain a unique position integrating data sets for new insights. For example, integrating subsets of regional climate runs at the watershed level, with hydrology models; atmospheric deposition to watersheds integrated with water quality models.

How Do You Propose Meeting or Complying with This Research Issue?

Director's Office support. Build LDRD's using LILAC.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

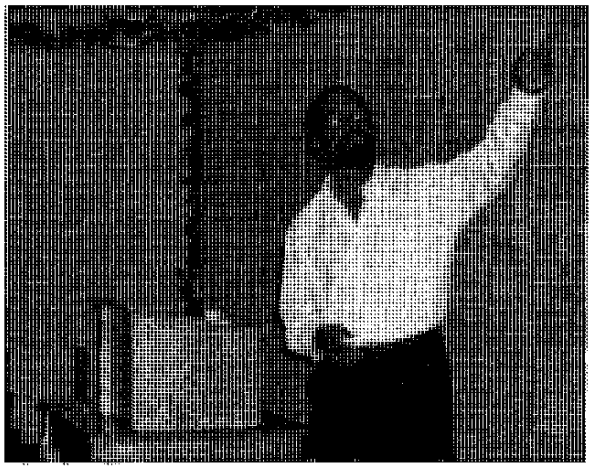
Importance:

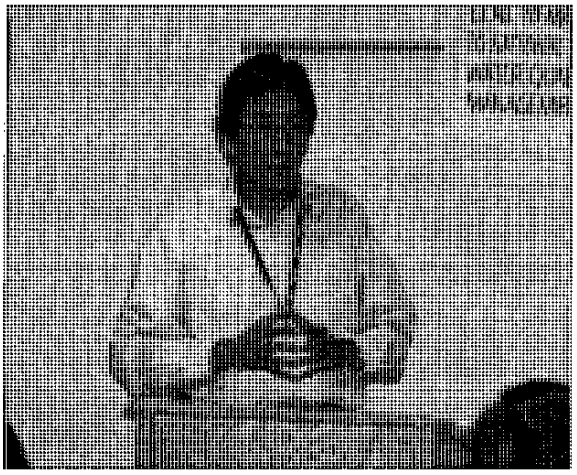
Inadequate funding = No program.

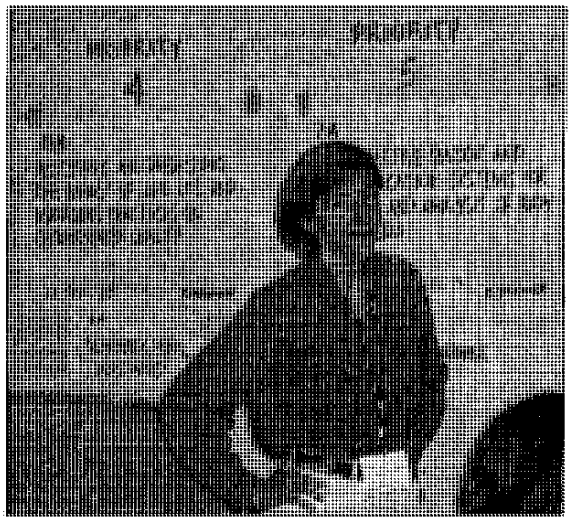
How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.

Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.







PRIORITY 3

Water Infrastructure Security

Originators:

Christiansen on behalf of himself, Cantwell, Coty, Folta, Grey, Moran, Rice, Rosenberg, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Water Infrastructure Security**

Originator: Christensen

Research Issue Description:

Water security is linked to energy security, and both are intimately linked to national security. Security requires solid risk analysis around those infrastructures, the development and deployment of advanced sensors/detectors/signaling systems, and strategically applying defense and response assets. The development of the risk analysis systems linked with advanced physical systems represents the challenge.

Importance:

Disruption of water assets, nationally or internationally, presents an important threat to national security and international stability.

How Do You Propose Meeting or Complying with This Research Issue?

Develop demonstration systems.

Title: **Water Security Analysis Via System-Level Vulnerability Assessments**

Originator: Cantwell

Research Issue Description:

- Adaptable, system-level vulnerability models for the entire scope of water systems within the U.S. have not been built, nor have vulnerability assessments of any sort on a national scale been conducted.

- Other sector infrastructure analyses have demonstrated that significant vulnerabilities, placing large numbers of citizens at risk, are only visible upon developing a model of the infrastructure that encompasses the largest scale of system boundaries possible.

Importance:

Water system vulnerabilities are pervasive and significant.

How Do You Propose Meeting or Complying with This Research Issue?

Capitalize on Livermore's unique capabilities in threat assessment, familiarity, and experience with biological weapons, chemical weapons and radionuclides, and responsibility for Homeland Security science and technology.

Title: **Transboundary Aquifer Management Tools**

Originator: Coty

Research Issue Description:

- Develop an aquifer management "tool box" that is GIS based and allows users to verify adherence to water allocations, assess efficient use, and optimize water resources. These GIS-based conceptual and modeling tools will allow users to manage aquifer issues in a graphical and simple manner.

- LLNL is in a unique position to provide objective and credible assessment tools such that stakeholders may enhance decision making.

Importance:

- Increased demand on water supplies greatly potentiates conflicts and misuses of valuable, yet shared, groundwater supplies.
- Limited supplies of water necessitate efficient use and the sustainable management of resources.
- Transboundary aquifer issues and water security are critical issues on an international scope.

How Do You Propose Meeting or Complying with This Research Issue?

- Require the integration of hydrogeology technologies, information management systems, decision-science technologies, and GIS tools.
- Provide a tool that quantifies water use, recharge, and storage in the aquifer while using information management and decision-science tools to evaluate the data and present this in a conceptually simple, but powerful, GIS interface.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Host a Tribal Nations' Water Conference in Partnership with the U.S. Department of Energy**

Originator: Grey

Research Issue Description:

Look at the traditional and technical aspects of water. We should target land-based tribes. Traditional leaders look at water from a sacred/religious view. Tribal technical people look at water as management and long-term use issues.

Importance:

We need to hear from tribal leadership along with traditional and tribal technical personnel. Fifteen percent of the natural resources reside on Indian lands. This could be LLNL's contribution to support the USDOE's Indian Policy. It could also prevent major water litigations that might arise due to non-tribal input.

How Do You Propose Meeting or Complying with This Research Issue?

Host a tribal national water conference and get the USDOE to fund it. We can also look to gaming and energy tribes to assist in funding such a conference. The USDOI could also be a potential partner.

Title: **Protecting Groundwater from Unintentional Water Recycling (in the Fastest-Growing Cities in the World)**

Originator: Moran

Research Issue Description:

Water recycling is carefully controlled in developed countries. In developing countries, untreated wastewater is used to irrigate large areas of farmland and is transported in infrastructure that is frequently compromised. Contamination of drinking water (especially groundwater) and food supplies by wastewater is an issue that has not received much attention by scientific researchers, given the magnitude of the health problems it causes.

Importance:

Every day, hundreds of millions of people are ill due to waterborne diseases. Some of these illnesses are the results of wastewater contamination of drinking water. Political and economic stability cannot be achieved when a significant portion of the population is ill or tending to ill relatives. In large cities with exploding populations (e.g., Mexico City, Lagos, Gaborone, Bombay, Shanghai), the construction of sewage treatment facilities or water recycling plants will be impractical over the next couple of decades (surface water supplies everywhere have to be treated – there is a chance to protect some highly valuable groundwater supplies before they are highly impaired).

How Do You Propose Meeting or Complying with This Research Issue?

Research should be focused on identifying the main pathways by which wastewater contaminates groundwater used for drinking water. Research should take place in a few large cities whose population growth is out of control and groundwater exploitation is likely to continue. Determine key parameters that govern virus/microbial transport; delineate areas where groundwater is vulnerable (using GAMA-like assessments, which are actually highly cost-effective) to contamination from unlined, leaking sewage drains. Optimize the use of water treatment technologies for the biggest payoff, focusing on health risks. A major challenge would be convincing USDOE that this is worthwhile for funding.

Title: **Re-Engineering of Water Capture Systems in the Urban Environment**

Originator: Rice

Research Issue Description:

Existing urban water drainage systems conduct water efficiently to the ocean and often limit recharge or capture for storage. These systems need to be reconsidered to increase capture and treatment when necessary to the meet water quality of intended use. This could include greater application of constructed wetlands or bioactive treatment systems on storm drains on a community level.

Importance:

Increased capture of run-off water can provide significant volumes of "new" water for the 21st century.

How Do You Propose Meeting or Complying with This Research Issue?

Partner with urban planners at a pilot city that is rapidly growing and has an increasing water need.

Title: **Transboundary Water Resource Conflicts as Opportunities to Promote Regional Security**

Originator: Rosenberg

Research Issue Description:

Rather than view water resource conflicts primarily as threats to regional security, one can view them as opportunities to promote greater understanding, cooperation, and ultimately greater stability and security. There are many ways to approach "environmental peacemaking." The issue here is to identify what types of problems and approaches to addressing these problems work best.

Importance:

Conflicts over water resources are increasing in many areas of the world, many of which are unstable and of strategic interest to the U.S.

How Do You Propose Meeting or Complying with This Research Issue?

Engage organizations (e.g., the State Department, military, NGOs) interested in this issue and form partnerships. LLNL brings the technical/scientific component to such a partnership as well as experience supporting national and international security matters.

Title: **Rapid Notification of and Response to Suspected Incidents of Intentional Water Contamination**

Originator: Rosenberg

Research Issue Description:

There is a need to quickly determine if water has been contaminated and, if so, the nature of this contamination and its likely consequences. Needs include early warning systems (e.g., sensors, communication, etc.) in water distribution systems, field kits for first responders to an event, sampling and analysis for rapid contaminant identification, and better understanding of the fate and transport of contaminants in a water supply system (including reactions with chlorine). This technology is dual-use (i.e., it would protect against non-intentional contamination as well).

Importance:

Concern with terrorist attacks on water supply systems.

How Do You Propose Meeting or Complying With This Research Issue?

Engage the USEPA, water utilities, and emergency response community, all of which are very interested in this issue.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Management Decision Tools for Optimizing Investment Choices to Increase Water System Security**

Originator: Woodward

Research Issue Description:

We have developed processes (practical environment restoration management [PERM]) to allow managers to estimate the impacts of investment choices on resources using a deterministic approach; however, investment choices to reduce risks from terrorist activities require probabilistic approaches. We need to expand the PERM process to integrate probabilistic input and to optimize choices.

Importance:

Water system managers need to transparently demonstrate the reason for their investment choices and to predict long-term operating and capital costs. By augmenting the PERM process

(which provides transparency) with probalistic approaches, managers can effectively demonstrate which investment choices will minimize operating costs.

How Do You Propose Meeting or Complying with This Research Issue?

Involve Decision Support, Engineering, Non-Proliferation and Arms Control (NAI), and municipal water system managers.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

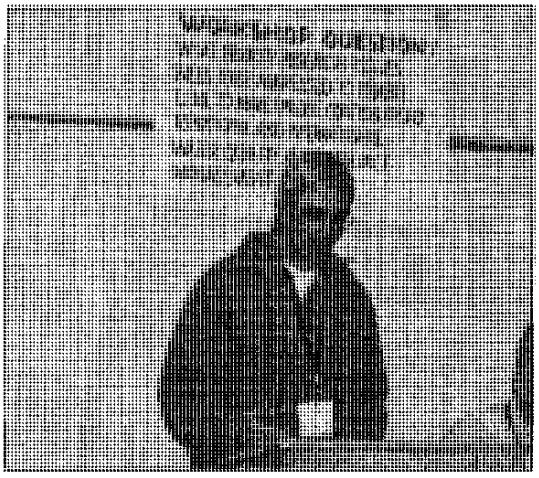
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

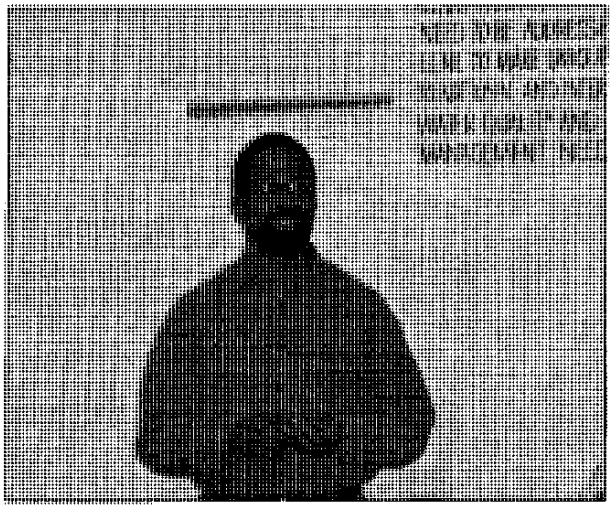
Importance:

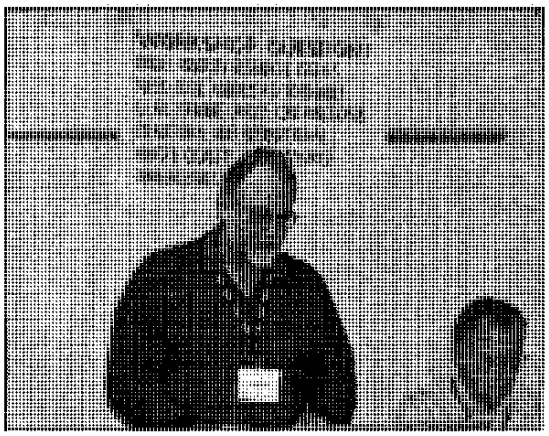
Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.







PRIORITY 4

Assess and predicting the Impact of Land Use and Managing Practices on Groundwater Quality

Originators:

Newmark (for Carle), Cody, Esser, Folta, Lamarre/Woodward, Rice, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Groundwater Quality Prediction for Water Supply Management**

Originator: Newmark (for Steve Carle)

Research Issue Description:

In California, much recent legislative effort and several modeling tools now facilitate management of the *quantity* of groundwater supplies; however, groundwater*quality* in groundwater basins is addressed primarily by monitoring approaches without emphasis on predictive capabilities. In the long-term, degraded groundwater quality may seriously diminish the *quantity* of groundwater available for beneficial use, as well as the usable storage capacity of groundwater basins.

Importance:

The issue of predicting long-term water quality in groundwater basins ties into several other important issues besides management of water supply quantity in California, including:

- Regulatory limits, which tend to decrease over time (e.g., arsenic).
- Use of groundwater basins to store and manage surface water supplies (conjunctive use).
- Intrusion of poor quality groundwater, saltwater, or brine as a result of excessive overdrafting.
- Salinization of aquifers as a result of surface irrigation by imported surface water.

- Recharge using reclaimed water (e.g., Orange County, California).
- Nonpoint source pollution (e.g. nitrate).
- Water supply for any arid or semi-arid region on earth (e.g., western U.S., the Middle East).
- Water supply for many nonarid regions on earth (e.g., Bangladesh).
- Global stability (water security).

Currently, water management models (e.g., CALVIN) consider groundwater but do not have a capability for groundwater quality prediction. This is especially important as the result of different land uses (urban, environmental agriculture).

How Do You Propose Meeting or Complying with This Research Issue?

LLNL possesses an array of analytical and simulation capabilities that could be interfaced with a water management model (e.g., CALVIN). Some of these capabilities, with key technical personnel in parenthesis, include:

- Use of water management models (Jeff Stewart, Alan Lamont, UC Davis).
- Groundwater age dating to evaluate susceptibility to pollution and improve the calibration of groundwater flow models (Bryant Hudson, Lee Davisson).
- Groundwater flow modeling (Steve Carle, Zafer Demir).
- Particle-based transport modeling (Reed Maxwell, Andy Tompson).
- Reactive transport modeling using GIMRT (Carl Steefel, Andy Tompson) or NUFT (John Nitao). This is especially important for land use-induced fluxes.
- Understanding land use impacts on water quality.

A possible way to initiate a program would be to target two study areas: one in California and one overseas. For California, find a progressive agency willing to work with LLNL (e.g., SCVWD or Orange County Water District [OCWD]). Help agencies apply for state grants (e.g., AB303 groundwater management [up to $350,000], Prop 13 groundwater storage [up to $5 million]). Note that collaboration with outside groups is encouraged for these state funding opportunities. For overseas, could we perhaps obtain funding from USDOE through a "water security" program? It is important to work with (local) managers to identify current and perceived management issues from the start.

Title: **Develop a Tool Box for Total Maximum Daily Loads (TMDLs) Management Tools**

Originator: Coty

Research Issue Description:

Develop a TMDL technology and management system tool box composed of integrated, yet multiple and separable, capabilities that fit user needs across the nation that includes:

- Coupled and unique (yet critical) water quality models (e.g., surface to groundwater; atmospheric to surface water; estuary).
- An allocation model.
- An economic analysis tool to assess alternative best management practices (BMPs) for the efficacy and efficiency of resource use (i.e., couple water quality model with economic model).
- A framework for decision making with uncertainty and incomplete knowledge.

Importance:

- It is burdensome (resource intensive) to mitigate non-point source pollution.
- It is resource intensive, contentious, and a slow process.
- There is a national need for tools that enhance resource-limited use and capabilities to quantify water quality issues; make difficult allocation decisions; understand uncertainty in analyses; and develop the best implementation plan to mitigate contamination.
- Forty-thousand TMDLs need to be addressed and within a contained timeframe.

How Do You Propose Meeting or Complying with This Research Issue?

Develop a program within the water resources research area that is multidisciplinary and uses a teamwork framework to develop integrated tools, including:

- Water models.
- Economic and decision science (allocation) models.
- Assessment tools for valuing of water quality for various uses.
- Geospatical Information System (GIS) tools and interfaces.
- Decision-making tools to deal with uncertainty and risk.

Work with multiple agencies and stakeholders in partnership to build the toolbox.

Title: **Water Resources Research, Integration, and Assessment Programs**

Originator: Coty

Research Issue Description:

Develop a water resources research integration and assessment program that assesses proposed water resource technologies and tools to provide guidance that ensures applicability, usefulness, and transferability.

An analogy to this proposed program is the example of a patent office. A patent office performs "market research" and provides guidance such that scientists modify their research so it may be patented. This water integration and assessment program would provide guidance on modifying and enhancing research to better ensure applicability and usefulness.

Importance:

- Enhance the interdisciplinary and integrated nature of water resources research and technologies at LLNL to fill gaps in water research arena.
- Maximize the potential for usefulness, applicability, and use of technology and research for intended water resource issues by stakeholders/clients.
- Bridge chasms between science and values by incorporating these in projects upfront.

- Carry out market research that guides how a problem is framed and addressed.
- Maximize the potential that better science will actually be used in the real world rather than have the science remain irrelevant to the issue resolution or decision-making.

How Do You Propose Meeting or Complying with This Research Issue?

- Form a committee within a Water Center or focus area at LLNL that develops this assessment program.
- Form an advisory board that includes multiple disciplines as well as external members from key agencies, NGOs, etc.

Title: **Assessing the Impact of Land Use and Management Practices in Groundwater Quality**

Originator: Esser

Research Issue Description:

Much attention has been paid to how land use affects groundwater recharge and, to some extent, salinity. Less attention has been paid to the impact on other groundwater quality parameters, especially nonpoint source pollutants. A simple approach to gaining insight into this issue is to assess how deep groundwater basins respond to changes in land management. To do this, we need a robust way to correlate changes in groundwater quality with changes in land use, agricultural or animal operation management practices, and water management practices (including artificial recharge). An integrated approach would:

- Use groundwater tracing (with noble gas tracers and tritium-helium ages).
- Determine of true groundwater ages (with groundwater models strongly coupled to apparent groundwater age).
- Develop source tracers (with isotope and trace inorganic and organic geochemistry).
- Apply reactive transport or particle-tracking modeling.

The goal is to be able to demonstrate the impact of different management plans on groundwater quality.

Importance:

Changes in the way the land surface is used and surface water is managed in groundwater recharge areas can have dramatic effects on groundwater basin water quality. As we become increasingly reliant on groundwater as a drinking water resource, understanding the trend toward suburbanization of agricultural lands, implementing precision agriculture and comprehensive nutrient management, and implementing conjunctive use will affect groundwater quality and becomes increasingly important. Many management practices are voluntary (e.g., best management practices in agriculture, methods of artificial recharge) and/or are costly (e.g., conversion from septic to sewer). Policy makers need strong evidence that changes are needed and are effective, and water managers need data to support analysis of tradeoffs between different management practices.

How Do You Propose Meeting or Complying with This Research Issue?

Difficulties with clear demonstration of impact include:

- The scale of management practice studies (which are generally conducted on short time scales and only encompass the soil zone).
- The longer time scales over which groundwater processes operate.
- The difficulty in determining the age and origin of young groundwater.

LLNL has leadership in age dating young groundwater. To leverage this leadership, we should:

- Develop groundwater models that are strongly coupled to apparent groundwater age, and that output true groundwater age.
- Develop source tracers and reactive transport models appropriate to the contaminants of concern.
- Demonstrate the applicability and effectiveness of the technique by conducting field studies where best management practices have been instituted, and land use has changed in the last 50 years.

We should pursue our contacts with UC Davis, the Alameda County Flood Control and Water Conservation District, SCVWD, and use their field sites and their problems to demonstrate the approach.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.

Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Adverse Impacts of Groundwater Pumping**

Originator: Lamarre/Woodward

Research Issue Description:

The issue is how to prevent or mitigate the adverse consequences of mining groundwater, such as land subsidence or loss of surface water bodies.

Importance:

Extensive groundwater pumping, primarily for agricultural irrigation, has resulted in a significant lowering of the water table in many regions, especially in California's Central Valley and in southern Arizona. Severe adverse impacts resulting from this have been subsidence and cracking of the ground surface, dewatering of previously free-flowing rivers and streams, and loss of habitat for aquatic and riparian species.

This issue is important because population growth, and the attendant need for increasing amounts of water for urban and agricultural use, will put more pressure on groundwater resources and require increased extraction from groundwater basins. The cost of repair to and maintenance of virtually all ground surface infrastructure (e.g., utility lines, buildings, streets and highways, airports and railroad lines, etc.) as it shifts and subsides in response to increased pumping could be immeasurable. The loss of surface water bodies for recreation (as their groundwater source declines) will negatively impact land values and quality of life. Many already-stressed ecosystems will cease to exist as the water table is drawn down.

How Do You Propose Meeting or Complying With This Research Issue?

I do not have the solution to this, but it is important enough to be addressed by the workshop. The Engineering Directorate may be able to contribute research ideas to mitigate against land surface subsidence.

Title: **Regional Scale Data-Driven Water Supply/Demand/Quality Forecasting and Optimization Models**

Originator: Rice

Research Issue Description:

Integrated, coupled atmospheric, hydraulic, biogeochemical models on a regional scale represent significant computational and information system challenges worthy of a national multidisciplinary laboratory.

Importance:

Development of a coupled, integrated modeling system will support water allocation and infrastructure investments to address future climate changes and to meet increasing water needs for the twenty-first century.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL should partner with the State of California to use GAMA, Geotracker data, and other data centers to use California water problems to develop model system functionality. Start with existing California water management codes and reimplement and integrate, and then add solute transport to them.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

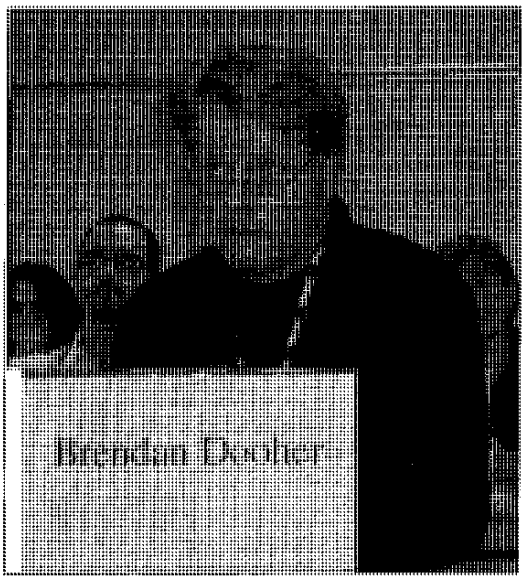
Inadequate funding = No program.

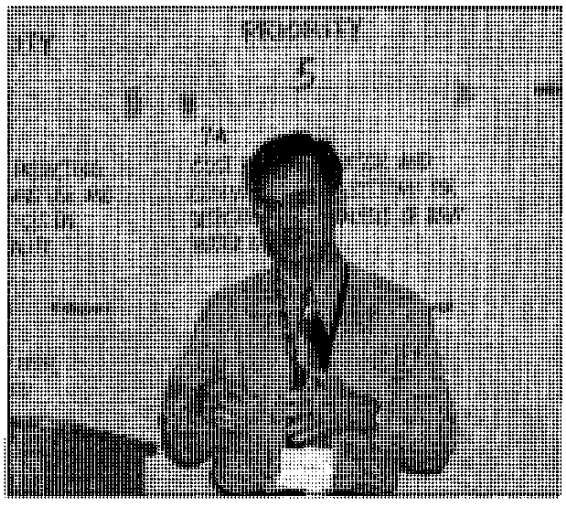
How Do You Propose Meeting or Complying with This Research Issue?

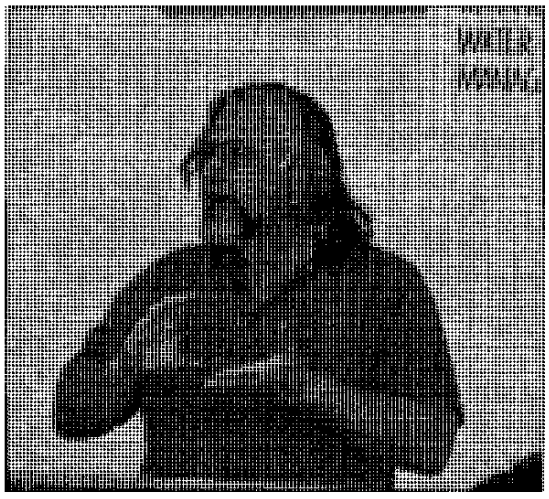
- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.

- Use LLNL Director's Office to publicize the Water Initiative and its successes.

- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.


Brendan Beasley






Jeanne Horn

PRIORITY 5

Cost-Effective Sensor and Communication Systems for Detection and Analysis of Raw Water Media

Originators:

Dooher on behalf of himself, Cantwell, Folta, Hoppes, Horn, O'Brien (for Kane), Rosenberg, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Near-Real-Time Water Sensor Development**

Originator: Dooher

Research Issue Description:

Use LLNL's expertise and technology to develop inexpensive, real-time or near-real-time data collection capabilities for water quality, water level, and water flow rates. Such sensors should be capable of storing and periodically tying into the internet using wireless standards and public protocols.

Importance:

An understanding of the dynamics of groundwater and surface water systems calls for more than quarterly data tracking. Near-real-time data collection of, at least, water levels in wells would be invaluable in tracking contaminant movement from point source releases, as well as to understanding the dynamics of nearby public, private, agricultural, and industrial extraction wells.

Additionally, developing a reliable, low-cost method to measure groundwater movement (as opposed to estimating groundwater velocities) and stream and river flow rates is necessary to understanding the system's dynamics.

Chemical sensors should be capable of accuracy levels of at least hundreds of parts per billion and work on a day-to-day basis. These chemical sensors could act as sentries for contaminant

movement and would be invaluable for not only contaminant sites, but for drinking water wells and riverine systems.

Manpower is often the greatest cost in assessing contaminants and monitoring drinking water sources, so developing low cost sensors would allow better monitoring of water quality and understanding of water systems.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has great programs that are already looking at sensor development. They should work with water utilities and regulators to understand their needs and direct attention to reducing the cost of monitoring the nation's water supplies and, thus, increasing their safety.

Title: **Multidisciplinary Teams for Real-Time, Continuous, Inexpensive Biomonitoring Systems for Any Aqueous Source**

Originator: Cantwell

Research Issue Description:

Major engineering and communication system challenges exist in producing a high fidelity, commercializable version of the above. No one has done it yet, primarily because most efforts have been scattered and under funded. In addition, I have to stress the significant challenges associated with building teams to develop these types of monitors. Multidisciplinary teams must be unified and work together side-by-side.

Usually, these types of projects require significant resource allocations to get to successful field trials.

Importance:

The need is huge and will only become more pressing as water resources are compromised due to use pressures. We will not only need to know bioconstituents, but we will also need to attribute source and understand how to mitigate problems.

How Do You Propose Meeting or Complying with This Research Issue?

Use proven LLNL capabilities in biodetection, microtechnology, water monitoring systems, genomics, assay development, and communication systems for large sensor networks.

Title: **Extend DNA Signature Efforts to Detect (Intentional) Water Contamination**

Originator: Folta

Research Issue Description:

Computational methods have been highly successful in developing candidate DNA signatures. These signatures are the basis of probes that uniquely identify pathogens and are recognized as the "gold standard" for the CDC. The process has been successfully deployed to detect airborne pathogens. Modification of this system to support the detection of water pathogens would leverage successful, well funded, more mature work.

Importance:

- Real-time identification of pathogen contamination in water.
- Leverage off very successful, well-funded program currently at LLNL. Same customers (CDD/USDOE, cities, etc.).

How Do You Propose Meeting or Complying with This Research Issue?

Partner Nina/Slezak/Fitch (CBNP Project).

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).

- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Portable Sensors for Monitoring Complex Water Media**

Originator: Hoppes

Research Issue Description:

Often, water resource professionals must make time-sensitive management decisions concerning water resources. These decisions must be based on water-quality information that cannot be delivered quickly.

Our current analytical capabilities often cannot answer some questions (e.g., What was released? How much was released? Where is it coming from? When did it start? Has it stopped? Is it there?) in adequate spatial and temporal resolution needed to take informed action.

The first challenge is to develop sensor and detector technologies that provide real-time analytical capability.

The second challenge involves engineering detectors that are free from the benchtop and can be deployed in the field, operated by a trained technician, remotely or in a wireless environment.

The third challenge is to get these sensors to work reliably in the field: in sewage, seawater, brackish water, stormwater, and in the places where it is difficult to get sensors to work, but where managers need information about water quality in real-time and of high quality.

Importance:

- There are needs that range from acute management actions, such as deciding whether to close beaches due to fecal coliform outbreaks.
- Source investigations benefit greatly from real-time field capabilities.
- There are approaches that would replace our currently single point-in-time, analyte-by analyte compliance approaches with real-time, online whole effluent toxicity or analyte specific monitoring.

How Do You Propose Meeting or Complying With This Research Issue?

- Create research team of professionals from LLNL and the State and Water Resource agencies to tackle a single tough project. LLNL has the capabilities in sensor technology and engineering. The agencies have the money and the need.
- Develop a real-time field portable sensor that would differentiate human fecal coliform from other sources in seawater samples (a challenge). A similar challenge would be the detection of classes of pesticides and certain organics in surface water runoff.

Title: **Disinfection and Monitoring of Biotic Contamination of Drinking Water**

Originator: Horn

Research Issue Description:

Are there better methods to ensure the sterility of drinking water? This is especially important for third-world countries. In addition, we must develop capabilities to monitor contamination in distribution systems.

Importance:

Contaminant-free water is extremely important in developing countries. In first-world countries, chlorine treatment is not always effective. Distribution system monitoring is also a homeland security and military/defense issue.

How Do You Propose Meeting or Complying With This Research Issue?

Develop new technologies.

Title: **Real-Time, Online Pathogen Detector**

Originator: O'Brien (for Kane)

Research Issue Description:

There is an urgent need for the rapid biological assessment of drinking water quality, particularly with regard to public health and public perception of water safety. Additionally, the increased use of recycled water may contribute to the risk (perceived or real) of exposure to pathogens (bacteria and viruses) that survive the wastewater treatment process. Present methodologies for analysis of biological agents in water are both time- and labor-intensive and have low efficiencies for detection in natural waters. Filter-based systems designed to remove biological contaminants from water do not provide for the adequate recovery and integrity of pathogens for subsequent analysis and are unsuitable for monitoring applications due to clogging. A comprehensive approach is needed that addresses all aspects of the sample collection, processing, and detection process in real water matrices (at relevant volumes) to provide highly reliable data in a rapid time frame.

Importance:

In today's climate, there is an increased awareness of the vulnerability of our drinking water supplies. In the event of a biothreat attack, pre-symptomatic action is required. Water distributors need to make costly and timely decisions based on accurate information concerning whether to divert a water supply from public consumption.

Standard methods today:

- Use Ultrafiltration membranes; use a system commercially available with tracer particles.
- Use tracer particles and laser detection to examine "log reduction," log (F_p / F_D), where F_p = particles upstream versus F_D=particles downstream. A log reduction of >5 is needed.
- Monitor at 2-to 3-week time intervals during the start-up of the plant. Done offline at that time.

- Have subsequent monitoring done monthly.
- Are neither real-time or online!
- Do not really test for pathogens.

The goal is a cost-effective, energy efficient system downstream from ultrafiltration. There is a need to detect at log reductions of 6 and lower. Expect these values to go down as time goes on. System would be downstream of ultrafiltration and other filters; therefore, would be dealing with relatively "clean water."

LLNL is a world-recognized leader in detection methodologies for pathogens in air. While this technology development can be leveraged, water has its own unique set of interferences for detection methodologies and engineering complexities for dealing with large volume samples. A rapid and quantitative means of separating and concentrating biological material from nonbiological material is needed. Further, the detection and quantification of biological agents is only part of the solution, since the real concern is whether the agents are viable and/or infective; therefore, the sample preparation steps need to preserve the integrity of the biological materials collected.

How Do You Propose Meeting or Complying with This Research Issue?

Preliminary research on MEMS-based DEP systems as a means of selectively concentrating biological material from raw water is already underway in the Center for Microtechnology at LLNL. Concentration by DEP is dependent on a dipole moment induced in each particle in a non-uniform electric field. A key advantage to DEP is that body forces can be exerted on biological particles without occluding channels, thus mitigating clogging, the biggest impediment to continuous monitoring. The forces can be applied using alternating current fields up to megahertz frequencies, allowing for the collection of bacterial cells at an electrode surface with a subsequent release of cells when the electric field is removed.

These types of sensors have been shown previously to be able to effectively separate DNA molecules in solution. Another advantage of DEP is that there can be some capture selectivity depending on the frequency of excitation. This technology may provide the front-end to a continuous autonomous pathogen detection instrument for water monitoring.

Other combination techniques (e.g., DEP coupled with ion exchange technology)need to be explored to better capture these moieties.

The key is to develop a:

- Collection system (perhaps DEP).
- Analysis system (derivative of autonomous pathogen detection system).

Phase I

- Explore the ability of this real-time system on a prototype level (low flow rates).
- Increase sensitivity through coating of electrodes.

Phase II

- Pilot-scale unit testing: unit designed to operate at 20 gallons per day.
- Couple with existing processes.

Phase III

- Demonstration phase at specific water plants.
- Matching funds from industry.

Need to involve:

- OEMs for membrane manufacturing.
- USEPA and the California DHS.
- Robin Miles, Betsy Cantwell, Kevin O'Brien, and Staci Kane.
- Other personnel in the LLNL Center for Microtechnology, the Biology and Biotechnology Program, and Nonproliferation, Arms Control, and International Security (NAI).

Title: **Rapid Notification of and Response to Suspected Incidents of Intentional Water Contamination**

Originator: Rosenberg

Research Issue Description:

There is a need to quickly determine if water has been contaminated and, if so, the nature of this contamination and its likely consequences. Needs include early warning systems (e.g., sensors, communication, etc.) in water distribution systems, field kits for first responders to an event, sampling and analysis for rapid contaminant identification, and better understanding of the fate

and transport of contaminants in a water supply system (including reactions with chlorine). This technology is dual-use (i.e., it would protect against non-intentional contamination as well).

Importance:

Concern with terrorist attacks on water supply systems.

How Do You Propose Meeting or Complying With This Research Issue?

Engage the USEPA, water utilities, and emergency response community, all of which are very interested in this issue.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.

Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.

PRIORITY 6

Brine Use and Management Technologies for Gas and Oil Production, Power Plants, and Wastewater Treatment Plants

Originators:

O'Brien on behalf of himself, Bourcier, Cantwell, Folta, Horn, Hudson, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Brine Reduction and Utilization**

Originator: O'Brien

Research Issue Description:

Water clean-up technologies range from RO to EDR to ion exchange. Most systems are a combination of separation processes (e.g., UF coupled with RO). In all these processes, waste streams (brine) are generated. Brine can only be reduced through a systems approach. This needs to be achieved in a cost-effective manner. The more efficient the process, the less brine is generated.

Importance:

In many situations, brine handling is the major driving economic factor. Many projects in the Central Valley in California were cancelled because of this factor alone.

This issue is mitigated with seawater RO systems since they are located near power plants, and the brine is discharged into the ocean. Land-locked brackish water systems do not have this route to mitigation. For example, the City of Phoenix, in Arizona, examined brackish water clean-up projects and were constrained by the handling of the brine.

It is important that we not exchange one non-usable resource for another (i.e., create non-reusable contaminants that will need to be handled).

How Do You Propose Meeting or Complying with This Research Issue?

Requires a combination approach:

- Increase the efficiency of existing processes (i.e., improve separation efficiencies in existing processes):
  - new membrane materials research
  - improved energy recovery processes

- Couple with new research into crops that could use the brine generated.

- Examine solutions, such as the transport of brine to other locations and dilute with seawater.

- Explore solutions that create revenue for the resulting water facilities. For example, power plants collect fly ash and sell this to the cement industry. This would help offset the expected increase in operating costs. Power plants have existing infrastructure that can be readily used, thereby reducing capital outlays. Revenue generation and sharing between power plants and water clean-up facilities could prove to be an overall economic advantage.

The first step would be to identify an area where a problem has been previously identified (e.g., Central Valley or the Navajo Nation). Next, work the proposed solutions in parallel. This requires working simultaneously with the scientific/engineering issues, policy issues, and overcoming parochial boundaries. LLNL is uniquely positioned because of its ability to bridge all of these areas. LLNL can act as a trusted third party. LLNL has worked issues in this fashion in the past. LLNL can then position itself as the KMPG Consulting firm for brackish water handling.

LLNL would need to interact with:

- NSF Science and Technology centers.

- Federal agencies (e.g., U.S. Bureau of Reclamation, USEPA).

- Large engineering firms responsible for plant construction.

- Original equipment manufacturers for water separation systems (e.g., IONICS, Hydronautics, KOCH, etc.).

- State legislators.

- Universities involved in genomics research, such as UC Davis.

Title: **What Is the True Value of Water?**

Originator: Bourcier

Research Issue Description:

Develop a method for determining the true cost of water in various uses at different points of use. Current water costs do not reflect the true value or real cost of water.

Importance:

In order to evaluate directions for possible research areas in water quality and resource management, we need to be able to identify problem areas that are most significant. A water value analysis helps determine the best direction for research.

How Do You Propose Meeting or Complying with This Research Issue?

Create a team of economists, system modelers, and technical people to develop a detailed model of rate costs

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Title: **New Technologies for Resource Extraction from Saline Solutions**

Originator: Bourcier

Research Issue Description:

- Develop new technologies for removing targeted minerals and metals from water.
- Focus on produced brines from oil, gas, and coal extraction that are very saline and contain useful resources, in addition to the brines produced by membrane separation technologies.

Importance:

- Improves the economics of water treatment by generating a marketable byproduct, in addition to a useful purified water stream.
- Reduces the need for energy-intensive mining operations.

How Do You Propose Meeting or Complying with This Research Issue?

- Target new water treatment research and development for the selective removal of elements.
- Leverage off "smart membrane" research and development in other disciplines.

Title: **Technologies to Treat Produced Waters from the Fossil Fuel Industry**

Originator: Bourcier

Research Issue Description:

These fluids have unique properties that make their treatment using existing technologies difficult:

- High organic content.
- High salinity.
- High concentration of toxic metals.

Importance:

- Large volume of produced water (10-million acre feet per year).
- Currently reinjected at average cost of $1 per barrel.
- USDOE has a vested interest in this area.
- Problematic reinjection wells due to scaling.
- Produce water suitable for agriculture (especially in the western U.S.).
- USDOE funds available now to work on this.

How Do You Propose Meeting or Complying with This Research Issue?

Need to develop improved technologies for dealing with problems unique to these fluids:

- High-pressure reverse osmosis using ceramic membrane.
- Down hole oil/water separation.
- Mineral extraction technologies.
- Antiscalants.

Title: **Integrated Water and Energy—Long-Term Planning and Conflict Resolution**

Originator: Cantwell

Research Issue Description:

Provide the ability to do long-term planning and "conflict resolution" for large-scale challenges between the uses and needs of power systems and the uses and needs of water systems.

Importance:

I expect that within the next 10 years, globally, and within the next 20 years in the U.S., we will see significant challenges associated with energy system limitations on our water availability, and vice versa.

How Do You Propose Meeting or Complying with This Research Issue?

- Anticipate problems using science-based analysis and modeling. Develop large-scale models that integrate between both "systems."
- Obtain new data and information to fill in the gaps. Understand system-level integration of vulnerability assessments and utility needs.
- Refine the understanding of the problem with further modeling and analysis.
- Assist policy makers in developing policy that helps to avoid the problem.
- Develop technology that changes or eliminates the problem(s).

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Microbial Effects on Membranes and Materials for Water Distribution**

Originator: Horn

Research Issue Description:

Membrane fouling and microbial effects on membrane integrity are important treatment problems. The corrosive effect of microbes on piping materials is an important issue as well.

Importance:

Microbiologically influenced corrosion (MIC) causes significant damage to piping/transport systems. Also, there is the problem of fouling of reverse osmosis and other purification membranes.

How Do You Propose Meeting or Complying with This Research Issue?

Already have a MIC program at LLNL. Look into corrosion-resistant materials research, biocides/inhibitor, or other methods to discourage fouling, degradation, and the corrosion of materials.

Title: **Advanced Technology to Support Wastewater Recycling**

Originator: Hudson

Research Issue Description:

Develop advanced real-time (or near-real-time sensors) to characterize the operation of water recycling facilities. Sensors should measure a variety of water quality parameters and be combined with a data management system capable of assimilating and evaluating the data. This effort will be highly synergistic with water security technology needs.

LLNL has previously demonstrated two enabling technologies for wastewater recycling: $^{3}H/^{3}He$ dating and enriched-isotope noble gas tracers. These techniques allow for the accurate tracking of recycled water after being released to the environment. This work was done in a laboratory

research setting and, while the work was economically viable in this setting, we need to develop practical/targeted methods to see that these technologies are truly usable and available.

Importance:

Water recycling represents one of the important sources of "new" water, especially in urban settings. There has been considerable public opposition to recycling water for indirect potable reuse. The two items above directly address important components of the public concern. These issues are also viewed as important by regulatory agencies. The tracer technology is also significant for economical issues since maximizing the use of environmental buffers requires the direct measurement of the flow-paths and flow-rates of recycled water in the subsurface environment (i.e., if you cannot measure it, you must be much more conservative – you cannot recycle as much water).

How Do You Propose Meeting or Complying with This Research Issue?

Focus efforts in advanced technologies, such as "smart" membranes, "gene-chips," and bioassays (Bourcier, Reynolds, Farmer, Kane, Beller).

Focus efforts on the development of small, inexpensive, and robust gas mass spectrometry systems. This effort will also be synergistic with water security technology needs (Hudson, Hutcheon, Krulevitch, Microtechnology Center).

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

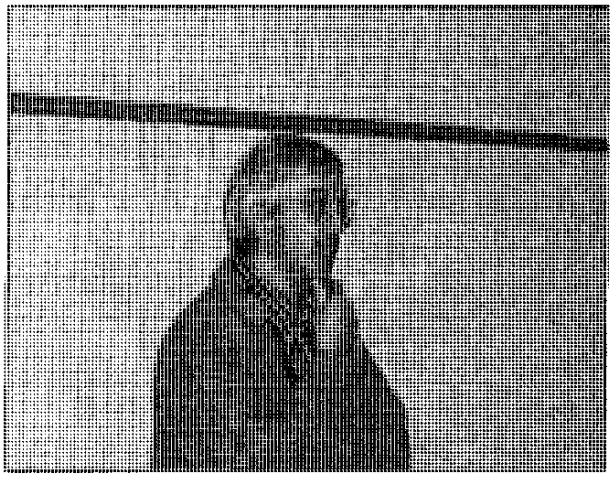
Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.

Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.




Kevin O Brien

PRIORITY 7

Innovative Approaches to Characterize, Manage, and Treat Nitrate Contamination in Groundwater

Originators:

Esser on behalf of himself, Folta, Hudson, O'Brien, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Innovative Approaches to the Characterization, Management, and Treatment of Nitrate Contamination in Groundwater**

Originator: Esser

Research Issue Description:

New technical approaches are needed to manage pervasive nitrate contamination in groundwater. The problem is multifaceted and will benefit from a multidisciplinary approach. Issues include:

- Characterizing the source, history, extent, and fate of current contamination.
- Quantifying nitrogen transport and biogeochemistry in the vadose and saturated zones (i.e., aquifer assimilative capacity).
- Understanding the economic consequences of different management/treatment approaches.
- Developing science-based approaches to source mitigation and treatment.
- Demonstrating the impact of different water management plans on groundwater quality.

LLNL has the analytical capabilities, expertise, and experience in building teams to solve large problems to make significant progress in each of these areas.

Importance:

The presence of high levels of nitrate in ground and surface water had adverse effects on human health and ecosystems. In California, nitrate contamination of groundwater consistently accounts for the highest number of exceedence of drinking-water standards of any single contaminant in public drinking supply wells. In ecosystem research, the largest and most poorly understood of all issues related to coastal eutrophication is the fate of nitrogen in aquifers. We do not understand the current extent of problem, the response of aquifers to different levels of nitrogen loading on the basin-scale, or the most cost-effective way of dealing with the problem. The SWRCB recognizes these issues and has asked LLNL's help in dealing with them.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has expertise in the following:

- Tracing groundwater (with ^{3}H- ^{3}H age-dating and noble-gas tracers).
- Characterizing contaminant sources and geochemistries (with inorganic mass spectrometry and trace organic analytical chemistry).
- Using molecular biology probes to understand biogeochemical processes in the subsurface.
- Modeling groundwater flow and the reactive transport of contaminants.
- Managing and visualizing large data sets.
- Optimizing the management of complex systems.

With respect to nitrogen biogeochemistry, we have developed membrane inlet mass spectrometry to allow for a fast, sensitive, and precise determination of the ultimate product of denitrification—nitrogen gas—and demonstrate the existence of autotrophic denitrification at a local field site. These techniques and capabilities should be integrated into a larger research effort to provide the science necessary to manage nitrate contamination at the field to basin-scale.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Improved Understanding of the Natural Attenuation of Nitrate in Groundwater**

Originator: Hudson

Research Issue Description:

Nitrate contamination of groundwater is a nearly ubiquitous and long-standing problem. However, recent studies (Beller et al., 2003) have demonstrated that, in some cases, natural attenuation of nitrate can be quite large. This result is generally in conflict with "common wisdom." LLNL has developed a collection of tools that can be used to investigate and resolve this issue.

Importance:

In seeking to address the issue of nitrate contamination and to apply wellhead purification technologies, we must make wise choices (i.e., good economic choices). We need to be able to recognize situations where denitrification is occurring and be able to make quantitative prediction about its transport and ultimate fate.

At the same time, a better understanding of denitrification may lead to improvements in nitrate management strategies.

How Do You Propose Meeting or Complying with This Research Issue?

Our present tool set includes:

- Being able to measure the isotopic composition of N and O in nitrate on macroscopic and microscopic samples to address sources and denitrification.
- Being able to accurately measure "excess" N_2 in groundwater as a quantitative measure of denitrification.
- Being able to quantitatively understand groundwater flow using modeling coupled to age-dating.
- Being able to detect co-contaminants in order to get additional information on nitrate sources.

We should apply these methods to two study areas (suggest Livermore Valley and Santa Clara Valley) to evaluate nitrate impacts on existing and future water supply wells and identify which wells will require wellhead treatment and which will not. (Esser, Beller, Moran, Hudson, McNab, and Tompson).

Title: **Molecular Engineering of Electrodialysis Membranes for Nitrate Removal**

Originator: O'Brien

Research Issue Description:

Previous research and developments in the area of EDR have shown that the transport properties of the membranes are major factors that drive the economics of the process. Increased selectivity to a given ion, as well as maintaining a low electrical resistivity, is critical to reduce energy requirements for the process. The goal of this effort would be to combine previously developed LLNL technology with new molecular engineering approaches to achieve a new ion-exchange based platform technology that will be cost-effective for cleaning up brackish water feed streams.

Importance:

A significant number of California public and, especially, private groundwater wells have nitrate levels that exceed or approach regulatory limits for drinking water, and a significant fraction of California's surface water supplies have nitrate concentrations that would preclude their use for groundwater recharge if draft California Department of Health Services regulations were adopted. In 1988, approximately 10 percent of the California groundwater analyses in the USEPA STORET database exceeded the drinking water maximum contaminant limit (MCL). Today, approximately 80 percent of the groundwater wells in the Stanislaus County database are impacted by nitrate contamination (i.e., have maximum concentrations greater than 3 milligrams per liter), and greater than 15 percent have maximum concentrations that exceed the drinking water limit.

How Do You Propose Meeting or Complying with This Research Issue?

Improving efficiency results in a cost-effective technology.

- Obtain current standards and set baseline: Asahi Glass Company and IONICS systems.
- Capitalize nanotechnology efforts within LLNL:
  - functionalize carbon nanotubes to assist in the transport of nitrates
  - examine the physical properties of materials
- Couple with molecular simulations to understand how functionalization affects transport.

- Fabricate on small scale and screen.
- The final result is a pilot-scale demonstration device that can be ported to a pre-determined site for testing.
- Need to simultaneously work the policy area and need to create funding sources.
- The goal is a ubiquitous system that can be adapted for treating various brackish water sources.

Requires:

- Interacting with universities/NSF centers.
- Municipal water suppliers.
- Major engineering firms.
- Coupling with University of California, Merced

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

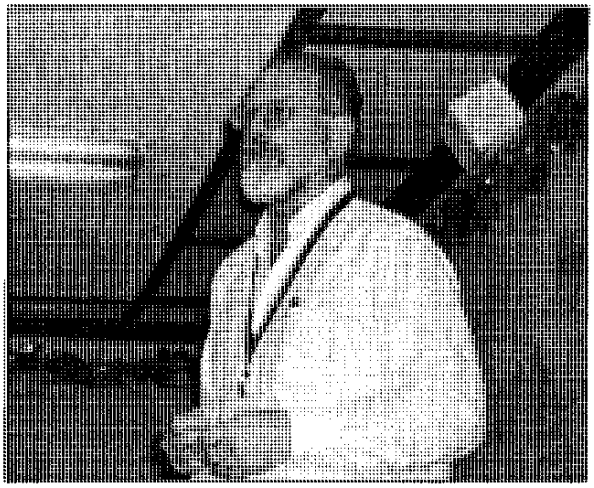
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

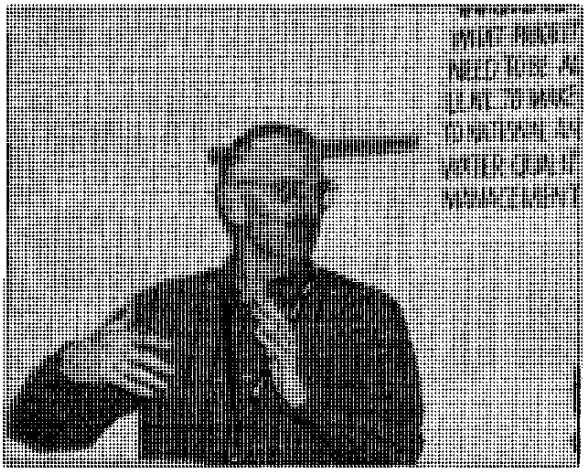
Importance:

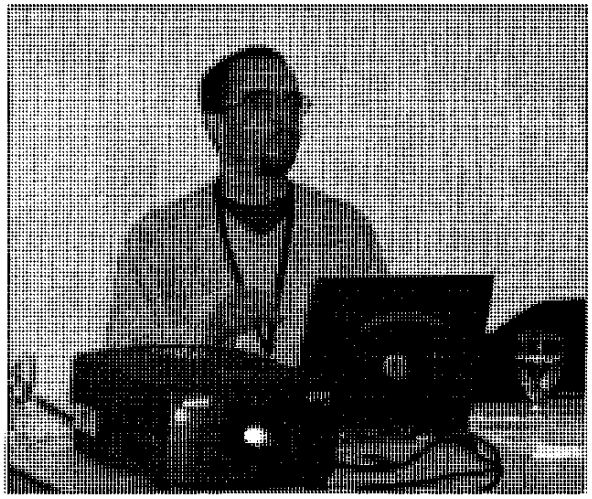
Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.







PRIORITY 8

Impact of Climate Change on Water Management and Infrastructure

Originators:

Lamont on behalf of himself, Folta, Layton (for Duffy), McNab, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Impact of Climate Change on Water Management and Infrastructure**

Originator: Lamont

Research Issue Description:

We can expect that climate change will cause changes in precipitation, patterns of precipitation and runoff, and soil moisture. In California and elsewhere, the infrastructure and patterns of water use have been developed to meet the requirements of the existing climate. When the climate changes, we will need to develop different management strategies, infrastructure, and patterns of use.

The impacts of climate change depend on how we respond to it. We cannot understand the long-term economic impact of climate change unless we first understand how to best manage the water under the new regime. From that, we can draw conclusions about the actual impacts of climate change.

This research will first identify optimal management and infrastructure responses to climate change in California. It will then evaluate the overall impact of climate change.

Importance:

Climate change may have substantial, possibly detrimental, impacts on water systems. We need to understand what these impacts might be and how we can best deal with them.

How Do You Propose Meeting or Complying with This Research Issue?

We will use the results from the proposed high-resolution climate modeling work for California. We can use these results to drive the CALVIN water economics model. This will identify the optimal water management strategies, given the existing infrastructure and the overall costs and benefits of those strategies. From the results of the optimization model, we can also understand the value of new infrastructure that will allow a greater range of management strategies.

Title: **Value of Long-Term Water Forecasts in Water Management**

Originator: Lamont

Research Issue Description:

The optimal water management strategies include allocations of water between years when water is plentiful and water is scarce. When we run water management optimization models, we assume that the water availability is known for each year. This provides an estimate of the very best that we can do through water management. This, of course, is not completely realistic. Water managers do not know the availability for future years and, thus, must hedge their strategies, which leads to less than maximum performance. Better water forecasts would help them reach the optimal level of performance.

The questions are:

- How important is accurate forecasting? It might be that the existing forecasts give us enough information to nearly achieve the maximum value.
- How good must the forecasts be? How accurate?
- What must be forecast? For example, the exact precipitation is probably not important; it may only be important to forecast the onset or end of droughts.

The result of this research will be recommendations for future research in climate modeling to improve multi-year forecasting.

Importance:

This will provide us with an understanding of the need for, and value of, further climate research and an identification of what needs to be forecast.

How Do You Propose Meeting or Complying with This Research Issue?

We need to adapt the water management models to first understand the way that uncertainty about future conditions affects current water management decisions and the long-term value of those decisions. We can then evaluate the impact of reducing the uncertainty and identify the most important aspects of uncertainty to address.

Then, working with the Climate Modeling Group, we can identify ways that these uncertainties might be reduced. We would like to identify a course of research that has a high probability of leading to an effective forecasting capability. Developing a research plan will require a balancing between the value of reducing an uncertainty and the feasibility of reducing that uncertainty.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Climate Change/Variability Effects on Water Supplies**

Originator: Layton (for Phil Duffy)

Research Issue Description:

The basic challenge of this research effort is to predict the nature and magnitude of climate change/variability impacts on water supply and demand in California and elsewhere in the country. In order to address this challenge, predictions of temperature, precipitation, and hydrologic responses to climate change and variability in major watersheds will be developed using a suite of models, including high resolution global and regional climate models and a watershed-scale hydrological model. Initial efforts of this effort would be to simulate present climate/hydrologic conditions (matching statistical and spatial climate/hydrologic attributes of selected regions) and then predict future climate change/variability impacts for different scenarios of greenhouse gas emissions.

Importance:

Changes in climate due to increased in greenhouse gases, combined with modes of natural climate variability (e.g., El Niño) will have potentially significant impacts on California's water supply system. Multibillion dollar investments in water infrastructure in California are typically based on the premise that historic climate/hydrologic conditions will persist into the future. Failure to plan for climate change impacts on future hydrologic conditions could result in water projects that do not operate as expected.

How Do You Propose Meeting or Complying with This Research Issue?

Phil Duffy has recently received LDRD funding to develop an integrated climate change and hydrologic impacts prediction capability. This will be developed and applied in collaboration with groups at other institutions in California. The proposed work would proceed along the lines noted above.

Title: **Assess the Feasibility of Large-Scale Aquifer Storage/Recovery (ASR) to Address Water Storage Needs in the Face of Climate Change**

Originator: McNab

Research Issue Description:

Impacts of climate change to California's water distribution system may include changes in the spatial distribution of rainfall and a reduction in the storage capacity offered by snowpack in the Sierras. Taking into account population growth, the need for significant additional storage capacity is obvious. Economic and environmental considerations may preclude significant new surface-water storage capacity, while the direct recharge of aquifers through recharge and infiltration may also be problematic for a variety of reasons.

Therefore, aquifer storage through injection may offer a practical means of establishing new, large reservoirs of water. Key issues, however, will need to be addressed:

- Where will we find the most economical sources of recharge water in a climate-altered California?

- What are the issues associated with long-term management of recharged aquifers and recharge will fields (e.g., aquifer geochemistry and well clogging)?

Importance:

ASR is likely to be a significant component of water management strategies in California in the future. Planning ASR on a large scale will be complex – who owns the water, who pays for the ASR system, etc.? A comprehensive, basin-scale assessment of ASR-related issues would be useful for state and local water agencies.

How Do You Propose Meeting or Complying with This Research Issue?

Leverage LLNL strengths in climate modeling and geochemical reactive transport modeling, along with applying coupled groundwater-surface water modeling (i.e., calibrated to groundwater age data collected under the GAMA study) to identify recharge strategies (e.g., infiltration versus injection) on a basin-scale across the state.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
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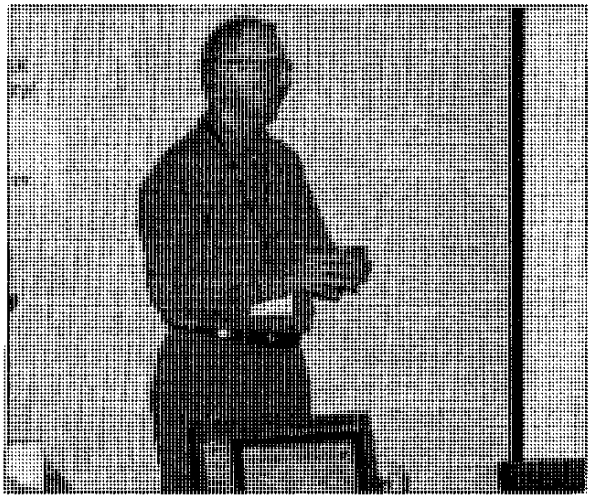
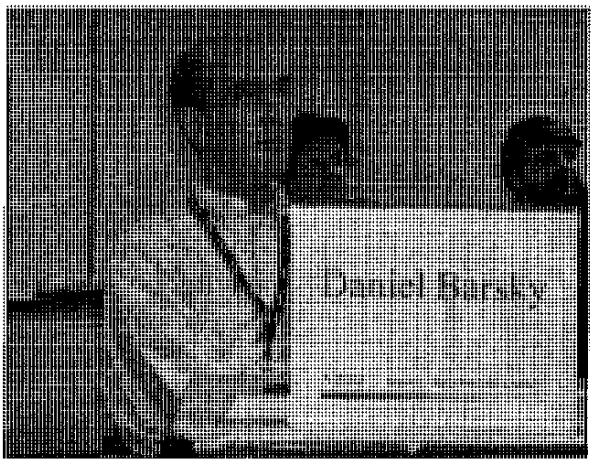



Daniel Barsky

PRIORITY 9

Molecular Studies of Biochemical Cycling of Aquatic Contaminants

Originators:

Beller on behalf of himself, Barsky, Esser, Folta, Horn, Stewart, Watz, and Woodward

The following research issues were consolidated under the above title:

Title: **Effect of Biogeochemical Cycling of Metals and Radionuclides on Water Quality**

Originator: Beller

Research Issue Description:

As a result of research, development, testing, and production of nuclear weapons, the USDOE is currently responsible for remediating 1.7-million gallons of contaminated groundwater and 40-million cubic meters of contaminated soil at its facilities. More than 60 percent of USDOE facilities are estimated to have groundwater contaminated with metals or radionuclides, such as uranium.

Oxidation state is a major control on the solubility and mobility of many metals and radionuclides in groundwater. In particular, uranium is highly insoluble in its (IV) oxidation state and is soluble in its (VI) oxidation state. Thus, microbially mediated reduction of uranium is being considered as a groundwater cleanup approach that would immobilize uranium *in situ*. This remediation approach is of great interest to USDOE, which awarded tens of millions of dollars in the fiscal year 2002 to several projects addressing metal/radionuclide reduction under the Genomes to Life program. Despite recent funding efforts, the biogeochemical cycling of uranium and other elements of concern to USDOE is not well understood beyond the phenomenological level.

Importance:

The large scope of USDOE's responsibility for remediating the metal and radionuclide contamination of aquifers was indicated above. Considering the serious attention that USDOE has paid to *in situ* reductive immobilization and the need for this restoration strategy to be

effective for thousands of years, it is essential to have a high degree of understanding of the complexities of biogeochemical redox cycling of metals and radionuclides.

How Do You Propose Meeting or Complying with This Research Issue?

Many aspects of topic require much more intensive study, including an understanding of:

- The metabolic ecology of aquifer bacterial communities that can oxidize, as well as reduce, metals and radionuclides.
- How environmental conditions are sensed by bacteria and how they control the expression of respiratory genes.
- How bacteria can respire using insoluble mineral phases that cannot be transported into the cell.

Many areas of scientific expertise are critical to the biochemistry of metals/radionuclides, including advanced radiochemical analysis, anaerobic microbiology (biochemistry and physiology), state-of-the-art genomic and proteomic techniques, surface analytical chemistry, inorganic geochemistry, and modeling of metal/radionuclide speciation.

Personnel in C&MS, BBRP, SSEP, E&E, and perhaps other directorates would need to collaborate on this research (strategic hires would also be necessary).

Title: **Assessing the Assimilative Capacity of Aquifers for Organic Contaminants**

Originator: Beller

Research Issue Description:

Groundwater contaminated with organic pollutants is a worldwide problem that effectively reduces the amount of potable water available. In the U.S., intrinsic bioremediation (or natural attenuation) by indigenous bacteria has been promoted as the most cost-effective approach to groundwater restoration, but the science underlying the application of this approach is less than rigorous at many sites. Even when intrinsic biodegradation is well documented, a particularly intractable aspect has been the estimation of *in situ* biodegradation rates, which must be distinguished from the effects of dilution and dispersion. Rigorous methods are needed to definitively demonstrate whether biodegradation is occurring at a given site and, if so, at what rate.

Importance:

If documented in a scientifically credible manner, intrinsic biodegradation can lead to highly cost-effective and productive restoration and management of groundwater. However, if inaccurate claims of intrinsic bioremediation (including overestimates of degradation rates) are accepted by regulators, this will either delay the necessary engineered cleanup or represent a risk to those who may be exposed to the contamination.

The NRC identified as a research priority to "understand [the] assimilation capacity of the environment and time course of recovery following contamination."

How Do You Propose Meeting or Complying with This Research Issue?

An interdisciplinary approach is required, involving emerging techniques in analytical chemistry, molecular biology, biogeochemistry, hydrogeology, and reactive transport modeling.

The approach would involve:

- Identification and *in situ* detection in groundwater of signature metabolites associated with specific contaminants.
- Identification and *in situ* detection of genes (and mRNA transcripts) associated with the degradation of specific compounds.
- Compound-specific isotope ratio mass spectrometry of parent compounds and metabolites *in situ.*
- Age dating of groundwater.
- Reactive transport modeling of specific contaminants in the subsurface that incorporates these and other data.

Implementation of this project would require the following:

- For some pollutants, biochemical elucidation of key metabolites in degradation pathways and highly sensitive and selective mass spectrometric methods for metabolite detection in groundwater (such as isotope dilution liquid chromatography-tandem mass spectrometry).
- For some pollutants, elucidation of genes that encode key degradation enzymes (e.g., based on comparative genomic studies for degrading bacteria) and highly sensitive and selective methods for detection of target nucleic acids in groundwater.
- For compound-specific isotope ratio mass spectrometry, purchase of the appropriate instrumentation would be required, as it is not currently available at LLNL.

H. Beller, B. Hudson, S. Kane, W. McNab, others in BBRP and CMS

Title: **Develop and Apply a Molecular-Level Understanding of Water-Material Interactions**

Originator: Barsky

Research Issue Description:

Water separation is integral to desalination and purification. This usually involves a membrane (e.g., RO, dialysis) and always involves selectively exploiting/removing water-solute or water-membrane interactions. Our knowledge of those interactions is currently limited and has not been applied to membrane design as well as other aspects of "water separation" (which is really water purification).

Importance:

In understanding and, therefore, designing better water separation technologies, we need to understand water-material interactions.

How Do You Propose Meeting or Complying with This Research Issue?

This issue could be addressed through a combined experimental/theoretical approach across LLNL. For example, we could develop a test-bed system to couple theory and experiment. Perhaps it is best to start at the "nano-scale," where experiment and simulation are beginning to meet.

Title: **Very New Isotopic Approaches to Understanding the Sources and Cycling of Metal and Nutrient Contaminants in Natural and Engineered Environments**

Originator: Esser

Research Issue Description:

Identifying contaminant source is important to distinguishing anthropogenic from natural components, to attributing liability, and to developing effective source mitigation. An understanding of contaminant cycling at different spatial scales is important in understanding the transport and fate of metals in the environment, in demonstrating natural attenuation, in understanding how watershed activities contribute to total maximum daily loads, and in evaluating remediation strategies.

The use of metal and nitrogen isotopic composition investigations in these fields is well established. Two recent advances in inorganic mass spectrometry are significant. Multi-collector magnetic-sector inductively-coupled plasma mass spectrometry (MC-ICPMS) is allowing us to determine isotopic composition of metals at precisions not previously obtainable, which will open up new metal source and cycling research. High spatial resolution secondary-ion-mass spectrometry will allow elemental and isotopic investigations at sub-micron scales, which will significantly improve our understanding of the biogeochemistry of metals and nutrients at the microbial scale. MC-ICPMS is a rapidly developing field; submicron-scale SIMS is a brand new field. Livermore has the instrumentation and expertise to play a significant role in developing these fields.

Importance:

Nonpoint source pollution is exceptionally difficult to attribute. Understanding contaminant metal chemistry at microbial scales will lead to new remediation technologies.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has a multi-collector ICPMS (MicroMass Isoprobe) and a high-resolution multi-collector SIMS (Cameca NanoSIMS). We are developing heavy metal stable isotope applications on a shoestring budget (e.g., working with the University of California, Berkeley, on a National Institute of Environmental Health Sciences [NIEHS] grant looking at mercury isotopes). We need to find ways to increase institutional investment in this capability. The NanoSIMS has just arrived and will be heavily used for biomedical research to understand the localization of targeted radionuclides in cells. We should leverage on the expertise gained from this research to explore metal biogeochemistry at the microbial scale. An obvious first target is microbial reduction of uranium as a method of *in situ* remediation, an application which has programmatic implications for USDOE clean-up. Other applications include studies of nutrient cycling at microbial scales.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Microbial-Induced Chemical Effects on Groundwater Quality: Interfacial Interactions at the Micron Scale**

Originator: Horn

Research Issue Description:

Examine the contribution of microorganisms to the groundwater chemistry of those chemical species of importance.

- Characterize the processes and effects, including effects under different environmental conditions.
- Explore mechanisms—this probably requires going to the pore-scale, looking at the interaction of microbes on surfaces (mineral/organic) with surrounding solution.
- Develop predictive capabilities to describe these interactions.

Importance:

This fundamentally affects water quality.

How Do You Propose Meeting or Complying with This Research Issue?

A substantial research effort is required. LLNL is well-suited to explore/characterize surfacial interactions at micron-to-millimeter scale, as well as modeling capability. Other groups include Montana State University's BioFilm Engineering Institute and other USDOE laboratories.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Develop a Scientific Basis for the Carrying Capacity of Aquatic Ecosystems to Provide a More Defensible Basis for Ecosystem Management**

Originator: Watz

Research Issue Description:

Characterize the carrying capacity of aquatic ecosystems with respect to key ecosystem receptors, such as bacteria, plant, and marine life. The assimilative capacity needs to be assessed on a spatial and temporal scale for inorganic and organic pollutants currently regulated and proposed for future regulation.

Importance:

Water discharge limits for point and nonpoint sources are highly contentious with uncertain outcomes. The cost of discharge compliance is extremely high and not economically efficient. If there was some way of assessing the assimilation of pollutants/contaminants into aquatic ecosystems; it could provide a more scientifically sound basis for developing economically efficient discharge limits.

How Do You Propose Meeting or Complying with This Research Issue?

NRC's Water Science Technology Board called this out as a key research issue. The solution to the proposed idea is highly complex and requires the integrated resources of a national laboratory.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

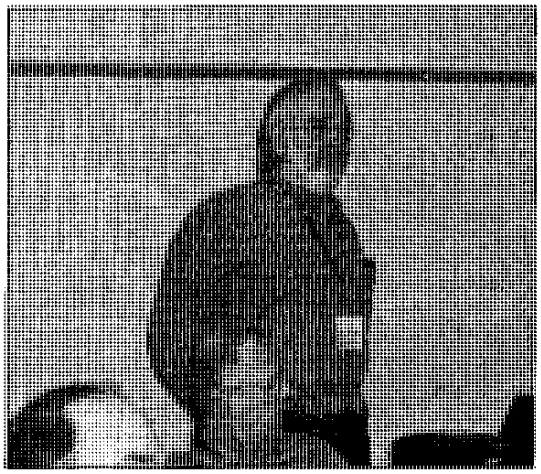
Importance:

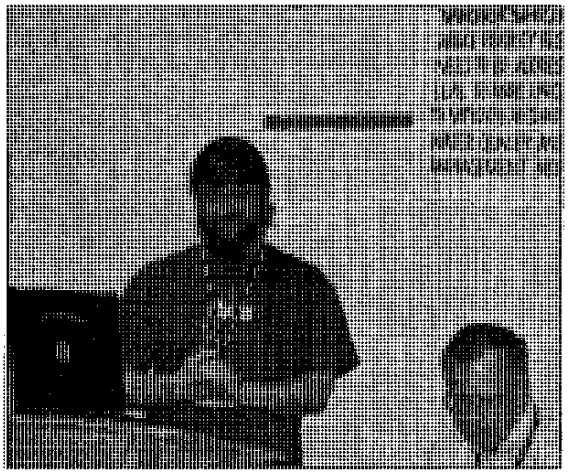
Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.


Jean Moran





PRIORITY 10

Optimize Conjunctive Use with LLNL's Advanced Analytical and Modeling Capabilities

Originators:

Moran on behalf of herself, Beller, Folta, Hudson, Stewart, McNab, and Woodward

The following research issues were consolidated under the above title:

Title: **Optimize Conjunctive Use with LLNL's Advanced Analytical and Modeling Capabilities**

Originator: Moran

Research Issue Description:

Conjunctive use and groundwater banking will become increasingly relied upon as new surface water storage has become unworkable. This is an underutilized and tempting option for water resource managers, but it should be approached with caution and with the best scientific evidence possible. Outstanding questions relate to:

- When and where artificial recharge is most productive (and when/where it may not be a good idea).
- Optimal operation of artificial recharge facilities (i.e., pond and in-stream operations, sedimentation versus infiltration rate).
- The time scales for turnover of the effective storage area of a groundwater basin.
- Changes in water quality during recharge and storage.

Importance:

Water resource managers, regulators, and legislators have recently come to the realization that groundwater banking and conjunctive use will be absolutely crucial to increasing the volume of high-quality water delivered as will be required as the population of the state increases. Past

experience with water banking and artificial recharge suggests that these projects can enhance water management options, but that there can be undesirable, unforeseen changes in water quality, or operational problems if key facets of basin hydrogeology and biogeochemical processes are unknown.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has developed and tested unique capabilities that offer crucial information about groundwater flow away from artificial recharge facilities (e.g., noble gas tracers) and about basin turnover times and which areas of a basin are part of the active flow system (e.g., groundwater age dating using the tritium-helium method). Flow models that can be used to predict basin turnover times and storage capacities that are based on these data would be used to optimize artificial recharge and pumping. Work with the State of California Department of Water Resources, the DHS, and water districts to identify potential conjunctive use and groundwater banking areas, and use integrated analytical/modeling approach to take out surprise elements.

Beneficial changes in water quality that may occur during recharge or storage include denitrification, reduction in total organic compounds (TOC), natural biodegradation, etc. Detrimental changes may include increased TDSs, the addition of arsenic or selenium, or the mobilization of relatively stagnant, pre-existing contaminants, and adverse effects on ecosystems. These questions can be addressed using advanced analytical techniques and coupled biogeochemical models.

Title: **Assessing the Assimilative Capacity of Aquifers for Organic Contaminants**

Originator: Beller

Research Issue Description:

Groundwater contaminated with organic pollutants is a worldwide problem that effectively reduces the amount of potable water available. In the U.S., intrinsic bioremediation (or natural attenuation) by indigenous bacteria has been promoted as the most cost-effective approach to groundwater restoration, but the science underlying the application of this approach is less than rigorous at many sites. Even when intrinsic biodegradation is well documented, a particularly intractable aspect has been the estimation of *in situ* biodegradation rates, which must be distinguished from the effects of dilution and dispersion. Rigorous methods are needed to definitively demonstrate whether biodegradation is occurring at a given site and, if so, at what rate.

Importance:

If documented in a scientifically credible manner, intrinsic biodegradation can lead to highly cost-effective and productive restoration and management of groundwater. However, if inaccurate claims of intrinsic bioremediation (including overestimates of degradation rates) are accepted by regulators, this will either delay the necessary engineered cleanup or represent a risk to those who may be exposed to the contamination.

The NRC identified as a research priority to "understand [the] assimilation capacity of the environment and time course of recovery following contamination."

How Do You Propose Meeting or Complying with This Research Issue?

An interdisciplinary approach is required, involving emerging techniques in analytical chemistry, molecular biology, biogeochemistry, hydrogeology, and reactive transport modeling.

The approach would involve:

- Identification and *in situ* detection in groundwater of signature metabolites associated with specific contaminants.
- Identification and *in situ* detection of genes (and mRNA transcripts) associated with the degradation of specific compounds.
- Compound-specific isotope ratio mass spectrometry of parent compounds and metabolites *in situ.*
- Age dating of groundwater.
- Reactive transport modeling of specific contaminants in the subsurface that incorporates these and other data.

Implementation of this project would require the following:

- For some pollutants, biochemical elucidation of key metabolites in degradation pathways and highly sensitive and selective mass spectrometric methods for metabolite detection in groundwater (such as isotope dilution liquid chromatography-tandem mass spectrometry).
- For some pollutants, elucidation of genes that encode key degradation enzymes (e.g., based on comparative genomic studies for degrading bacteria) and highly sensitive and selective methods for detection of target nucleic acids in groundwater.
- For compound-specific isotope ratio mass spectrometry, purchase of the appropriate instrumentation would be required, as it is not currently available at LLNL.

H. Beller, B. Hudson, S. Kane, W. McNab, others in BBRP and CMS

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify high performance computing (HPC) and modeling/simulation needs – integration.

Title: **Noble Gas Tracers to Support Water Banking and Noble Gas Isotope Separation**

Originator: Hudson

Research Issue Description:

LLNL has demonstrated the use and effectiveness of tagging groundwater with enriched noble gas isotopes (tracer cost is $1 per acre foot or 1,200 cubic meters of water) for groundwater recharge operations in Orange County, Los Angeles County, and Alameda County. These tracers are permanent and non-hazardous. Many different isotopes are available at approximately the same cost (we have used xenon most extensively – 9 stable isotopes).

We need to improve measurement techniques and develop new tracer introduction methods. We need to look at new methods for noble gas isotope separation to further reduce tracer costs and improve availability.

Importance:

Storage of water in the subsurface (water banking) is and will be an important part of water management. However, putting water in a water bank today is a lot like putting money in an unaudited bank.

How Do You Propose Meeting or Complying with This Research Issue?

We need to develop a small, simple, inexpensive, and robust gas mass spectrometer system to make this method more practical and available. We need to investigate new tracer introduction methods (i.e., permeable membranes with pressure and flow regulation to achieve constant concentrations). We need to investigate the development of "tuned" permeable membranes to enhance the isotopic separation of noble gas isotopes (especially xenon) (Hudson, McNab, Bourcier, Ruiz).

Title: **Explore the Issues Associated with Conjunctive Use of Urban Runoff Water**

Originator: McNab

Research Issue Description:

Investigate four key issues associated with using urban water runoff for aquifer recharge in select test locations around California:

- Evaluate distributions of organic and inorganic chemicals in urban groundwaters.
- Evaluate possible recharge mechanisms into shallow aquifers (generally not used for drinking water), either from infiltration basins or collection and injection.
- Look into the assimilative capacity of shallow aquifers to attenuate contaminants.
- Look at the rates of recharge (if any) from shallow aquifers into deeper aquifers that may be used for drinking water.

Importance:

Urbanization and a growing population will require ever more resourceful uses of water to meet domestic demands. An integrated study of urban runoff conjunctive use will shed insights into the feasibility of injecting and treating urban water in the context of managing water supply aquifers.

How Do You Propose Meeting or Complying with This Research Issue?

Leverage other proposed LLNL water initiative studies that address assimilative capacity of shallow aquifers, as well as applying data-driven basin-scale groundwater models to examine inorganic and organic chemical fluxes through the subsurface.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.

PRIORITY 11

Identify Research Efforts to Support Focused Water, Reuse, and Conservation

Originators:

Woodward on behalf of himself, Beller, Christensen, Folta, Hudson, and Stewart

The following research issues were consolidated under the above title:

Title: **Identify Research Efforts to Support Focused Water Conservation**

Originator: Woodward

Research Issue Description:

Focus research efforts where they would likely have the most significant effect. This would probably be in the agricultural area.

Importance:

Conservation, in effect, is like having new water sources.

How Do You Propose Meeting or Complying with This Research Issue?

- Research which parts of the agricultural industry use the most water.
- Examine practices that have high potential for reduced use by alternative methods, rates of application, etc.
- Develop research programs to demonstrate effectiveness of alternate water saving methods.

Title: **Water Reuse: Characterization of Analytically Intractable Disinfection Byproducts**

Originator: Beller

Research Issue Description:

Water is a limited resource in many regions of the world, and recycling wastewater is an attractive option for enhancing supply. Although tertiay-treated wastewater could be demonstrated to meet primary and secondary drinking water standards before potable reuse, there is the possibility that currently unregulated compounds could survive wastewater treatment and potentially result in detrimental human health effects. Among the compounds of concern are endocrine disruptors (i.e., natural and synthetic compounds that stimulate or inhibit normal hormonal activity), pharmaceuticals, and disinfection byproducts. A current LDRD project is assessing endocrine disruptors in groundwater as a result of the nonpotable reuse of wastewater, so that topic will not be further addressed here.

One particularly poorly understood class of compounds is halogenated disinfection byproducts of high molecular weight (e.g., >500 Da). Laboratory studies have shown that a significant portion of the mutagenic activity of chlorinated organic material is in this molecular weight range. Conventional analytical techniques are inadequate for characterizing such compounds, which can constitute up to 50 percent of the total organohalogen disinfection byproducts.

Importance:

The availability of drinking water in the U.S. is threatened by population increases, which are occurring disproportionately in arid regions of the Southwest. The NRC listed "increas[ing] the safety of wastewater treated for reuse as drinking water" as a research priority. The USEPA, and other federal and state regulatory agencies, have acknowledged that there are important and unresolved issues surrounding the potable reuse of treated wastewater. Accordingly, there has been significant public opposition to such projects (often derided as "toilet to tap" projects) throughout the U.S.

How Do You Propose Meeting or Complying with This Research Issue?

More thorough characterization of analytically intractable disinfection byproducts is one step in gaining public acceptance of the potable reuse of treated wastewater. LLNL has excellent resources for the chemical and genotoxic characterization of high molecular weight disinfection byproducts. Chemical characterization could take advantage of LLNL expertise in mass spectrometric analysis of complex biomolecules; techniques could include liquid

chromatography-electrospray ionization-tandem mass spectrometry and MALDI-TOF mass spectrometry.

Mass spectrometrists in C&MS, H. Beller, BBRP biochemists specializing in genotoxicity

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Title: **Water Reuse: Focused Use Planning Together with Focused (Selective) Purification Technology**

Originator: Christensen

Research Issue Description:

Today, we aggressively purify and treat water for the tap. Much of this water is used for purposes where such high quality is not necessary. In fact, such high purity may cause deleterious impacts to the environment. Our greatest concern is the fact that much water is used only once after having invested heavily in purification. Focusing the tailoring contaminant purification/separation technologies represents an opportunity to improve the efficiency of water reuse.

Importance:

- Tailoring the quality of water to the use can result in lower cost and improvements in water use efficiency.
- Improved planning, in terms of staging water use, results in leveraging the investments made in purification.

How Do You Propose Meeting or Complying with This Research Issue?

- This requires the custom development of water separation technologies, sensors and control technologies, and developing Green Building and/or Green Community concepts designed to optimize the reuse of water.
- It also requires custom analysis of water quality versus water use in order to optimize, stage water use, and minimize cost.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Advanced Technology to Support Wastewater Recycling**

Originator: Hudson

Research Issue Description:

Develop advanced real-time (or near-real-time sensors) to characterize the operation of water recycling facilities. Sensors should measure a variety of water quality parameters and be combined with a data management system capable of assimilating and evaluating the data. This effort will be highly synergistic with water security technology needs.

LLNL has previously demonstrated two enabling technologies for wastewater recycling: $^{3}H/^{3}He$ dating and enriched-isotope noble gas tracers. These techniques allow for the accurate tracking of recycled water after being released to the environment. This work was done in a laboratory research setting and, while the work was economically viable in this setting, we need to develop practical/targeted methods to see that these technologies are truly usable and available.

Importance:

Water recycling represents one of the important sources of "new" water, especially in urban settings. There has been considerable public opposition to recycling water for indirect potable reuse. The two items above directly address important components of the public concern. These issues are also viewed as important by regulatory agencies. The tracer technology is also significant for economical issues since maximizing the use of environmental buffers requires the direct measurement of the flow-paths and flow-rates of recycled water in the subsurface environment (i.e., if you cannot measure it, you must be much more conservative – you cannot recycle as much water).

How Do You Propose Meeting or Complying with This Research Issue?

Focus efforts in advanced technologies, such as "smart" membranes, "gene-chips," and bioassays (Bourcier, Reynolds, Farmer, Kane, Beller).

Focus efforts on the development of small, inexpensive, and robust gas mass spectrometry systems. This effort will also be synergistic with water security technology needs (Hudson, Hutcheon, Krulevitch, Microtechnology Center).

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

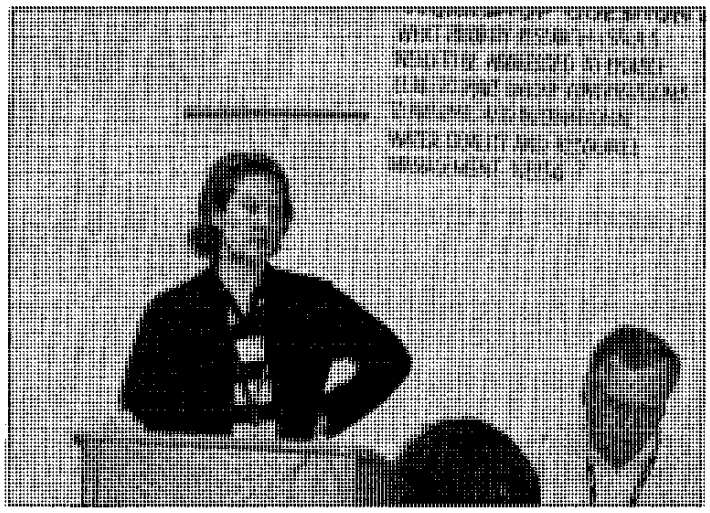
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.



PRIORITY 12

Integrated Water and Energy – Long-Term Planning and Conflict Resolution

Originators:

Cantwell on behalf of herself, Folta, Grey, Stewart, Watz, and Woodward

The following research issues were consolidated under the above title:

Title: **Integrated Water and Energy—Long-Term Planning and Conflict Resolution**

Originator: Cantwell

Research Issue Description:

Provide the ability to do long-term planning and "conflict resolution" for large-scale challenges between the uses and needs of power systems and the uses and needs of water systems.

Importance:

I expect that within the next 10 years, globally, and within the next 20 years in the U.S., we will see significant challenges associated with energy system limitations on our water availability, and vice versa.

How Do You Propose Meeting or Complying with This Research Issue?

- Anticipate problems using science-based analysis and modeling. Develop large-scale models that integrate between both "systems."
- Obtain new data and information to fill in the gaps. Understand system-level integration of vulnerability assessments and utility needs.
- Refine the understanding of the problem with further modeling and analysis.

- Assist policy makers in developing policy that helps to avoid the problem.
- Develop technology that changes or eliminates the problem(s).

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Economic Growth and the Political and Legal Issues Surrounding Them**

Originator: Grey

Research Issue Description:

Look at the long-term uses of water for both human and industrial use. We need to study their direct impacts to the environment. The study should include ground and surface waters.

Importance:

Certain groups are not given input to water issue, yet development and growth continue to impact their way of life. Certain groups feel that they have senior water rights and need to be acknowledged. Five hundred fifty federally recognized tribes have some claim to water rights.

How Do You Propose Meeting or Complying with This Research Issue?

Establish grassroots committees for input, including a number of tribal organizations that work on Indian water rights and issues.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Couple Power Generation and Water Treatment Facilities to Take Advantage of Economics of Scope**

Originator: Watz

Research Issue Description:

In the spirit of last night's State-of-the-Union address and the President's call for hydrogen-fueled transport, the only seemingly reasonable way to produce H_2 is electrolytically from water. If this is done on a large enough scale (via nuclear or renewables), pure oxygen is also generated as a process byproduct, which can be used as part of a water purification/treatment process. Developing integrated power/water systems potentially reduces the cost of both products.

Importance:

The costs of both power production and water treatment are rising steadily with concomitant environmental repercussions. There is a greater need for evaluating integrated systems for major commodities to decrease system costs and increase system efficiency.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has a long history of hydrogen system modeling capable of being augmented to effectively evaluate the technical and economic benefits of this approach. We also have engineering and scientific capabilities for developing innovative water treatment technologies using oxidation.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.

PRIORITY 13

Advanced Watershed Characterization and Diagnostics to Support Hydrologic Simulations

Originators:

Layton on Behalf of himself, Folta, Hoppes, Hudson, Moran, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Advanced Watershed Characterization and Diagnostics to Support Hydrologic Simulations**

Originator: Layton

Research Issue Description:

A simulation of distributed geohydrologic/geochemical processes requires spatial and temporal information on the system being addressed. Hence, the cost-effective acquisition and analysis of relevant data are essential parts of developing realistic and valid simulations of a given system. There are two components to this challenge. The first is the identification and acquisition of relevant data, and the second is the processing of that data to provide the necessary model input parameters and associated revisions from calibration exercises. Existing data can come from well data (e.g., logs, pump tests, tracers, and isotopic composition of water), historic hydrologic and climatic data, and remote sensing information (e.g., land uses, InSAR, etc.). The analytical software should directly support the LLNL models used to simulate geohydrologic/biogeochemical processes.

Importance:

Acquisition and analysis of geohydrologic data are probably the most expensive parts of model development but are essential to the generation of model predictions that a user can have a high degree of confidence in. If LLNL can both enhance and cut the costs of these parts of the model development process, then simulation approaches will be more widely adopted to support critical water management decisions in California and elsewhere.

How Do You Propose Meeting or Complying with This Research Issue?

This effort would involve a multidisciplinary team who are experienced in the collection of relevant geohydrologic and chemical data, as well as those familiar with geostatistical/quantitative techniques for processing data.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Link Air Contaminant Transport Pathways to Urban Watersheds**

Originator: Hoppes

Research Issue Description:

- Loadings to surface water can have an air transport component.
- To what degree do management actions, or regulatory actions that are designed to manage a facility, impact surface-water loadings in a watershed basis?

Importance:

Waste load allocations in non-point source discharge is an important issue. Air quality controls can be incorporated as an element of these assessments.

How Do You Propose Meeting or Complying with This Research Issue?

Case study – What is available already?

Title: **Couple Groundwater Modeling with $^{3}H/^{3}He$ Dating**

Originator: Hudson

Research Issue Description:

Groundwater flow models are traditionally calibrated using groundwater elevation data that is only weakly coupled to the flow system. Thus, equally well calibrated groundwater models can have drastically different flow patterns (see Tompson et al., Water Resources Research, 1997). Groundwater dating using the $^{3}H/^{3}He$ method provides a new source of data for calibrating flow models. The age-dates are strongly coupled to the flow system.

Age-dating measurements also greatly benefit from having a flow model to provide age-distribution evaluations that are necessary to accurately interpret the measurements and turn "apparent" ages into true ages.

Importance:

Currently, LLNL is a leader in both groundwater modeling and groundwater age-dating. By combining these two activities, we significantly strengthen both and guarantee our unique position in the field of understanding groundwater flow. Age-dating is an important part of on-going funded activities (California Ambient Groundwater Monitoring and Assessment Program). By adding a modeling component, the value of the age-dating measurements will be significantly increased. Finally, while age-dating is a fairly direct measurement of the flow system "today," well-calibrated models are necessary to predict "tomorrow."

How Do You Propose Meeting or Complying with This Research Issue?

The principal issue is to develop and implement efficient numerical methods to use the age-dating measurements, both in the construction of models (inverse – modeling) and the ultimate calibration and validation of groundwater flow models. It will be important to link model construction with information databases (GeoTracker) and geographic information systems (Tompson, Carle, McNab, Demir, Hudson, Dooher, Hall).

Title: **Calibrate "Old" Groundwater Dating Techniques and Determine Sources of Salinity in Groundwater**

Originator: Moran

Research Issue Description:

GAMA program data show the surprising fact that a large fraction of water used in California is pre-nuclear age (and the related surprising fact that even in urbanized environments, such as Los Angeles and San Jose, many wells are completely free of anthropogenic contaminants). Characterization of this large volume of water has received little research attention and remains mysterious. Many tools and tracers are available for characterizing young water. This volume of water is well monitored partly because consulting work focuses on shallow groundwater. While some produced water is highly saline, there is a gradient, and some produced water is fresh enough to use for agriculture or even drinking water. Increasing salinity in groundwater is a growing water resource management issue.

Importance:

This "old" groundwater is heavily exploited and is generally free of contaminants. One needs to know the time-scale for recharge since this water is being mined here in California (Central Valley) and in the Great Plains (Kansas, Oklahoma, Texas). One needs to quantify salt sources in water being exploited today – whether from "old water", seawater intrusion, or agricultural return water

(an insidious, slowly approaching problem). This research would also address the issue of distinguishing anthropogenic versus natural sources for contaminants.

How Do You Propose Meeting or Complying with This Research Issue?

Use existing data (GAMA) to find this water in areas where "old" water is being used. Calibrate ^{4}He using other radiometric dating techniques, since this covers a relevant age range. Develop ^{14}C age dating capability on compound specific organic C. Use long-lived isotopes like ^{36}Cl and ^{129}I for age dating/salinity source tracing (uses the LLNL accelerator mass spectrometry facility).

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.

PRIORITY 14

Improve the Scientific Basis of Risk Assessment, Risk Management, and Risk Communications for Water Systems

Originators:

Dooher on behalf of himself, Folta, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Improve the Scientific Basis of Risk Assessment, Risk Management, and Risk Communications for Water Systems**

Originator: Dooher

Research Issue Description:

The public understanding of risk is often based on what people may feel are voluntary or non-voluntary risks, or of risks that are distorted by public interest groups, who may have a desire to gain publicity or see legislation be passed. The internet can be used to pass information to the public that shows the science behind risk assessment, how the risk is to be managed, and to place the risk in context to the public in ways that they are better able to understand.

Importance:

Resources for water assessment and remediation are often distorted because the public does not have the time nor the capability to assess the true risks associated with contaminants. An advanced version of GeoTracker (an internet GIS and database system), developed as an educational device, would go a long way towards helping the public understand how and why economic resources are distributed to deal with water contamination. This could eventually lead to a better direction of economic and manpower resources, and better management of our groundwater systems.

How Do You Propose Meeting or Complying with This Research Issue?

Provide an integrated presentation of data, with the risks placed in various levels of understanding. Instead of stating that a chemical may give a 10^{-6} chance of getting cancer over a lifetime, the risk could be stated in terms of incidents that people understand in everyday life, in terms of economic costs, or of alternative remediation or environmental needs that cannot be accomplished because resources are being directed to the lower risk issue.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

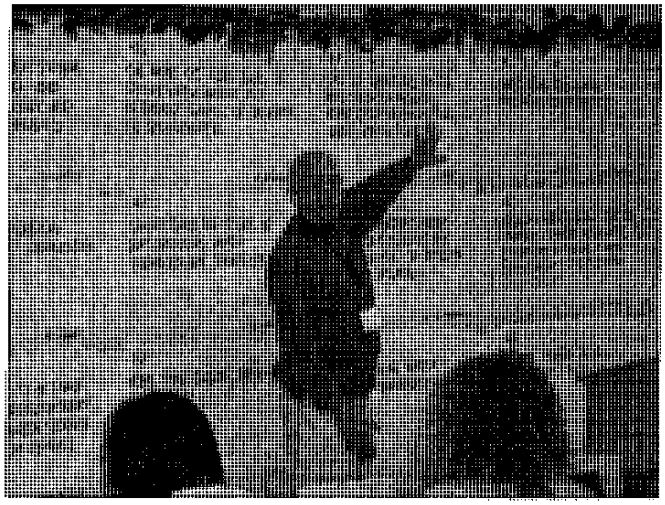
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

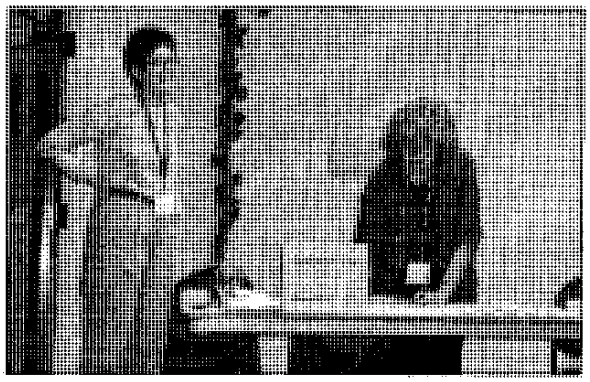
Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.





PRIORITY 15

Water Quality Indicators to Quantitatively Apportion Anthropogenic Loadings of Constituents of Concern

Originators:

Hoppes on behalf of himself, Coty, Esser, Folta, Moran, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Water-Quality Indicators to Quantitatively Apportion Anthropogenic Loadings of Constituents of Concern**

Originator: Hoppes

Research Issue Description:

Source investigations are one of the more difficult undertakings in water resource management. This is made more difficult when the constituent of concern has both natural and multiple anthropogenic sources. Heavy metals and other contaminants of groundwater and surface water can have loadings from both sources. Is the dioxin in your stormwater runoff from an unknown release, an industrial process, or a controlled grassland burning on your site? A toolbox of techniques that allows water managers to identify the natural contribution to loading of constituents of concern would be an important addition in guiding source investigations.

Importance:

Am improved ability to differentiate natural loadings would allow for more targeted allocations of resources to address water-quality issues.

How Do You Propose Meeting or Complying with This Research Issue?

Develop a white paper on the available techniques in water media, including gap analysis and toolbox needs, followed by targeted research efforts to cost-effectively fill in gaps.

Title: **Develop a Tool Box for Total Maximum Daily Loads (TMDLs) Management Tools**

Originator: Coty

Research Issue Description:

Develop a TMDL technology and management system tool box composed of integrated, yet multiple and separable, capabilities that fit user needs across the nation that includes:

- Coupled and unique (yet critical) water quality models (e.g., surface to groundwater; atmospheric to surface water; estuary).
- An allocation model.
- An economic analysis tool to assess alternative best management practices (BMPs) for the efficacy and efficiency of resource use (i.e., couple water quality model with economic model).
- A framework for decision making with uncertainty and incomplete knowledge.

Importance:

- It is burdensome (resource intensive) to mitigate nonpoint source pollution.
- It is resource intensive, contentious, and a slow process.
- There is a national need for tools that enhance resource-limited use and capabilities to quantify water quality issues; make difficult allocation decisions; understand uncertainty in analyses; and develop the best implementation plan to mitigate contamination.
- Forty thousand TMDLs need to be addressed and within a contained timeframe.

How Do You Propose Meeting or Complying with This Research Issue?

Develop a program within the water resources research area that is multidisciplinary and uses a teamwork framework to develop integrated tools, including:

- Water models.
- Economic and decision science (allocation) models.
- Assessment tools for valuing of water quality for various uses.
- GIS tools and interfaces.
- Decision-making tools to deal with uncertainty and risk.
- Work with multiple agencies and stakeholders in partnership to build the tool box.

Title: **Very New Isotopic Approaches to Understanding the Sources and Cycling of Metal and Nutrient Contaminants in Natural and Engineered Environments**

Originator: Esser

Research Issue Description:

Identifying contaminant source is important to distinguishing anthropogenic from natural components, to attributing liability, and to developing effective source mitigation. An understanding of contaminant cycling at different spatial scales is important in understanding the transport and fate of metals in the environment, in demonstrating natural attenuation, in understanding how watershed activities contribute to total maximum daily loads, and in evaluating remediation strategies.

The use of metal and nitrogen isotopic composition investigations in these fields is well established. Two recent advances in inorganic mass spectrometry are significant. Multi-collector magnetic-sector inductively-coupled plasma mass spectrometry (MC-ICPMS) is allowing us to determine isotopic composition of metals at precisions not previously obtainable, which will open up new metal source and cycling research. High spatial resolution secondary-ion-mass spectrometry will allow elemental and isotopic investigations at sub-micron scales, which will significantly improve our understanding of the biogeochemistry of metals and nutrients at the microbial scale. MC-ICPMS is a rapidly developing field; submicron-scale SIMS is a brand new field. Livermore has the instrumentation and expertise to play a significant role in developing these fields.

Importance:

Nonpoint source pollution is exceptionally difficult to attribute. Understanding contaminant metal chemistry at microbial scales will lead to new remediation technologies.

How Do You Propose Meeting or Complying with This Research Issue?

LLNL has a multi-collector ICPMS (MicroMass Isoprobe) and a high-resolution multi-collector SIMS (Cameca NanoSIMS). We are developing heavy metal stable isotope applications on a shoestring budget (e.g., working with the University of California, Berkeley, on a National Institute of Environmental Health Sciences [NIEH] grant looking at mercury isotopes). We need to find ways to increase institutional investment in this capability. The NanoSIMS has just arrived and will be heavily used for biomedical research to understand the localization of targeted radionuclides in cells. We should leverage on the expertise gained from this research to explore metal biogeochemistry at the microbial scale. An obvious first target is microbial reduction of uranium as a method of *in situ* remediation, an application which has programmatic implications for USDOE clean-up. Other applications include studies of nutrient cycling at microbial scales.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Calibrate "Old" Groundwater Dating Techniques and Determine Sources of Salinity in Groundwater**

Originator: Moran

Research Issue Description:

GAMA program data show the surprising fact that a large fraction of water used in California is pre-nuclear age (and the related surprising fact that even in urbanized environments, such as Los Angeles and San Jose, many wells are completely free of anthropogenic contaminants). Characterization of this large volume of water has received little research attention and remains mysterious. Many tools and tracers are available for characterizing young water. This volume of water is well monitored partly because consulting work focuses on shallow groundwater. While some produced water is highly saline, there is a gradient, and some produced water is fresh enough to use for agriculture or even drinking water. Increasing salinity in groundwater is a growing water resource management issue.

Importance:

This "old" groundwater is heavily exploited and is generally free of contaminants. One needs to know the time-scale for recharge since this water is being mined here in California (Central Valley) and in the Great Plains (Kansas, Oklahoma, Texas). One needs to quantify salt sources in water being exploited today – whether from "old water", seawater intrusion, or agricultural return water (an insidious, slowly approaching problem). This research would also address the issue of distinguishing anthropogenic versus natural sources for contaminants.

How Do You Propose Meeting or Complying with This Research Issue?

Use existing data (GAMA) to find this water in areas where "old" water is being used. Calibrate ^{4}He using other radiometric dating techniques, since this covers a relevant age range. Develop ^{14}C age dating capability on compound specific organic C. Use long-lived isotopes like ^{36}Cl and ^{129}I for age dating/salinity source tracing (uses the LLNL accelerator mass spectrometry facility).

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

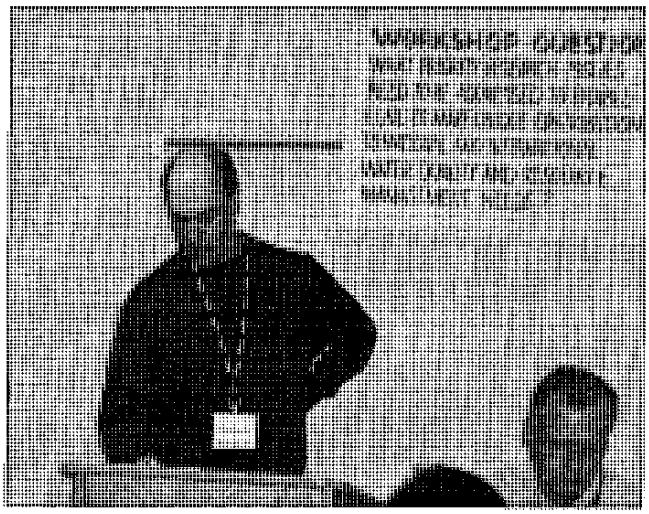
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

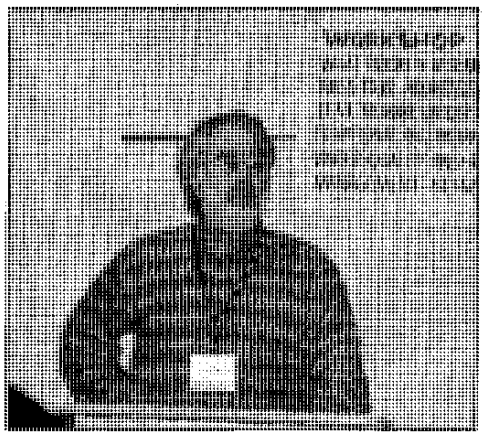
Importance:

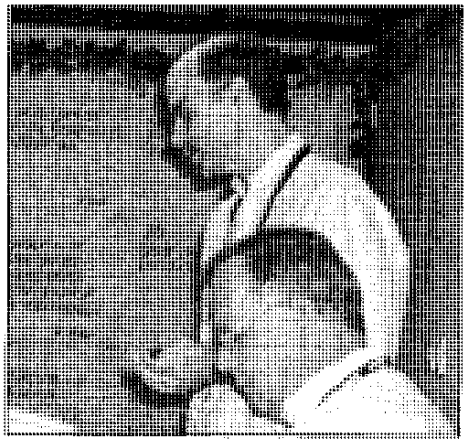
Inadequate funding = No program.

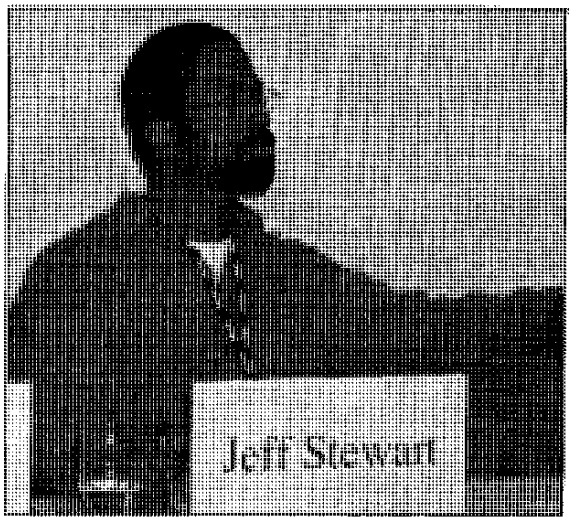
How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.








Jeff Stewart

PRIORITY 16

Apply Biological Ion Selectivity to Membrane Separation Technology

Originators:

Barsky on behalf of himself, Beller, Folta, Stewart, and Woodward

The following research issues were included under the above title:

Title: **Water Lessons from (Structural) Biology**

Originator: Barsky

Research Issue Description:

As we focus on material-water interactions and desired separations, we can learn much from biological systems, especially membrane transport systems and metal binding. By understanding biological systems, we may be able to mimic their effectiveness. Examples include ion channels and metal binding proteins, and even high saline resistance in archi-bacteria.

Importance:

Water purification and, in particular, selective separations are of great social and economic importance.

How Do You Propose Meeting or Complying with This Research Issue?

- Conduct workshops/seminars to discuss fine examples from biology.
- Understand/rationalize how biomolecules accomplish feats of separation:
  - experiments (mutagenesis, spectroscopy)
  - calculation/simulation, including molecular dynamics and *ab initio* quantum chemistry methods (static and dynamic)

Title: **Investigation of Applying Biotechnology to Desalination**

Originator: Beller

Research Issue Description:

Desalination is internationally viewed as a promising method for enhancing water supply. One limitation of existing desalination technology (i.e., reverse osmosis) is that it is highly energy intensive.

Importance:

Clearly, the development of more energy-efficient desalination approaches would be of enormous benefit worldwide. Accordingly, the NRC recently recommended improvement of existing technologies for desalination.

How Do You Propose Meeting or Complying with This Research Issue?

Caveat – I have no firm grasp of the feasibility of this idea, but it might be worth consideration.

Some bacteria contain membrane-bound proteins that pump sodium ions across a biological membrane to create a membrane potential. If the relevant proteins could be fixed to membranes used for desalination, it might be possible to enzymatically pump Na^+ ions to the other side of the membrane, effectively removing a major seawater ion from solution. Although reverse osmosis treatment might still required after this treatment, the reverse osmosis energy requirements should be lower because the osmotic pressure will be reduced.

Depending on how much of the cellular "machinery" could be incorporated into the membrane, there could be some distinct advantages in terms of energy sources and greenhouse gas emissions; some of these sodium-pumping bateria use hydrogen as an energy source and consume carbon dioxide.

Biology and Biotechnology Research Program and Chemistry and Materials Science.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
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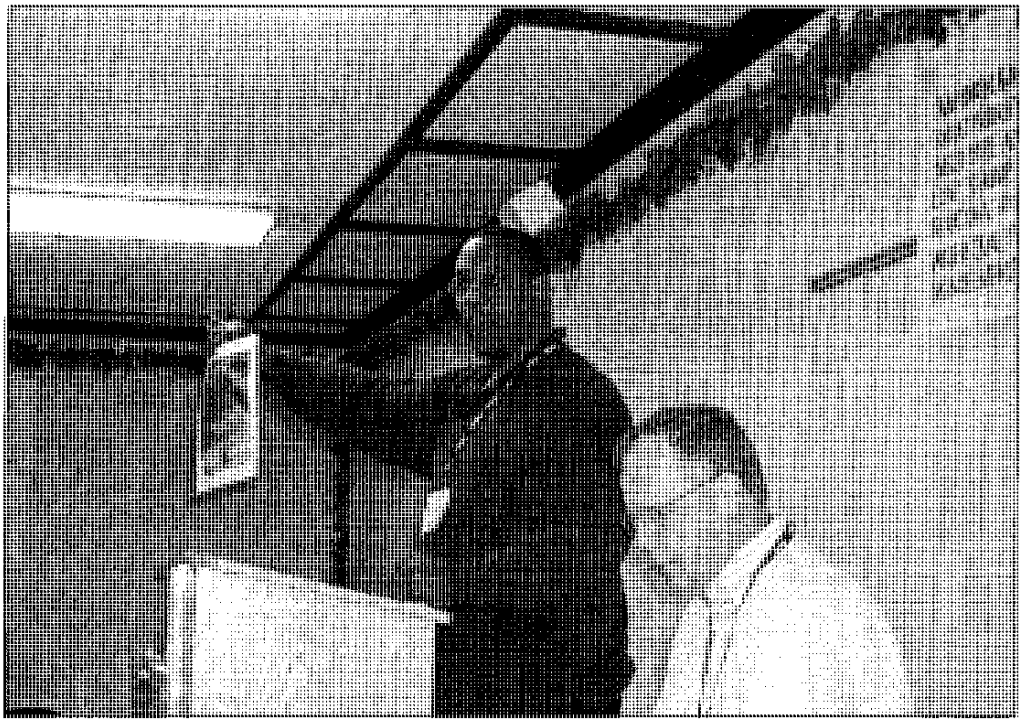

PRIORITY 17

Water Technology Transfer

Originators:

Cantwell on behalf of herself, Folta, Mack, Newmark, Rice/Cherepy, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Water Technology Transfer**

Originator: Cantwell

Research Issue Description:

There are three success factors in transferring technologies for the acquisition of new data and for the mitigation of water management challenges to those who can and will use it. These include:

- State, industry, and LLNL partnerships that provide test beds and field demonstration opportunities that all parties will trust.
- Early involvement of potential commercial partners in the technology development cycle. This will require true innovation in developing new models for dealing with business partners, along with a high tolerance for risk.
- As mentioned, a high quality, well-thought-out marketing effort.

Importance:

The technology or fundamental knowledge that we want to develop will not be highly utilized unless we carefully structure partnerships to transfer our knowledge.

How Do You Propose Meeting or Complying with This Research Issue?

Create a water industry initiative in partnership with state agencies. An alternative is to create a Center for Water Technology Transfer.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Capacitive Deionization (CDI) Technology – National/International Marketing**

Originator: Mack

Research Issue Description:

CDI with carbon aerogel electrodes can be used to remove anions and cations, including heavy metals and radioisotopes, from aqueous streams at USDOE and the USDOD facilities, as well as at a variety of civilian industrial plants. Such deionization processes generate large volumes of corrosive secondary waste that must be treated, including spent anion and cation exchange resins, contaminated acids, and contaminated bases. For example, solutions of H_2SO_4 are used for the regeneration of cation columns used in metal finishing facilities, while HNO_3 is used for the regeneration of cation columns in plutonium processing plants. During plutonium processing, resins and solutions of HNO_3 become contaminated with PuO_2^{++} and other radioisotopes. Every pound of cation exchange resin requires approximately 100 pounds of 10 weight percent H_2SO_4 or HNO_3 and 2 to 3 pounds of rinse water for regeneration. Similarly, solutions of NaOH are used to regenerate anion exchange resins. Given the high cost of waste disposal, there is a tremendous incentive for reducing the volume of waste. This new technology, aerogel-based capacitive deionization, eliminates waste generation by substituting nontoxic and nonpolluting electricity for the acids, bases, and salts that are normally used for the regeneration of ion exchange resins.

Importance:

If fully developed, the CDI process could have the following important applications:

- Removing various ions from wastewater without generating acid and base secondary wastes.
- Treating boiler water in nuclear and fossil power plants.
- Producing high-purity water for semiconductor processing.
- Providing low-cost, electrically-driven water softener for homes.
- Removing salt from water for agricultural irrigation.
- Providing lower cost seawater desalination systems with reduced maintenance.

How Do You Propose Meeting or Complying with This Research Issue?

Secure funding internally to support LLNL-based marketing efforts.

Title: **CDI Technology – Technology Transfer**

Originator: Mack

Research Issue Description:

To date, CDI has been licensed to CDT Systems (Arizona) and WB Solutions (Wyoming). CDT is investigating a variety of applications, including replacing existing reverse osmosis plants. WB Solutions is investigating reducing mineral deposits that contaminate groundwater deemed harmful to soils, vegetation, and water resources. These mineral deposits occur during the development of coal bed methane wells. Coal bed methane production has existed in the U.S. for the past several years, and the U.S leads the world in coal bed methane exploration and development. The process of coal bed methane extraction involves the dewatering of underground coal seams, which relieves the pressure confining the available methane within the seam. As the groundwater is extracted, methane gas migrates upwards through the well and is collected, compressed, and transported for use. Current industry and state regulatory estimates suggest that the number of wells developed for coal bed methane production will range from 80,000 to nearly 140,000 over the next 10 years. WB Solutions is currently testing a filter based on LLNL's original design. They are also interested in designing a filter based on a fluidized bed reactor design patented by LLNL. Suez-Oneo subsidiary in the U.S. is actively talking to LLNL.

Importance:

- Maintain, protect, and expand agricultural land use.
- Ensure vendors that licensed CDI will succeed by providing the necessary engineering expertise and support.

How Do You Propose Meeting or Complying with This Research Issue?

Expand technology transfer efforts and market technology to appropriate commercial concerns.

Title: **CDI Technology — Potential-Swing Ion-Adsorption Control Algorithm Development**

Originator: Mack

Research Issue Description:

A potential-swing ion adsorption control algorithm was developed and patented by LLNL. The design consists of a continuous-flow pilot plant with two CDI cell stacks or filters arranged in parallel. One stack will be regenerated (discharged) while the other stack separates (charges). This mode of operation is analogous to pressure-swing gas absorption. The stacks are charged and discharged like electrolytic capacitors. Additionally, stack electrode polarities are reversed during each discharge cycle. Regenerating stacks are discharged to the alternate stack to affect energy recovery, thus reducing the process electricity operating costs. The total capacitance of a stack assembly is directly computed from the aerogel volumetric capacitance and the total stack assembly aerogel volume. This control algorithm can be easily extended to any number of paired stack assemblies connected in parallel.

Importance:

- The process is more robust and the electricity operating costs are reduced.
- The ion removal efficiency is improved.

How Do You Propose Meeting or Complying with This Research Issue?

Secure funding from the USDOE or another federal agency, and establish a research program at LLNL.

Title: **Understand the Implementability Issues of Water Management Strategies**

Originator: Newmark

Research Issue Description:

LLNL has expertise and experience in fundamental research, predictive simulations, and technology development. The transfer of our technologies into the sponsor community has received mixed success. Water issues span perhaps a greater range than previously encountered: technical, engineering, economic, customer, cultural, political, and philosophical.

Importance:

To be successful in impacting the evolving water landscape, we must be able to implement our ideas/creations. Some solutions will involve both technical and political aspects (e.g., Salton Sea).

How Do You Propose Meeting or Complying With This Research Issue?

- Improve communication: workshops, advisory panels, and partnering with regulatory and management agencies, NGOs, and industry.

- Conduct academic forums to carry out this effort
  - LLNL's new Center for Societal Impacts
  - University of California, Merced

Title: **Water Purification Via Advanced Oxidation Technologies**

Originator: Rice/Cherepy

Research Issue Description:

Cost-effective advanced oxidation technologies are needed for applications such as:

- Industrial effluent purification prior to discharge.
- Drinking water purification of chemical as well as microbial contaminants.
- Industrial water purification (e.g., for ultrapure water used in semiconductor manufacture).

Advanced oxidation technologies involve chemical and electrochemical processes to degrade both chemical and biological contaminants in water.

Importance:

Water supplies are limited; contamination by industrial waste, pesticides, etc., further limit usable water. Current drinking water supplies still use old technologies, primarily filtration and chlorination, to eliminate microbial contamination and particulates. Advanced oxidation technologies are relevant for industries that need to limit their discharge of pollutants and for those who need ultrapure water for processing. Concerns in the U.S. about drinking water quality suggest demand for improved technologies to ensure the purity of drinking water that current technology cannot provide.

How Do You Propose Meeting or Complying with This Research Issue?

If there is sufficient interest in this topic, it would be worthwhile to identify potential collaborators at LLNL, University researchers, industrial sponsors, and managers of municipal water supplies. There is significant active research in this area, though not at LLNL.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
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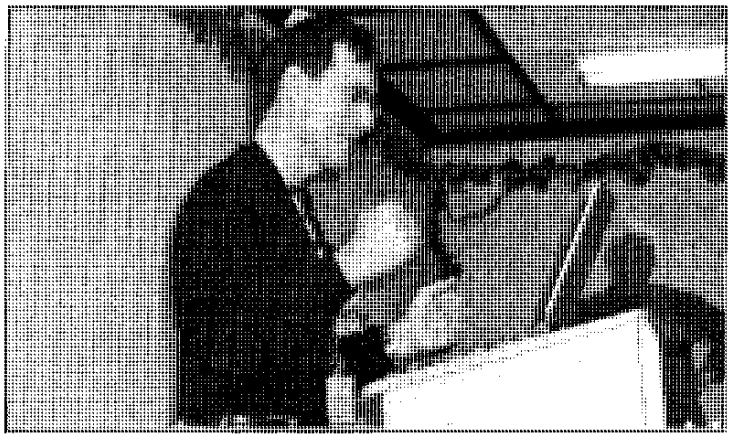


PRIORITY 18

Deep and Practical Understanding of Osmosis

Originators:

Barsky on behalf of himself, Christensen, Folta, Hudson, O'Brien, Stewart, and Woodward

The following research issues were consolidated under the above title:

Title: **Deep and Practical Understanding of Osmosis**

Originator: Barsky

Research Issue Description:

Currently, while better RO membranes are sought, there is a poor understanding of osmosis itself (this problem is over 100-years old). With respect to flow across the membrane, is it dominated by diffusion or bulk (viscous) flow? Is there an understandable relation to the size and chemical nature of pores?

Importance:

This research would be fundamental to water purification and, in particular, to improved membrane performance.

How Do You Propose Meeting or Complying with This Research Issue?

- Conduct workshops/seminars with outside speakers to understand the problem.
- Develop an experimental test bed, having "regular" pores (e.g., electron microscopy drilled membranes or carbon nanotube arrays).
- Develop simulation capabilities, especially non-equilibrium molecular dynamics methods where we are currently falling behind. Fortunately, even hard-sphere simulations have been able to capture diffusion versus viscous flow.

Title: **Water Reuse: Focused Use Planning Together with Focused (Selective) Purification Technology**

Originator: Christensen

Research Issue Description:

Today, we aggressively purify and treat water for the tap. Much of this water is used for purposes where such high quality is not necessary. In fact, such high purity may cause deleterious impacts to the environment. Our greatest concern is the fact that much water is used only once after having invested heavily in purification. Focusing the tailoring contaminant purification/separation technologies represents an opportunity to improve the efficiency of water reuse.

Importance:

- Tailoring the quality of water to the use can result in lower cost and improvements in water use efficiency.
- Improved planning, in terms of staging water use, results in leveraging the investments made in purification.

How Do You Propose Meeting or Complying with This Research Issue?

- This requires the custom development of water separation technologies, sensors and control technologies, and developing Green Building and/or Green Community concepts designed to optimize the reuse of water.
- It also requires custom analysis of water quality versus water use in order to optimize, stage water use, and minimize cost.

Title: **How Does LLNL Leverage High Performance Computing (HPC) and World-Class Computer Science Research to Develop LLNL-Unique Program Elements?**

Originator: Folta

Research Issue Description:

- LLNL has the fastest computer in the world; it will only get faster.
- USDOE Office of Science is a strong supporter of LLNL computer science research.
- LLNL's role in water research must be justifiable (overhead).
- Support program elements (think big), including:
  - large computational problems requiring HPC
  - data integration (system level)
  - data mining
  - state → national → global integrated modeling and simulation

Importance:

- Justify funding – why must this be done at LLNL?
- Identify needs so that we have solutions/resources in a timely manner (hardware and algorithms).

How Do You Propose Meeting or Complying with This Research Issue?

- Work with program elements identified here today.
- Identify HPC and modeling/simulation needs – integration.

Title: **Advanced Technology to Support Wastewater Recycling**

Originator: Hudson

Research Issue Description:

Develop advanced real-time (or near-real-time sensors) to characterize the operation of water recycling facilities. Sensors should measure a variety of water quality parameters and be combined with a data management system capable of assimilating and evaluating the data. This effort will be highly synergistic with water security technology needs.

LLNL has previously demonstrated two enabling technologies for wastewater recycling: $^{3}H/^{3}He$ dating and enriched-isotope noble gas tracers. These techniques allow for the accurate tracking of recycled water after being released to the environment. This work was done in a laboratory research setting and, while the work was economically viable in this setting, we need to develop practical/targeted methods to see that these technologies are truly usable and available.

Importance:

Water recycling represents one of the important sources of "new" water, especially in urban settings. There has been considerable public opposition to recycling water for indirect potable reuse. The two items above directly address important components of the public concern. These issues are also viewed as important by regulatory agencies. The tracer technology is also significant for economical issues since maximizing the use of environmental buffers requires the direct measurement of the flow-paths and flow-rates of recycled water in the subsurface environment (i.e., if you cannot measure it, you must be much more conservative – you cannot recycle as much water).

How Do You Propose Meeting or Complying with This Research Issue?

Focus efforts in advanced technologies, such as "smart" membranes, "gene-chips," and bioassays (Bourcier, Reynolds, Farmer, Kane, Beller).

Focus efforts on the development of small, inexpensive, and robust gas mass spectrometry systems. This effort will also be synergistic with water security technology needs (Hudson, Hutcheon, Krulevitch, Microtechnology Center).

Title: **Molecular Engineering of Electrodialysis Membranes for Nitrate Removal**

Originator: O'Brien

Research Issue Description:

Previous research and developments in the area of EDR have shown that the transport properties of the membranes are major factors that drive the economics of the process. Increased selectivity to a given ion, as well as maintaining a low electrical resistivity, is critical to reduce energy requirements for the process. The goal of this effort would be to combine previously developed LLNL technology with new molecular engineering approaches to achieve a new ion-exchange based platform technology that will be cost-effective for cleaning up brackish water feed streams.

Importance:

A significant number of California public and, especially, private groundwater wells have nitrate levels that exceed or approach regulatory limits for drinking water, and a significant fraction of California's surface water supplies have nitrate concentrations that would preclude their use for groundwater recharge if draft California Department of Health Services regulations were adopted. In 1988, approximately 10 percent of the California groundwater analyses in the USEPA STORET database exceeded the drinking water maximum contaminant limit (MCL). Today, approximately 80 percent of the groundwater wells in the Stanislaus County database are impacted by nitrate contamination (i.e., have maximum concentrations greater than 3 milligrams per liter), and greater than 15 percent have maximum concentrations that exceed the drinking water limit.

How Do You Propose Meeting or Complying with This Research Issue?

Improving efficiency results in a cost- effective technology.

- Obtain current standards and set baseline: Asahi Glass Company and IONICS systems.
- Capitalize nanotechnology efforts within LLNL:
  - functionalize carbon nanotubes to assist in the transport of nitrates
  - examine the physical properties of materials
- Couple with molecular simulations to understand how functionalization affects transport.

- Fabricate on small scale and screen.
- The final result is a pilot-scale demonstration device that can be ported to a pre-determined site for testing.
- Need to simultaneously work the policy area and need to create funding sources.
- The goal is a ubiquitous system that can be adapted for treating various brackish water sources.

Requires:

- Interacting with universities/NSF centers.
- Municipal water suppliers.
- Major engineering firms.
- Coupling with University of California, Merced.

Title: **Annual LLNL Water Research Workshop/Training**

Originator: Stewart

Research Issue Description:

Train the water community on successful water tools at LLNL.

Importance:

- Many LLNL ideas do not get the exposure necessary to benefit LLNL.
- Input from Stakeholders.

How Do You Propose Meeting or Complying with This Research Issue?

Set-up water workshops for the public, universities, other agencies, and NGOs.

Title: **Marketing LLNL Water Resource Capabilities**

Originator: Woodward

Research Issue Description:

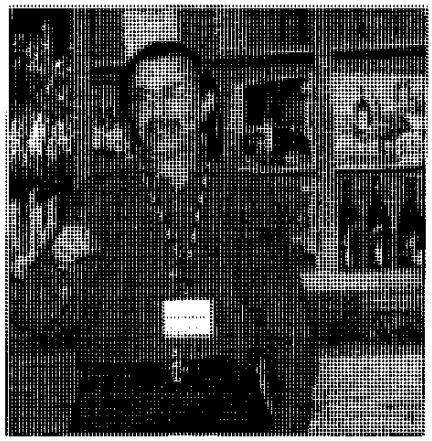
Our water initiative will not be successful unless we master the marketing of LLNL capabilities and resources. In other words, marketing is integral to the funding of research if the water initiative is to grow into a major LLNL program.

Importance:

Inadequate funding = No program.

How Do You Propose Meeting or Complying with This Research Issue?

- Involve potential future research funders as current research partners.
- Identify and strongly support those research efforts that may quickly influence policy decision changes, such as leaking underground fuel tanks.
- Sponsor onsite and offsite seminars where LLNL capabilities can be highlighted.
- Strongly support key federal and state legislators and their staff.
- Identify international water resource problems where LLNL can quickly and inexpensively (hopefully) provide solutions.
- Use LLNL Director's Office to publicize the Water Initiative and its successes.
- Make research investment decisions focus on problems that need to be solved as opposed to our skills seeking problems to work on.



STRENGTH OF FEELING ANALYSES OF PARTICIPANTS AND SUBGROUPS OF PARTICIPANTS

The following table gives a quantitative sense of the degree of agreement (or disagreement) among the workshop participants regarding the importance of each identified and prioritized research issue. Table 1 is organized according to the priority ranking by all 25-workshop participants of all 18 major research issue areas on which they voted.

To create these tables, each of the 25 participants voted individually for the 10 highest priority responses to the workshop question: ***What priority research issues need to be addressed to enable LLNL to make unique contributions to national and international water quality and resource management needs?***

The table lists the research issues in descending order of importance, the issue title, the times it was voted for (picked), the total number of points received from the balloting, and finally, the strength of the group's feeling, expressed as a percentage.

TABLE 1

Issues (18) Ranked by All Participants (25)

Rank	Title	Times Picked/Pts	Strength of Feeling
1.	What Is the True Value of Water?	21/145	83.8%
2.	Regional Scale, Data-Driven Water Supply/Demand/Quality Forecasting and Optimization Models	17/123	71.1%
3.	Water Infrastructure Security	17/115	66.5%
4.	Assess and predict the Impact of Land Use and Managing Practices on Groundwater Quality	20/113	65.3%
5.	Cost-Effective Sensor and Communication Systems for Detection and Analysis of Raw Water Media	18/95	54.9%
6.	Brine Use and Management Technologies for Gas and Oil Production, Power Plants, and Wastewater Treatment Plants	18/95	54.9%
7.	Innovative Approaches to Characterize, Manage, and Treat Nitrate Contamination in Groundwater	16/90	52.0%
8.	Impact of Climate Change on Water Management and Infrastructure	18/86	49.7%
9.	Molecular Studies of Biochemical Cycling of Aquatic Contaminants	10/82	47.4%
10.	Optimize Conjunctive Use with LLNL's Advanced Analytical and Modeling Capabilities	16/76	43.9%
11.	Identify Research Efforts to Support Focused Water, Reuse, and Conservation	14/70	40.5%
12.	Integrated Water and Energy – Long-Term Planning and Conflict Resolution	15/57	32.9%
13.	Advanced Watershed Characterization and Diagnostics to Support Hydrologic Simulations	9/56	32.4%

Rank	Title	Times Picked/Pts	Strength of Feeling
14.	Improve the Scientific Basis of Risk Assessment, Risk Management, and Risk Communications for Water Systems	8/54	31.2%
15.	Water-Quality Indicators to Quantitatively Apportion Anthropogenic Loadings of Constituents of Concern	10/41	23.7%
16.	Apply Biological Ion Selectivity to Membrane Separation Technology	5/28	16.2%
17.	Water Technology Transfer	8/28	16.2%
18.	Deep and Practical Understanding of Osmosis	3/14	8.1%

APPENDICES

APPENDIX A

ACRONYMS

ASR	aquifer storage/recovery
AWWARF	American Water Works Association Research Foundation
BBRP	Biology and Biotechnology Research, LLNR
BMP	Best Management Practice
CALFED	CALFED Bay Delta Program
CALSIM	Water resources simulation model for evaluating operational alternatives of large, complex river basins (developed by State of California, Department of Water Resources)
CALVIN	CALifornia Value Integrated Network
CDC	Centers for Disease Control
CDI	Capacitive DeIonization
C&MS	Chemistry & Materials Science, LLNR
CMU	Carnegie Mellon University
COE	U.S. Army Corps of Engineers
DARPA	Defense Advanced Research Projects Agency
DEP	dielectrophoresis
DHS	(State of California) Department of Health Services
EDR	electodialysis reversal
E&E	Energy and Environment, LLNL
EPD	Environmental Protection Department, LLNL
EPRI	Electric Power Research Institute
FERC	Federal Energy Regulatory Commission
GAMA	Groundwater Ambient Monitoring and Assessment
GIEMS	Georeferenced Integrated Environmental Management Systems
GIS	Geospatial Information System
HPC	high performance computing
IGSM	Integrated Groundwater-Surface water flow Model
ISO	International Organization for Standardization
LDRD	Laboratory Directed Research and Development
LLNL	Lawrence Livermore National Laboratory

MC-ICPMS	Multi-Collector-Magnetic-Sector Inductively Coupled Plasma Mass Spectrometry
MCL	maximum contaminant limit
MEMS	MicroElectroMechanical Systems
MIC	microbiologically influenced corrosion
MODFLOW	MODular three-dimensional finite-difference groundwater FLOW model
MTBE	methyl tertiary butyl ether
NARAC	National Atmospheric Release Advisory Center
NIEHS	National Institute of Environmental Health Sciences
NGO	Non-Governmental Organization
NORM	Naturally Occurring Radioactive Material
NRC	National Research Council
NWRI	National Water Research Institute
OEA	Office of Energy Assurance, USDOE
OEM	Original Equipment Manufactures
OCWD	Orange County Water District
PERM	Practical Environment Restoration Management
PLUHA	PLUme History Analysis
ppm	parts per million
R&D	research and development
RDD	radioactive dispersal device
RO	reverse osmosis
SCVWD	Santa Clara Valley Water District
SIMS	Secondary Ion Mass Spectrometer
SSEP	Security and Environmental Protection, LLNL
SWRCB	State Water Resources Control Board
TDS	total dissolved solids
TMDL	total maximum daily loads
TOC	total organic compounds
UC Davis	University of California, Davis
UF	ultrafiltration
USBR	U.S. Department of the Interior, Bureau of Reclamation
USDA	U.S. Department of Agriculture
USDOD	U.S. Department of Defense
USDOE	U.S. Department of Energy
USDOI	U.S. Department of the Interior
USEPA	U.S. Environmental Protection Agency

APPENDIX B

PREVIOUS NGT WORKSHOPS CONDUCTED BY NWRI

Life Cycle Environmental Impacts Associated with Different Fuel Options. Report of a workshop sponsored by NWRI in cooperation with Clarkson University, Lawrence Livermore National Laboratory, and USEPA – Office of Research and Development. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, February 15-17, 2002. 202 p.

Issues in Methanol Research. Report of a workshop sponsored by NWRI in cooperation with the American Methanol Institute. Hilton Hotel, Costa Mesa, CA, October 5-7, 2001. 173 p.

Chino Basin Organics Management. Report of a workshop sponsored by NWRI in cooperation with the Inland Empire Utilities Agency, and the Southern California Alliance of Publicly Owned Treatment Plants. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, April 18-20, 2001. 205 p.

Desalination Research & Development. Report of a workshop sponsored by NWRI in cooperation with the United States Bureau of Reclamation. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, January 19-21, 2001. 185p.

Knowledge Management. Report of a workshop sponsored by NWRI. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA January 5-7, 2001. 169 p.

Oxygenate Contamination. Report of a workshop sponsored by NWRI in cooperation with the United States Bureau of Reclamation. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, September 15-17, 2001: 258p.

Utility Leadership. Report of a workshop sponsored by NWRI in cooperation with Malcolm Pirnie, Inc., the University of Southern California, and the University of South Florida. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, October 24-26, 1999: 154p.

Non-potable Water Recycling. Report of a workshop sponsored by NWRI in cooperation with Irvine Ranch Water District and the Orange County Water District. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, May 23-25, 1999: 174p.

Conjunctive Use Water Management Program. Report of a workshop jointly sponsored by NWRI, Association of Ground Water Agencies, and the Metropolitan Water District of Southern California. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, May 27-29, 1998: 157p.

Barriers to Providing Safe Drinking Water Through Small Systems. Report of a workshop jointly sponsored by NWRI, Pan American Health Organization, and NSF International/WHO Collaborative Center. Pan American Health Organization Headquarters, Washington, D.C., May 13-15, 1998: English report: 175p., Spanish report: 188p. (Bound in a single volume.)

Barriers to Harvesting Stormwater. Report of a workshop jointly sponsored by NWRI, Los Angeles County Department of Public Works, County of Orange Public Facilities & Resources Department, Southern California Coastal Water Project, and the American Oceans Campaign. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, September 22-24, 1997: 159p.

Groundwater Disinfection Regulations Benefits Conference. Report of a conference sponsored by NWRI. Arnold and Mabel Beckman Center, National Academies of Sciences and Engineering, Irvine, CA, March 17, 1997: 75p.

Groundwater Disinfection Regulation. Report of a workshop jointly sponsored by NWRI and the USEPA. Arnold and Mabel Beckman Center, National Academies of Sciences and Engineering, Irvine, CA, January 6-8, 1997: 209p.

Membrane Biofouling. Report of a workshop jointly sponsored by NWRI, UNESCO Centre for Membrane Science and Technology, and CRC for Waste Management and Pollution Control, LTD. UNSW Institute of Administration, Sydney, Australia, November 15-17, 1996: 176p.

The Santa Ana River Watershed. Report of a workshop jointly sponsored NWRI and the Santa Ana Watershed Project Authority. Co-sponsors included: City of San Bernardino Water Department, City of Riverside, Western Municipal Water District, and Orange County Water District. Kellogg West Conference Center/Hotel, California State Polytechnic University, Pomona, CA, August 23-25, 1995: 182p.

The New River. Report of a workshop jointly sponsored by NWRI and the County of Imperial, California. Barbara Worth Country Club, Holtville, CA, May 19-21, 1995: English report: 134p., Spanish report: 134p. (Bound in a single volume)

Establishment of The Middle-East Water and Energy Research and Technology Centre. Report of a workshop jointly sponsored by NWRI and the Sultanate of Oman through the Worldwide Desalination Research and Technology Survey. Muscat, Oman: September 21, 1994: 29p.

Risk Reduction in Drinking Water Distribution Systems. Report of a workshop jointly sponsored by NWRI and the Environmental Criteria and Assessment Office of the USEPA. Arnold and Mabel Beckman Center, National Academies of Sciences and Engineering, Irvine, CA, February 27-28, 1994: 142p.

Fouling and Module Design. Report of a workshop jointly sponsored by NWRI and the National Science Foundation (NSF). Virden Conference Center of the University of Delaware, Lewes, DE, October 30 – November 1, 1993: 115p.

Groundwater Disinfection Rule. Report of a workshop jointly sponsored by NWRI and the USEPA in collaboration with the Weston Institute. Virden Conference Center of the University of Delaware, Lewes, DE. June 7-8, 1992: 103p

APPENDIX C

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APPENDIX D

WORKING GROUPS' VISUAL PRESENTATIONS

LLNL Water Resources Simulator: A Coupled, Scaleable, Data-driven, System to Optimize Water Management Solutions

Dave Layton, Jeff Stewart, Betsy Cantwell, Brendan Dooher, Jessie Coty, Dave Rice

21st Century Water

LLNL WateRSim: Problem statement

Supply
- ✓ Nearly a third of the world's population will face severe water shortages by 2025
- ✓ Economic growth in the Western U.S. has been sustained by large water projects, but supply/demand imbalances will limit future growth
- ✓ Climate changes will significantly change water utilization world-wide

Quality
- ✓ 1.2 billion people (20%) drink polluted water
- ✓ 5 million people die annually from water borne diseases

Security
- ✓ Water supply systems are not designed to resist acts of terror

21st Century Water

LLNL WateRSim: Goals:

- ✓ Improve global water quality and supply in the 21st century by addressing compelling scientific challenges in water treatment, hydrologic cycle characterization & system management.
- ✓ Discover optimal solutions to critical water resource problems such as:
  - •Development of realistic TMDL goals
  - •Identify impaired waters that can be cost effectively treated to create clean new water, e.g., nitrates
  - •Support cost benefit analysis for the application of emerging treatment technologies
  - •Conjunctive use
  - •Salinity management

21st Century Water

LLNL Water Resources Simulator Components

- Dynamic Data Warehouse
  - Access to distributed data
  - Data mining tools (LILAC)
  - Sensor data
  - Geims/GAMA data
  - Land use data
- Data Analysis and Processing Rule Sets
  - Spatial scale
  - Data fusion
  - Geo statistical interpolation
  - Inverse techniques
  - Statistical approaches

21st Century Water

LLNL Water Resources Simulator Components

- Water Resources Simulator
  - Scaleable, Coupled Simulation Capability
  - Enhanced leveraged existing models (PC based)
    - Calvin
    - ISGM
    - NUFT
  - Computationally intensive LLNL owned models
- User Friendly Interface
  - Permits "options gaming" by water policy decision makers
  - Allows clients to see how they may use the system
  - Enables efficient problem set up.

21st Century Water

LLNL WateRSim: Implementing Team

•Strong experience in:

- •Computations and information systems integration
- •Geo spatial interpretation
- •Hydrogeologic systems including water movement in saturated and unsaturated flow
- •Interpetation of advance water characterization data
- •Biogeochemical environmental interactions

21st Century Water

LLNL WateRSim: Level of Effort

- •Dynamic Data Warehouse - 1.5 FTE/yr ($300K)
- •Data Analysis and Processing Rule Set - 3 FTE/yr ($600K)
- •Scaleable, Coupled Simulation Capability - 3 FTE/yr ($600K)
- •User Friendly Interface - 0.5 FTE/yr ($100K)
- •Total $1000K

•Workshops
•Add calSim
•Modflow
•Downward projection to lower resolution
•Hardware costs
•Action Plan

21st Century Water

WORKING GROUP 4

Water Initiative Workshop: Priority Group 4

ASSESSING AND PREDICTING THE IMPACT ON WATER QUALITY OF CHOICES IN LAND USE AND MANAGEMENT PRACTICES

Bill Hoppes, Robin Newmark, Dick Woodward, *with cameo appearances by Brad Esser and Bryant Hudson*

Managers need science-based tools to guide policy decisions in land use planning and choices in management practices.

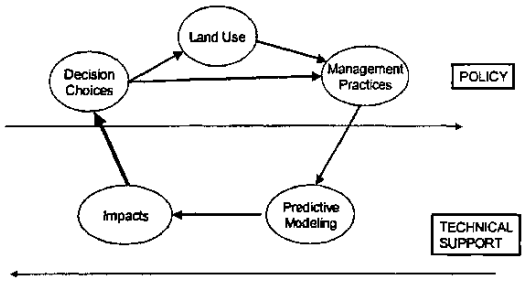
Needed: a robust means to correlate changes in groundwater quality and quantity with

- ⇨ changes in land use,
- ⇨ agricultural operation management practices and
- ⇨ water management practices (including artificial recharge).

Portions can be addressed by specific models (i.e., groundwater flow or water allocation models), but integrated tool suites are necessary to assess the impact of such decisions on overall water quality and quantity.

A multi-faceted approach is needed.

ASSESSING AND PREDICTING THE IMPACT ON WATER QUALITY OF CHOICES IN LAND USE AND MANAGEMENT PRACTICES



How will we address this issue?

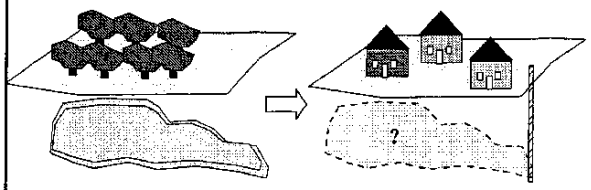
- Develop a capability that includes coupled model systems that encompass the range of atmospheric/surface/ground water interactions that control water quality. Temporal and spatial scales need to be able to reflect realistic cases.
- Validate the process through demonstration in historic case analyses in which management decisions can be tested through a combined experimental/simulation analysis in partnership with water resource agencies and agricultural interests.

Coupled model systems are required

- Atmospheric precipitation driving models coupled through the surface
- Groundwater flow models
- Particle-based transport modeling
- Reactive transport models, with appropriate biogeochemistry
- Need to address fluxes resulting from specific land uses: *parameterization will be important*
  - **natural ecological sources**
  - **urban/industrial runoff**
  - **agricultural runoff**
  - **point and non point source discharges**
- Scenarios must be able to simulate outcomes from different management practices, at the appropriate time scales. These include choices in water use and discharge restrictions specific to each land use. These models must be field-testable using a suite of groundwater tracers and age dating techniques, coupled with groundwater flow models.

Historic Case Analysis of Land Use Change: Santa Clara Valley, California

Land use change over past 40 years from agricultural (primarily orchards) to suburban setting: nitrate reduction expected in young (<40 yr old) water.



Validation through historic case analysis: Santa Clara Valley

- Use groundwater tracing (with noble gas tracers and tritium-helium ages)
- Determine the true groundwater ages (with groundwater models strongly coupled to apparent groundwater age)
- Develop and demonstrate source tracers (with isotope and trace inorganic and organic geochemistry)
- Develop and run forward simulation scenario
- Analyze and compare results

Factors affecting water quality and quantity in California that can be addressed through this work

- Regulatory limits (tend to decrease over time (e.g., arsenic))
- Use of groundwater basins to store and manage surface water supplies (conjunctive use)
- Intrusion of poor quality groundwater, saltwater or brine as a result of excessive pumping
- Salinization of aquifers resulting from surface irrigation by imported surface water
- Recharge using reclaimed water (e.g., Orange County, Ca)
- Nonpoint source pollution (e.g., nitrate)
- Water supply
- Changes in surface water elevation due to groundwater drawdown, often accompanied by surface subsidence.

Who needs to participate?

- **Interdisciplinary technical team**, including members from the technical community (hydrogeology, atmospheric and surface water modeling, computations, geochemistry, ecology, economics, information management specialist, land use specialist).
- **User communities** (e.g., State Water Resources Board, water managers (e.g., Santa Clara Valley Water District), University of California, Davis, Alameda County Flood Control and Water Conservation District, water suppliers, Agricultural Extension Service (USDA), land planning agencies).
- NGOs such as the Sierra Club and Friends of the River

Budget

$4 million over 3 years

This involves **technical components** such as model evolution, field survey design and performance and analysis as well as substantial **interactions**, problem definition, data collection and exchange.

Trust us; we're worth it!

Epilogue

- Issues discussed: Who is the sponsor and what is our product?
  - **Water resource agencies**
  - **Case studies**
- How to package our results? Can we do optimization?
- Does not include: economics and water allocation models

Cost-Effective Sensor and Communication Systems for Detection in Raw Water Media and Analysis of the Result

4 separate solutions: chem., bio, physical parameters (velocity) and communications networking.

Elizabeth Cantwell, Brendan P. Dooher, Peggy Folta, William Hoppes, Joanne Horn, Kevin O'Brien, and Nina Rosenberg

Research Issue Description

- There's an urgent need for rapid chemical, biological, and physical assessment of environmental water quality and properties.
- Present methodologies for analysis of chemical and biological agents in water, and the physical properties of groundwater and surface water systems, are time- and labor-intensive, expensive, and especially for the biochem detection systems, have low efficiencies in natural waters.
- A comprehensive approach is needed that addresses all aspects of the sample collection, processing, and detection process in real water matrices (at relevant volumes) to provide highly reliable data in a rapid time frame.

Challenges

- Develop field deployable detectors that can, if needed, be operated remotely. These sensors must work reliably in sewage, seawater, brackish water, stormwater, and in the places where it is difficult to get sensors to work, but where managers need information about water quality in real-time and of high quality.
- Development of sensor and detector technologies that provide real-time or near real-time measurement and analytical capabilities for water quality, water level, and water flow rates.

Importance

- Understanding of the dynamics of groundwater and surface-water systems calls for more than quarterly data tracking.
- There is an increased awareness of the vulnerability of our drinking water supplies, and the need for pre-symptomatic action in the event of a biothreat attack against water resources or water systems.
- As water distributors need to make costly and timely decisions based on accurate information concerning whether to divert a water supply from public consumption, real time and near-real time data collection and assessment are critical.

Data Collection Needs

- Well water levels in order to track contaminant movement from point source releases in order to understand the dynamics of nearby public, private, agricultural, and industrial extraction wells;
- Development of reliable, low-cost methods to measure groundwater movement (as opposed to estimating groundwater velocities) and stream and river flow rates is necessary to understanding the system's dynamics;
- Chemical sensors capable of accuracy levels of at least hundreds of parts per billion (with capabilities in the parts to tens of parts per billion for critical areas) and report at least on a day-to-day basis, or send instantaneous alerts if there is a detection;
- Development of real-time field portable or in-situ sensors that differentiate human fecal coliform from other sources in seawater samples (admittedly, a challenge);
- Real-time identification of pathogen contamination in water;
- Bio-sampling downstream from ultrafiltration with a detection of log reduction of 6 and lower;
- A system for rapid and quantitative separation and concentration of biological materials from non-biological materials; and
- Sample preparation steps that preserve the integrity of the biological materials collected.

Why Livermore?

- LLNL is a world-recognized leader in detection methodologies for pathogens in air
- Livermore is a world leader in the detection and quantification of biological agents
- In addition to human health per se, distribution system monitoring is also a homeland security and military/defense issue.
- Livermore has experience developing field portable sensor systems
- Livermore has a significant effort in sensor system communications
- Livermore has a large body of water experts in-house and water agency collaborators externally

Meeting the Research Challenge

- Specific project to develop pathogen detection capability
  - **Phase I**
  - Explore the ability of this real-time system on a prototype level (low flow rates).
  - Increase sensitivity through coating of electrodes.
  - **Phase II**
  - Pilot-scale unit testing: unit designed to operate at 20 gallons per day.
  - Couple with existing processes.
  - **Phase III**
  - Demonstration phase at specific water plants or in other field studies.
  - Develop matching funds from industry.
  - **Need to involve:**
  - Original equipment manufacturers for membrane and filter manufacturing.
  - USEPA, water utilities, emergency response community, the California Office of Emergency Management, and the California Department of Health Services.
  - Robin Miles, Betsy Cantwell, Kevin O'Brien, Staci Kane, Nina Rosenberg, Tom Slezak, and Pat Fitch.
  - Other personnel in the LLNL Center for Microtechnology, the Biology and Biotechnology Program, and Nonproliferation, Arms Control, and International Security (NAI).

Meeting the Research Challenge

Problem Solution	Cost to Solve	Minimum Time to Solve
Bio-sensor	$1.5-$2 M	3-4 years to integrated instruments
Chem-sensor	$800 K - $1 M	2-3 years to integrated instruments
Low Flow Velocity Sensor	$500 K	1-2 years
Sensor communication systems and networking	$2 - $4 M	4-5 years (intense)

Brine Utilization and Management Technologies for Gas and Oil Production, Power Plants, and Wastewater Recycling Operations

Kevin O'Brien, Bryant Hudson

Outline

- The Problem
  - Oil, Natural Gas, Coal Bed Methane
  - Power Plants
  - Waste Water / Desal Plants
- The Solution
- The Team
- The Cost

Brine generated from gas, oil, and coal bed methane production

- Naturally occurring radioactive materials (NORM) such as 226Ra, 238U. These contaminants could be a special challenge.
- Toxic elements such as arsenic, chromium, selenium
- Toxic naturally occurring organic compounds (e.g. benzene)
- Bulk of effluent would be sodium, calcium, magnesium, chloride, carbonate
- Some produced waters have TDS ~ 1000, therefore nearly usable as produced, thus the water content makes these "brines" especially valuable.
- DOE funding is available to examine this issue.

Brine from Pre-Treating boiler/steam system

- (NOTE: quality of water supplied INTO the boilers will be MORE STRINGENT than potable standards)
- Bulk of effluent would be sodium, calcium, magnesium, chloride, carbonate. NOTE: expect more similar levels of sodium, calcium and magnesium.
- Since the starting water is relatively good, high efficiency in the "polishing" treatment can be especially effective at reducing the volume of the brine effluent.
- Identified as one of the major issues for the Power Plant industry at a recent DOE Combustion Science Meeting in Salt Fork, Ohio, August 2002
- Funding available through DOE to approach this issue

Brine from Desal and Waste Water Treatment

- **Bulk of effluent would be sodium, calcium, magnesium, chloride, carbonate**
- **Expect several hundred ppm of a vast array of different organic compounds some of which will be toxic**
- **Microorganisms present, especially from backwash**
- **Pathogens could potentially be present**

Typical Methods to Dispose of Brines

- Surface water discharge
  - ↗ Cost of conveyance
- Discharge to sewer
  - ↗ Site dependent, shared outfall is attractive
- Deep well injection
  - ↗ Only used for high concentration flow rates and only in Fl
- Evaporation ponds
  - ↗ Land Intensive
- Spray irrigation
  - ↗ Requires Blending
- Zero liquid discharge
  - ↗ High Energy Costs

Major Issue

- A major surface water disposal issue in the State of Florida since 1992 has been the occurrence of major ion toxicity (Mickley, 2000) in several concentrates from desalting plants using groundwater sources.
- Deep well disposal of industrial wastes (including membrane concentrate and backwash) is not permitted in many states.
- Microorganism removal by MF and UF processes results in concentration of the microorganisms in the backwash from these processes.
- There are, however, no water quality standards prohibiting or limiting discharge of such backwash to surface waters.

Issues Extend Across All Processes

Table 6.1 Characteristics of Concentrate and Backwash Streams

Membrane Process	Feedwater TDS (mg/L)	Typical Operating Pressure (psi)	Typical System Recovery	System Ion Rejection (%)	What is Concentrated
PROCESSES HAVING CONCENTRATES					
Seawater RO (SWRO)	18,000 - 45,000	800 - 1,200	20 - 50	99+ (TDS)	Salt, Dissolved organics, Viruses, Spores, Bacteria, Cysts, Particulates
Brackish RO (BRO)	500 - 3,500 low pressure; 3,000 - 10,000 high pressure	150 - 600	60 - 85	85-95 (TDS) 90 - 98 (Hardness)	Salt (lesser extent than SWRO), Most dissolved organics, Viruses, Colloids, Bacteria, Cysts, Particulates
Nanofiltration	Up to 500	50 - 150	75 - 90	90 - 98 (Hardness)	Salt (lesser extent than BRO), Dissolved organics, Viruses, Colloids, Bacteria, Cysts, Particulates
Electrodialysis	Up to 7,000	Not applicable	75 - 90+	50-70% monovalent ion removal due to size	Salt, Some polar organics
PROCESSES HAVING BACKWASHES					
Ultrafiltration	< 500 (not used to remove TDS)	Below 100	95+	Zero rejection of TDS	Some organics, Some viruses, Some colloids, Bacteria, Cysts, Particulates
Microfiltration	< 500 (not used to remove TDS)	Below 100	95+	Zero rejection of TDS	Some bacteria, Cysts, Particulates

Key Efforts to Achieve Goal

- Increase % recovery beyond % achieved by current membrane systems.
- If brine is transported, then volume reduction directly relates to ENERGY and INFRASTRUCTURE costs.
- Methods to economically separate radionuclides and toxic transition metals need to be developed. Work done by Coleman (EPD) and Reynolds (CMS) using functionalized aerogels mixed with granular activated charcoal show promise.
- Explore the use of the bulk constituents to produce a higher value added material, e.g. building material (equivalents of concrete blocks and dry wall). This generates REVENUE and reduces disposal costs. Need to examine properties of final end products produced with these recycled materials.

Key Efforts to Achieve Goal

- Explore the concentrations of valuable metals present in the brine such as cobalt and vanadium. These may represent economically valuable ores which are already in solution.
- Expect a SYSTEMS APPROACH will be required, i.e. linking power plants, building materials plants, water treatment facilities, etc. Need to leverage handling equipment which is already in place.
- Economic analysis will be specific to a specific geographical areas and specific brine compositions, e.g. how close to oil field, power plant, waste facility, etc
- Key will be to select appropriate targets UPFRONT then work closely with stakeholders to show success. This would serve as a model for future interactions at additional sites

External Team Members

- Engineering Firm(s)
- Power Plant Facility for demonstration testing (Northern Az. perhaps)
- Waste Water facility (Southern CA water recycling project)
- Boiler Original Equipment Manufacturers (OEMs)
- Chevron / Texaco (Coal Bed Methane, Power River Basin)

Effort is HIGHLY LEVERAGED OFF EXISTING INDUSTRIAL CONTACTS

Internal Team Members

- Membrane scientist
- Chemical Engineer
- Chemist
- Economist
- Molecular modeler
- Regulatory
- Civil Engineering
- Geoscientist
- Microbiologist

Budget

	YR1	YR2	YR3	TOTAL
FTEs	6	8	9	23
Funding (Thousands)	$1,500	$2,000	$2,500	$6,000

Innovative Approaches to the Characterization and Management of Nitrate Groundwater Contamination

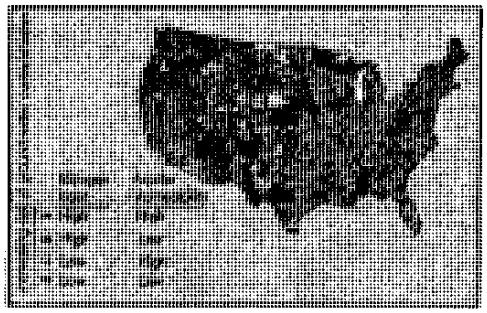
NWRI Working Group 7: Brad Esser, Steve Grey
January 30, 2003

Brad Esser, Bryant Hudson, Jean Moran,
Harry Beller, Brendan Dooher, , Dave Rice,

Nitrate and Human Health

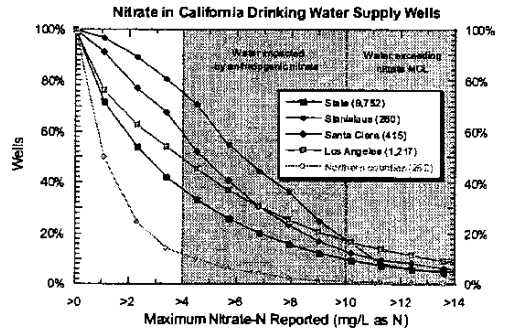
- **Demonstrated health effects**
  - —Infant methemoglobinemia: strong evidence
  - —Cancer: weak evidence, ongoing studies
- **Nitrate in drinking water is regulated**
  - —10 mg/L nitrate-N (Federal) = 45 mg/L as nitrate (State MCL)
  - —10 mg/L nitrate+nitrite-N (Federal MCL, State MCL & PHG)
- **No movement to change standard**
  - —Federal EPA six-year review nearing completion

Nitrate contamination is a national problem

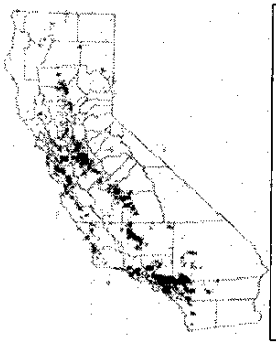


Nolan B. T., Hitt K. J., and Ruddy B. C. (2002) Probability of nitrate contamination of recently recharged groundwaters in the conterminous United States. Environmental Science & Technology 36(10), 2138-2145.

The nitrate problem in California groundwater



Nitrate in California



- California public drinking water supply wells are being lost at an alarming rate (8,000 out of 24,000 since 1988). **Nitrate** is the most common reason for abandonment.
- Since 1988, **nitrate** has consistently accounted for the highest number of MCL exceedences of any single contaminant in public drinking supply wells.

Potential LLNL contributions to nitrate research

TOOLS
- Aquifer assimilative capacity: denitrification
- Source attribution & co-contaminant characterization
- Age-coupled groundwater modeling

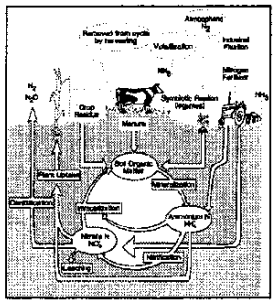
APPLICATIONS
- Nitrate management assessment
- Groundwater basin assessment

MANAGEMENT
- Optimization of management options
- New treatment technology

Aquifer assimilative capacity is unknown

- **Assimilative capacity is important**
  - Groundwater basin assessments
  - CNMPs and discharge permits
  - Subsurface water storage
- **Most research in soil zone**
  - Best management practices
  - Field scale models
  - Surface water concerns
- **Denitrification in subsurface?**
  - Limited by low DOC and high O_2?
  - Heterotrophic denitrification slow?
- **New tools are available**
  - Dual isotope approach (community)
  - Excess nitrogen by MIMS (LLNL)
  - Molecular biology tools (could be developed at LLNL)

Denitrification is the ultimate nitrate sink



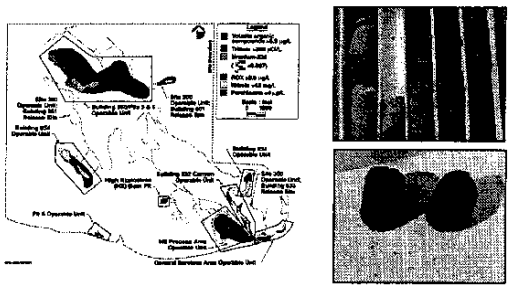
- **Denitrification requires**
  - Denitrifying bacteria
  - Low oxygen conditions
  - An electron donor
- **Heterotrophic denitrification**

$$5\ CH_2O + 4\ NO_3^- \rightarrow 2\ N_2 + 4\ HCO_3^- + CO_2 + 3\ H_2O$$

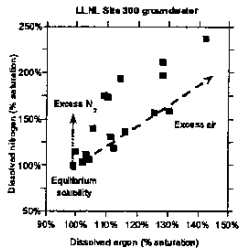
- **Autotrophic denitrification**

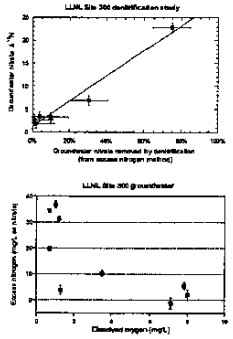
$$5\ FeS_2 + 14\ NO_3^- + 4\ H^+ \rightarrow 7\ N_2 + 10\ SO_4^{2-} + 5\ Fe^{2+} + 2\ H_2O$$

Denitrification: Site 300, a natural laboratory



Excess nitrogen: a valuable tool





- **Membrane inlet mass spectrometry**
  - — Nitrogen, argon, oxygen
  - — Allows determination of excess nitrogen
  - — Fast, portable and inexpensive

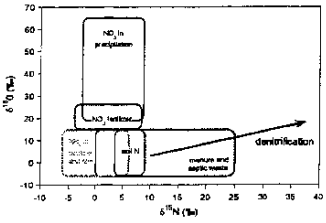
Denitrification: aquifer assimilative capacity

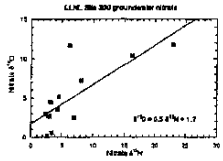
- Field studies of denitrification in individual basins using excess nitrogen, nitrogen isotopes and groundwater age
- Survey of denitrification in a subset of GAMA wells (stable isotopes, excess nitrogen)
- Microcosm studies of autotrophic denitrification by bacteria using pyrite (FeS2) as an electron donor
- Development of a molecular (DNA-based) method to estimate populations of denitrifying bacteria in aquifer material
- Development of appropriate proxies to assess aquifer assimilative capacity in groundwater basins
- Development of rate constants for input into reactive transport models
- Resources: SCVWD, Alameda County Zone 7, Thomas Harter (UC-Davis), Brenda Erkwurzel (U Arizona), Site 300, GAMA

Source attribution and co-contaminants

- **Develop and source tracers**
  - **—Nitrate co-contaminants**
  - **—Nitrate nitrogen & oxygen isotopes**
- **Evaluate the usefulness of source tracers for**
  - **—source attribution,**
  - **—susceptibility assessment,**
  - **—assessment of management practices**
  - **—remediation planning**

Stable isotopes: Source and Process Tracers





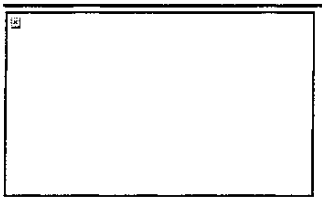
- Traditional isotope approach uses only nitrate-$\delta^{15}N$
  - Cannot distinguish source from process
- Dual isotope approach also uses nitrate-$\delta^{18}O$
  - Potential for distinguish source from process

Denitrification is occurring at Site 300

$$\delta^{15}N = [(^{15}N/^{14}N)_{sample}/(^{15}N/^{14}N)_{standard} - 1] * 1000$$

$$\delta^{18}O = [(^{18}O/^{16}O)_{sample}/(^{18}O/^{16}O)_{standard} - 1] * 1000$$

Nitrate Co-Contaminants: A Human Health Risk?



- "Xenobiotics" covers a wide range of chemicals
  - Different transport characteristics
  - Different wastewater treatment characteristics
- DHS: model for emerging contaminants of concern
  - No idea how to establish public health goals

- **Nitrate sources**
  - Irrigated agriculture: fertilizer
  - Confined animal operations: manure
  - Septic systems
- **Current research focus**
  - Endocrine disruptors
    - Pharmaceuticals
    - Personal Care Products
  - Occurrence
    - Surface waters
    - Treated wastewater
- **Opportunity**
  - Agricultural sources
  - Groundwater occurrence & geochemistry

Age-coupled groundwater flow models

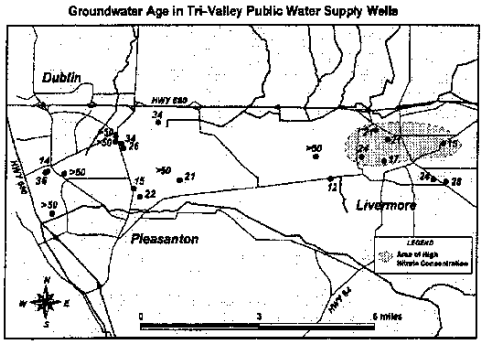
- **LLNL has leadership in tracing young groundwaters**
  - Tritium-helium age dating
  - Noble gas tracers
- **We should develop flow models strongly coupled to age**
  - Unique solutions
  - Less data intensive than traditional hydrogeologic approach
  - Initial calibration with stochastic engine
    - Then ported to desktop application
- **A unique LLNL capability**
  - Analytical leadership
  - Modeling leadership

Nitrate management assessment

GOAL: Demonstrate correlation between changes in land use or management practice and groundwater quality

- **Use CAS groundwater ages to demonstrate land use effects**
- **Perform focused field studies**
  - Nitrate plume characterization (source, history, future)
  - Groundwater flow path studies
  - Agricultural management field studies
  - Artificial recharge field studies
- **Resources:** SCVWD, Alameda County Zone 7, Thomas Harter (UC-Davis), Brenda Erkwurzel (U Arizona), Site 300, GAMA

Nitrate and CAS in Livermore Valley



Groundwater basin assessment

- **Use the existing CAS database**
- **Import nitrate-specific data into the GEIMS database; Build visualization and analysis tools for the Geotracker GIS**
- **Characterize the nitrate distribution in groundwater basins; Develop a comprehensive monitoring plan**
- **Assess the susceptibility of groundwater basins and individual wells to nitrate contamination at a useful scale**
- **Model future nitrate distribution in groundwater basins**

Products

- A toolkit for **assessing aquifer assimilative capacity**
- A toolkit for **determining nitrate source**
- A new and more **robust modeling approach** to constraining groundwater flow
- A robust method for **assessing the impact of land use** and management on nitrate in groundwater
- An approach to **assessing the current state of nitrate contamination** in State of California groundwater
- A tool for optimizing management & treatment of nitrate-contaminated groundwater in the State of California

What is the LLNL role?

- **LLNL has a strong relationship with the State Board**
  - GAMA/CAS is our most recent and largest effort
  - LLNL is seen as disinterested, customer-oriented, and technically innovative
  - LLNL has access to secure water data
- **AB599 requires a comprehensive groundwater plan**
  - *Groundwater Quality Monitoring Act of 2001*
  - Requires a comprehensive monitoring and basin assessment plan
  - Provides no funding
- **Proposition 50 provides a funding source**
  - *Water Security, Clean Drinking Water, Coastal and Beach Protection Act of 2002*
  - Passed November 2, 2002 (55.4% Yes, 44.6% No)
  - Allows the State to sell $3.44B in bonds
  - $50M earmarked for Comprehensive Basin Assessment

People

- **LLNL**
  - —**CMS:** Esser, Hudson, Moran
  - —**EE:** Kart, Bourcier
  - —**EPD:** Bellar, Kane, McNab, Demir, Dooher
  - —**Engineering:** Lamont, Stewart
- **Collaborators**
  - —Santa Clara Valley Water District
  - —Alameda County Zone 7
  - —UC-Davis Agricultural Extension (Thomas Harter)
  - —U Arizona (Brenda Erkwurzel)

Plan and budget

- **Stategic plan**
  - —Develop new tools (LLNL funding)
  - —Collaborate with water districts & universities on field studies (LLNL and matching funds/resources)
  - —Approach State Board for role in basin assessment
    - Leverage GAMA and inclusion of "ages" in AB599 plan
  - —Market tools through an LLNL water organization
- **Budget**
  - —**2-4 FTE/year**

WORKING GROUP 8

Impact of Climate Change on Water Management and Infrastructure

Alan Lamont
Peg Folta

Climate change affects on water management and infrastructure

- Climate change will affect precipitation and runoff
- New water management strategies will be needed
- New infrastructure may be needed
- Could have significant impacts on groundwater aquifers
- Better forecasting may improve management

We can address this through a set of coupled models

- High resolution climate and hydrology models
  - inflows to water management system
- Calvin water management model
  - Optimal allocations and storage use
- Coupled groundwater-surface water-geochemistry models
  - Chemical and physical impact of cycling groundwater aquifers

Improving forecasts

- Improved forecasts may improve water managent strategies
  - More likely that managemetn decisions are correct for future conditions
- We can use the water mangement models to assess the impact of uncertainty on the management strategies
- Identify the key parameters that must be forecast accurately to improve management
- work with Climate Modeling Group to assess feasibility of making improvements
  - Arrive at research plan for developing better forecasts

Budget

- Total effort: about 6 FTEs
  - 2 climate modeling
  - 2 management modeling
  - 2 aquifer modeling
- High resolution climate modeling already partly covered under LDRD

Assessing artificial recharge, groundwater banking, and conjunctive use with LLNL's advanced analytical and modeling capabilities

Working group members: Jean Moran, Walt McNab and Greg Mack
Possible participants: McNab, Moran, Tompson, Carle, Hudson, Beller, Kane, Dooher, Esser, Steefel, Davisson

The Need ...

- Lack of viable surface water storage
- Impending increased demand in urban areas + desire to increase groundwater proportion

Water agencies, permitters, regulators need to know ... what will happen when groundwater banking is undertaken?

Research Issue Description

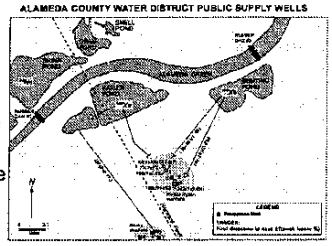
- Apply advanced analytical and modeling techniques to questions of artificial recharge, water banking, and conjunctive use on a basin or sub-basin scale
  - What is the nature of the groundwater and recharge water – quantity and quality?
  - What is the relationship between the recharge water and the basin hydrogeology?
  - What are the key biogeochemical processes that affect the fate of chemical constituents in the recharge water?

Nature of Recharge Water

- Recharge Sources
  - Diverted excess streamflow
  - Recycled water
  - Surplus agricultural water
- Groundwater/Recharge Water Quality
  - Nitrates
  - TDS
  - Organics/pesticides/xenobiotics

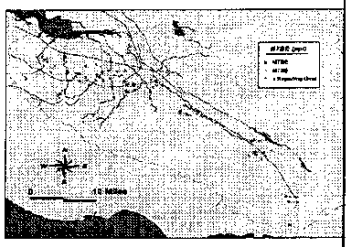
Hydrogeology

- Infiltration
- Pumping strategy
- Sustainable yield
- Near field flow
- Cross aquifer recharge
- Storage capacity/residence time
- Land subsidence
- Seawater intrusion mitigation



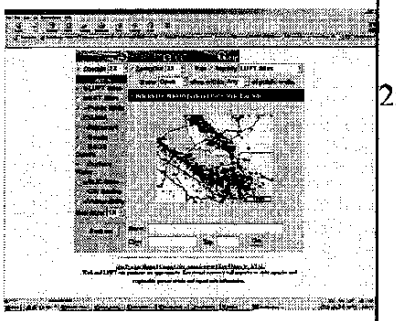
Water Quality Changes

- Water-rock interactions
  - Dissolution
  - Ion exchange
- Aquifer assimilative capacity
  - Nitrate
  - Organics
- Unwanted mobilized species
  - Fe, Mn, As, Se, Cr
  - Disturbing existing anthropogenic contaminants



Nature of Groundwater and Recharge Water – Action Items

- Set up liaison with water agency /stakeholders
- Data integration and information management
  - Assimilate and utilize existing data
  - **Construct GIS database**



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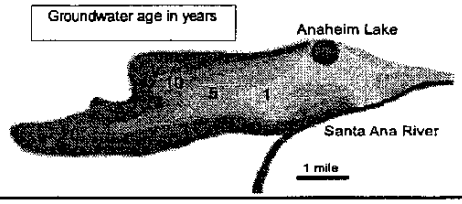
Hydrogeology – Action Items

- **Use isotopically-enriched noble gas tracers for determination of near-field flow**
- **Use GAMA ages for determining basin-scale flow field**
- Calibrate integrated groundwater-surface water flow model (IGSM) to tracer and age data



Water Quality Changes – Action Items

- **Construct reactive transport model coupling a groundwater-surface water flow model (IGSM) with solute transport and geochemical speciation (PHREEQC) components.**
  - Flow & transport
  - Aqueous and surface complexation, mineral precipitation/dissolution, ion exchange, redox
  - Reaction kinetics (PHREEQC uses a flexible scripting language)
  - **Specific IGSM capabilities (surface water, land subsidence, etc.)**
- Assimilate existing pertinent kinetic data for transformations involving chemicals of concern
- **Conduct targeted research to fill data gaps**
  - **N isotopes/excess N for denitrification studies**
  - **Signature metabolites of specific contaminants**

Workplan

- Conduct pilot project with Santa Clara Valley Water District
  - Jointly funded
  - Tailored to specific technical concerns of the SCVWD
  - Run model scenarios
    - Water balances
    - Track recharged water
    - Chemical evolution of groundwater under recharge
    - Land subsidence issues
  - Calculate value of additional storage capacity
  - Enlist DWR/ DHS/ RWQCB/ SWRCB as advocates
- Market full service program to other agencies/basins
  - Sacramento Area Metropolitan Water Agencies (SAMWA)
  - Northern CA counties
  - Central Valley irrigation districts
  - High growth urban areas
- Budget
  - 3 FTEs over 3 years (1 from SCVWD)

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