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The Actinide Research Quarterly

Nuclear Materials Research and Technology

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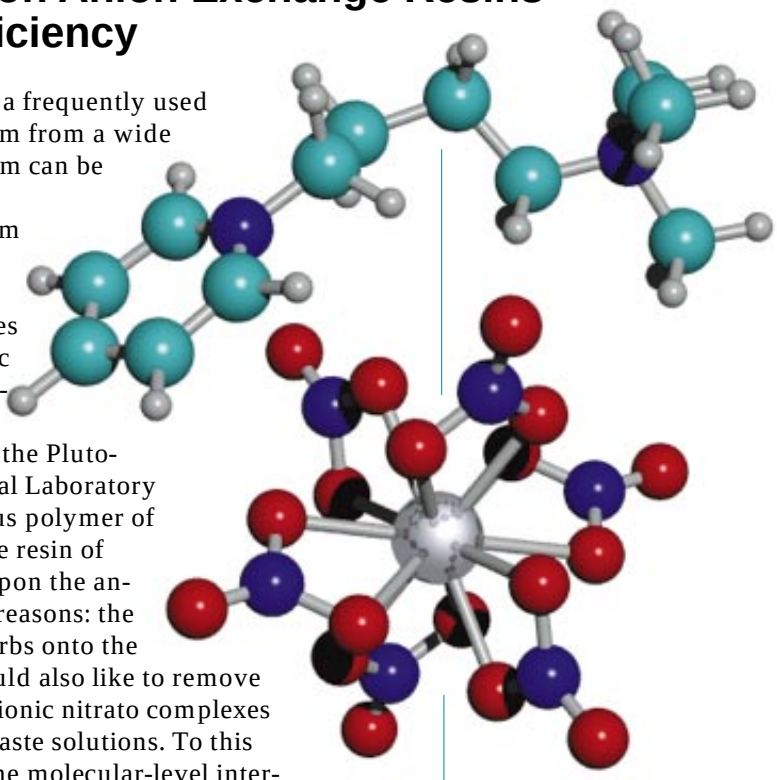
In This Issue

Modeling Plutonium on Anion Exchange Resins Helps Separation Efficiency



"Docked" configuration of the plutonium hexanitrato dianion and a model bifunctional dication (nitrogen atoms in blue).

Anion exchange in nitric acid is a frequently used process for the recovery of plutonium from a wide range of impure materials. Plutonium can be selectively removed from dissolved residues (for example, salt cakes from electrorefining) because the large complexation sphere and high charge/radius ratio of Pu(IV) enables it to form anionic complexes in nitric acid where few metals form competing species. This unique chemical behavior has long been exploited at the Plutonium Facility at Los Alamos National Laboratory where Reillex HPQ™, a macroporous polymer of N-methylated 4-vinylpyridine, is the resin of choice. We would like to improve upon the anion-exchange process for two main reasons: the rate at which the Pu(IV) complex sorbs onto the resin is unusually slow, and we would also like to remove americium, which does not form anionic nitrato complexes as readily as plutonium, from the waste solutions. To this end, we are developing models of the molecular-level interactions of actinide anions with the resin sites. Accurate models will help us to understand the mechanisms of sorption and ultimately allow us to design resins for a variety of anions under a variety of conditions.

Anion-exchange resins are polymers that contain positively-charged (cationic) functional groups bound in the solid matrix. Under typical anion-exchange conditions, sorption of a dianionic species requires complexation to two separate cationic resin sites. The orientation and availability of these sites for cooperative interactions with a dianion is not well controlled. Spectroscopic studies suggest that plutonium sorption onto the resin may occur via a process in which an uncharged tetranitrato complex in solution is converted to a dianionic hexanitrato complex at the resin surface, acquiring two nitrate groups in the process. We hypothesized that a resin that could facilitate the uptake process, for example by positioning the two nitrate groups in the proper configuration, could provide superior binding properties and selectivity for plutonium nitrato complexes, exhibit enhanced kinetics for plutonium uptake from solution, and encourage the formation of weaker nitrato complexes.

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Modeling Plutonium on Anion Exchange Resins Helps Separation Efficiency *(continued)*

The principal developers of this project are **Mary E. Barr, Eddie Moody,** and **Gordon Jarvinen** (NMT-6); **S. Fredric Marsh** (NMT-6 emeritus); and **Richard A. Bartsch** (Texas Tech University).

To test our "facilitated uptake" hypothesis, we synthesized and evaluated a series of bifunctional resins in which the structure of the anion-receptor site is well-defined; the two anion-exchange sites are separated by a fixed distance in a fixed orientation. These resins are synthesized via modification of poly(4-vinylpyridine) resins with a second cationic site such that the two anion-exchange sites are linked by "spacer" arms of varying length and flexibility. Plutonium sorption data from nitric acid media indicate that this controlled geometry of the anion-exchange sites has a positive impact upon the sorption of the plutonium dianion. Most notably, a ''spacer" length of 4–5 methylene units generally provides the best plutonium uptake conditions regardless of the functionality of the second cationic site.

Modeling the dianion / dication interactions is a complex, multistage process. The first step of this modeling is a proper description of the actinide complex. We recently developed refined MM2 parameters for Pu(IV), U(IV), Np(IV) and Th(IV) hexanitrato complexes. Ideally, we like to describe actinide complexes with as few parameters as possible, which allows for faster structural optimization times and / or the ability to model larger systems in the same amount of time. Our parameters are optimized to allow maximum structural flexibility for the dianion in order to determine what structural distortions may occur upon "docking" of the dianion with cationic sites. For this work, we used solution EXAFS (extended x-ray absorption fine structure) data acquired by LANL researchers to establish initial structural parameters for the plutonium hexanitrato dianion. Estimated van der Waals radii were used to extend the model to the analogous thorium, uranium, and neptunium complexes. The excellent agreement between the models and experimental single-crystal x-ray structures of the four complexes gives us some confidence in the efficacy of this method, and we plan to extend our modeling to other systems that lack solid-state structural data.

Determination of the distribution of charges for each atom of the dianion and dication is critical to the calculation of their electrostatic attraction. The simplest method is to use "formal charges" for all the atoms. However, formal charges are really just a way to keep track of the total charge and do not accurately reflect the actual charge distribution of a complex molecule. To calculate the partial-charge distribution for the large, unwieldy plutonium hexanitrato dianion, we had to use a theoretical neutral "compound," the triradical $Pu(NO_3)$. To model the bifunctional resin sites, we replace the polyvinylpyridine "backbone" with a pyridine molecule. There are many different ways to calculate partial charge distribution for organic molecules, all providing very different answers. To some extent, we rely on "chemical intuition" and internal consistancy to help us decide which method provides the best charge metrics.

Once we decide what set of charges to use, we determine the optimized anion / cation configuration for each of the "docked" ion pairs using molecular mechanics and calculate the net force by summing the attractive (opposite charges) and replusive (same charges) forces between the anion / cation pair. This "stickiness factor" (SF) is then correlated with the experimental plutonium distribution coefficients (K_d) found for the corresponding resin. We have found that the strongest (most attractive) SF tends to correspond to the highest experimental K_d. Using formal-charge metrics, the models accurately predict that a 4–5 atom "spacer" between the cationic sites is the best for complexation of the plutonium hexanitrato dianion. We are currently refining our models to incorporate more chemically realistic partial charges. Our models cannot yet predict a K_d for a specific system, but they can determine trends within a system, and we would like to develop a method for *a priori* prediction of distribution coefficients.

Division Completes Science and Technology Assessment

NMT Division successfully completed its yearly science and technology assessment (May 11 through 13). It was the first in a new three-year cycle that covers all division operations. The formal review this year concentrated on four focus areas: materials stabilization, Seaborg Institute and LDRD projects, plutonium disposition, and collaborations (internal, international, and across DOE, universities, and industries). The report of the 11-member review committee (see box, page 4) will go to Laboratory Director John C. Browne and the University of California Science and Technology Panel of the Office of the President.

In the first session Division Director Bruce Matthews (standing in for Associate Laboratory Director for Nuclear Weapons Steve Younger) gave the committee an overview of the division's place in the restructured Laboratory organization. He then gave a division profile—its people, organization, resources, and major programs and significant accomplishments during the past year. Over the remainder of the first two days division scientists made 26 oral presentations and gave 22 poster papers, demonstrating the depth and breadth of NMT's science and technology in this year's four focus areas.

The committee spent the third day formulating its assessment after meeting with several selected groups of individuals representing the technical staff, program managers, and Laboratory senior managers.

The division is evaluated on review criteria that have been agreed upon by the UC Science and Technology Panel and the Laboratory: quality of science and engineering, relevance to national needs and agency missions, performance in the construction and operation of major research facilities, and programmatic performance and planning. Although the assessment report will not be completed and submitted until sometime after this issue of the *Actinide Research Quarterly* goes to press, the committee's comments at the close-out session were uniformly positive. The successful review was a tremendous effort over many months on the part of the division's scientific, support, and management staff with a record number of NMT members and members of other Laboratory support organizations participating.

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Reported by **Ann Mauzy,** CIC-1.
Photos by **Gary Warren,** CIC-9.

Division Review Committee Members (left to right) Dr. Susan Wood, Dr. Tony Thompson, Dr. Stephen Carpenter, Dr. Darleane Hoffman.

Division Completes Science and Technology Assessment *(continued)*

The accompanying photos show some of the review committee members, division participants, and activities in the annual review.

Division Review Committee
Dr. Ned A. Wogman, Chair
Associate Director, National Security and Defense
Battelle, Pacific Northwest Laboratories

Dr. Richard A. Bartsch
Department of Chemistry and Biochemistry
Texas Tech University

Dr. Rohinton K. Bhada
Director, Waste Management Education and Research Consortium
Associate Dean of Engineering
New Mexico State University

Dr. B. Stephen Carpenter
Director, Office of International Affairs
National Institute of Standards and Technology

Dr. Gregory R. Choppin
Department of Chemistry
Florida State University

Dr. Darryl D. DesMarteau
Department of Chemistry
Clemson University

Dr. Darleane C. Hoffman
Charter Director of the Seaborg Institute
Professor of Graduate School
Lawrence Berkeley National Laboratory

Dr. Todd LaPorte
Department of Political Science
University of California, Berkeley

Dr. W. Lamar Miller, invited guest
Department of Environmental Engineering Science
University of Florida

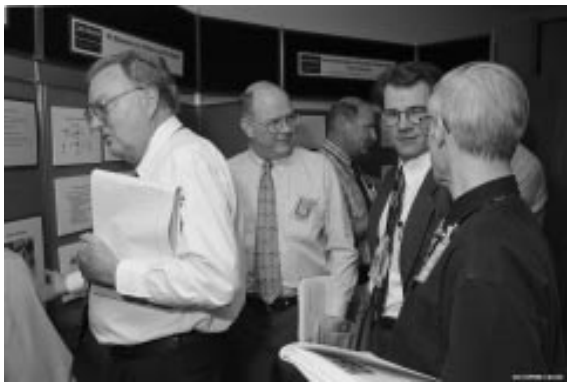
Dr. Anthony W. Thompson
Materials Science Department
University of California, Berkeley

Dr. Robert Uhrig
Nuclear Engineering Department
The University of Tennessee

Dr. Susan Wood
Vice-President and Director
Savannah River Technology Center
Westinghouse Savannah River Company

Photos (from top to bottom) John Hemminger and Jim Porter, Bruce Matthews and Karl Staudhammer, Sophie Vigil, Todd LaPorte and K. C. Kim, Richard Bartsch, Todd LaPorte, Ned Wogman, and Darryl DesMarteau

NMT Science and Technology Assessment Papers and Poster Presentations



The following talks were presented at the NMT Division Science and Technology Assessment, May 11–13: T. Allen, "Container Inspections"; L. Avens, "The NMT Integrated Approach to Combustible TRU Waste Treatment"; R. Wieneke, "Waste Certification"; T. Blair, "Thermal Treatment of Weapons-Derived PuO_2 to Reduce the Gallium Content"; D. Brandt, "Packaging Nuclear Materials for Storage at Los Alamos"; T. Nelson, "Fabrication of MOX Fuel for DOE's Plutonium Disposition Program / Russian Interaction on MOX"; D. Christensen, "Managing Skills During a Period of Transition"; D. Clark, "Seaborg Institute / LDRD"; T. Cremers, "Nondestructive Assay—a Joint United States and Russian Activity"; T. Hayes, "Current Aqueous Operations and Near-Term Upgrades"; D. Horrell, "Material Characteristics and Issues for Storage"; C. Hoth, "Container Designs for Intermediate and Long-Term Storage"; G. Jarvinen, "A New Paradigm in Separations: Molecular Recognition Membranes"; D. Kathios, "Pyrolysis"; M. Lopez, "MOX Fuel for Parallex from PuO_2 Converted by LANL"; S. McKee, "The National Material Stabilization R&D Program"; T. Nelson, "Pu Disposition / ARIES"; A. Neuman, "MOX Fuel for ATR Irradiation Test Using PuO_2 Converted by LLNL"; L. Pansoy-Hjelvik, "Nitrate Anion Exchange in 238-Pu Scrap Recovery Operations"; K. Ramsey, "Molten Salt Oxidation"; L. Schulte, "Effluent Polishing Techniques for Nitrate and Chloride Operations"; J. Williams, "Plutonium Recovery / Purification Flowsheet for the Future"; T. Nelson, "Russian I nteractions on Pit Disassembly and Conversion"; L. Worl, "Development of Hydrothermal Plutonium Combustible Waste Treatment Process"; and T. Nelson, "The United States Pit Disassembly and Conversion Facility."

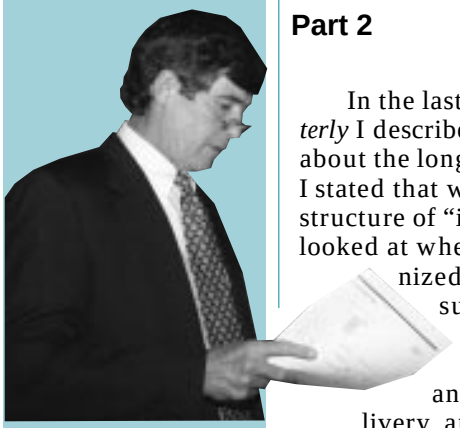
The following posters were presented at the NMT Division Science and Technology Assessment, May 11–13: W. Brown, "Pit Bisection to Achieve ALARA Goals"; A. Carrillo and A. Morales, et al., "MOX Fuel Fabrication Using Plutonium from Weapons for Irradiation Testing in the Advanced Test Reactor"; K. Chidester. C. James, et al., "Thermal Removal of Gallium from Weapons Grade Plutonium Oxide"; K. Chidester, K. Ramsey, et al., "Development of Advanced Mixed Oxide Fuels for Plutonium Management"; D. Clark, et al., "Actinide Complexes under Highly Alkaline Conditions"; B. Cort, et al., "Plutonium Aging: Investigation of Changes in Weapon Alloys as a Function of Time"; C. Davis, et al., "Characterization of Rocky Flats and Hanford 94-1 Materials"; K. Fife, "Pu Residue Stabilization and Scrap Recovery"; J. FitzPatrick, D. Knobeloch, et al., "ULISSES, The Uranium Line for Separation Science, from Concept to Reality"; B. Flamm, et al., "Alpha Ingot Thermal Cycling / Alpha Beta Phase Transformation"; B. Flamm, et al., "Hydride-Dehydride—the Second Generation System"; L. Foster, et al., "Moisture Probe Based on Neutron Moderation"; C. James, "Weapons Grade Plutonium Metal to Oxide Conversion for MOX Fuel"; T. Knight, et al., "Thermal Analyses of Plutonium in BNFL Containers"; D. Kolman, "94-1 Core Technology Corrosion Research: Correlating Crystallographic Orientation"; J. Lloyd, "Small Molecules Adsorbed at U and UO_2 Number 1: H_2O, CO_2, and CH_3OH"; R. Mason and T. Baros, "Materials Characterization of MOX Powders and Fuel"; E. Moody, M. Barr, et al., "Molecular Modeling of Cation / Anion Interactions"; L. Morales, and J. Haschke, "Investigation of the Plutonium Oxide-Water Reaction"; J. Morris, et al., "Fiberscopic Examination of Pit Interiors"; C. Smith, M. A. Martinez, and K. Veirs, "Quantitative Analysis of Gallium in Plutonium using Laser-Induced Breakdown Spectroscopy"; K. Veirs, et al., "Acoustic Sensing in Storage Containers"; D. Wedman, et al., "Decontamination of Surface Transuranic from Uranium"; and S. Yarbro, et al., "Using Distillation to Recover Nitric Acid and Actinides from Radioactive Liquid Waste."

Photos (left) Kirk Veirs and Gerd Rosenblatt, (top) Lamar Miller, Richard Bartsch, Tim Nelson, and Todd LaPorte, (bottom) Eddie Moody, Stephen Carpenter, Mary Barr, Richard Bartsch, and Gordon Jarvinen.

Editorial

Institutional Constancy Guides NMT's Future

Part 2



Bruce Matthews,
NMT Division
Director

"We ultimately work for the U.S. taxpayers, and we are the stewards of their plutonium."

In the last issue of *Actinide Research Quarterly* I described why NMT must be concerned about the long-term impact of its activities, and I stated that we should be introducing an infrastructure of "institutional constancy." I then looked at where we should be in 2010, organized according to five constancy-assuring capabilities and activities: skilled people, excellence in actinide science, safe and compliant operations, solid record of delivery, and stakeholder involvement. In this editorial I look at where we are now in each of the five areas.

Skilled people: A cadre of skilled people, trained in actinide sciences and nuclear facility engineering, is a necessary element of constancy for the future. Given the year-to-year budget uncertainties combined with a paucity of institutions that train and educate people in nuclear materials disciplines, attracting and retaining educated employees has become a complex challenge. Past practices have been to transfer people internally and to hire new employees to meet the latest programmatic need. Strategic hiring, a key objective for the future, has not been well managed. While a number of activities (such as those noted below) have begun to help build the numbers of skilled people, additional, similar activities will be needed to execute future nuclear materials missions.

- NMT Division has acquired the data needed to formulate a long-term recruiting action plan and, in doing so, developed a predictive tool to enable recruiting and hiring of people with critical skills for projected future needs.
- NMT Division has introduced employee development plans, and the NMT Training Team has begun to offer training in the fundamentals of chemistry and physics. The Laboratory has established a student mentoring program.
- The Los Alamos Branch of the Seaborg Institute has developed a strategy for engaging university faculty and students to do research on actinide materials. NMT Division currently supports more than 70 postdoctoral associates and graduate and undergraduate students. Two dozen collaborating universities provide opportunities for students to gain experience with nuclear materials.
- NMT Division has tasked HR experts to evaluate the compensation of fissile materials handlers here compared with those at other nuclear facilities.

These activities will support a strategic hiring plan that targets 25% of new hires as entry-level hiring aimed at filling the skills required for anticipated future NMT Division programs and facilities.

Excellence in actinide science: The overall objectives of our sponsors and program offices are oriented towards short-term results. The overall objectives of assessors and regulators are compliance and rigorous formality in all operations. These objectives do not produce an environment that is particularly nurturing for sustained advances in actinide science. Nevertheless, our dual operational challenges of (a) certifying the safety and performance of the enduring stockpile without testing and (b) manufacturing a limited number of pits for nuclear warheads have heightened the importance of understanding the fundamental properties of plutonium. Science-based stockpile stewardship is not just a clever name for the work of sandbox physicists, chemists, and materials scientists; it is essential for certifying the reliability of the enduring stockpile, of whatever size. NMT must continue to expand activities that complement the shorter-term emphases of sponsors and regulators with rigorous, high-quality scientific work for the long term.

The DOE Defense Programs Office has begun supporting new programs designed to study the special properties of plutonium. The Pit Surveillance Project, pit certification activities, and enhanced surveillance studies are a foundation for future programs in the fundamentals of plutonium materials science. Materials scientists are making measurements of plutonium's properties—crystal structures, structural changes and melting, surface, mechanical, and shock properties—and how these change over time. These measurements will enable physicists to model and predict the long-term behavior of plutonium. New approaches in actinide-separations chemistry are being explored to produce in-specification metal for the stockpile, as well as to minimize waste at the source, protect residues, and secure excess plutonium metal and oxide for long-term storage.

The Associate Laboratory Director for Nuclear Weapons has launched an important initiative called "Outward Look" that will give NMT Division further incentive to ensure that the best science and technologies are applied to plutonium programs. Current division-wide activities such as the Plutonium Futures Conference, the Los Alamos branch of the Seaborg Institute, and the division's annual science and technology assessment will be the foundation for the division's part in Outward Look.

Safe and compliant operations: No future activities are possible unless we have a safe operating facility that complies with regulations. Our DOE sponsors have supported that need. NMT's facility management, nuclear materials control and accountability, waste management, training, radiation protection, industrial safety, and performance assurance are building a strong foundation for implementation of integrated safety management in our nuclear facilities. We continue to formalize improvements in facility operation based on internally identified issues and clearly articulated expectations of high performance. We think that, with sustained effort, these activities will prepare TA-55 and the CMR Building for future external regulation.

The recent integration of the CMR Building into NMT presents a strong challenge in preparing for future operations that will stress NMT's nuclear operations infrastructure. As we apply the best of TA-55 formality-of-operations practices, combined with the Lab-wide Integrated Safety Management Program at CMR, we will achieve operations that are safe and in-compliance there. We recognize the need to upgrade aging and inoperable facility-safety systems and have developed programs (the Nuclear Materials Storage Facility, the Capability Maintenance and Improvement Project, and the CMR Upgrades Project) that should provide for a solid operational foundation for the future.

Solid record of delivery: For years TA-55 has excelled in small-scale, innovative, high-quality, manufacturing of nuclear material components for weapons programs, nuclear energy programs, and disposal programs. The key to continued success and achievement of institutional constancy in the future will be the on-schedule, in-budget delivery on all such NMT projects. A number of large projects are being managed with modern project-management tools with the result that they meet cost and delivery commitments. In the future, as federal budgets are constrained, as DOE becomes an ever more demanding customer, and as public expectations and requirements for accountability increase, continued improvement of planning, scheduling, and delivery will be necessary.

Stakeholder involvement: The DOE's initiatives in openness and attempts to gain public trust through the Site-wide Programmatic Environmental Impact Statement have heightened public awareness of Los Alamos' activities and the impact of these activities on the public and the environment. This report, combined with NMT's expanded mission, has increased the public's demands on the Laboratory. We must take aggressive measures to engage our stakeholders and gain their trust and confidence. After all, we ultimately work for the U.S. taxpayers, and we are the stewards of their plutonium. We have paid too little attention to this most important element of institutional constancy in the past, despite some positive, minor attempts to do so. However, until the University of California, the Laboratory, and NMT apply resources toward improved external relations, the continuing success of our nuclear materials programs is threatened.

In conclusion, the answer to the question, "Are we in NMT Division becoming fit for the future?" is "Yes, we have started." We are striving vigorously in most areas, but success requires continued diligence and additional and sustained effort. If the current initiatives continue and are successful and if we continue to introduce new activities and initiatives in these areas, the 2010 vision for skilled people, excellence in actinide science, safe and compliant operations, and solid record of delivery will be achieved. My greatest concern lies in the challenge of gaining public trust and confidence through formal activities in stakeholder involvement.

Bruce Matthews

The recommendations in this editorial are mine; they do not represent the opinion of Los Alamos National Laboratory, the University of California, the Department of Energy, or the U. S. Government.

LANL Eyes Requirements for Highly Enriched Uranium (HEU)

With the integration of TA-55 and CMR nuclear facilities, the scope of NMT's programmatic activities has increased and significantly expanded beyond plutonium. This article introduces one aspect of the uranium program, for example, carried out at CMR.

A significant part of maintaining the nation's enduring nuclear stockpile is the management of nuclear materials, including HEU. Issues involved when stockpile decisions are made include material disposition methods that ensure waste minimization and cost-effective, efficient operations. DOE evaluated alternatives for performing its nuclear weapons mission in 1995. The protocol for this evaluation, the Stockpile Stewardship and Management Programmatic Environmental Impact Statement (SSM PEIS), addressed alternatives for the various segments of the nuclear weapons mission. SSM PEIS criteria impact weapon fabrication, stockpile surveillance, remanufacturing of components, dismantlement of retired units, and the disposition and storage of weapons materials. Their impacts are felt in ongoing work at all sites in the nuclear weapons complex (NWC)(see figure, next page).

In order to meet these requirements, we must have the capability to understand the characteristics of HEU, the capacity for reworking the material, and reliable chemical processing that ensures a "steady-state" flow of material through the various processes to meet stockpile needs. Just what this steady state is will also be affected by changing nuclear weapon programmatic requirements and the push to channel material disposition efforts toward the fabrication of mixed oxide fuel for nuclear reactors. A balance in safety, operating costs, physical configuration, and technology will need to be defined for current and future HEU chemical processing operations.

The Oak Ridge Y-12 Plant, managed by Lockheed Martin Energy Systems, Inc., continues to support every weapon in the stockpile along with other related activities including the Stockpile Life Extension Program and the disposition and storage of weapons materials. As the DOE Lead Laboratory for Uranium, Lawrence Livermore National Laboratory supports the Y-12 mission. This assignment offers a link between the National Laboratories and the "plant," along with connections to DOE Headquarters and the various DOE area offices. Los Alamos National Laboratory works directly with Livermore in support of the goal to offer technology enhancements to the uranium-handling chemical processes. However, Livermore's technical capabilities are focused more on metal forming and shaping; Los Alamos plays a stronger support role for uranium process chemistry, including integrated manufacturing, material inventory management and disposition, and assistance with other DOE site issues including those at Rocky Flats.

Under the DOE integrated manufacturing initiative, future weapons manufacturing processes will be conducted in a drastically altered environment. Baseline requirements arising from the SSM PEIS include minimum floor space usage, maximum utilization of available equipment, and a significant reduction in total production expenses while using regulation-compliant systems that function effectively in flexible, batch-operating modes. Several aspects of the SSM PEIS baseline requirements match expertise we have already demonstrated at Los Alamos with our extensive capability in glove box operations. This expertise includes the use of batch-operating modes in which process throughput is scaled to chemical operations that can be completed in one day rather than continuous operations that require larger equipment and longer operating times.

The challenge is the maintenance of a robust and competitive manufacturing environment where science is integrated and matched to production requirements, and technology developments are focused on producing products. Thus, the interaction between Los Alamos and the Oak Ridge Y-12 Plant is moving towards a shared approach in technology development and demonstration. Initially, we are looking at chemical process enhancements that offer low risk and moderate payoff in terms of alternative processing capabilities. In the longer term, we are addressing SSM PEIS goals with technology developments that trade off high risk and high payoff for more cost-effective, smaller, and more flexible chemical process operations.

One of the major goals of our uranium chemistry activities is to develop state-of-the-art capabilities for uranium chemical processing and recovery in support of metal making and fabrication for both HEU and depleted uranium (DU). ULISSES, the Uranium Line for

Special Separation Science, was first conceived as an attempt to recapture the uranium process technology that existed at Los Alamos until 1984. Now, it is apparent that there are new techniques, processes, equipment, and chemistry available that would be beneficial for processing HEU and DU in a more environmentally friendly and reliable manner. Thus, the ULISSES concept is now being developed as a "test-bed" capability to develop and demonstrate new chemical process technologies. A variety of new chemistries and techniques have been investigated including those for dissolution, separation, conversion, and metal making. The ULISSES Program's high-priority goals are to reduce the current inventory of HEU residues at Los Alamos and to introduce processes that will curtail waste and residue generation in support of future manufacturing operations.

To help the DOE meet various goals outlined in the SSM PEIS, as well as those of START I & II stockpile limits, Los Alamos will need to implement plans to address the NWC's approximately 3-metric-ton HEU inventory. Such plans involve the disposition and storage of a large portion of this inventory at the Oak Ridge Y-12 Plant. Thus, material transfer and storage issues between Y-12 and Los Alamos will need to be resolved. Work has already been initiated to address these issues through negotiations for Memoranda of Understanding and Memoranda of Agreement) between Los Alamos and Y-12. Preliminary estimates indicate that approximately two-thirds of LANL's HEU inventory will be available for transfer to Y-12 from Los Alamos. The remaining material will be used to support Los Alamos missions in the SSM program.

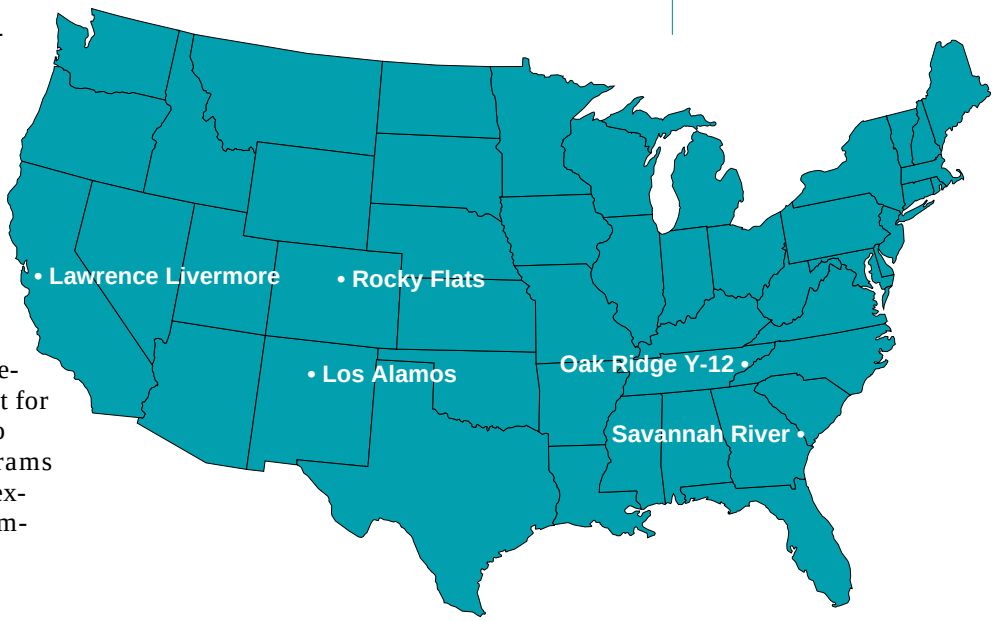
Other DOE sites, specifically Rocky Flats and Savannah River, will have similar issues to address concerning HEU materials and residues. It will also be important for them to transfer material to the Y-12 site to support the variety of ongoing HEU programs that are an integral part of the NWC. For example, HEU inventories at Rocky Flats comprise approximately 6 metric tons, and Savannah River has approximately 13 metric tons. We need to make sure the NWC has the capabilities necessary to transfer and store its HEU inventories at the Y-12 Site.

To address HEU site returns from Pantex, Y-12 has already implemented a new long-term storage system based on modular concrete pallets. These pallets can be stacked and are adaptable for various types of storage containers and facilities. This is one example of NWC technology-support activities from which Los Alamos would derive direct benefit. Material transfer between DOE sites will require continued support for fabrication and certification of shipping containers, storage facilities at Y-12, and a DOE-coordinated material transfer schedule to ensure that sufficient secure transport vehicles are available.

In summary, Los Alamos plays a key role in the implementation of the SSM PEIS and DOE Office of Fissile Materials Disposition program thrusts to manage the DOE HEU inventory. An important aspect is our ability to transfer part of the Los Alamos HEU inventory to Y-12 for disposition and/or storage. In addition, we will work with Y-12 to implement various strategies that support Y-12's ability to dispose of waste materials at off-site locations. The need to help establish a DOE-wide discard limit for HEU is a high priority for both Y-12 and Los Alamos.

This article was contributed by **D. Knobeloch** (NMT-2), **J. Fitzpatrick** (CST-7), and **K. Abney** (CST-11).

Concern for the management of HEU is shared among several members of the DOE nuclear weapons complex.



Recent Publications, Presentations, and Reports (April 1998–June 1998)

Journal Publications, In Press

B. C. Benicewicz, G. D. Jarvinen, D. J. Kathios, and B. S. Jorgensen, "Open-Cell Polymeric Foam Monoliths for Actinide Separations," *J. Radioanal. Nucl. Chem*.

J. M. Berg, D. K. Veirs, R. B. Vaughn, M. R. Cisneros, and C. A. Smith, "Plutonium (IV) Mononitrate and Dinitrate Complex Formation in Acid Solutions as a Function of Ionic Strength," *J. Radioanal. Nucl. Chem*.

D. C. Christensen and M. A. Robinson, "Development and Implementation of Attractiveness Level E Criteria and the Plutonium Disposition Methodology" (LA-UR-98-967), *J. Nucl. Mater. Mgmt.*, Summer, 1998.

M. E. Cournoyer, W. Sandoval, L. Bustos, L. Ortega, and D. Quintana, "A New Waste Minimization Method For Radiological Volatile Organic Analysis" (LA-UR 97-1263), *J. Radioanal. Nucl. Chem.*

F. M. de Rege, W. H. Smith, B. L. Scott, J. B. Nielsen, and K. D. Abney, "The Electrochemical Properties of bis-Dicarbollide Uranium Dibromide," *Inorg. Chem*.

L. Drake and C. Mahan, "Direct Analysis of TRU Waste Using a DC-Arc CID Spectrograph," *Methods Development.*

L. Drake and C. Mahan, "Direct Analysis of TRU Waste Using a DC-Arc CID Spectrograph," *Trace Analysis.*

M. P. Eastman, P. G. Eller, K. D. Abney, W. H. Woodruff, S. A. Kinkead, and R. J. Kissane, "Thermal Decomposition Kinetics of Gaseous Dioxygendifluoride," *J. Fluorine Chem*.

P. G. Eller, L. B. Asprey, S. A. Kinkead, B. I. Swanson, and R. J. Kissane, "Reactions of Dioxygendifluoride with Neptunium Oxides and Fluorides," *J. Alloys and Compounds.*

P. G. Eller, J. G. Malm, B. I. Swanson, and L. R. Morss, "Reactions of Hexafluorides of Uranium, Neptunium, and Plutonium with Nitrogen Oxides and Oxyfluorides. Synthesis and Characterization of (NO)[NpF_6] and (NO)[PuF_6]," *J. Alloys and Compounds.*

W. K. Hollis , K. Velarde, J. Lashley, L. Bustos, M. Cournoyer, and R. Villarreal, "Gas Generation from Contact of Radioactive Waste and Brine," *J. Radioanal. Nucl. Chem.*

D. G. Kolman and J. R. Scully, "Comparison of Anodic Current Transients Resulting from Film Rupture on a Dynamically Strained Metastable b-Titanium Electrode to Those Observed Following Fractured Thin Film and Scratch Depassivation," *J. Electrochem. Soc.*

S. R. Luthi, H. U. Gudel, M. P. Heheln, and J. R. Quagliano, "Electronic Energy-Level Structure and Correlation Crystal Field Effects of Erin CsLuCl," *Phys. Rev. B.*

S. F. Marsh, G. D. Jarvinen, R. A. Bartsch, J. Nam, and M. E. Barr, "New Bifunctional Anion-Exchange Resins for Nuclear Waste Treatment- Part II," *J. Radioanal. Nucl. Chem*.

A. M. McCraig, D. M. Wayne, and J. M. Rosenbaum, "Changing Fluid Flow Regimes During Thrusting in the Pyrénées: Pb Isotope Evidence," *Geol. Soc. Am. Bull.*

L. D. Schulte, J. Espinoza, K. Ramsey, G. H. Rinehart, G. L. Silver, G. M. Purdy, and G. D. Jarvinen, "Purification of $^{238}PuO_2$ Scrap for Heat Source Fuel," *Sepa. Sci. Tech.*

B. F. Smith, R. R. Gibson, G. D. Jarvinen, M. M. Jones, M. Lu, T. W. Robison, N. C. Schroeder, and N. Stalnaker, "Preconcentration of Ultra-Low Levels of Actinides from Waste Waters by Water-Soluble Metal-Binding Polymers with Ultrafiltration," *J. Radioanal. Nucl. Chem*.

B. F. Smith, R. R. Gibson, G. D. Jarvinen, T. W. Robison, N. C. Schroeder, and N. Stalnaker, "Evaluation of Synthetic Water-Soluble Metal Binding Polymers with Ultrafiltration for Selective Concentration of Actinides," *J. Radioanal. Nucl. Chem*

D. R. Spearing and J. Y. Huang, "Zircon Synthesis via Sintering of ZrO_2 and SiO_2," *J. A. Ceram. Soc.*

L. Tandon and G. V. Iyengar, "A Review of Radiologically Important Trace Elements in Human Bones," *App. Radiat. Isot.*

Invited Talks

Gordon Jarvinen, "Technology Needs for Actinide and Technetium Separations Based on Solvent Extraction, Volatilization, and Other Processes," NATO Advanced Study Institute: Chemical Separation Technologies and related Methods of Nuclear Waste Management: Applications, Problems, and Research Needs, Dubna, Russia, (May 1998).

K. C. Kim, "Plutonium Futures - The Science," Department of Nuclear Engineering, Oregon State University, Corvallis, OR (June 1998).

Conference Papers (Division Assessment papers are listed on page 5.)
The following were presented at the Actinide Separations Conference, Chatanooga, TN (April 1998): M. S. Blau, "Levitation Zone Refining and Distillation of Plutonium Metal" (LA-UR-98-0241); V. A. Hatler, C. Brown, Jr., A. D. Guillen, K. D. Abney, M. R. Cisneros, and L. D. Schulte, "Americium Beryllium Neutron Sources Dissolution Study" (LA-UR-98-0892); D. Kolman, C. A. James, D. P. Butt, Y. Park, and M. Stan, "Thermally-Induced Gallium Removal from Plutonium Dioxide for MOX Fuel Production"; D. Padilla, L. A. Worl, S. J. Buelow, D. Harradine, L. Le, and J. H. Roberts, "Hydrothermal Processing of Radioactive Combustible Waste" (LA-UR-98-1605); D. Padilla, "Hydrothermal Processing Of Radioactive Combustible Waste" (LA-UR-98-1605); and L. D. Schulte, R. R. Salazar, J. E. Farnham, M. M. Fowler, and R. E. Gritzo, "Development of a Solution In-Line Alpha Counter for Actinide Process Control Applications" (LA-UR-98-1007).

The following were presented at the 193rd meeting of the Electrochemical Society, San Diego, CA (May 1998): D. Costa and W. Smith, "The Nature of Uranyl Chloride in RTMS Melts" (LA-UR-98-1862) and W. Smith, G. M. Purdy, and S. D. McKee, "Comparison of Silver(II), Cobalt(III), and Cerium(IV) as Electron Transfer Mediators in the Mediated Electrochemical Destruction of Cation Exchange Resin in 6 *M* Nitric Acid."

M. E. Cournoyer, "Metal Separation Technologies for the Iron Oxide Industry" (LA-UR 97-1481), Iron Oxides 98: for Hard / Soft Ferrites, Pittsburgh, PA (June 15, 1998).

P. Noll, "Copper Skarn Development in Moat Sediments of the Taum Sauk Caldera, Southeastern Missouri, U.S.A.," Geological Association of Canada Annual Meeting, Quebec City, Quebec, Canada (May 18–20, 1998).

P. G. Eller, L. R. Avens, and G. D. Roberson, "Plutonium Stabilization / Storage Research in the DNFSB 94-1 Core Technology Program," American Nuclear Society Meeting, Nashville, TN (June 7–11, 1998).

M. Martinez and K. Veirs, "Determination of Gallium in Plutonium Using Laser Induced Breakdown Spectroscopy" (LA-UR-97-3917), High Power Laser Ablation Conference, Santa Fe, NM (April 1998).

D. Spearing and J. Y. Huang, "Synthesis and Characterization of $PuSiO_4$: A Potential Ceramic for Pu Disposition" (LA-UR-98-1070), American Ceramic Society, Cincinnati, OH (May 1998).

R. Selvage, et al., "Maintenance of AB During Major Modifications," 1998 Safety Analysis Working Group (SAWG) Workshop, Energy Facility Contractors Group, Park City, Utah (June 1998).

Conference Proceedings
The following were published in the proceedings for the 46th American Society for Mass Spectrometry (ASMS) Conference for Mass Spectrometry and Allied Topics, American Society for Mass Spectrometry, Santa Fe, NM: V. Majidi, Y. Duan, C. Lao, R. Steiner, and D. Wayne, "Capillary Electrophoresis Inductively Coupled Plasma Mass Spectrometry for Chemical Speciation"; J. A. Olivares, Y. Duan, V. Majidi, R. Steiner, and D. Wayne, "The Thermal Ionization Cavity Source, Theory and Performance"; and R. E. Steiner, V. Majidi, D. Wayne, Y. Duan, J. Olivares, and J. Cuadrado, "Characterization of a Miniature Thermal Ionization Cavity Source for Mass Specrometry."

B. F. Smith, T. W. Robison, and G. D. Jarvinen, "Water-Soluble Metal-Binding Polymers with Ultrafiltration: A Technology for the Removal, Concentration, and Recovery of Metal Ions from Aqueous Streams," ACS Symposium Series, *Advances in Metal Ion Separation and Preconcentration*, R. Rogers, A. Bond, and M. Dietz, eds., American Chemical Society, Washington, DC (1998).

Technical Reports
J. M. Berg and P. G. Eller, "Literature Survey of Methods to Determine Moisture Levels in Impure Plutonium Materials," Los Alamos National Laboratory report LA-UR-98-2223 (May 1998).

G. Jarvinen, S. F. Marsh, and M. E. Barr, "New Anion Exchange Resins For Improved Separations Of Nuclear Materials," Los Alamos National Laboratory report LA-UR-98-2295 (May 1998).

M. Schanfein, C. Bonner, D. Vigil, M. Padilla, L. Ticknor, M. Newell, G. Auchampaugh, R. Lucero, and J. Caldwell, "Performance Validation of the Pajarito Scientific Corporation Mobile Waste Assay System" Los Alamos National Laboratory report LA-UR-98-1985 (May 1998).

A. Toupadakis, L. Foster, D. Horrell, C. Martinez, R. Mason, J. Trujillo, C. Davis, and B. Bender, "Materials Identification and Surveillance Project Item Evaluation: Item: Impure Plutonium Oxide (011589),"Los Alamos National Laboratory report LA-UR-98-2005 (May 1998).

NewsMakers

■ **Senator Pete Domenici** visited the Laboratory on April 6. During his visit, he was given a tour of ARIES, the Advanced Recovery and Integrated Extraction System at TA-55. On April 20, 1998, Senator Domenici sent a thank you letter to Division Director Bruce Matthews, stating in part, "The lunch was superb, and I found the tour of ARIES extremely interesting. I look forward to application of the ARIES system as we move ahead with critical bilateral weapon dismantlement and conversion agreements with the Former Soviet Union. Your staff at TA-55 is clearly and justly proud of their contributions to the nation's security, with tremendous responsibilities for many aspects of our nuclear stockpile."

■ On April 22 the Laboratory held a ceremony honoring individuals and teams who qualified for 1998 Pollution Prevention Awards. The awards recognize significant contributions to the Laboratory's effort of minimizing or reducing waste streams through good practices. NMT winners are **James J. Balkey**, **Charles L. Foxx, Kathleen M. Gruetzmacher**, and **Lorenzo A. Trujillo** (NMT-7); **Laura A. Worl** (NMT-6); and **Perla Davis** (NMT-8).

Two New Award Programs Recognize Excellence

NMT Division is happy to announce two new award programs that will honor employees for excellent achievements. Exceptional contributions made by members of the division are now being recognized by The William J. Maraman Award in Operations Excellence and The Richard D. Baker Award for Science and Technology.

NMT's core capabilities—nuclear facilities operation and nuclear materials science and technology—are taking on increasing importance. Both of the awards will be given to honor those whose outstanding achievements have contributed to these capabilities in support of the Laboratory mission. The first of these awards seeks to encourage and promote operational or engineering excellence in the division by recognizing an NMT employee or team whose work represents especially meritorious performance in the operation of nuclear facilities. The second award will encourage and promote technical excellence by recognizing especially meritorious technical contributions by an NMT staff member.

For information on the nomination criteria for both of these awards and the selection process, contact K. C. Kim, NMT Division Office (phone: 7-7753, e-mail: kck@lanl.gov).

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