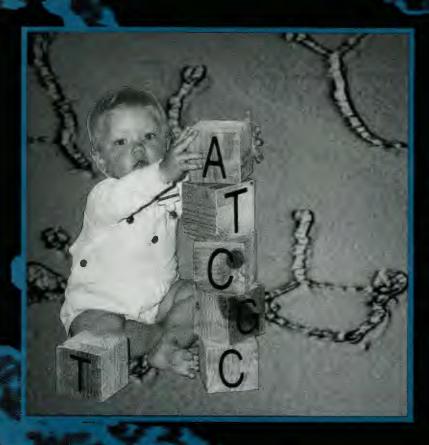
Martin Marietta Energy Systems, Inc.

Oak Ridge National Laboratory

# Val. 25, Na. 1, 1992



PROBING
LIFE'S
BUILDING
BLOCKS

DOE'S CANARY IN A CAGE

FUTURE BATTLEFIELD TECHNOLOGY

#### ON THE COVER

ORNL is developing technologies to more rapidly determine the order of life's building blocks—the bases of DNA—for the national Human Genome Project. One of its achievements has been imaging plasmid (circular) DNA molecules (sample images surround the baby) using an atomic force microscope. For details, see the articles starting on p. 18 and p. 22.

The Oak Ridge National Laboratory Review is published quarterly and distributed to employees and others associated with ORNL. The address of the editorial office is Bullding 4500-South, M.S. 6144, Oak Ridge, TN 37831-6144. Telephone: internal, 4-7183 or 4-6974; commercial, (615) 574-7183 or (615) 574-6974; FTS, 624-7183 or 624-6974.

If you have changed your address and want to remain on the mailing list, please notify the editorial office.

ORNL is managed by Martin Marietta Energy Systems, Inc. for the Department of Energy under contract DE-AC05-84OR21400

Printed in the United States of America. Available from National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161.

ISSN 0048-1262

**Editor** 

Carolyn Krause

**Associate Editor** 

Jim Pearce

**Consulting Editor** 

Alex Zucker

Designer

Vickie Conner

**Technical Editing** 

Mike Aaron

**Electronic Publishing** 

Bob Eldridge

Photography, Graphic Arts, and Printing and Duplicating departments



#### **FEATURES**

2	Walker Branch Watershed: DOE's Canary in a Cage  Michael Huston The effects of pollution and climate change on forests are being studied in Oak Ridge.
10	Technology for the Future Battlefield  Katie U. Vandergriff and James H. Hannah  ORNL's automated techniques could improve the safety and efficiency of rearming battle tanks.
18	New Technologies for DNA Sequencing  Bruce Jacobson  ORNL is developing new technologies for rapidly determining the structures of human genes.
22	Covering All the Bases: ORNL Probes the Human Genome  Jim Pearce  Researchers conduct DNA sequencing and genome mapping studies at ORNL.
40	ORNL as a Supercomputer Research Center  Jim Pearce  ORNL's new parallel supercomputer will be used for alloy design and groundwater modeling.
44	Paving the Way to Superconcrete  A. J. Mattus  Using the polystyrene of throwaway cups, ORNL researchers have developed a very strong concrete
51	A New Look at Supercritical Water  Carolyn Krause  Waste treatment technologies and steam systems may benefit from basic supercritical water studies.
54	Small Mammals as Environmental Monitors  Sylvia Talmage and Barbara Walton  Small mammals, such as shrews, can be reliable bioindicators of chemicals in the environment.

#### **DEPARTMENTS**

58	Awards and Appointments
62	Pick a Number—Joseph Fourier and his heat flux law
64	User Facilities—A new mission for Holifield Heavy Ion Research Facility
68	Educational Activities—New training opportunities for students and university faculty
71	<b>R&amp;D Updates</b> —Bulk Shielding Reactor permanently shut down; CO <sub>2</sub> claim disputed by ORNL model; studies of Brazil's rain forest; ORNL's corrective action plan approved; report on advantages of demand-side management; cold neutron source for Advanced Neutron Source promising
77	<b>Technical Highlights</b> —Fuzzy-logic chip for controlling robot; studies of vegetation regrowth at Mt. St. Helens; global chemical pollution; space conditions simulated at ORNL
86	Technology Transfer—CRADA signing at ORNL witnessed by President Bush; new microwave furnace developed; CRADA involving ORNL, UT, and Dow Chemical; Optics MODIL CRADA; licenses for check valve technology and Raman spectral library



## Walker Branch Watershed: DOE's Canary in a Cage

By Michael A. Huston

ew people realize that in the middle of one of the nation's largest Superfund sites lies one of the nation's oldest and best-known ecological research areas. Walker Branch Watershed. Like the proverbial canary in a cage carried by miners to detect the presence of poisonous gas, Walker Branch Watershed provides an indication of the ecological condition of the Oak Ridge environment, as well as a vardstick to measure the health and recovery of streams and forests damaged by past activities. Because Walker Branch Watershed is an ecosystem, composed of interacting plants, animals, soils, and water, it serves as a barometer of many different components of environmental health.

Walker Branch Watershed, named for the pioneer family whose homestead gave the stream, or "branch," its name, was established as a research site on the Oak Ridge Reservation by the Atomic Energy Commission (AEC) in 1967 for three purposes: (1) providing baseline values for unpolluted natural waters, (2) contributing to

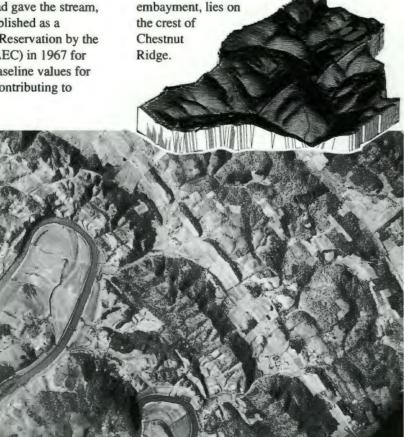
knowledge of the movement (cycling) of chemicals in and their losses from natural ecosystems, and (3) enabling the construction of models for predicting the effects of human activities on the landscape.

To meet these general goals, the AEC and Department of Energy (DOE) have funded the Walker Branch Watershed project for more than 20 years and expanded research efforts to include the much larger area of the Oak Ridge National Environmental Research

Park. Over this time, the Walker Branch Watershed project has addressed such problems as the effects of atmospheric sulfur pollution on forests, the transport of contaminants through soils, and the role of forests in the carbon cycle (and potentially the greenhouse effect).

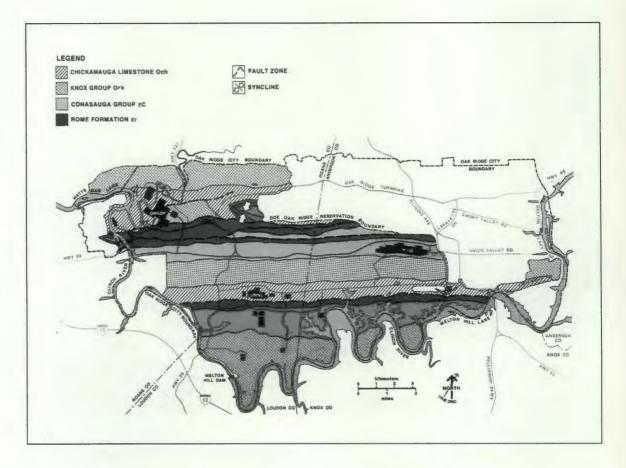
Walker Branch Watershed is located near the center of the Oak Ridge Reservation on a diagonal between Oak Ridge National Laboratory and the Oak Ridge Y-12 Plant. The lower portion of the Walker Branch Valley has been flooded by the Tennessee Valley Authority's (TVA's) Melton Hill Reservoir, forming an embayment that is passed daily by thousands of ORNL employees on their way to and from work. The Watershed Research Area, which is





uphill from the

A 3-D computer image of Walker **Branch Watershed** is superimposed on a pre-1940 aerial photo of Chestnut Ridge, Bethel Valley, and the Clinch River. This topographical map shows the sub-watersheds that integrate biogeochemical processes across the landscape and characterizes ecosystem variability. The 97.5-ha site has an elevation range of 265 to 360 m (870 to 1180 ft) and is forested with oak and hickory trees and some pine and cove hardwoods.



The location of the Walker Branch Watershed and the geology of the area are shown here. ORNL is underlain by the Chickamauga Limestone Formation.

Because of the repeated pattern of ridges and valleys caused by thrust faults in the Oak Ridge area, the soils and geology of the Knox group dolomite on which Walker Branch Watershed is located are virtually identical to those of Black Oak Ridge, on which most of the city of Oak Ridge is built.

The watershed is essentially a suburban forest located in the greater Knoxville metropolitan area, surrounded by DOE's research and production facilities and several industrial parks, and within sight of two of TVA's large coal-burning power plants. Its suburban location makes Walker Branch unique among the nation's major watershed research areas because the rest are located in remote mountainous regions used primarily for recreation and timber production. Were it not for the unusual history of the Oak Ridge Reservation and its role in the Manhattan Project, the Walker Branch Watershed Research

Area would probably be the Walker Hills subdivision.

### Monitoring the Health of Forests and Streams

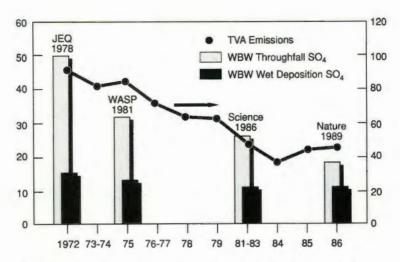
Although research issues on Walker Branch have changed over the years, the project has continued to collect basic data on the condition and health of the forest and streams. The guiding principle of watershed research is that the condition of an ecosystem can be monitored by measuring changes in its chemical composition. ORNL scientists in the Environmental Sciences Division (ESD) determine how the chemical composition of the 250 forested acres of the Walker Branch Watershed is changing by calculating the amount of an element that comes into the watershed in rainfall and subtracting the amount that leaves the watershed in the stream.

This method, known as "mass balance," can indicate whether the ecosystem is accumulating or losing a particular element or whether the amount of that element in its composition is at a steady state. At other watershed research sites, changes in stream chemistry, such as increased nitrate concentrations, have provided the first warning that insects were defoliating trees in parts of the forest. The effect of insects was detected in the stream chemistry because

removal of leaves reduced the amount of nitrogen being taken up by trees, while insect droppings released nitrate that moved rapidly into the streams.

Long-term monitoring at Walker Branch has documented the beneficial effects of the pollution-control devices installed by TVA on its local coal-burning power plants. ESD researchers demonstrated that as much as half the sulfur released from burning coal is returned to the landscape in a dry form, as sulfate particles that settle onto leaves and branches, rather than as sulfuric acid in rainfall. By measuring the amount of sulfate that washes off leaves during rainstorms, Steve Lindberg of ESD documented a decrease in sulfate deposition onto Walker Branch that corresponds with the decline in sulfur emissions from TVA's power plants.

Two of the major advantages that Walker Branch ecologists have over researchers at other sites are the local expertise and experience in the use of radioisotopes and a controlled site where radioisotopes can be used safely. Radioisotopes of phosphorus, sulfur, and hydrogen (tritium), as well as radon gas, have been used to investigate both the movement of water through the soils and in the stream and the cycling of elements through the vegetation.



Long-term monitoring shows that sulfate deposition on the Walker Branch Watershed has declined in proportion to decreases in Tennessee Valley Authority sulfate emissions.

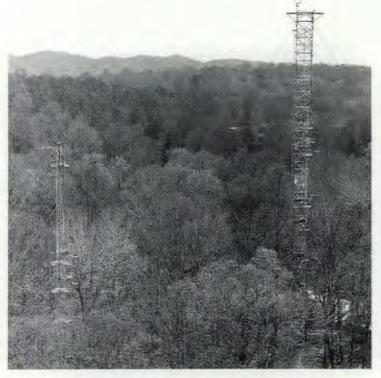
A fundamental piece of evidence in the sulfur pollution story was provided by an experiment conducted by ESD's Steve Lindberg and Chuck Garten in which whole trees on Walker Branch Watershed were labeled with radioactive sulfur-35. Low levels of radioactivity in the sulfate washed off the tree leaves by rainstorms demonstrated that the source of most of that sulfate was *not* the tree itself but rather deposition from the atmosphere.

### **Investigations from Above and Below**

Basic research on Walker Branch extends both above the forest canopy and below the soil surface. On the crest of Chestnut Ridge is a tower of aluminum scaffolding that extends some 20 m above the forest canopy. The tower was built by the Atmospheric Turbulence and Diffusion Division (ATDD) of the National Oceanic and Atmospheric Administration (NOAA), which has a laboratory in Oak Ridge. NOAA scientists, working in collaboration with Walker Branch Watershed project staff, have investigated various interactions between the forest canopy and the atmosphere. Examples are the penetration and absorption of solar radiation; the exchanges of

"ORNL scientists... determine how the chemical composition of the 250 forested acres of the Walker Branch Watershed is changing."

"Two of the major advantages that Walker Branch ecologists have over researchers at other sites are the local expertise and experience in the use of radioisotopes and a controlled site where radioisotopes can be used safely."



The ATDD tower extends far above the canopy of the Walker Branch Watershed forest.

carbon dioxide among the soil, the forest canopy, and the atmosphere; and the movement and deposition of such automobile-related pollutants as nitrogen oxides.

Not far from the ATDD tower is an unusual subterranean research facility known as the subsurface weir. Similar to the surface weirs on Walker Branch where the volume and chemistry of stream flow are measured, the subsurface weir collects water flowing laterally through the soil. Originally used for the purpose of studying movements of simulated contaminants through forest soils, the subsurface weir is now part of a network of sampling stations across the watershed that measure changes in the volume and chemistry of water as it moves down the landscape. An identical facility, located southeast of ORNL in Melton Branch Watershed, has allowed comparisons of the patterns and mechanisms of

stream flow generation on two watersheds that have contrasting geological structures.

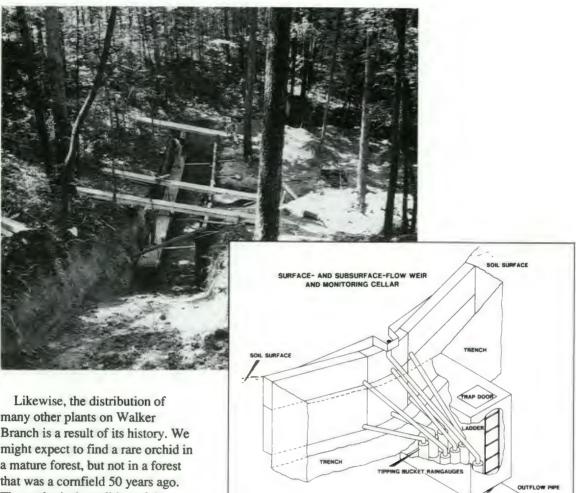
#### Monitoring Forest Growth and Succession

In addition to the chemical inputs to and outputs from the watershed, scientists on the Walker Branch Watershed project monitor the growth and productivity of trees and the changing composition of the forest as it has responded to insect outbreaks and the drought of the 1980s. However, many of the changes in the forest are not the result of any particular stress or disturbance. They are simply the effects of natural succession as the forest takes over the fields and pastures that covered this area before the Manhattan Project.

Although the Oak Ridge area is heavily wooded today and is probably the largest forested

area in East Tennessee outside of the mountains, in 1940 it was a patchwork quilt of small farms and communities. Most of the valleys were covered by fields, and the ridges were a mosaic of fields, pastures, and woodlots. A farm was present at the highest water source in each little valley along Chestnut Ridge, and Walker Branch was no exception. The fallen remains of log cabins and associated outbuildings can still be seen on both the East and West Forks of Walker Branch.

Understanding the history of the forest on Walker Branch is critical to understanding its ecology and biogeochemistry today. Most of the pine trees that have died in Walker Branch during the 1980s were short-lived Virginia pines that grew up on the plowed fields that were abandoned in 1940. They died not as the result of atmospheric pollution or some natural disaster, but primarily as a result of old age.



Construction of a surface- and subsurface-flow weir and monitoring cellar is shown in this 1985 photograph. Superimposed on it is a drawing of the weir and monitoring cellar.

Likewise, the distribution of many other plants on Walker
Branch is a result of its history. We might expect to find a rare orchid in a mature forest, but not in a forest that was a cornfield 50 years ago.
The ecological condition of the current forest on Walker Branch is being investigated using old aerial photographs that show the condition of the landscape 50 years ago. This information, along with computer models of stream flow and forest succession, is being used to predict the future appearance of our landscape and possible forest responses to climate change.

## **Climate Change** and Forests

The climate change that may result from increasing amounts of carbon dioxide in the atmosphere has been a long-term research concern of DOE. Past Walker Branch research has investigated many of the processes of the carbon

cycle, including the decomposition of leaves and dead wood, the accumulation of carbon in living trees, changes in the amount of carbon stored in the soil, and carbon dioxide uptake and release by plants.

A major new multiyear experiment to investigate the effect of climate change on forest ecosystems will be initiated on Walker Branch Watershed in 1992. Change in rainfall amount is expected to be one of the most serious impacts of climate change on agricultural and forest productivity. Although existing climate models cannot predict with any confidence how much precipitation will change in any particular area,



Glenn Wilson (formerly of ESD, now at the University of Tennessee) checks the water flow in the subsurface weir.

several models agree in the prediction that the southeastern United States will become drier.

The Walker Branch researchers will investigate the effects of both increased and decreased precipitation using an experimental design that intercepts water before it reaches the ground in one plot and drains it onto another plot. Through a system of plastic troughs that cover 25% of the ground in an area of forest roughly the size of three football fields, one area of forest will be made 25% drier and a nearby area will become 25% wetter than current conditions. Conditions on the dry plot will be comparable to those during the driest years of the 1980s.

Many different properties of the forest are expected to change in response to increased or decreased rainfall. ORNL scientists, in collaboration with researchers from NOAA, the U.S. Forest Service, and a variety of universities and colleges, will monitor basic ecosystem responses such as forest productivity and nutrient cycling and conduct research on specific issues such as changes in the susceptibility of trees to insect attack. One specific concern is the development of methods to detect impending changes in ecosystem processes before they



Pat Mulholland checks an experiment on the effect of increased light on stream algae in Walker Branch.

become irreversible. By monitoring the biochemical condition of trees and soil microbes, scientists may detect changes in their physiology that can serve as early indicators of ecosystem change. For example, conversion of starch into sugars in tree roots can indicate that the tree is under stress and may also make the tree more susceptible to fungal infections.

In addition to its role as a nationally and internationally known watershed research site. Walker Branch Watershed also has an important local role. Because it has the same history and geology as most of the Oak Ridge area, it can serve as a "control" site for comparison with the health of the rest of our environment. The success of remedial actions being conducted to clean up the streams of the Oak Ridge Reservation is being evaluated by comparing the quality of the water in the remediated streams with that of the unpolluted natural streams of Walker Branch and other natural ecosystems of the region. Continued monitoring of DOE's canary in a cage can reassure us about the health of our local environment, as well as provide early warning of local and global environmental problems.

#### Biographical Sketch



Michael Huston stands among the plastic troughs used to investigate the effects on forests of both increased and decreased precipitation that might result from climate change.

Michael A. Huston is leader of the Walker Branch Watershed project. He seeks to integrate the results of watershed-scale ecosystem studies and experiments with recent theoretical developments in community ecology and with methods for addressing regional and global issues. He received a B.A. degree in biology from Grinnell College in 1973 and a Ph.D. degree in biological science from the University of Michigan in 1982. His doctoral dissertation examined the effect of light and nutrients on tropical rain forest succession in Costa Rica. In 1983 he joined ORNL's Environmental Sciences Division as a Wigner Fellow.

Huston's research interests include forest succession, population dynamics, nutrient cycling, disturbance effects, and species diversity. He has field experience in tropical and temperate forests, tropical coral reefs, and North American prairies. He is best known for his theoretical contributions in the area of species diversity, plant succession, and population size structure. His work on nonequilibrium competitive dynamics and individual-based models of populations, communities, and ecosystems continues to have significant influence on the field of ecology.

A recent article in *BioScience* by Huston and his co-workers in the Environmental Sciences Division describes a new approach to ecological modeling that has the potential to integrate ecological processes ranging from suborganismal physiology to global vegetation dynamics. In 1992 the Cambridge University Press Ecology Series will publish Huston's book *Biological Diversity: The Coexistence of Species*, which addresses an issue of urgent global concern.

## Technology for the Future Battlefield

By Katie U. Vandergriff and James H. Hannah



Ammunition is currently loaded by hand one piece at a time through the tank's hatch. This laborintensive activity exposes soldiers to weapon fire and nuclear, biological, and chemical agents.

uring Operation Desert Storm, the ground war lasted only four days, minimizing the need for U.S. armored forces to reload ammunition. However, if battle conditions had been different or if Iraq had made good on its threat to use nuclear, biological, and chemical (NBC) weapons, the process of manually reloading ammunition into armored fighting vehicles would have been a much more dangerous task.

This problem was noticed long before Operation Desert Storm, however. Since the mid-1970s the U.S. Army has been looking at the difficulties of rearming armored and mechanized vehicles on the battlefield in light of various combat scenarios and computer models. Under some of these battle conditions, the necessity of manually reloading ammunition could limit the effectiveness of U.S. armor.

Currently, the world's most lethal battle tank, the M1A1 Abrams, must be rearmed one piece of ammunition at a time through a hatch on top of the tank. Under battle conditions, when the tank is running low on ammunition, the tank commander asks the base to send a Heavy Enhanced Mobility Tactical Truck (HEMTT, pronounced him-it) to meet with the tank well behind the fighting line. When the tank and HEMTT meet, the tank hatch is opened, the HEMTT crew and tank crew dismount, and ammunition reloading begins. Crew members remove the tank ammunition from storage cans and pass it up to the top of the tank where other soldiers lower it down through the hatch. Inside the tank, a soldier places the ammunition into storage honeycombs. Under the best conditions, this procedure is a tiresome task; under battlefield conditions it is also dangerous

because the crew and equipment may be exposed to deadly weapon fire and NBC agents.

#### **ORNL's Role**

An ORNL group is part of a national team working to improve the safety and efficiency of this essential element of armored warfare by developing critical technology for automated reloading of armored vehicles. This technology will be demonstrated using the Future Armor Rearm System (FARS). Under the project guidance of ORNL's Robotics and Process Systems Division (RPSD), staff members from RPSD, the Central Engineering Division at Martin Marietta Energy Systems, Inc., and ORNL's Plant and Equipment Division have joined together to help develop automated reloading technology.

The development of the FARS technology is sponsored by the U.S. Army's Project Manager for Ammunition Logistics (PM-AMMOLOG) through the Work for Others Office. The charter of PM-AMMOLOG is to identify logistics problems in the U.S. Army's ammunition chain and find solutions. Ammunition reloading for heavy armored systems is a proven logistical problem within the Army's armored systems. "The FARS program," says project sponsor Nelson Gravenstede, "is intended to develop, integrate, and demonstrate technologies capable of moving ammunition from a rearm vehicle into the tank."

To develop and demonstrate the FARS technology, PM-AMMOLOG has put together a team consisting of personnel from ORNL and several other Army facilities. The team members were selected based on their individual expertise. The ORNL group was chosen based on our experience with robotic and remote systems, our advanced controls and integration capabilities, and our ability to design systems to operate in hazardous environments, such as nuclear fuel reprocessing facilities and outer space. Other team members include the Human Engineering Laboratory at Aberdeen Proving Ground, Maryland, and the Tooele Army Depot at Tooele,

Utah. We are also collaborating with Benet Weapons Laboratory of Watervliet, New York, designer of the autoloader that will fit inside the advanced tank. We are working with these groups to develop the many subsystems of the FARS automated reloading system. ORNL is responsible for the ammunition handling and storage system, the overall controls, systems integration, and final technology demonstration.

#### A Look at the FARS

The FARS will consist of a tracked, armored chassis and a specialized mission module. The mission module will house systems for storing and transferring ammunition into the tank bustle. Automated reloading, which will be demonstrated with FARS technology at ORNL, will not only ease the manual burden on the soldier but will also provide a safer, faster, and more efficient means of reloading heavy armored systems. The use of FARS technology will eliminate the possibility of exposing soldiers to enemy fire or NBC agents during the reloading operation.

With the FARS technology, when a tank is running low on ammunition, the tank commander will communicate that need to the base, which will send a FARS to meet the tank. Because the FARS will be on a tracked chassis, it will be able to negotiate the same sort of terrain as tanks, and, with its armored protection, the FARS will be able to meet the tank closer to the fighting line than the HEMTT. The FARS operator will approach the tank and dock the transfer arm to the port located on the tank bustle. While performing the docking operation, the operators will stay safely inside the FARS cab, relying on camera viewing and joy-stick control of the transfer arm to remotely guide it. Once the docking is completed, the connection between the tank and the FARS will be purged to remove any possible contamination by NBC agents during reloading, and a communication link with the tank will indicate when ammunition transfer can begin.

Ammunition will be housed in the FARS in individual storage cells. These cells will be

ORNL's automated techniques could improve the safety and efficiency of reloading ammunition in armored tanks.

The FARS technology will make possible fully automated ammunition transfer, which is faster, safer, and more efficient than current rearming methods.



mounted on a rotating carousel to allow access to any desired type and sequence of ammunition. The tank commander will be able to choose from several types of ammunition, depending on the nature of the target. For example, different types of ammunition are fired at heavily armored and lightly armored targets. When the tank commander specifies the desired combination of ammunition, the FARS will send the ammunition from the carousels to a lift table and through the transfer arm into the bustle of the tank. Once inside the tank, the round will be transferred into an autoloader mechanism that will store ammunition and feed it into the main gun.

#### **Benefits of Automated Reloading Technology**

Automated reloading technology being developed will provide many benefits over the current manual method. It will increase safety, reduce the size of armor support crews, and increase the battlefield availability of armored fighting vehicles.

Soldier safety will be improved because crews from both vehicles can remain under full armor protection during the entire reloading process. The technology also protects the systems from NBC contamination. Also, the soldiers are less vulnerable because automatic reloading is faster than the current method.

The second main area to benefit is crew size. The current method is labor intensive and lengthy. Soldiers from both crews must dismount and handle the ammunition as they move it from HEMTT storage, to the tank, down the hatch, and into the tank storage system. Automated ammunition reloading will reduce crew size because, once the FARS leaves the supply base, the ammunition never again has to be manually handled.

The third major benefit of automated reloading is improved battlefield availability for the fighting vehicles. Because the automated reloading vehicle is armored and tracked, it can move closer to the fighting line than the current reloading vehicle. The goal for the entire automated reloading sequence is 10 minutes or less, a significant improvement over the current manual method. Combining the increase in loading speed and the ability to perform reloading operations in closer proximity to the fighting line would result in approximately a 20% increase in the number of tanks on the battlefield.

## Demonstration of FARS Technology

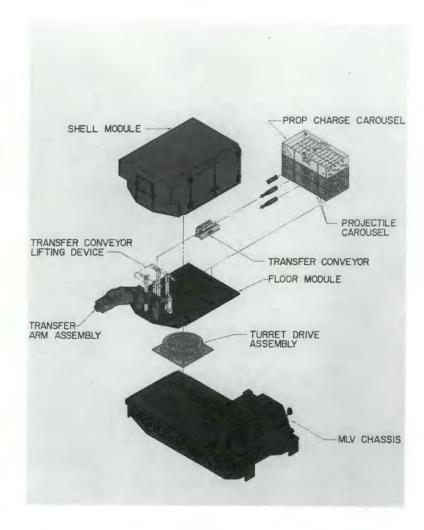
Although the FARS concepts apply to a fully developed rearm vehicle, the demonstration will concentrate on the critical areas of technology. A fullsize advanced tank will be included in the FARS technology demonstration. which will take place at ORNL in the fall of 1992. The FARS will approach, dock. communicate, and transfer ammunition into the tank's automated loading system. The technology developed with the FARS will feed into the Army's Advanced System Modernization program for the Future Armor Resupply Vehicle as a fielded system.

The FARS team members have dedicated many hours of company and personal time to the project. Bob Oliver of the Central Engineering Division made scale FARS and tank models on his own time.

These models have been used

in briefings to top Army officials and others. For his initiative and effort, Oliver received special recognition from the PM-AMMOLOG Deputy Director. "Building military models has been one of my hobbies for many years," says Oliver. "Being named principal engineer for a full-scale prototype like this has been the highlight of my career at ORNL."

The FARS project results will demonstrate a variety of new and advanced technologies for the Army community. The control system currently under development will enable the FARS operator to access any desired piece of ammunition by coordinating the various systems into an integrated operation. Rick Glassell, an RPSD controls engineer, has helped design the control



The automatic ammunition reloading system will consist of subsystems now being developed by various FARS team members. The system will be demonstrated using a full-size advanced tank in the fall of 1992 at ORNL.

system for the FARS. "Developing the controls system required to coordinate this many different operations has been a challenge," says Glassell. "Communicating with the tank and remotely controlling the ammunition transfer arm are two of the major goals we are working on for the demonstration."

The ammunition handling and transfer system, which was designed by ORNL, is the first of its kind to be able to remotely handle ammunition produced using the Army's advanced combustible-case ammunition technology. The ability to remotely dock and communicate with the tank is also a technological advancement. Systems exist that assist with reloading specific types of ammunition; however, these systems



Claude Benge, Katie Vandergriff, Terry Ray, and P.R. Long work together to assemble the ammunition storage carousel. Teamwork has been an essential element in the success of the FARS project.

Craftsmen Jimmy Watson, John Stout, and Dennis Tilley put the finishing touches on a hardware test setup. The FARS technology has been demonstrated at the Fort Knox Armor Conference, the Army Material Command Technology Exposition, and the Army's Logistic Research Exposition.





Animated computer graphics by Michelle Hollis not only help to visualize the FARS concepts but also aid with the design process. Designs can be verified and clearances can be checked before the actual hardware is built.

require a soldier in the rearming loop to complete the operation. The fully automated FARS, from the storage cells to the firing of rounds from the tank's cannon, will be a technological first.

The Army plans to employ FARS technology after the year 2000 on its next generation of tanks. However, the advanced technology being developed by the FARS program will likely have applications in other areas of military rearming.

The innovative application of advanced technology to FARS has been a significant technical challenge. It has required a total integrated systems approach using a broad range of ORNL expertise and capabilities, particularly in remote systems, telerobotics, and advanced automation. The FARS team and ORNL staff members are strongly contributing to meeting the technology needs of the U.S. military.



The FARS armored chassis has been fitted with the ammunition transfer arm and adjoining systems. The ammunition handling carousel and other FARS hardware and controls will be installed and integrated at ORNL.



Bob Oliver, Walt Glover, and Jim Poston examine the ammunition storage carousel during the hardware integration.



Rick Glassell is developing the **FARS** controls system to enable the multiple subsystems to work in an integrated operation. ORNL's expertise in advanced controls and system integration has been widely recognized in the military community.



FARS team members work on the ammunition storage system and integrated controls. From left are Hannah, Glassell, Glover, Oliver, and Vandergriff.



Jim Hannah and Bob Oliver work out reloading scenarios with scale models. Oliver built the FARS models in his spare time to illustrate the FARS design concepts. These models have been used in briefings for top U.S. Army officials and others.



The work done by ORNL
on the Future Armor Rearm
System has helped to earn
ORNL recognition as an
outstanding engineering and
development laboratory.
"The FARS project sponsor refers to
us as a 'world class' R&D organization,"
says Jim Hannah, manager of ORNL's
Ammunition Logistics Program. He credits the
success of the program to the enthusiasm of the
team members and the complete team atmosphere.
Hannah cites the technical contributions of the Remote

Systems Development Section and the Telerobotic Systems Section of RPSD as well as the Central Engineering Division and the fabrication shops. He places special emphasis on the individual efforts by the many craftsmen and support personnel working on the PM-AMMOLOG projects. "Pride in workmanship and dedicated support for the U.S. armed forces," he says, "are obvious in these individuals."

Colonel Thomas Tobin, the Army's Project Manager for Ammunition Logistics, recognized ORNL's significant contributions by presenting certificates of appreciation. Receiving the certificates for ORNL were Alex Zucker, ORNL associate director for Nuclear Technologies; Dick Davis, associate director for Army Programs under the Space and Defense Technology Program; Jim Hannah, RPSD manager of Ammunition Logistics; and Katie Vandergriff, FARS project manager. Both Hannah and Vandergriff accepted the awards on behalf of the whole team.

"The excellent work on the FARS project has significantly influenced the Army sponsor to use the expertise and broad technology base of ORNL in several other development projects," says Hannah. "We currently have five active projects in addition to FARS in the Ammunition Logistics Program. This new work area has become an excellent opportunity to broaden our technology base as well as share the 'world class' R&D capabilities of ORNL, especially in telerobotics and remote systems, through DOE's Work for Others Program."

#### Biographical Sketches

Katie Vandergriff is

project manager for the **Future Armor Rearm** System. She joined the ORNL staff in 1987 as a member of the Robotics and Process Systems Division. She received her B.S. degree in mechanical engineering from Tennessee Technological University and worked as task leader for the Radiation Effects and Component Hardening (REACH) project before joining the FARS project. She also represents Martin Marietta Energy Systems, Inc., as a technical recruiter and serves as teamwork chairman of ORNL's Values Committee.

A native of Anchorage, Alaska,
Vandergriff is Tennessee state chairman of
the Young Engineers Committee through
the Tennessee Society of Professional
Engineers. She currently serves on the
steering committee for the Tennessee Math
and Science Education Initiative, is an
organizing member of the Greater Knoxville
Math/Science Coalition, and was chairman
for the 1992 Engineer's Week Activities for
Knoxville, Oak Ridge, and surrounding
areas. Vandergriff has been chosen as one of
the Outstanding Young Women of America.

Jim Hannah is manager of the Ammunition Logistics Program in ORNL's Robotics and Process Systems Division. He earned a B.S. degree from the University of Tennessee in mechanical engineering. He



Jim Hannah, Alex Zucker, Katie Vandergriff, and Dick Davis display awards they received from the U.S. Army for their contributions to the FARS project.

came to ORNL in 1967 and has worked at all three DOE sites in Oak Ridge over the past 24 years. He was development engineer and development group leader during his 14 years at the Oak Ridge Gaseous Diffusion Plant and served as the department head of Dimensional Inspection Engineering at the Oak Ridge Y-12 Plant from 1985 through 1987.

Hannah returned to ORNL in 1987 and has managed a wide variety of engineering projects in the Robotics and Process Systems Division. He is currently group leader of the division's Systems Engineering and Integration Group. Hannah also serves as the technical coordinator of a cooperative agreement between the DOE and the French Commissariat à l'Energie Atomique in the field of remote systems technology.

Number One, 1992 17

## New Technologies for DNA Sequencing

By K. Bruce Jacobson

Tom Thundat, Bruce Jacobson, and Dave Allison inspect the head of an atomic force microscope, used to obtain detailed images of DNA molecules.



t is a momentous occasion when several fields of science come together to focus on a single problem. This is one of those times. Determining the structure of the human genome has caught the fancy of people in many scientific areas. An unprecedented ferment has resulted as scientists throughout the world attempt to understand one another and do meaningful experiments together.

Within ORNL the Human Genome Project (HGP), supported by the Department of Energy, is focused on two areas: the analysis of the mouse genome with emphasis on human similarities and the development of new technologies for genome analysis. This article will be restricted to the latter.

One goal of the HGP is to sequence the deoxyribonucleic acid (DNA) in the human genome, which contains a total of six billion bases. Sequencing involves determining the order of these nitrogen-containing bases attached to

DNA's phosphate backbone. The order of these bases can determine the order of amino acids in more than 50,000 different proteins that carry out life's processes. Each gene has a particular sequence of bases, and being able to recognize that structure helps researchers understand what makes a gene function normally-or abnormally. In 1987 a good day's work for a team of researchers would result in the identification of 2000 bases on one strand of DNA; now it may be 5000 for a single worker. An important objective of the HGP

has been to develop faster and less expensive ways to determine DNA sequencies. (For background, see "Pursuing Biology's Holy Grail," *Review*, Numbers Three and Four, 1989, p. 32.) For details on ORNL's human genome studies, read the article starting on p. 22 in this issue.

#### **Stable Isotope Sequencing**

Several innovative techniques for DNA sequencing are under development at ORNL. A visiting expert noted that we have more technological development under way than any other laboratory or university.

In 1988 I conceived of a way to sequence DNA using stable isotopes rather than radioactive isotopes to reduce worker exposure to radiation. Hal Schmitt of Atom Sciences, Inc., of Oak Ridge, and I planned to use resonance ionization spectroscopy (RIS) to determine the positions of bases in labeled DNA bands following

conventional separation by gel electrophoresis. RIS is a laser-based technique invented in Oak Ridge. It can be used to identify and quantify most elements by ionizing atoms of each with light of a characteristic wavelength and then detecting and counting the removed electrons to measure the concentration of the target atoms. Combined with mass spectroscopy, it can distinguish between isotopes of an element based on differences in their masses.

Although we first proposed using four stable isotopes of sulfur because the chemistry for attaching it to DNA bases was already known, we found that the stable isotopes of tin are much more useful because 10 different ones are available. Because this work required the development of new chemistry for attaching tin to DNA, we sought the help of ORNL chemists. Rick Sachleben and Gil Brown, both of the Chemistry Division, have accomplished this goal and are working on, or have proposed, several additional methods.

Bob Foote and Fred Sloop, both of the University of Tennessee, have attached the tin to DNA bases, and Rick Woychik and Frank Larimer, both of the Biology Division, have employed tin-labeled bases in standard molecular biology experiments, demonstrating that the new labels perform as they should. Finally, Norbert Thonnard and Heinrich Arlinghaus, both at Atom Sciences, adapted RIS procedures to detecting the tin-labeled bases produced by Larimer and Woychik.

To ensure the accuracy of our sequencing technique, we must select stable isotopes that are not abundant in the environment to avoid background interferences in our measurements. For example, we will not use iron because it is abundant in machinery and the earth's crust. Because of their low availability in the environment, we will test rare earths for sequencing. A complexing agent that will allow us to attach a number of rare earth isotopes to DNA bases is being synthesized by Martha Garrity, a postdoctoral fellow in chemistry from the University of North Carolina.

Currently, the gel electrophoresis procedure is being retrofitted to RIS by Mitch Doktycz, a recent postdoctoral fellow in biology from the University of Illinois. Debbie Czarniecki, a participant in the Great Lakes Colleges Association undergraduate research program from Lawrence University, is developing and evaluating alternative ways of attaching tin to DNA.

Another novel approach to this problem is sequencing by hybridization (SBH). Several groups have proposed new SBH methods, one of which was reported back to Oak Ridge from Valencia, Spain, by my son, Dan, who had met a group from Belgrade, Yugoslavia, that was considering this approach. As this new approach was studied by the stable isotope group, Foote recognized the need for innovative chemistry to make it a practical procedure. He has been developing this chemistry with the assistance of K. P. Stengele, a recent arrival from Germany who has broad experience in DNA chemistry. The Belgrade group has now moved to Argonne National Laboratory to develop the SBH method, and the Affymax Research Institute is also working on the technique.

#### STM View of DNA

Yet another unconventional approach to DNA sequencing is being pursued by Tom Ferrell, Bruce Warmack, and Dave Allison, all of the Health and Safety Research Division (HASRD). I joined forces with them to provide advice and expertise on DNA. The goal is to stretch a strand of DNA out on a flat surface and observe the individual bases directly to determine their sequence by simply taking a picture of them. Getting DNA to hold still while its picture is being taken has proven to be a vexing problem.

When Larry Bottomley came here from the Georgia Institute of Technology this past summer, he demonstrated that DNA can be immobilized on a gold surface. Reproducible pictures can now be obtained by Allison with a scanning tunneling microscope and by Tom Thundat of HASRD with an atomic force microscope. The group is very enthusiastic over this success.

#### **Mass Spectroscopy Sequencing**

In the classical method for DNA sequencing, the DNA molecule of interest is replicated (copied) by an enzyme, DNA polymerase, to produce a set of

ORNL is developing new technologies for rapidly determining the structures of human genes.

Number One. 1992

DNA molecules that represents a series of sizes that differ by only a single nucleotide. By subjecting the mixture of these DNA molecules of varying sizes to gel electrophoresis, the molecules are arranged by size. (Gel electrophoresis involves placing pieces of DNA in a conductive gel and placing a voltage across the gel. The electric potential causes the DNA pieces to move through the gel at varying rates, depending on their size. Eventually this process results in the ordering of pieces by size.) From this array, and information obtained from the method of their production by DNA polymerase, the sequence is obtained.

The mass spectroscopists have proposed that their instruments can produce such an orderly array of different sizes, using the same mixture as gel electrophoresis, and can distinguish among the molecules of different sizes by detecting differences in their masses or other properties. Thus, they should be able to determine the sequence directly.

Michelle Buchanan and Bob Hettich, both of the Analytical Chemistry Division, have used laser desorption Fourier transform mass spectroscopy to sequence DNA molecules having four to six bases. Gary Glish and Scott McLuckey, also of the Analytical Chemistry Division, have used tandem mass spectrometry (MS/MS) to successfully detect a short DNA molecule, called an oligonucleotide.

Winston Chen of HASRD has recently proposed the use of ferrocene-labeled DNA to facilitate ionization of the DNAs in the mixture of sizes and the detection of individual species of the different sizes by a high-resolution reflectron time-of-flight mass spectrometer. Jack Davidson of the Instrumentation and Controls Division has proposed yet another approach that is yet to be

tested. These, along with all the other approaches mentioned here, have the potential to increase the rate of DNA sequencing by orders of magnitude.

#### GRAIL

From a lexical viewpoint, interpreting an array of 500,000 letters (consisting of the A, G, C, and T of the DNA alphabet) is a challenge. Where are the words, the sentences, and the paragraphs? Where do messages embedded in the DNA start and stop? Some DNA sequences have been interpreted, and these are being used by Richard Mural and Ed Uberbacher of the Engineering Physics and Mathematics Division to train computers that are equipped with neural networks. This training enables the computer to recognize precise information encoded in the DNA sequence, separating the genetically useful "words" from the intervening, meaningless groups of letters. This computer program, called GRAIL (Gene Recognition and Analysis Internet Link), is available on electronic mail networks. DNA sequence data from many laboratories around the country are now being interpreted by GRAIL, helping researchers find genes among the other information.

New technologies for DNA sequencing have been the focus of the Human Genome Program and may continue to be supported for two to four more years. The current plan is eventually to select the most promising methods and underwrite them for use in the long-term effort to sequence the human genome. As more powerful methods become available, they will also be used to study the genomes of other animals and plants. The knowledge of genome sequence and structure can be employed in treating disease and developing superior food sources.



Reinhold Mann and Ed Uberbacher, both of the Engineering Physics and Mathematics Division, and Richard Mural of the Biology Division have developed an intelligent computer system known as GRAIL (Gene Recognition and Analysis Internet Link) to identify the genetically useful portions of DNA sequence data.

#### Biographical Sketch

K. Bruce Jacobson has been a member of the research staff of ORNL's Biology Division since 1958 and a professor in the University of Tennessee–Oak Ridge Graduate School of Biomedical Sciences since 1968. He has a Ph.D. degree from Johns Hopkins University and had a postdoctoral appointment at the California Institute of Technology. His research interests include the mechanism of enzyme action, the structure-function relationships for transfer ribonucleic acid (RNA), pteridine metabolism, and the development of new technologies for DNA sequencing.

Number One, 1992 21

## Covering All the Bases: ORNL Probes the Human Genome

By Jim Pearce

esearch into the human genome at ORNL is focused on genome mapping and DNA sequencing. The genome is subdivided into chromosomes, each of which contains thousands of genes.

Determining the order of these genes and the spacing between them is called mapping.

Understanding a gene's function involves unraveling the codes it contains for specifying protein structure and for turning the gene on and off. The codes are specific sequences of nucleic acid bases, so determining the order of these bases is the goal of DNA sequencing.

This delving into human genetic roots has yielded information on thousands of genes, including those responsible for such disorders as muscular dystrophy, cystic fibrosis, and Huntington's disease. Researchers are hopeful that, as they uncover the causes of genetic diseases, they will also be able to develop genetic "fixes" for these conditions.

An individual's genetic information is normally recorded on 46 chromosomes (23 from Mom and 23 from Dad). These chromosomes comprise roughly three billion pairs of bases, throughout which are scattered the estimated 50,000 to 100,000 genes of the human genome.

Despite these daunting numbers, there are only four kinds of DNA bases—adenine (A), thymine (T), cytosine (C), and guanine (G). These bases are arranged in sets of three (for instance, AAA, CGC, or GAC), called codons. Each codon corresponds to a particular amino acid or regulatory signal to the cell. Genes, then, are strings of amino acids that build proteins and regulate cell function.

For practical purposes, think of the DNA molecule as a ladder with a strand of phosphate and sugar molecules on each side and pairs of bases between the strands for rungs. Because DNA bases come in matched pairs (A bonds with T, and C bonds with G), knowing the

The four bases—adenine (A), thymine (T), cytosine (C), and guanine (G)—are the building blocks of DNA.

#### AGCT

Amino acids are the components of proteins. The DNA bases are arranged in sets of three, called codons, each of which corresponds to a particular amino acid or regulatory message to the cell.

#### AAA CGC GAC CGA

**Genes** are strings of thousands of amino acids that build proteins and regulate cell function.

#### -ACGAAAATCCGCGCTTCAGATACCTTA-

Chromosomes are strings of thousands of genes, along with "filler" material—bases that aren't used for building proteins or regulating cell function. Normally individuals have 46 chromosomes, 23 from each parent.



The genome of an organism is its complete set of genetic information—the sequence of all the bases on all the chromosomes.



Source: Office of Technology Assessment

22

"This

human

delving into

genetic roots

has vielded

information

of genes,

including

responsible

disorders as

muscular

dystrophy,

fibrosis, and

Huntington's

disease."

cystic

for such

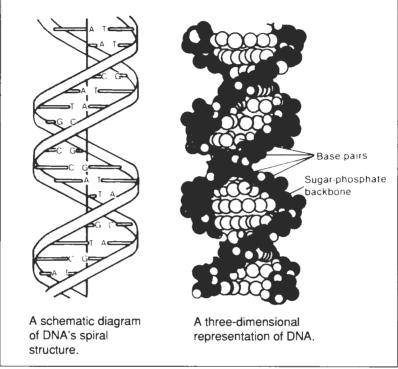
those

on thousands

sequence of the bases on one side of the ladder makes it possible to determine the sequence of the other.

ORNL researchers have adopted a number of approaches to sequencing and mapping DNA. Some methods are the highly efficient descendants of techniques that have been used for years, such as gel electrophoresis and radiolabeling; others employ nontraditional technologies, such as laser ionization and computer modeling.

The result is a wide array of research programs that spans several research disciplines. Many of these programs are described below.



Source: Office of Technology Assessment

### Microscopic Sequencing of DNA

If it were possible to take a picture of a DNA molecule, then the order of its bases might be easily determined. Dave Allison and Bruce Warmack, both of the Health and Safety Research Division, are taking this unconventional approach to sequencing DNA.

"Researchers in our group are using a new class of microscopes to develop sequencing technologies," Warmack says, "and, for the first time, we're enjoying a good deal of success at imaging complete DNA molecules." Allison and Warmack are working with two scanning probe instruments, an atomic force microscope (AFM) and a scanning tunneling microscope (STM), to

determine whether DNA strands can be imaged well enough to identify individual DNA base pairs.

The AFM drags a fine metal probe (about 10 to 50 nm in width—a fraction of the diameter of a human hair) across a sample bound chemically to a supersmooth surface. The AFM measures variations in the height of the probe as it is dragged across the surface of the sample using a laser focused on the probe's tip. After the AFM makes 400 passes across the sample at 1-nm intervals, the data it produces are converted to a computer-generated image.

The STM, in much the same way as the AFM, uses an electromagnetic probe to scan a sample at narrow intervals and construct a computer image of the resulting data.

Sample preparation for the AFM requires little more than evaporating DNA out of a water solution

"For practical purposes, think of the DNA molecule as a ladder with a strand of phosphate and sugar molecules on each side and pairs of bases between the strands for rungs."

An atomic force microscope (AFM) was used to create this image of gene-containing bacterial plasmid DNA. The twisted appearance of the plasmids is the result of the characteristic spiral structure of DNA molecules. (Micrograph by University of Tennessee Associate. Thomas Thundat)



onto a mica substrate, but a persistent problem with the STM has been developing a procedure for the routine preparation of samples. Because the substrate used with the STM must be an electrically conductive material, such as gold and mica, nonconductive materials with "sticky" surfaces have been ruled out. Recent progress in this area has been the development of an organic molecule that binds to both the gold substrate and the DNA.

The group has yet to determine exactly how they will distinguish among the various bases that make up DNA once they are imaged, although they have some schemes in mind. "Up until now," says Allison, "the challenge has been just finding a way to routinely see the DNA."

It appears their efforts are beginning to pay off; in October, the research group became the first in the world to image an entire genomic (gene-containing) molecule using an STM; in this case the molecule was a plasmid (a

circular DNA molecule) from an *E. coli* bacterium.

"We are also looking forward to using the STM to observe biological reactions as they occur," Warmack says. "No other microscope can do that."

#### DNA Sequence Analysis by Hybridization

Although it sounds rather mysterious, according to Bob Foote of the Biology Division, hybridization is simply the bonding of complementary pieces of DNA. The technique of sequencing by hybridization employs an array (a geometric arrangement) of short DNA segments of known sequence,

representing all possible sequences of a given length. An unknown sequence of DNA is broken into pieces, which are then added to the array. Theoretically, the pieces will "stick," or bond, to the complementary segments in the array. For example, because the DNA base A bonds with T and C bonds with G, the sequence A-C-T-G bonds with T-G-A-C.

Foote and his colleagues, including Rick Sachleben of the Chemistry Division, have proposed a way of making arrays of DNA segments to carry out many hybridizations simultaneously. "We had the idea of doing this on a microscopic scale with an array that measures

1 to 2 cm on a side," says Foote. "Considering that there are four different DNA bases and that we wanted to work with 8-mers (8-base-long pieces of DNA), we have 48, or 65,536, possible combinations of bases.

"If we tried to synthesize these combinations one at a time, it would take about half a million steps," says Foote. "Using photolithographic methods, the same process used to make microchips, we can synthesize them all in 32 steps."

To accomplish this feat, strings of bases are built up in stages by treating the array with DNA bases containing a photolabile (light-sensitive) blocking group. The bases bond to the array, and the blocking group prevents further reaction until it is removed from selected sections by exposing them to light. Then a second base is applied to the array, bonding only where the blocking group is absent. This process is repeated 32 times, producing a  $256 \times 256$  array of bases containing all possible 8-mer sequences.

containing all possible 8-mer sequences.

Once this process of synthesizing arrays has been mastered, Foote and his colleagues will label pieces of an unknown DNA sequence with radioactive or fluorescent tags and add them to an array. If everything works as it should, they will bond with their complementary sequences. The radiation or fluorescence of the unknown pieces bonded to the array makes possible the location and identification of the complementary sequence

to which the unknown sequence bonds.

"This process is not perfect," says Foote.
"Errors can occur in hybridization. For instance, the DNA base A could be paired with C instead of T. Depending on where the mismatch occurs, it may not be enough to disrupt the double-stranded structure of the DNA. However, most mismatches can be eliminated by doing this under stringent conditions, and the redundancy of this method allows a certain degree of error in the individual hybridizations."

When the hybridization is complete and the sequence of the unknown DNA segments has been determined, computational techniques are used to put these pieces back together to determine the sequence of the entire unknown DNA segment.

"Originally we were going to develop the techniques to do this ourselves," Foote says, "but



Bob Foote places a glass sample plate into the synthesis cell of a DNA synthesizer. The synthesizer manufactures specific sequences of DNA bases for use in hybridization research.

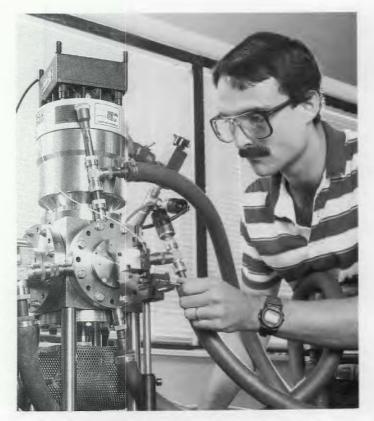
we found out that researchers at Argonne National Laboratory, who originated much of the theory behind this type of research, have developed some computer algorithms for determining the overall sequence. We've maintained contact with them for two years, and, when we can do some actual hybridization with our arrays, we may be doing something more formal with them."

For the near future, Foote's main focus will be on refining the chemistry of synthesizing the arrays to improve the efficiency of these steps. "Once we get the chemistry done," says Foote, "we'll be testing the accuracy of hybridization on these small arrays and working with Jack Davidson of the Instrumentation and Controls Division and others at ORNL on detection methods."

## It Slices, It Dices, It Sequences DNA

ORNL's portable ion trap is rapidly becoming the high-tech equivalent of the Veg-A-Matic<sup>®</sup>. This versatile device, which is also used to sniff out explosives and analyze water and soil samples, is now part of a highly sensitive method of sequencing DNA.

"ORNL's portable ion trap is rapidly becoming the high-tech equivalent of the Veg-A-Matic."



Scott McLuckey and his colleagues have used their ion traps for everything from sniffing out explosives to sequencing DNA. Here McLuckey adjusts one of the traps in preparation for analyzing ionized DNA fragments.

Scott McLuckey, Gary Glish, Gary VanBerkel, and Rose Ramsey, all of the Analytical Chemistry Division, use a technique called electrospray ionization to ionize DNA fragments for analysis in the ion trap. There they are subjected to multiple stages of mass spectrometry, which separates them according to mass and charge.

The electrospray process involves dissolving the DNA fragments in a solvent (usually water) and then sending them through a high-voltage needle. At the end of the needle, the solution becomes electrostatically unstable, breaking into a fine mist or spray of charged droplets, known as an electrospray.

"Electrospray is an extremely soft ionization method," McLuckey says. "Historically, it has been very difficult to ionize DNA because it is very fragile. Most ionization methods require an energetic beam—a laser or an ion beam. This type of process usually transfers enough energy to the DNA's internal structure to cause it to break into pieces. We get around this problem by tricking the ion into entering the gas phase in the form of a charged droplet. When the solvent evaporates, a bare ion is left."

As these droplets dry off, their surface charge becomes very large and the ions are desorbed. The ions are then injected into the ion trap, which provides a mass spectrum. "From this spectrum, you can determine the molecular weight of the sample," says McLuckey. "It turns out that all combinations up to 14 bases have unique masses, so once we know the mass, we can determine the base composition—but not the order."

The order of the bases is determined by selecting a DNA ion and energizing it until it breaks into pieces. By analyzing how the ion falls apart, the sequence of its bases can be determined. Repeating this process with other ions allows the

entire DNA fragment to be sequenced.

Currently, this approach can handle sequences up to 12 bases long without any serious technical problems. "We're really a long way from sequencing sections of DNA as large as 500, but that's our goal," says McLuckey. "This research is less than a year old, so we're working our way up."

The value of this method lies not only in its potential as a sequencing tool but also in its ability to determine the precise composition of a sample. For example, some DNA bases are modified by methylation, a condition known to influence certain cell characteristics, although how this occurs is not well understood.

"Other techniques used to sequence DNA typically cannot identify a modified base," says

McLuckey. "Using mass spectrometry, the modified base stands out like a sore thumb.

"Down the road, the most valuable aspect of this technique may be its applications for locating and identifying modified DNA. I think it will probably be highly useful in cancer research once the genome is sequenced—once we know what's right, this will be very useful in identifying what's wrong."

#### Sequencing by Fourier Transform Mass Spectrometry

Another variation on the theme of sequencing by mass spectrometry is offered by Bob Hettich and Michelle

Buchanan, both of the Analytical Chemistry
Division. While most approaches to sequencing
DNA using mass spectrometry focus on measuring
molecular masses, Hettich and Buchanan are
applying Fourier transform mass spectrometry
(FTMS) to investigating the structure of modified
DNA segments. The ion-trapping and manipulation
capabilities of FTMS combined with its highly
accurate measurement capabilities suggest that this
technique has tremendous potential for
investigating the structure of organic molecules.

The fragile nature of DNA molecules makes them difficult to study using conventional mass spectrometry. Hettich and Buchanan are avoiding this problem by using a technique known as matrix-assisted laser desorption, originally developed for examining proteins and peptides. For this method, the DNA segments are first mixed with a matrix compound (nicotinic acid) and then dried onto the tip of a stainless steel probe. The mixture is then desorbed with a 266-nm beam from a Nd:YAG (neodymium: yttrium aluminum garnet) pulsed laser.



Bob Hettich and Michelle Buchanan examine a DNA sample disk before it is placed in the FTMS for laser desorption.

Because the nicotinic acid strongly absorbs electromagnetic radiation at 266 nm, it serves as a buffer between the laser and the DNA, allowing the DNA segments to be carried into the gas phase with minimal fragmentation. The resulting DNA ions are then trapped in the FTMS cell where they can be studied in detail to determine their molecular weights and sequences.

Once the molecular weights of the ions have been determined, they can be selectively fragmented by filling the FTMS cell with argon gas and studying the resulting collisions between the ions and the argon molecules. The fragmented ions provide detailed information about the sequence and structure of the original DNA segment. This approach has been used successfully to determine the sequence of segments up to six bases long. Improvement of the process should allow detection and characterization of even larger segments.

In addition to determining the order of bases in each DNA segment, this process also determines the types and locations of chemical modifications "The main thrust of studying modified bases is to understand the molecular changes that occur in DNA as a result of cancer or mutation."

Number One, 1992 27

"We may be able to do separations that used to take several hours using gel electrophoresis in less than than one

second."

of the DNA, such as the addition of alkyl groups to the DNA bases. "The main thrust of studying modified bases is to understand the molecular changes that occur in DNA as a result of cancer or mutation," Hettich says.

Currently, research is focused on two specific tasks. First, Hettich and Buchanan want to optimize the matrix-assisted laser desorption technique to allow investigation of larger DNA segments. "Nicotinic acid absorbs energy well at 266 nm," says Hettich, "but, unfortunately, so does DNA. The trick is to find another suitable laser matrix that absorbs energy well at a wavelength at which DNA does not. This should allow us to desorb larger pieces of DNA without them breaking up."

Secondly, they want to extend the instrumental capability of the FTMS to detect and examine larger DNA ions. "Developments in matrix-assisted laser desorption FTMS," Hettich says, "should help determine the potential of this technique for the measurement and structural characterization of large DNA fragments required for DNA sequencing."

#### **VUV Mass Spectrometer Shows Promise**

One of the more unlikely players in the DNA sequencing game is Winston Chen of ORNL's Health and Safety Research Division. "We had been using lasers to do research in the physical sciences," Chen explains, "and we wanted to see if we could expand into biological and environmental research."

Chen, Marvin G. Payne, also of the Health and Safety Research Division, and Bruce Jacobson of the Biology Division are developing a new high-resolution mass spectrometer equipped with a vacuum ultraviolet (VUV) photoionizer to sequence ferrocene-tagged DNA. This approach could eliminate the need for both gel electrophoresis and radioactive tagging while sequencing DNA segments that are thousands of bases long.

In this procedure, a primer (a small molecule to which DNA bases are added) is labeled with an organometallic compound, such as ferrocene. Then new DNA segments that terminate at each occurrence of a particular DNA base (A, G, C, or T) are built up on the primer using the original DNA as a template.

To ionize these fragile molecules without breaking them up, the group is using a technique known as laser desorption from a cryogenic matrix. In this technique, DNA segments are placed on a thin layer of solid argon that has been cooled to about 20 K on a cryogenic copper finger. A laser is then used to warm the finger to 100 K, causing both the argon and the DNA to vaporize and flow into the ionizer. Argon's low vaporization point makes fragmentation of the DNA segments during ionization very unlikely. Chen and his colleagues have sequenced DNA segments up to 34 bases long with a single laser pulse using this method. The system they are developing has 50 times the resolution of the current system and is expected to be able to sequence DNA segments up to 103 to 105 bases

When the DNA segments reach the ionizer in the new system, they will be ionized by a weak vacuum ultraviolet (VUV) beam. Preliminary studies on other fragile organic molecules indicate this process is very unlikely to result in fragmentation of the DNA segments. Also, this method has the advantage of being energetic enough to ionize ferrocene-tagged DNA, but not energetic enough to ionize untagged DNA or other possible impurities.

Finally, DNA ions resulting from VUV ionization are sent on to a high-resolution time-of-flight mass spectrometer where their masses and sequences are determined. "This type of mass spectrometer makes possible a greater separation between pieces of DNA at the detector," Chen says, "and makes it easier to distinguish between segments that differ by only one base."

The value of this novel technique is its potential for improving efficiency on several fronts. "This method has the potential for sequencing 10,000 times as many bases as gel electrophoresis," says Chen. "Our technique could also significantly reduce preparation time

and processing time and avoids the use of gels, radioactive materials, and fluorescent dyes.

"For instance, with gel methods the speed of molecules can be measured in meters per hour. Using the vacuum method, the speed can be measured in kilometers per second. As a result, we may be able to do separations that used to take several hours using gel electrophoresis in less than than one second."

#### Supercomputer Analysis of DNA-Carcinogen Interactions

It is widely believed that the process that leads to cancer can be initiated when certain biochemically active chemicals bind to DNA to form a combination molecule called an adduct. This reaction can disrupt the normal double-helical shape of the DNA, causing mutations when the DNA replicates, when the cell's DNA repair mechanisms fail to work properly, or when other unusual genetic events start the cellular process that leads to the development of cancer. As a result, an understanding at the atomic level of the effect of chemicals on DNA structure is critical to understanding chemical carcinogenesis.

Researcher Brian Hingerty of the Health and Safety Research Division describes the challenge of determining the relationship between various chemicals and cancer: "If one could establish structural hallmarks that distinguish DNA bound by a malignant chemical from DNA bound by a benign one, it might be possible to employ computational tools instead of bacterial or animal testing to screen chemical substances for mutagenic and tumorigenic potential."

One chemical substance of particular interest is benzo[a]pyrene, a material present in automobile exhaust and, therefore, common in the



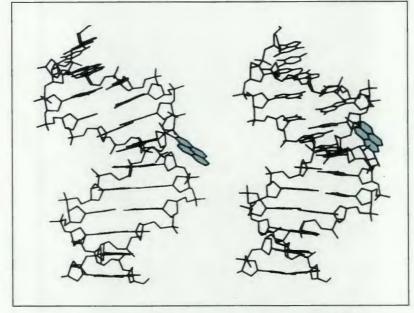
Kai Tang, a doctoral student in physics from Vanderbilt University, adjusts the optics of a laser used to vaporize DNA segments in the mass spectrometer's sample chamber.

environment. Once ingested, this chemical becomes activated, forming a number of derivatives, including a pair of mirror-image molecules called (+) and (-) antibenzo[a]pyrene-diol-epoxide (BPDE).

Interestingly, these mirror-image molecules have very different biological effects; in studies with mice, the (+) version has proven to be tumorigenic, whereas the (-) variant is apparently benign.

Both of these molecules can bind to DNA at the amino group of the base, guanine. In fact, this particular type of BPDE-bound DNA is the most common adduct formed by the tumorigenic (+) BPDE and is believed to be responsible for benzo[a]pyrene's carcinogenic effect. Determining at the atomic level how this (+) adduct differs in structure from its benign (-) mirror image is a first step in understanding why these two chemicals have such divergent biological properties.

Using computer-modeling methods at DOE's National Energy Research Supercomputer Center at Lawrence Livermore National Laboratory, Hingerty and his collaborator,



The computed structure (shown in color) of the (+) anti-BPDE DNA adduct (left) and the (-) anti-BPDE DNA adduct (right) aligned in opposite directions in the "minor groove" of double-helical, right-handed DNA.

"An understanding at the atomic level of the effect of chemicals on DNA structure is critical to understanding chemical carcinogenesis."

Professor Suse Broyde of New York University, explored the differences between the two adducts by determining the molecular structure of both chemicals in a short piece of DNA. They found that both the (+) and (-) versions of BPDE are positioned in the "minor groove" of double-helical, right-handed DNA; however, they point in opposite directions.

This structural difference between the two bound adducts could produce different treatments by the enzymes involved in DNA replication and damage repair, resulting in only one of the adducts being tumorigenic. "Our future plans," says Hingerty, "include examining other substances related to the benzo[a]pyrenes, some of which are tumorigenic and others not, to learn whether the distinction we have uncovered is more general."

#### Luminescent Labeling for DNA Sequencing

The need for labeling and detection methods that could be easily automated to greatly increase the rate of sequencing DNA fragments is the

motivating factor behind the luminescent labeling system being developed by Gilbert M. Brown of the Chemistry Division. The system uses the lanthanide ions samarium(III), europium(III), terbium(III), and dysprosium(III), bound by a chelating agent, as labels for the four DNA bases.

Luminescence from these rare-earth ions is generated by exciting the napthalene group attached to the chelating agent. "This is an energy transfer process," says Brown. "We shine a light on the napthalene, which has a long-lived excited

state. It eventually gives up this excitation energy to the lanthanide ion, which responds by emitting light." Because of the way the lanthanide ions are linked to napthalene, a single wavelength of light can excite all four labels, each of which emits light of a characteristic wavelength.

DNA fragments are conventionally labeled with radionuclides, such as sulfur-35 or phosphorus-32. The labeled fragments are then separated by electrophoresis, and the position of each fragment is detected by autoradiography. This approach provides high sensitivity for detection but also presents problems, including the potential for radiation exposure, high disposal costs, and limited shelf lives of radionuclides. Using lanthanide ions eliminates these problems.

Lanthanide ions offer several advantages over the fluorescent organic dyes currently in use. The fluorescent dyes have emission bandwidths that overlap, sometimes making it difficult to distinguish between bases. The emission bandwidths of the lanthanide ions are narrow, even at room temperature in fluid solution, allowing them to be detected simultaneously with minimum overlap.

"We are interested in designing a labeling system in which multiple labels could be detected simultaneously," Brown says. "From the sharp nature of the emission spectra, these elements appear ideal for detection."

Because the lifetimes of the excited states of these ions are relatively long, emission detection can be time-gated, virtually eliminating signals from background sources. "In time-gated detection, a pulsed excitation source allows a time delay between excitation and detection," says Brown. "After excitation, we delay turning on the detector until sources of interfering light, such as scattered excitation light, Raman scattering, and impurity fluorescence have died down, allowing us to identify bases with greater accuracy."

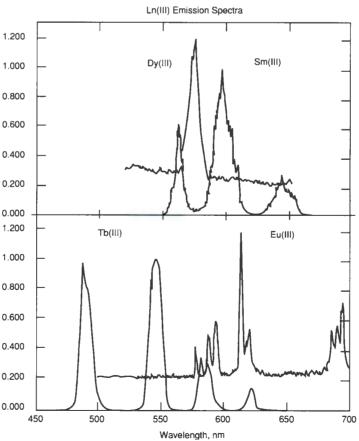
Another advantage of this system is that it is compatible with both capillary gel electrophoresis, which is considerably faster than conventional sequencing using slab gel electrophoresis, and computer collection and analysis of sequence data. "We'll be able to use a computer to look at the luminescence of the labeled DNA as it goes by," says Brown. These factors, combined with the certainty provided by the sharp spectral emission lines of the lanthanide ions, should provide a sequencing rate that is considerably higher than that achieved using conventional methods.

"This is the poor man's way to increase sequencing rates," Brown says. "It's not the fastest method around, but for researchers who don't have a half million dollars' worth of equipment, it ought to be a big improvement."

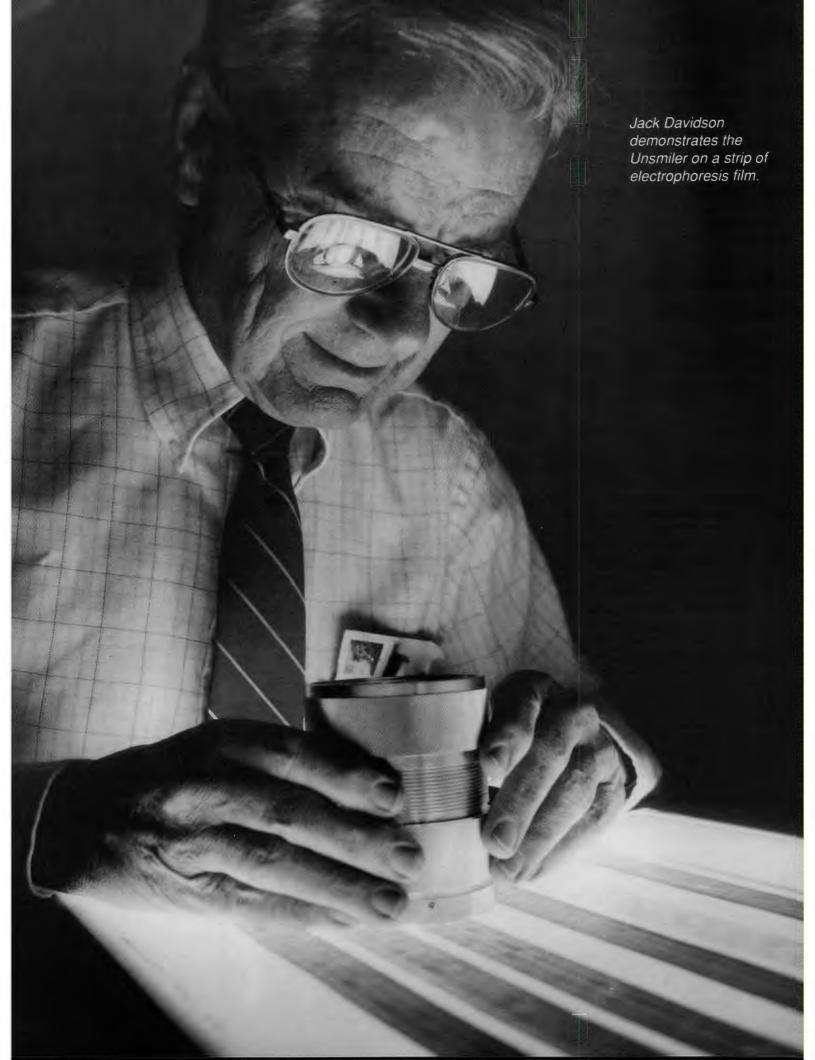
## Jack-of-All-Trades Approach to Sequencing Instruments

Jack Davidson of the Instrumentation and Controls (I&C) Division is hedging his bets on sequencing techniques by working on instrumentation for three different approaches: conventional electrophoresis film methods, a relatively new method known as sequencing by hybridization, and his idea for a high-speed gelless system.

For the conventional film method, his goal is to develop an inexpensive semiautomatic scanner that will read the sequence of DNA



The narrow bandwidths of the four lanthanide ions allow the corresponding bases to be easily distinguished, even in solution at room temperature.



bases quickly and directly from film without using sophisticated software and computing. A prototype now under construction is aimed at individuals and smaller groups who don't need or can't justify the more elaborate automated systems.

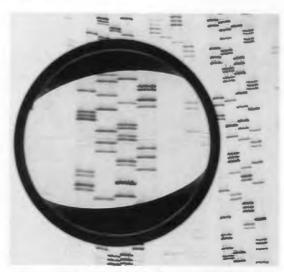
A couple of unforeseen by-products have resulted from Davidson's research in film sequencing methods. Working with Wil Allen of I&C and Reggie Miles of the Plant and Equipment Division, he has developed the Unsmiler and the Undimmer. The Unsmiler was developed in response to a condition known as "smiling" that occurs when the parallel bands on the film become tilted, making it difficult to visually determine their sequence. The Unsmiler is a hand-operated combination of lenses that both magnifies and "unsmiles," or straightens out, the bands, making them easier to sequence and improving the definition of closely spaced bands.

The Undimmer tackles the problem of lowcontrast, hard-to-read films by supplying a method of doubling the contrast of faint images, allowing these objects to be detected faster and more easily. The Undimmer uses a reflector under the film, rather than a light box. As a result, the viewing light comes from above and passes through the film twice rather than once, doubling the apparent density of objects on the film. The color of the reflector (yellow) is chosen to match the peak of the eye's photopic sensitivity, further enhancing the effect. Davidson also envisions possible applications of the Undimmer in medical and industrial radiography where it is desirable to see faint objects on a nearly transparent film background. In a recent demonstration of the device for the Oak Ridge Radiology Group, the Undimmer was used to turn a discarded, substandard mammogram into a "good, readable film," according to one radiologist.

In sequencing by hybridization, Davidson is lending his support to the research efforts of Bob Foote of the Biology Division. Foote's research involves synthesizing all possible combinations of 8-base-long sequences of DNA (8-mers) and arranging them on a slide in a known pattern. An



A strip of film viewed through an ordinary magnifier exhibits a curvature known as "smiling," caused by the unequal migration of DNA fragments.



The same film viewed through the Unsmiler. The sequence of the fragments is easier to determine when the "smiling" has been corrected.

unknown DNA sequence is then added to the slide where it hybridizes, or "sticks," to the corresponding 8-base-long sequences that are already there.

Because the unknown DNA is labeled with a radioactive or fluorescent tag, all of the 8-mers that make up the unknown segment should be detectable, and, in theory, their order in the

"The Undimmer was used to turn a discarded, substandard mammogram into a 'good, readable film.'"

unknown DNA could then be computed. From this information, the sequence of the entire unknown DNA segment can be determined. Davidson, using his "lensless" radiation microscope, which employs a combination of scintillators, fiber optics, and low-light-level television, is trying to develop a high-resolution, position-sensitive detector to locate and identify the hybridized 8-mers.

Finally, Davidson, with the help of Diedre Falter of the I&C Division and David Donohue, formerly of the Analytical Chemistry Division, is working on a high-speed, gel-less sequencing system that could potentially improve sequencing speed by orders of magnitude. Instead of the slow conventional method of separating DNA fragments in a thin layer of gel, the fragments would be separated by a time-of-flight mass spectrometer in milliseconds instead of hours. The sequence could then be determined by order of finish in a race over a known distance. Although much work remains to be done, the approach shows considerable promise, as evidenced by related approaches begun independently in other laboratories.

## **Intelligent Computer Tracks Down Genes in DNA Sequences**

The sequence of DNA bases that makes up the human genome is a coded message containing a huge amount of information. However, after sequencing a region containing a single gene out of perhaps 100,000 genes in the genome, the result is a string of thousands of A's, G's, T's, and C's, from which biological meaning must somehow be derived. Separating the biologically relevant information from the rest of the sequence is further complicated by the fact that only 3 to 5% of the bases in the region of a gene actually contain instructions for the manufacture of proteins—the molecules that govern the chemical processes necessary for life. Determining which portions of the sequence are biologically relevant is a significant challenge in this area of research.

Although the technology to locate these relevant sequences, or "exons," is critical to the success of the Human Genome Project, it has

never been clear how this would be accomplished or even if it would ever be possible. However, ORNL researchers Richard Mural of the Biology Division and Ed Uberbacher, Ralph Einstein, Reinhold Mann, and Xiaojun Guan, all of the Engineering Physics and Mathematics Division, have taken a major step toward putting the pieces of this puzzle together.

They have developed an intelligent computational system called GRAIL (Gene Recognition and Analysis Internet Link), which integrates biological insight into a state-of-theart, computer-based artificial intelligence system. Mural characterizes the effort as "a hybrid effort combining the computational and biological sciences—a realm of science that ORNL has not dealt with before."

"At a basic level, there's a new kind of biology going on here, based on genetic sequence data in which all the information used by living cells is stored." Uberbacher says. "Learning how to computationally extract the important biological information stored in these sequences is a tremendous challenge with great rewards." So far, ORNL researchers have correctly predicted the locations of at least 80% of the genes in the 5 million bases they have analyzed. The team's work was featured in the November 8, 1991, issue of *Science* magazine.

The GRAIL system first analyzes a genetic sequence using a group of mathematical algorithms that measure properties of DNA sequences that code for proteins and then combines the results of these algorithms using a neural network. "A neural network is a computer simulation of how neurons in the brain function and learn to recognize objects," Uberbacher says. "Machine learning is accomplished in the neural network by showing the system many examples of exons. Eventually the network learns the characteristics that distinguish exons from the rest of the DNA sequence." After its "training" process, the neural network learns how to identify exons in uncharacterized regions of sequence.

"What distinguishes our approach is that we are combining many features of sequences that are known to encode proteins," says Mural. "We become partners in the neural network," says Uberbacher. "We provide what we know about the biology of exon sequences, and the neural network learns how best to use the information—each partner contributes knowledge to the process."

Although traditional statistical and mathematical methods exist for analyzing sequences, these often result in large numbers of "false positives"—areas identified as exons that really are not. Because each area identified as "positive" must be experimentally verified, there is a premium on selecting an effective, yet conservative, method of analysis—one that locates a high percentage of the total number of exons, with a low false positive rate. The GRAIL system provides such a method.

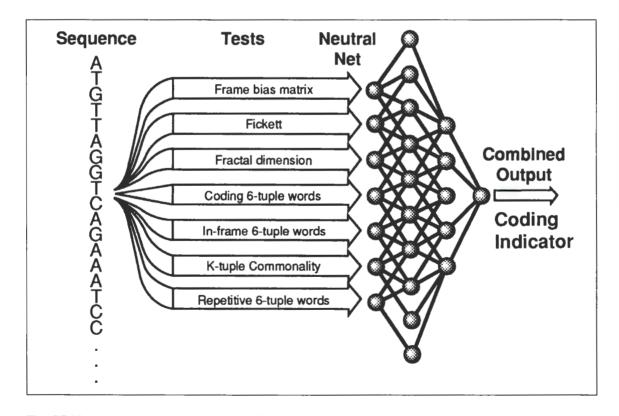
Recently, GRAIL was used to analyze a sequence of bases thought to contain the

Huntington's disease gene. The system located a number of potential exons, clustered in such a way as to suggest several genes. Subsequent experimental work based on GRAIL's predictions has verified exons at 80% of the predicted locations. Once the location of an exon is found, a combination of experimental and informational techniques can be used to determine the portion of the sequence that makes up the gene.

To encourage researchers outside ORNL to take advantage of GRAIL, users can send electronic mail files of DNA sequences directly to the system and it will automatically e-mail its analysis back. Turnaround time is usually only a few minutes for sequences containing fewer than 100,000 base pairs, and single or multiple sequences may be sent.

Over 200 laboratories worldwide currently take advantage of the GRAIL system in their search

"We provide what we know about the biology of exon sequences, and the neural network learns how best to use the informationeach partner contributes knowledge to the process."



The GRAIL system analyzes sequences of DNA bases using seven algorithms or tests to determine the likelihood that a given sequence contains all or part of a gene. A neural network then combines the results of these analyses to identify relevant portions of the sequences.

"Studying the mouse genome could provide some of the missing pieces of the genomic puzzle."





Insertional mutagenic techniques were used to create the mutation seen in the mouse paw on the left, known as polydactyly of the thumb. The equivalent human condition is shown on the right. When the location of the gene responsible for the mouse mutation is determined, researchers may be able to look at the corresponding area on a human chromosome and locate the functionally equivalent human gene. Photo on right is from Beighton, Peter, *Inherited Disorders of the Skeleton*, Churchhill Livingstone, 1978.

for the causes of genetic diseases such as Huntington's disease, various muscular dystrophies, and fragile X syndrome. Mural attributes GRAIL's increasing popularity to its ease of use. "It's very simple for the users. They can do some very simple procedures and get some highly interpretable results."

According to Mural and Uberbacher, the future holds an upgraded version of GRAIL that will incorporate feedback from the system's users. They are also working on a companion system to GRAIL that will allow users to assemble model genes from the exons found throughout the sequence, using a machine-learning approach similar to that employed by GRAIL.

## Of Mice and Men: Probing the Mouse Genome

Rick Woychik of the Biology Division can tell you almost anything you want to know about mouse genes. So, what does this have to do with sequencing the *human* genome? Well, as it turns out, there are a number of similarities (perhaps more than we'd like to admit) between mouse genes and human genes. And, as a practical matter, it's a lot easier to conduct a controlled study of a mouse in a lab than a man on the street.

Woychik looks at efforts to sequence the human genome as the first step in understanding

how the genetic code actually works. "Once we've sequenced and analyzed all the DNA bases of the human genome," he says, "we will know where all the genes are, but we won't know what they do." Studying the mouse genome could provide some of the missing pieces of the genomic puzzle.

"If we determine the function of a particular mouse gene whose location we know," Woychik says, "we can often look at the corresponding area on a human chromosome and locate the functionally equivalent human gene."

One of the techniques Woychik uses to probe the mouse genome is known as insertional mutagenesis. In this technique, hundreds of identical pieces of DNA are injected into mouse zygotes (fertilized eggs) in the hope of creating mutations in the resulting offspring. The DNA fragments, or "transgenes," are then incorporated, seemingly at random, into the zygote's genetic code. More often than not, this process results in normal laboratory mice, but every so often an unusual variation in the appearance or physical structure of one of the offspring, such as malformed limbs or internal organs, suggests that a mutation has occurred. "When we see an abnormality in the appearance of the offspring," Woychik says, "we test to determine whether the gene that was interrupted by a transgene is responsible for the change in appearance."

Another technique used to investigate the function of various mouse genes is known as targeted mutagenesis. In contrast to the random mutations introduced by insertional mutagenesis, targeted mutagenesis allows researchers to determine the effect of introducing a mutation at a specific site on a selected gene.

This degree of accuracy is achieved by introducing changes in the chromosomal DNA of cultured embryonic cells using a process called homologous recombination. In this approach, altered genetic material is inserted back into the context of a living mouse by microinjecting the manipulated cells into a host blastocyst (a 4-day-old mouse embryo).

Uncovering all the functional parallels between the genes of mice and humans could easily occupy several research lifetimes, but Woychik and his group have a more modest goal. Says Woychik: "We hope we can begin to establish molecular connections between individual genes on the genome and specific developmental processes in both mice and men."

## The Mouse as a Model For Human Genetics

Gene Rinchik and his group in the Biology
Division investigate mouse-human homologies—
mouse genes that are functionally equivalent to
human genes. "Geneticists have found that the
human and mouse genomes are very similar,"
says Rinchik, who has spent the past 13 years
working with mice. "We have also found that
research into the mouse genome can answer a lot
of questions about the human genome because
large blocks of genes have been conserved
throughout evolution and remain remarkably
similar."

Because the mouse is well understood genetically, easy to work with, and similar to humans in many ways, including genome size and structure, it has become the major model for the study of human genetics and biology. Rinchik's group is analyzing about 2 to 3% of the mouse genome. "That doesn't seem like much progress," Rinchik says, "but we're also trying to determine the function of individual genes in the sequence as we go."

The aim of Rinchik's research is to develop physical, functional, and mutation maps for the mouse genome and to use this information to predict the functions of the corresponding regions of the human genome. "You can't determine this information simply from sequencing the bases in a segment of DNA," Rinchik says. "Sequencing can provide important information on products of certain genes and reveal their biochemical functions, but it does little to predict the function of the gene product in the whole organism."

To determine how a gene functions in the organism as a whole, Rinchik uses heritable mutations that alter the quality or quantity of the gene product and studies the effect of these alterations on the whole organism. One approach

"Continued research into these genomic similarities may eventually permit a "surrogate" human genetics to be developed in the mouse."



Gene Rinchik and research assistant Linda Taylor display one of the quarter-million mice in ORNL's Biology Division. The study of functionally equivalent genes in mice and humans may enable researchers to identify the genetic components of many human genetic diseases.

to inducing mutations is to use chemical mutagens to introduce point mutations along a section of DNA that contains genes of interest.

"We look at the effect of the mutations on the mouse's whole life cycle—from fertilization, through fetal development, and into reproductive life," says Rinchik. "Unfortunately, because of space limitations, we usually can't keep the mice around long enough to study late-onset diseases or other conditions related to aging."

Another approach is to use radiation to delete pieces of DNA from a particular region of the mouse genome. This type of mutation is being used to study a set of human genetic diseases called contiguous gene syndromes. These syndromes are usually attributed to genetic deletion, resulting in missing sections of DNA. One of these diseases, known as Prader-Willi Syndrome (PWS), occurs in children and is

characterized by a range of symptoms, such as delayed development, feeding problems in infancy, lack of muscle tone, obesity, hypopigmentation, and small hands and feet. Any or all of the symptoms may be present in a PWS child.

Rinchik and his group are analyzing deletion in mice having symptoms that are somewhat similar to those observed in PWS children. By determining the locations of these deletions in mice, researchers hope to identify the individual genetic components in the human genome that contribute to PWS.

Continued research into these genomic similarities may eventually permit a "surrogate" human genetics to be developed in the mouse, accelerating the development of both physical and functional maps of corresponding regions of the human genome.

### **Human Genome Management Information System**

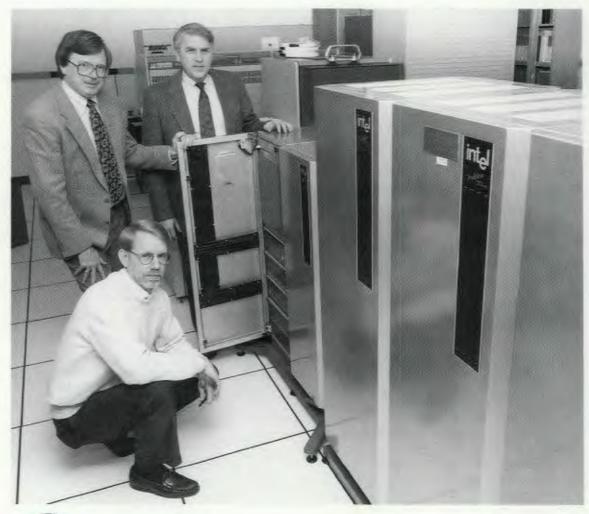
Providing behind-the-scenes assistance for much of the DNA mapping and sequencing research at ORNL and elsewhere is the Human Genome Management Information System (HGMIS) of the Health and Safety Research Division. Sponsored by both DOE and the National Institutes of Health, HGMIS helps communicate genome-related issues and research to contractors, grantees, and the public, and it provides a forum for information exchange among researchers in both the DOE Human Genome Program and the international Human Genome Project.

In the course of this work, HGMIS produces workshop reports; a bimonthly newsletter, *Human Genome News*; and a traveling exhibit; and it provides administrative support to genome-related projects. A textual data base of information on the human genome is also being developed.

HGMIS invites comments and suggestions from the research community and the public about its documents and services, which are available upon request and without charge.

# ORNL as a Supercomputer Research Center

By Jim Pearce



Richard Sincovec (left), Bob Ward, and Michael Leuze (front) at the Intel iPSC/2 and iPSC860 parallel computers, forerunners of the new Paragon supercomputer at ORNL.

RNL has been chosen as one of two Department of Energy high-performance computing research centers; the other is Los Alamos National Laboratory. The purpose of the centers is to enable scientists to explore the applications of new, high-performance computer systems to areas of scientific, economic, and environmental importance. The two centers will also support both interdisciplinary work and collaborations among institutions.

ORNL researchers will use a new highperformance parallel computer to design new materials and alloys and to model the movement of pollutants in groundwater. The computer is also expected to be used to solve other complex scientific problems classified as "Grand Challenges."

The establishment of a supercomputing research center at ORNL, called the Center for Computational Science, is the culmination of an effort to restore the Laboratory's position as a leader in computing research, a position it held throughout the 1950s. "In 1983, ORNL decided to pursue parallel computing," says Bob Ward, director of the Engineering Physics and Mathematics (EPM) Division. "We decided that there was no reason to try to compete with the traditional supercomputing groups using vector computers at Los Alamos and Lawrence Livermore

national laboratories. We simply moved on to the next technology—parallel computing. ORNL Director Al Trivelpiece deserves a lot of the credit for our success because he accelerated the use of this new technology by our computational scientists, which was one of the deciding factors in the competition."

"The competition was very tough because our competitors had great resource advantages," said Trivelpiece. "So I am pleased that ORNL was one of the two sites selected."

The ORNL center will be a collaborative effort among three DOE facilities—ORNL, Ames Laboratory, and Brookhaven National Laboratory—and six major universities: UT, Vanderbilt University, Rice University, State University of New York at Stony Brook, Texas A&M University, and the University of South Carolina. The Oak Ridge center will also work with Sandia National Laboratories on supercomputer-based mathematics and science education programs.

"In terms of doing scientific computing on parallel machines, we have the best staff of any group in the country," says Ward. "All of our partners in the new center have put their top researchers and scientists on the project."

This summer, ORNL will receive the latest thing in number crunching—a prototype of a Paragon supercomputer from Intel Corporation of Beaverton, Oregon. This "massively parallel" computer will be installed in stages and should be complete by mid-1993. The ORNL computer and a Thinking Machines CM-5 being installed at Los Alamos are expected to be the two most powerful parallel computers in existence.

The Intel iPSC/860 that has been used for parallel computing at ORNL until now is scheduled to be traded in on the new machine, but Intel has indicated they will donate the machine to UT. It will remain at the Laboratory for the use of ORNL researchers and UT students and faculty and will be used to develop and debug programs for the Paragon.

### What is Parallel Computing?

Today, the term massively parallel refers to computers that have 1000 or more processors

working together, or "in parallel." The Paragon supercomputer has 2000 processors, whereas its predecessor, the Intel iPSC/860, has only 128.

"Actually, it would be easier for the researcher to work with a single processor," says Al Geist, a computer scientist in the EPM Division. "There's a great deal of work to be done by the computer scientist who has to divide up a problem for solution on a parallel machine. It's like building a house—you can do it all yourself, working on one thing at a time, or you can get a bunch of people to help you. If you have people helping you, you have to decide who's going to do what so everybody isn't running into each other."

Interest in parallel processing has increased in recent years because of two major barriers to building single-processor machines to handle massive amounts of data. First, the speed of processors is limited—electrons can move no faster than the speed of light. Processing speed can be increased by miniaturizing the processors, thereby shrinking the distance the electrical signals must travel, but the cost of these microcomponents can be prohibitive. Not surprisingly, the second factor is cost. "You could build a machine with a single processor that is just as fast as one with 1000 processors," says Geist, "but it might cost 100 times as much."

"The price of parallel machines is lower because they use lower-tech chips than single-processor supercomputers," says Malcolm Stocks of the Metals and Ceramics Division, "but they use lots of them, and they are connected very efficiently. These chips are similar to those currently used in computer workstations."

Despite these attractive advantages, parallel computers are not likely to become the computational equivalent of the Swiss Army knife. "They can't do everything," says Stocks. "Parallel machines are best-suited for problems that involve massive computation and minimum communication between processors. Researchers have to learn how to restructure their problems to take advantage of this computational power.

"That's the refreshing thing about parallel architecture—it often forces you to rethink the whole way you do things," says Stocks. "It's a bit of an amusing business."

"This is a great chance for people from different disciplines to work together and make something happen that none of us could do individually."

## Supercomputers and Superconductors

The Paragon supercomputer promises to dramatically expand the boundaries of modeling for researchers like Stocks. "Currently, several areas of inquiry in materials science are limited by computing power," he says. "This is because the computing power required to model a system of electrons and nuclei is roughly equal to the cube of the number of atoms in the system. So, if we have been modeling a system of 2 atoms and we decide to look at a system of 20 atoms, increasing the size of the system by a factor of 10, the amount of computing power required will be 10<sup>3</sup>, or 1000, times greater."

Materials researchers use supercomputers to study the structure of disordered materials whose normal structure has been disrupted by the substitution of one type of atom for another. This kind of disorder occurs in scientifically important materials, such as high-temperature superconductors and metallic alloys.

"Supercomputers allow researchers to construct complex models of the forces that come into play on the atomic level in these materials," Geist says. "This technique has already resulted in a clearer understanding of the basic properties that are responsible for superconductivity."

Another advantage of increased computing power is that interactions between atoms can be modeled more accurately. "At one time, we used very simple models to study interactions between atoms, based on simple interactions between pairs of atoms," Stocks says. "Now, parallel processing enables us to use quantum mechanics to model atomic interactions with much greater precision.

"Of course, the more precise you make it, the more rapidly you run out of computing power. But if you want to model the details of how atoms interact, you have to use quantum mechanics. Otherwise, you'll never convince yourself that you've solved the problem properly."

### **Groundwater Modeling**

The new supercomputer will also be used to develop more sophisticated models that describe the transport of hazardous waste in groundwater. Using a prototype model called P-FEM, which has been adapted for use in a parallel computing environment, Laura Toran and Libby Reyes, both of the Environmental Sciences Division, and EPM

computer scientist Ed D'Azevedo are preparing to model groundwater transport in ORNL's Melton Valley.

"This is a great chance for people from different disciplines to work together and make something happen that none of us could do individually," says Toran in support of the center's interdisciplinary approach. "There aren't many places that offer both the opportunity and the funding for this kind of project."

The sheer computational power of the new machine will allow complex processes, such as groundwater transport, to be studied in much greater detail. "In the past, we've tried to model groundwater flow and

Al Geist (left) and Malcolm Stocks discuss the advantages of using the new Paragon computer for alloy design.



geochemical reactions," Toran says, "but when we tried to include several chemicals and reactions in the model, we ran into computing limitations. The supercomputer will allow us to model more processes in much greater detail.

"For example, most groundwater models have been two-dimensional or were very limited in the third dimension. Now we'll be able to look at an area with a real three-dimensional model and answer questions like, 'How does groundwater flow in tilted bedding?,' 'What is the relative importance of physical, chemical, and biological processes for transporting dissolved substances?,' and 'How can we simplify the

models we run on non-parallel computers?"

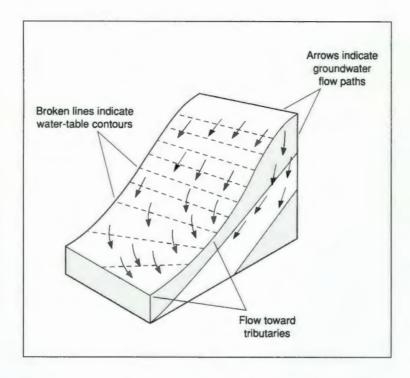
Eventually Toran hopes to be able to model other more complex physical processes, such as the underground movements of dense, non-aqueous liquids, such as the commonly used solvent trichloroethylene and oils containing polychlorinated biphenyls (PCBs).

### **Grand Challenges**

A Grand Challenge is "a fundamental problem in science or engineering, with potentially broad scientific, social, and economic impact, that could be advanced by applying high-performance computing resources."

Researchers from ORNL, UT, and other organizations who have been working with the Intel iPSC/860 to address portions of several Grand Challenge problems are expected to continue this work on the new Paragon supercomputer. Some of these Grand Challenges are:

 Particle physics—simulating particle interaction processes for the development of massive detectors for the Superconducting Super Collider. Designing experiments to study the



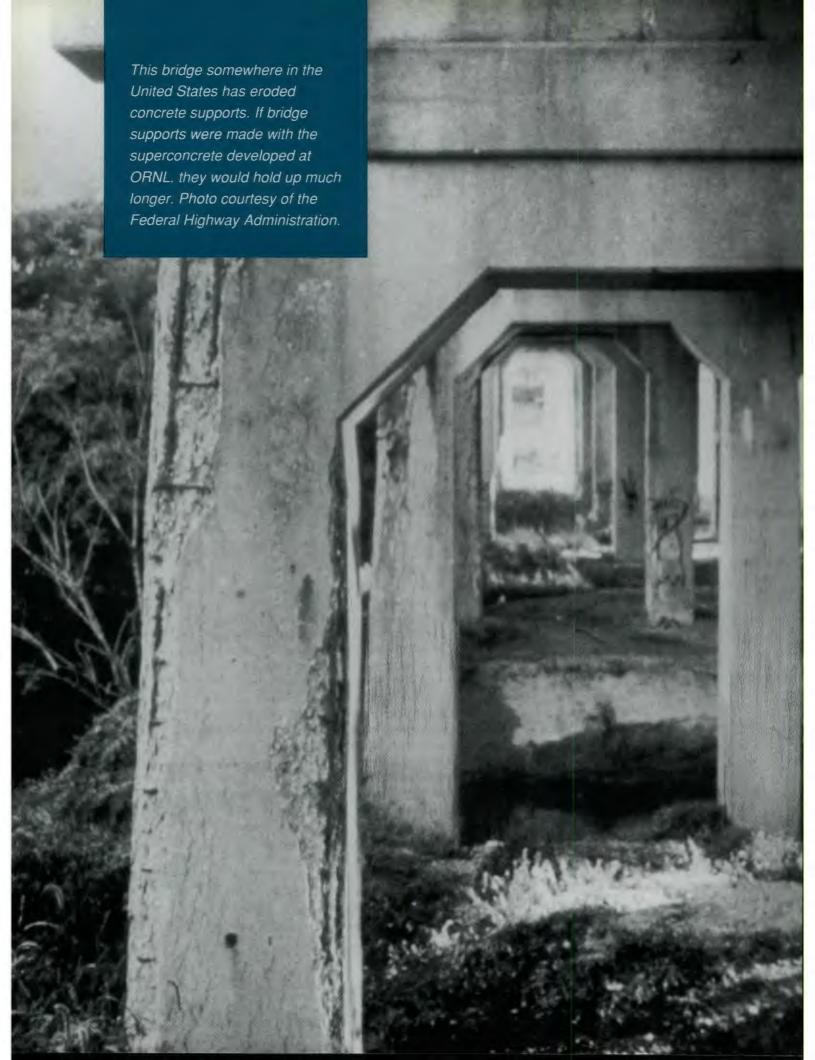
Increased computing power will enable groundwater researchers to use three-dimensional models to study both surface flow and underflows, as well as other physical, chemical, and biological variables.

plasmas of quarks and gluons in the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory

- Human genome—applying parallel network models to chromosomal band patterns
- Global climate change—modeling the coupled atmosphere, ocean, and biosphere system to understand the impact of chemical and energy releases on weather patterns
- Heavy-ion physics—modeling the production of lepton pairs, a phenomenon important to ion beam stability and focusing during high-energy, heavy-ion nuclear collisions.

In announcing the establishment of the new supercomputer research centers, Secretary of Energy James D. Watkins said, "These labs are well suited to apply new computer technologies to research on critical problems, ranging from environmental cleanup to climate modeling, that require massive computing power to solve.

"I expect these centers to set new standards for collaboration and interdisciplinary research in this field with all its ramifications for our country's economic competitiveness."



# Paving the Way to Superconcrete

By A. J. Mattus

Editor's Note: In early July 1991, Al Mattus of ORNL received a call from Jon Van, a reporter with the Chicago Tribune. Van had read about ORNL's success in making "superconcrete" using polystyrene, the material in the familiar throwaway cups and burger boxes that has become environmentally unacceptable because it does not degrade in landfills. The source of Van's information was What's Happening in Chemistry?, a compilation of easy-to-read reports on recent achievements in chemistry published for journalists and other lay readers by the American Chemical Society (ACS). The report by science writer Michael Woods, who learned about this development from the ACS, indicated that ORNL had ended "a century-long search for a practical way of producing polymer-impregnated concrete (PIC)," also known as superconcrete. In other words, ORNL had developed the pick of the PICs.

As a result of his interview with Mattus, Van wrote an article for the July 5, 1991, issue of the *Chicago Tribune* entitled "Researchers on road to superconcrete." The article was picked up by the Associated Press and led to other newspaper and trade press articles, including one in the August 12, 1991, issue of *Plastics News*.

Journalists found the ORNL development quite appealing because it offers potential solutions to the nation's environmental and infrastructure problems, as reflected in Van's two lead paragraphs:

"In the form of cups and packaging 'peanuts,' plastic foam often draws environmentalist scorn, but a new discovery may convert this familiar material from villain to hero among ecologists.

"Recycled polystyrene foam apparently can be mixed with cement to make a superconcrete that won't erode when exposed to water and other natural elements. If testing confirms the stability of plastic-enhanced cement, it could be used to contain toxic wastes safely, as well as to build sturdier and lighter-weight bridges and to pave highways that need fewer repairs."

As the result of this publicity, 54 organizations expressed interest in acquiring more information about and even commercializing the ORNL technology of making superconcrete. ORNL's development of a practical method for making polymer-impregnated concretes is discussed in the following article.

oncrete—first used extensively by the ancient Romans to build roads, bridges, aqueducts, and other massive structures—has been a reliable building material for centuries. But this familiar material so important for sidewalks, driveways, interstate highways, sports stadiums, and the foundations of buildings is far from perfect. For example, wastes that are disposed of by mixing them with cement-based grouts are leached out by water, and concrete bridges are weakened by exposure to seawater and other harsh environments. Hence, researchers have long sought to improve concrete's properties.

A "superconcrete" that is stronger, impermeable to water, and resistant to environmental chemical attack has been a major goal for almost a century. To achieve it, researchers have tried to fill, or impregnate, the pores of concrete with polymers, substances such as plastics that are made of giant molecules formed by the union of simple molecules called

monomers. These materials are known as polymer-impregnated concretes.

Until our recent success at ORNL, impregnating concrete with various types of polymers to obtain desirable properties has been limited substantially by the water it contained. Success has been realized only by use of complete drying and high-pressure entry methods. However, these methods have been shown to be highly uneconomical for full-scale practical use; as a result, only specialized, limited use is made of polymers in, for example, construction concrete and processed waste.

In the Chemical Technology Division, Roger Spence and I have found a simple way to make polymers enter dense, cement-based grout containing liquid waste. This development could potentially be applied to other materials using various polymers. Our method, which has rendered alkaline, cement-based grout impervious to attack by even concentrated acid, is still being evaluated. We achieved total saturation of the

Using the polystyrene of throwaway cups, ORNL researchers have developed a very strong concrete.

"A PIC is a hybrid product of a technology as old as the Egyptian pyramids and modernday polymers"



Mattus (right) and Spence make the point that a strong polymer concrete can be formed using polystyrene foam, the material in the inverted white coffee cup shown here.

concrete with polymer by using pore-entry particles that open a network of channels inside very dense materials, such as cement-based grout, despite the presence of water. The method requires no special equipment and appears to be easily adaptable to practical industrial scale-up. Applications may include lighter-weight concretes for bridges and grouts that completely immobilize toxic wastes.

### **Past Attempts and Problems**

The concept of using a polymer to impregnate concrete or other dense materials is not new; researchers have strived to develop a practical process since the beginning of this century, as shown by the published results of many studies of polymer-impregnated cements. In almost every case, the need to impregnate cement-based solids was dictated by the use of cement-based materials in environments that result in chemical

degradation and destruction of these materials. A few of the proposed uses for PIC are (1) reinforced concrete structures that have improved physical properties, (2) waterproofing and anticorrosion coatings, (3) waste form matrices

(3) waste form matrices that are nearly impermeable to water, and (4) grouts or concretes that are resistant to chemical degradation in reactive environments.

A PIC is a hybrid product of a technology as old as the Egyptian pyramids and modern-day polymers. Since ancient times, concrete has been made by mixing crushed stone, gravel, or some other suitable material with sand, water, and a

cementing material such as lime or, more recently, Portland cement. It was hoped that a polymer could improve concrete by filling the voids created during the curing stage of cement when concrete is kept wet to strengthen it. Voids are formed when amorphous gels, which occupy large volumes when the concrete is wet, shrink and crystallize into various minerals as it dries. If such voids could be filled with a polymer, then the highly porous concrete would gain added strength and be more resistant to chemical attack from the environment.

Although the task of introducing polymer reactants into such pores may at first seem trivial, it has plagued researchers since the inception of the idea. Impregnating a dense concrete solid is difficult for two major reasons: (1) just as oil will not mix with water, the organic reactants needed to form the polymer are hydrophobic, so their entry is blocked by both water and entrained gas pockets in the concrete; (2) the concrete solid,

although quite porous, is not very permeable to entry by liquids that are relatively viscous compared with water.

A number of different approaches have been tried to overcome these two major limitations. The problem associated with the presence of water is usually addressed by simply drying the concrete solid and then using a vacuum to remove any gases to facilitate polymer entry. A low-viscosity monomer is then forced into the solid mass under high pressure in preparation for polymerization.

This approach is not practical at all because of the amount of time and energy required to remove all the water from a mass, especially if it is a major component of a waste stream. In addition, because the denser concretes are made to be as impermeable to the movement of water as possible, extremely high pressures must be used to force the organic reactants inside. This approach is currently in use only for the production of waste storage casks and some pipes.

Attempts have been made to mix the organicbased reactants directly with the slurry of cement and other dry solids and then to cure the resulting mass. This approach has not worked because the organic reactants coat the surfaces of the solid cementitious particles, blocking the necessary hydration by water. The end result is a crumbly mass that has little strength and organic-lined channels and cracks leading to the surface.

Another approach to impregnation has been to use only cement and the theoretical amount of water-containing waste necessary to hydrate the cement. In this approach, cement is mixed with water and tumbled in a container until the cement is hydrated, forming a gravel-like, porous bed in which the organics could be poured and polymerized. This approach has been applied in waste disposal only for immobilizing tritium as the water used to hydrate the cement. Such an approach results in a solid containing mostly polymer and only a small amount of water and cement. This type of material would not be suitable for immobilizing wastes containing large amounts of water because the volume increase in the product waste form would be several thousand percent.

Another type of PIC is produced by mixing stabilized emulsions of latexes or other highmolecular-weight polymers into a cement slurry before curing it. The emulsion approach, when used properly, only imparts a very limited pore-blocking effect, and upon curing of the concrete, the gel portion of the cement shrinks as minerals are formed, leaving behind a small sphere of polymer in the center of a larger void. The resulting product is less permeable, but it is still not impervious to water or chemical attack from the outside. In addition, the product does not possess enhanced physical properties because the polymer particles sit in separate pores and lack the interconnections needed to provide added strength.

### **Initial Approach**

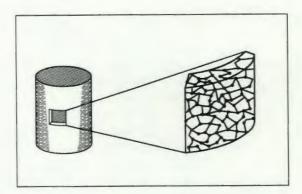
In 1988, we performed laboratory tests using a nitrate-based surrogate waste representing an actual waste found at ORNL. Initially, our tests were directed at observing the effects of the densification of cement-based waste forms on the leachability of nitrate. Nitrate is well known to be a difficult waste to isolate because of its mobility when the waste form comes in contact with water. Our goal was to examine the benefits of increasing the length of the path taken by nitrate anions (negative ions) to the outside of the waste form. This work expanded to include the use of polymers to aid in blocking the internal pores of the grout waste form to slow the movement of nitrate.

At that time we made an extensive literature search of government reports, chemical abstracts, and pertinent journals to learn about polymer impregnation. After studying the results, we decided to use styrene as a monomer to form polystyrene because of its low viscosity, which would facilitate pore entry, and its ability to be highly cross-linked, making it insoluble in most organic solvents and resistant to chemical attack.

In our initial tests, we did not remove pore water in the cement-based grout. We soaked the solid forms containing waste for various lengths of time in the styrene monomer, a catalyst, and a cross-linking agent as well as a red dye to track the movement of the polymer. We removed and sectioned the samples to measure the depth of

"In 1988, we performed laboratory tests using a nitrate-based surrogate waste representing an actual waste found at ORNL."

This is an exploded view of a concrete surface showing pore entry by ORNL's method of polymer impregnation.



entry of the polymer solution. Results indicated that penetration was limited to only 1 mm into the waste form.

We thought that if small channels about 2 mm apart could be formed throughout the waste form solid by some material, then the permeated polymer overlapping this material would completely impregnate the concrete. So we tried using very fine fibers of thread, obtained from the floors of sewing factories, as tiny wicks to create these channels. We mixed the fibers with the grout paste, cured it, and soaked it in the polymer solution. Our results revealed that the polymer solution followed the fibers only to a limited degree and on a random basis, so we discarded this method.

### The Polystyrene Solution

We then considered adding particles of material that is dissolved quickly by the organic monomer to provide a means of entry. We knew that the polystyrene used in manufacturing drinking cups and plastic peanuts for packaging is quickly dissolved by liquid styrene monomer, so we decided to try this material. Because the polystyrene foam in such cups and packing material is not chemically cross-linked and contains air in small pockets, it dissolves at an amazing speed, even in the presence of only the organic vapors. We found that, after the polystyrene pore-entry particles are dissolved, they become part of the polymer matrix material.

For our first experiment we used a wire brush to remove polystyrene foam from packaging

material. We mixed the foam (measuring less than 1 mm thick) at various volume ratios with the thick grout slurry, which we cast in Teflon tubes representing waste containers. Some grout samples were cured in an oven to accelerate the process; others were cured at room temperature. After the samples were cured, we poured the liquid mixture of styrene monomer (vinylbenzene), the catalyst (benzoyl peroxide), and the cross-linking agent (divinylbenzene) on top of the waste form in the tube. The container was sealed and placed in an oven at between 70 and 80°C for 12 hours.

This method proved very successful at all ratios of foam to waste-form volume. Complete impregnation was achieved, even to the walls and outside of the waste form surface. Further tests showed that penetration could be achieved in only a few hours and that all particles of foam were dissolved. Although the laboratory-scale samples were only 13 cm long, the entry appears to have no scale-up limitation judging from the rapidity of entry, even when using the most dense waste-form mixes with material approaching structural grade concrete in composition.

The styrene monomer appears to quickly dissolve the pore-entry polystyrene particles, forming a polymer matrix that permeates out radially from each particle and into the interconnecting channels between particles forming a network throughout the solid. The figure on this page depicts, by way of an exploded view, what is occurring within the solid.

To test our new impregnated material, we randomly broke it into pieces that we placed in concentrated hydrochloric acid to see if the surfaces were protected. In addition, an unimpregnated sample was placed in the acid. The polymerimpregnated samples remained intact in the acid until it evaporated away in two months, whereas the unimpregnated material fell apart in only a few hours.

Using visible light and scanning electron microscopes (SEMs), we observed the waste form surfaces to determine if the impregnated surfaces were completely protected. As shown in the SEM photomicrograph of an internal surface on the next page, the pores of the grout appear to have been effectively plugged by the polymer; in fact, the cement and the polymer appear to have become a

effectively plugged by the polymer; in fact, the cement and the polymer appear to have become a composite. That is, the polymer has moved within the space once occupied by the polystyrene foam particles and around cementitous gel phases that hold free water inside the pores. thereby minimizing the adverse effect of water. We found evidence for this composite formation when using colored dyes to track the movement of the polymer in earlier phases of the test program. The polymer not only follows channels between poreentry particles but also diffuses outward from these channels about 1 mm into the surrounding solid.

It would appear that the degree of penetration in the concrete by the polymer is governed by two major constraints: (1) the pressure necessary to overcome capillary forces, which limit monomer entry, and (2) the size and distribution of pore-entry particles. Because our study did not involve any overpressure but relied upon gravity alone, the size of the pores that could be filled with polystyrene was surely limited and appears to be between 1 to

limited and appears to be between 1 to 5 microns. As for the pore-entry particles, they must not be too small or capillary forces will limit the entrance of liquid monomer, and, if they are too large, the distance between particles will be too great.

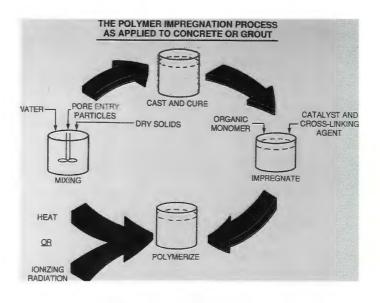
### **Possible Uses**

We originally developed this PIC process to enhance the properties of cement-based waste forms; however, we envision other uses for this PIC. In fact, the process might be found to work well with other polymers, such as polyvinyl-chloride, in which the monomer is capable of dissolving particles of polystyrene or even particles of another polymer.

Following further testing and development, this process might be used by the waste-processing



A scanning electron photomicrograph of an internal surface of a cement-based grout showing polystyrene plugging macropores.



A schematic process diagram showing the possible use of the pore-entry technique with cement-based grout in the waste-immobilization industry.

industry without the need for special equipment. As shown in the figure above, the pore-entry particle technique might be used in the field to immobilize waste in cement-based grout.

Although this developmental work has centered around the use of cement-based waste forms, the polymer entry technique might be used in a number of other areas: (1) to protect rebar in concrete from corrosion by seawater, (2) to produce a lighter-weight concrete for uses in the construction industry, such as making building facades, (3) to waterproof various solids or protect them from harsh chemical environments, and (4) to aid in immobilizing spent-ion exchange resins in various types of solids, such as in gypsum or cement.

On May 9, 1989, a U. S. patent was granted for this process of making superconcrete. Patent

rights have been waived from the Department of Energy to Martin Marietta Energy Systems, Inc. The company's Office of Technology Transfer is trying to identify interested companies that might want to have an exclusive license to the technology or to enter into a cooperative research and development agreement (CRADA) to make

the technology commercializable. A company in Jacksonville, Florida, is currently testing the process on undisclosed cement-based materials. Because of industrial interest in the process and because of its simplicity, one of the exciting materials down the road is likely to be superconcrete.

### Biographical Sketch

A. J. Mattus is an engineer in the Waste Treatment Group of the **Engineering Development** Section of ORNL's Chemical Technology Division. He has a B.S. degree in chemistry and an M.S. degree in hydrometallurgy, both from the New Mexico Institute of Mining and Technology in Socorro, New Mexico. He is currently working with various methods of altering or treating wastes using various chemical and electrochemical methods. He had worked for four years with techniques to immobilize wastes in cementbased grout and bitumen. His interests center around using chemical and physico-chemical methods to treat wastes, and his broad interests range from material science to applied physical chemistry. He tries to solve complex problems by applying simple scientific principles.



Al Mattus (right) and Roger Spence believe superconcrete could improve waste management and the nation's infrastructure.

## A New Look at Supercritical Water

By Carolyn Krause



Bob Mesmer (left), Hank Cochran, and Mike Simonson inspect the feed system of the hightemperature flow calorimeter used to study the properties of supercritical aqueous solutions.

esearchers at ORNL and the University of Virginia have been studying the behavior of solutions in supercritical water. This basic research may lead to improved understanding of new treatment technologies for hazardous wastes, the steam systems of fossil-fuel-fired power plants, and the formation of minerals and ores in the earth.

Depending on the temperature and pressure, water may exist as a solid (ice), liquid, or gas (steam). Above 374.1°C, all differences between liquid and gaseous water disappear. The resulting fluid state of water is called supercritical water. Many properties of supercritical water, like those of any supercritical fluid, change dramatically with very small changes of pressure or

temperature or with small quantities of dissolved substances.

#### **Basic Research Results**

The ability of water to dissolve various substances can be changed in striking ways. For example, oil becomes much more soluble and salt becomes less soluble under supercritical conditions than under normal conditions. Thus, supercritical water's role as a solvent is a topic of current interest.

The properties of solutions in supercritical water are being studied by Hank Cochran of ORNL's Chemical Technology Division and Mike Simonson and Bob Mesmer, both of ORNL's

Waste treatment technologies and steam systems may benefit from basic supercritical water studies. Chemistry Division, in collaboration with Peter Cummings of the University of Virginia, using computer codes developed by members of Cummings' group at the university. These studies include the first molecular simulations of supercritical aqueous solutions and reveal details of the structure of these solutions at a molecular level not previously studied.

In particular, their studies revealed that ionsfor example, the positive and negative ions (Na+ and Cl-) of common table salt, sodium chlorideform clusters of water molecules around themselves. The local water density in the vicinity of a sodium or chlorine ion is high relative to the average water density. For example, the average number of water molecules in the first solvation shell (water volume surrounding the dissolved ion) around a sodium ion in supercritical water is about 10.0, compared with a value of about 4.3 at ambient conditions. In contrast, the local water density in the vicinity of atomic argon is lower than the average water density. Molecular species such as methanol or water itself may form local regions of increased water density but at densities not nearly as high as around ions.

Some of the important properties of ordinary liquid water—particularly its properties as a solvent—are strongly influenced by water's special ability to form loose, roughly tetrahedral networks of hydrogen bonds (a tetrahedron has four faces, like a pyramid). In liquid water some dissolved substances such as argon tend to increase the extent of hydrogen bonding among neighboring water molecules, whereas others such as Na\* and Cl-tend to reduce it.

The molecular simulation studies are the first to provide evidence that, in supercritical water, the extent of hydrogen bonding is determined most strongly by temperature. The local density and the identity of the neighboring particle—whether atomic argon, ionic sodium or chloride, molecular methanol, or water itself—have little or no effect on the average number of hydrogen bonds in which nearby water molecules participate. In fact, though the number of water molecules in the first solvation shell surrounding a sodium ion is about three times the number in the first solvation shell around an argon atom, the researchers detected no

difference in the extent of local hydrogen bonding around either substance in supercritical water.

This new insight into the structure of solutions in supercritical water may improve understanding of the unusual behavior of supercritical water as a solvent. Other important properties, such as transport rates by diffusion and reaction rates, are also strongly affected by the local solution structure.

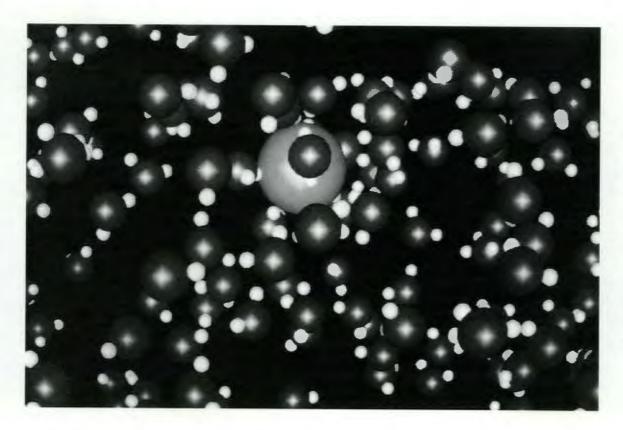
This work was initiated during the summer of 1990 when Cummings visited ORNL as an Oak Ridge Associated Universities Summer Faculty Research Participant. The research in this area by Simonson, Mesmer, Cummings, and Cochran is supported by the Division of Chemical Sciences of the Department of Energy's Office of Basic Energy Sciences. Supplemental funding for supercomputer calculations and researcher visits was provided by DOE's Division of Chemical Sciences and ORNL's Exploratory Studies Program.

### **Applications**

One possible application of the properties of supercritical water is a new technique for combustion of hazardous materials. The technique, developed by Mike Modell, founder and president of Modell Development Corporation, uses oxidation in supercritical water to treat the hazardous materials that had been candidates for incineration before the mounting public opposition to incinerators for waste disposal. The technique is being tested in pilot plants supported by the Department of Defense at Los Alamos National Laboratory and Sandia National Laboratories.

Supercritical water is particularly good for oxidizing wastes containing about 1 to 10% organic matter. Wastes containing other proportions of organics may be better treated by activated carbon or incineration. Oxidation in supercritical water converts organics to carbon dioxide and water and converts inorganic substances to salts that can be separated out and disposed of.

The technique could help DOE deal with its problem of treating mixed aqueous wastes in an



Computer simulation at the molecular level of a single chloride ion (big white ball) in supercritical water at the same conditions as pure water. Note that the concentration of water molecules is higher near the chloride ion than away from it. Developed by Peter Cummings of the University of Virginia.

acceptable way. Mixed aqueous wastes—
solutions or suspensions in water of hazardous
chemicals mixed with radioactive isotopes—
cannot legally be disposed of in the same way as
low-level radioactive waste.

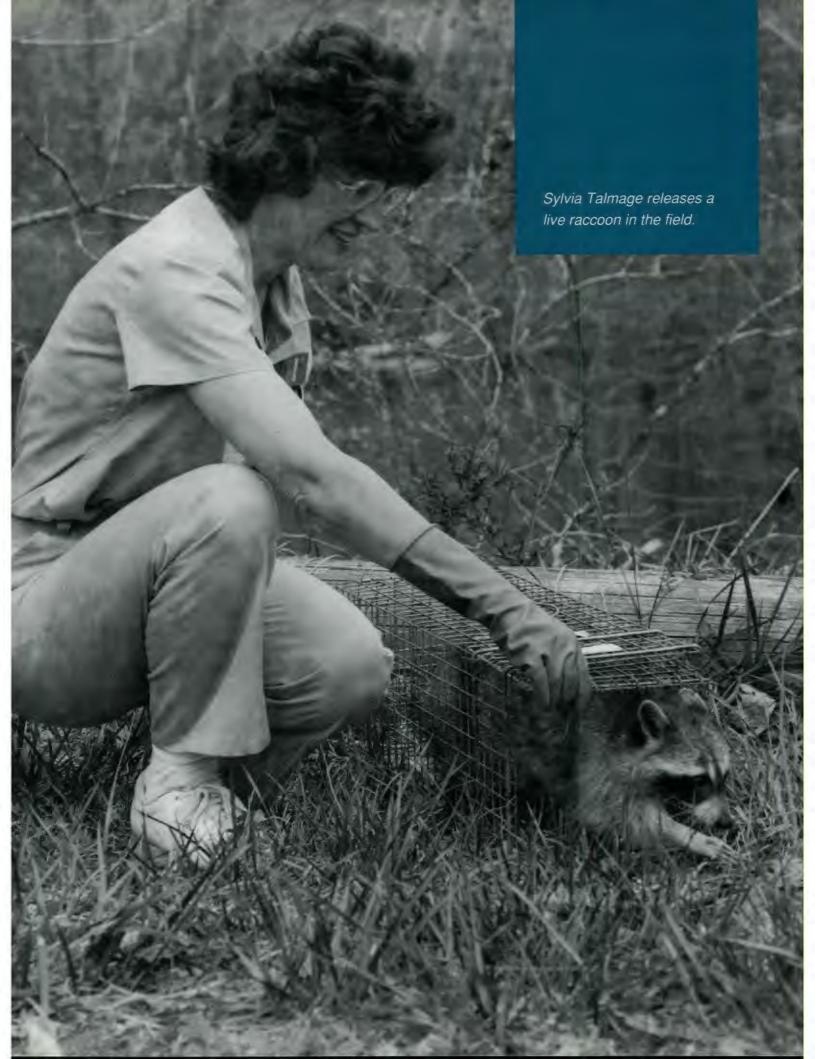
For example, at DOE's Hanford Engineering Development Laboratory, millions of gallons of mixed aqueous waste—solutions in water of organic chemicals, solvents, and radioactive actinides—might be treated by oxidation in supercritical water to produce a clean water stream and a solid, inorganic radioactive waste. The use of oxidation in supercritical water may be more economical than other waste treatment methods.

The behavior of supercritical water is also of interest to researchers trying to find cost-effective ways of operating coal-fired, oil-fired, and gasfired power plants. To use the energy from fuel more efficiently in producing electricity, many of these plants have supercritical steam topping cycles—turbines operating on the hottest steam

(i.e., supercritical water) produced from the burning fuel. Because of its special abilities to dissolve, transport, and deposit salts and other impurities on metal surfaces, supercritical water behaves differently from liquid water or ordinary steam. It is important to understand its properties because of their effects on the economically important problems of corrosion and fouling of steam generator tubes and turbine parts.

Geochemists are also interested in the work on supercritical water because it may help them better understand processes in the earth's crust. The transport and deposition of materials, the permeability of rock formations, the production of geothermal steam, and the analysis of reservoir chemistry are all geochemical problems. Solving them depends partly on knowledge of the properties of supercritical aqueous solutions.

The author gratefully acknowledges the assistance of Hank Cochran in preparing this article.



# **Small Mammals as Environmental Monitors**

By Sylvia Talmage and Barbara Walton

any contaminants released to the environment or stored at hazardous waste sites pose potential threats to natural wildlife populations. Scientists have been charged with developing methodologies for characterizing contaminated sites and assessing the potential effects of exposure to these contaminants on both human and wildlife populations. One approach to the characterization of contaminated sites is analyzing soil and water samples. Although such chemical analyses can provide information on the concentrations of contaminants present, they do not take into account the biological availability of the contaminants to the plants and animals or the interaction of the contaminants within the organisms.

Another approach to ecological assessment is residue analyses of biota—plants and animals at the site. The underlying assumption is that if animals are exposed, some of the chemical will be found in the tissues of their bodies. Thus, residue analyses of biota (or, more specifically, the target tissue of the chemical in the biota) collected at the site can be a more meaningful analytical approach in that it reveals not only that the contaminant is present, but also whether it is biologically available to produce a response. This approach raises several questions. Are all animals at a site equally suitable for monitoring? Do differences in food habits and habitat matter? Should the choice of species depend on the chemical of interest?

Small mammals, such as mice, rats, and voles, living in contaminated environments are exposed to contaminants over time and space and across media. Therefore, small mammals are realistic "bioindicators" of exposure to chemicals. Results of an extensive literature survey and field studies conducted in the vicinity of ORNL demonstrated to us the feasibility of using small mammals as monitors of environmental contaminants. This was the subject of Sylvia Talmage's recent doctoral dissertation undertaken in the Ecology Program at the University of Tennessee in Knoxville. The

research was conducted at ORNL under the supervision of Barbara Walton of the Environmental Sciences Division.

### Why Small Mammals?

Compared with larger animals having extensive home ranges and low reproductive rates, small mammals are convenient and useful monitors because of their small size, abundance, small home range, short lifespan, early sexual maturity, high reproductive rate, and short gestation period. In addition, many are easy to trap. Unlike deer, small mammals do not migrate long distances; thus, their point of capture can be used to characterize the extent of contamination and identify sources, or "hot spots," of contamination.

Furthermore, because different species of small mammals have varying food and habitat preferences, the species chosen as the monitor could be important. Insect-eating mammals, for example, might be better monitors than grasseating animals. Our research proved this to be true. The insectivores, such as shrews, with a position near the top of a food chain by nature of their diet, were generally the best monitors for most contaminants. Omnivores, such as white-footed mice and deer mice, were also suitable monitors for many contaminants; these species consume vegetation, seeds, and insects. Herbivorous animals such as cotton rats and voles were suitable monitors only for contaminants that are taken up by vegetation or deposited directly onto vegetation in aerosol form-for example, automobile exhaust or smokestack and factory emissions.

Most contaminants are taken up by target organs or target tissues. For example, mercury will concentrate in the kidneys and liver and radioactive strontium will appear in the bone. Many organic compounds such as pesticides are stored in fat tissue. Evidence of an animal's exposure to a certain contaminant can be determined by an analysis of the target organ or tissue.

Small
mammals,
such as
shrews, can
be reliable
bioindicators
of chemicals
in the
environment.

Number One, 1992

Talmage's research at ORNL involved extensive field work trapping small mammals at chemically contaminated sites on the Oak Ridge Reservation and in the city of Oak Ridge to determine whether all species were equally useful as indicators of chemical contamination in the environment. A total of nine species were trapped, and the most commonly trapped species were the omnivorous (vegetation-, seed-, and insect-eating) white-footed mouse and the insectivorous shorttail shrew.

#### **Insect Eaters and Metals**

We found that insectivorous animals were the best monitors for metals deposited in the soil. One of our study areas for inorganic contaminants was a mercury-laden floodplain in the city of Oak Ridge. Mercury generally remains in the soil and is not taken up by vegetation to a great extent. Thus, herbivorous and omnivorous species that eat primarily vegetation are likely to ingest less of the metal than insectivorous species such as shrews. Shrews eat soil-ingesting earthworms and carnivorous spiders and beetles that feed on soilinhabiting invertebrates; all of these contribute to the high levels of mercury in shrews' bodies. In addition, they burrow in soil, whereas many of the other species live above ground. In this study, all animals trapped at the mercury-contaminated site had higher concentrations of mercury than those trapped at an uncontaminated reference site. At the contaminated site, the mean concentration of mercury in the kidneys of shrews was significantly higher than the mean concentration in the kidneys of white-footed mice.

Monitors for Lead and Radionuclides

Our literature review revealed many published studies on the relationship between past lead emissions from road vehicles and lead in the bones and other organs of several species of small mammals. For example, the concentrations of lead in small mammals decreased as distance from roads increased. Lead concentrations were also directly proportional to traffic density. Because the lead from gasoline was deposited directly onto

vegetation, the difference between herbivorous and insectivorous animals as sentinels became less pronounced. Vegetation-eating mice and voles accumulated lead in their bones; shrews fed on insects that had already accumulated significant amounts of lead and thus had higher body burdens than the other species. Although herbivorous animals were suitable monitors, insectivores remained the best indicators of lead contamination.

In the case of lead, the large data base on the effects of lead on small mammals as determined in laboratory studies allowed us to compare the concentrations that result in toxic effects with concentrations in animals trapped at field sites. In a few cases, concentrations in the bodies of field-collected animals approached toxic levels as determined by the laboratory studies.

Talmage also trapped animals living on the Solid Waste Storage Area (SWSA) 4 site on the Oak Ridge Reservation to study the accumulation of radionuclides. In this case, the contaminant of interest was strontium-90. Strontium has a naturally occurring isotope, but the radioactive form was present in soil at the site because of radioactive waste buried there. Strontium, which acts similarly to calcium in biota, is taken up by vegetation. It was also present in water "seeps" from the waste trenches. Because it was ingested by all animals through vegetation, soil, and water, no species studied exhibited an appreciably higher level than any other. All of the animals had measurable levels of strontium-90 in their bones. and mean concentrations at SWSA 4 were significantly higher than concentrations at a reference site.

### **Importance of Habitat**

At this study site, habitat influenced contaminant concentrations in the different species. Because SWSA 4 is a grassy field, it is a suitable habitat for the herbivorous harvest mouse and cotton rat. Individuals of these two species had the highest concentrations of strontium-90. Shrews and white-footed mice probably spent less time in this area and more time in the adjacent, less contaminated, brushy area. Individuals of all

"Shrews eat soil-ingesting earthworms and carnivorous spiders and beetles that feed on soil-inhabiting invertebrates."

species trapped along a creek downstream of the seep area also had measurable, but very low, concentrations of strontium-90 in their bones, indicating the usefulness of monitors for following the migration of a contaminant from its source.

These studies provide strong evidence that food habits and habitats of small mammals are major factors influencing exposure to chemical contamination under field conditions. We believe that knowledge of the contaminants available to mammals and their routes of uptake into the body may help scientists better predict the risks posed to humans by hazardous wastes. Our work significantly adds to the data base on biomonitoring. Enough data on contaminated sites may one day bring an understanding of which sites pose the greatest hazards to both the environment and public health and which ones have been successfully cleaned up.



A white-footed mouse searches for food on the Oak Ridge Reservation.

### Biographical Sketches

Sylvia S. Talmage is a technical information specialist in the Biomedical and Environmental Information Analysis Section of ORNL's Health and Safety Research Division. She has been employed at ORNL since 1975. She received a Ph.D. degree in environmental toxicology from the University of Tennessee at Knoxville. She is a native of West Lawn, Pennsylvania. Her research focuses on chemical hazard evaluation and wildlife toxicology, specifically the use of small mammals as monitors of environmental contaminants. Currently, she is preparing human and environmental risk assessment reports on chemicals for both private and federal regulatory agencies.



Barbara T. Walton is a research staff member in the Environmental Biotechnology Section of ORNL's Environmental Sciences Division (ESD). She also holds an adjunct faculty position in the Ecology Program and the Graduate Program in Environmental Toxicology at the University of Tennessee. Walton received a Ph.D. degree from the University of Illinois in entomology and environmental toxicology. She joined ESD in 1977. She is a native of Latrobe, Pennsylvania.

Walton is a diplomate of the American Board of Toxicology (certified in general toxicology), a member of the board of directors of the American Board of Toxicology, and a member of the editorial board of Environmental Toxicology and Chemistry. From 1984 to 1988 she served as editor of special publications for the Society of Environmental Toxicology and Chemistry. She is also a past president of the Society of Environmental Toxicology and Chemistry.

## RE: Awards & Appointments



Liane and William Russell

William L. Russell, founder of the Mammalian Genetics Section of ORNL's Biology Division, was honored by a recent issue of the international science journal Mutation Research. In this special issue on "Mammalian Germ-Cell Mutagenesis," it was stated that "no single person has contributed more to the field of mammalian mutagenesis, and thus to genetic risk assessment in man, than Dr. W. L. Russell." The editor of the special issue, which was published in tribute to Russell on his 80th birthday, was his wife, Liane B. Russell.

William W. Carpenter has been named chairman of the Advisory Board of the National Technical Information Service.

Thomas Wilbanks has been elected vice president of the Association for American Geographers.

**David B. Reister** has been reappointed associate editor of *Energy—The International Journal*.



**Thomas Wilbanks** 

Ernest Silver, editor-in-chief of Nuclear Safety, has been awarded a presidential citation by the American Nuclear Society in recognition of the -publication's contributions over the past 30 years.

Vivian M. Baylor has been named chairman of the Technology Transfer Committee of ASM International, a worldwide materials society.

John Hayter was recognized in the local press for designing and building a neutron spin echo spectrometer that was used to test the polymer theories of Pierre-Gilles de Gennes of the College de France, Paris. The polymer work helped de Gennes win the 1991 Nobel Prize for Physics. The spectrometer, located at the Institut Laue-Langevin in Grenoble, France, is the highest-resolution neutron spectrometer in the world.

Jackson B. Richard has been named chairman of the Association for Excellence in Reactor Operations.



**Ernest Silver** 

V. A. Protopopescu has been appointed to the editorial boards of two journals, Mathematical Models and Methods in Applied Sciences and Transport Theory and Statistical Physics.

Curtis C. Travis has been named a member of the Committee on Remedial Action Priorities for Hazardous Waste Sites of the National Research Council.

A. W. Renshaw has been named a member of DOE's Counselor for Science and Technology staff.

Michael H. Ehinger has been named chairman of the Technical Subcommittee on Nuclear Material Safeguards, Isotopes, and Radiation Division of the American Nuclear Society.

Kenneth E. Plummer has been elected vice chairman of the Nuclear Engineering Division of the American Institute of Chemical Engineers.

Anthony V. Palumbo has been named a member of the editorial board



Vivian Baylor

of the new international journal *Ecotoxicology*. He also has been elected co-chair of the American Society for Microbiology's National Meeting Short Course on Innovative Bioremediation Technologies.

David L. Greene has been appointed a member of the National Cooperative Highway Research Program Project Panel of the Transportation Research Board of the National Research Council. He also has been named a member of the National Academy of Science/National Academy of Engineering Committee on Fuel Economy of Automobiles and Light Trucks.

T. S. (Tom) Kress has been appointed a member of the Advisory Committee on Reactor Safeguards of the Nuclear Regulatory Commission.

Lynn A. Boatner has been elected a fellow of ASM International.

Mary Brown, a part-time ORNL staff member and a professor at



Jack Richard

Knoxville College, received the college's Outstanding Teacher Award for 1990.

Gary T. Mays has been named head of the newly created Operational Performance Technology Section of ORNL's Engineering Technology Division.

**Scott M. Pearson** has been awarded a 1991 Alexander Hollaender Distinguished Postdoctoral Fellowship.

Bruce L. Kimmel has been appointed a member of the scientific review panel for the National Science Foundation's Experimental Program to Stimulate Competitive Research.

Michael S. Bronzini has been elected chairman of the National Research Council Transportation Research Board's Committee for the Study on Lakeside Access to U.S. General Cargo Ports.

**Robert Hawsey** has been appointed director of ORNL's High Temperature Superconductivity Pilot Center.



**David Greene** 

Louis K. Mansur, Kenneth Farrell, and Roger E. Stoller received the 1990 DOE Materials Sciences Research Competition Award for Significant Implications for their cooperative work in reactor vessel embrittlement.

Duane Larson has been named head of the Nuclear Data Measurement and Evaluation Section of ORNL's Engineering Physics and Mathematics Division.

Stephen H. Stow has been appointed the first secretary-treasurer for the newly formed Education Division of the Geological Society of America.

**Robert D. Hatcher** has been elected vice president of the Geological Society of America.

James Sand and Edward Vineyard have received a "best paper" award from the American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) for their paper entitled "Experimental Performance of Ozone-Safe Alternative Refrigerants."



**Bruce Kimmel** 

John Jones has been appointed to the Boston Edison Company Technical Advisory Council, which provides technical review and advice to Boston Edison Company's senior executives.

Brenda Ramsey and Marilyn
Langston, both of ORNL's Health
and Safety Research Division, have
been presented Distinguished
Achievement Awards by division
director Steve Kaye. Ramsey received
the award for the "exemplary
administrative support" she provided
the division during the past year.
Langston was honored for her
"exemplary technical support"
through computer applications during
the same period.

Robert S. Burlage, an Oak Ridge Associated Universities postdoctoral appointee in ORNL's Environmental Sciences Division, has been named to the editorial board of the *Journal of Microbiological Methods*.



John McCarthy

John F. McCarthy has been appointed to the Scientific Advisory Committee of the Marine Mammal Action Program of the United Nations Environmental Program.

W. R. Garrett and C. E. Klots have been elected fellows of the American Physical Society.

**Prem C. Srivastava** has received a Distinguished Scientist Award from the United Nations World Development Program.

Robert N. Compton has received the 1991 Jesse W. Beams Medal and a Certificate of Merit for significant research in physics from the Southeastern Section of the American Physical Society.

Paul Rohwer is president-elect of the American Academy of Health Physics.

Carolyn Hunsaker has been recognized by the Water Pollution Control Federation for her "outstanding service" in chairing its Ecology Committee.



**Paul Rohwer** 

Barbara T. Walton has been elected to a second three-year term on the editorial board of the journal Environmental Toxicology and Chemistry.

Steven Lindberg has been named associate editor of *Environmental Reviews*, a journal of the National Research Council of Canada.

Carolyn Krause is Chapter Public Relations Competition Manager for the international Society for Technical Communication.

Charles Scott has been appointed director of the Laboratory's newly established Bioprocessing Research and Development Center.

Rufus H. Ritchie has been elected vice chairman of the Southeastern Section of the American Physical Society and will automatically become chairman at the next annual meeting to be held in November 1992.

**Duane Larson** has been appointed head of the Nuclear Data



**Robert Compton** 

Measurement and Evaluation Section of ORNL's Engineering Physics and Mathematics Division.

Philip J. Maziasz has been presented the Significant Contribution Award by the Materials Science and Technology Division of the American Nuclear Society for his paper "Microstructural Evolution of Martensitic Steels during Fast Neutron Irradiation."

Jacqueline M. Grebmeier has been elected to the National Science Foundation's Division of Polar Programs Advisory Committee.

W. Ray Garrett has been elected a fellow of the American Physical Society.

Todd A. Anderson has received the Student Travel Award to attend the 12th Annual Meeting of the Society of Environmental Toxicology and Chemistry Foundation.

Thomas Burns has received the Robert C. Anderson Memorial Award



Steven Lindberg

from the University of Georgia Research Foundation.

James Turner has been elected president-elect of the American Academy of Health Physics.

Lee Shugart has been named as a consultant to the U.S. Environmental Protection Agency's Science Advisory Board.

Annetta Watson was a finalist in the 1991 YWCA Tribute to Women, sponsored by the YWCA of Knoxville, Tennessee.

Jonathan Woodward is chairman-elect of the executive committee of the Biochemical Technology Division of the American Chemical Society.

The presentations of Fran
Sharples, Glenn Suter, and Kaye
Sigmon were cited among the top ten
best at the Seventh Annual DOE
Model Conference on Waste
Management and Environmental
Restoration.



**Annetta Watson** 

Donald Lee has been appointed chairman of the Air and Radiation Management Committee of the Environmental Engineering Division of the American Society of Civil Engineers.

Tom Ashwood has been invited to serve on a Local Governments Oversight Committee to provide local input to programs relating to DOE operations on the Oak Ridge Reservation.

Joseph Herndon has been named DOE's Office of Space representative to the Space Technology Interdependency Group robotics and artificial intelligence.

C. L. Fu, M. H. Yoo, C. J. Sparks, and G. E. Ice received DOE Materials Science Awards for 1991 for their work in metals and ceramics.

J. R. Thompson, D. K. Christen, R. Feenstra, C. E. Klabunde, and H. R. Kerchner received 1991 Materials Science Awards for their work in solid state physics.

## : Pick A Number

5

## Joseph Fourier and His Flux Law

By Alan Solomon

our ability to

understand and

control physical

processes through the

development of the major techniques of

what we now call applied mathematics. Chances are, as you read this note, someone nearby is using a fast Fourier transform to

analyze data arising from some experiment, somebody else is analyzing the vibrational

behavior of a structure using Fourier series,

while yet another person is simulating heat

nder the moonlit Egyptian sky Jean-Baptiste Joseph Fourier (1768-1830) thought about the wonders of the world in which he lived. A member of Napoleon's expedition to Egypt from 1798 through 1801, Fourier belonged to a generation of scientists who had inherited from Newton, Euler, and others a variety of mathematical tools (e.g., calculus, differential equations, and series representations), instruments and techniques for measurement and observation of physical and natural phenomena, and a growing understanding of many physical processes. In just a few years this young revolutionized

flow in a novel machine using tools based on Fourier's flux law.

In the area of heat transfer. Fourier's name is identified with an equation for the flux of heat being transferred by conduction in a body. The "flux" of something is the rate at which it flows across the surface area. Thus, the flux of water across a cross section of a pipe is the number of liters per minute flowing across a square meter of that cross section. Because heat is measured in joules or British thermal units (Btus), the flux of heat across a surface would be in units of joule per second per square centimeter or Btu per square foot per hour.

Moving from the observation that heat moves from points of higher to lower temperature and is roughly inversely proportional to the distance between these points, Fourier in 1807 produced an expression for the flux in the form

Heat flux = -k dT/dx

with k as the thermal conductivity of the body and dT/dx the derivative, or rate of change of temperature, with respect to distance. The minus sign corresponds to the flow of heat from higher to lower temperatures. Fourier's "Despite its almost universal acceptance as the basis of a model of heat transfer diffusion, the Fourier flux law is flawed."

law is the basis for all classical models of heat transfer in bodies and, hence, all computer software simulating such processes. Using such models we predict the thermal performance of walls in buildings, structures in nuclear reactors, and airplane wings in flight.

The Fourier flux law assumes the same form when in place of heat we speak of materials in diffusion processes or flow of water in porous media. In these cases the flux law is referred to as Fick's Law, after the physicist A. Fick, or D'Arcy's Law, after the hydrologist H. D'Arcy, who developed these relations in 1855 and 1856, respectively.

Despite its almost universal acceptance as the basis of a model of heat transfer diffusion, the Fourier flux law is flawed. It is merely an approximation of reality that works well when temperature differences are not overly great and heat transfer processes are not overly rapid, because it predicts an infinite speed of propagation of thermal energy, which is impossible.

According to this model, if we light a match somewhere in a room, an instantaneous change in temperature occurs everywhere. For most heat transfer processes, the error of this prediction is so small that it cannot be measured. However, in recent years, heat transfer processes have become extremely rapid in areas ranging from laser technology to nuclear safety. In these situations, the Fourier flux law needs to be replaced by a more realistic but complex relation.

Despite its occasional flaws, the work of the young man who wondered about how to represent the physical world in mathematical models is, and will remain, of vital importance to our technological growth. It is safe to assume that in a few years space colonists will be making use of Fourier's flux law, Fourier series, and fast Fourier transforms while viewing the earth from the moon that 200 years ago shone upon Joseph Fourier.

### **RE:** User Facilities

## Holifield's New Mission: Reaching for the Stars

The radioactive, or "exotic," beams produced at the revamped Holifield Heavy Ion Research Facility will add over 200 isotopes to the facility's repertoire, expanding nuclear structure studies and providing the Holifield with an important astrophysics capability.



RNL's Holifield Heavy Ion Research Facility, recently facing budget cutbacks or even shutdown, has received both a new lease on life and an expanded research mission. The 12-year-old nuclear structure facility will curtail experimental operations for two years, beginning in the fall of 1992, while it undergoes a \$3 million conversion that will enable it to accelerate not only beams of stable ions, but also radioactive ion beams to probe the intricacies of the atomic nucleus.

The radioactive beams produced at the revamped Holifield facility will be made up of nuclei that haven't occurred naturally on the earth, or even in the solar system, for billions of years. Despite their absence on the earth, these elements are constantly being created throughout the

universe—in the burning of cataclysmic binary star systems and in the terminal blasts of supernovae. Holifield's ability to create these elements will also provide it with an important astrophysical capability.

Investigating stellar nucleosynthesis. One of the new directions taken by the exotic beam facility will be to study the astrophysical process of stellar nucleosynthesis—the formation of "new" elements in and around stars. In these reactions, nuclei of lighter elements are combined to form heavier elements. This line of research will become even more important as new observation platforms, such as the Hubble Space Telescope and the Gamma Ray Observatory, provide detailed information on sites of nucleosynthesis.

In describing the broad scope of the astrophysical research proposed for the Holifield, Jerry Garrett of the Physics Division refers to a recent book about the physics of the creation of the universe, called *The First Three Minutes*. "After the first three minutes," Garrett says, "the universe had cooled sufficiently to allow protons and neutrons to bind together to form deuterons. Once this happened, most of the physics wasn't particle physics anymore, but nuclear physics. What we'll be looking at is not the first three minutes of the universe, but the next 16 billion years."

"A typical question in this area is, 'Why is the earth's crust 3% oxygen; why isn't it 10%?' says David Olsen of the Physics Division. "Or we might want to know, 'Why does <sup>16</sup>O make up over 99% of the total oxygen on earth while two other stable isotopes, <sup>17</sup>O and <sup>18</sup>O, account for only 0.2%?' or 'Why are these percentages different in stars and meteorites?'"

The answers to these questions are directly related to the history of the early universe. How and where were these elements made? What were the temperature and density? How much energy was being produced? "To answer these questions we need to know more about the processes that produce these isotopes in nature," Garrett says.

One of the processes researchers will be able to study with the improved facility is "rapid hydrogen burning," which is responsible for synthesizing many of the light elements, up to iron. This process is thought to occur in binary star systems in which one of the stars is a red giant, made mostly of hydrogen, and the other is a white dwarf, made mostly of heavier elements. At some point, the red giant becomes so large that the white dwarf can pull hydrogen away from the giant. This hydrogen is fed down to the surface of the white dwarf, where it produces a thermonuclear explosion, causing jets of proton-rich heavy elements to shoot out into space (see illustration and photo, p. 67).

ORNL's radioactive beam facility will produce beams of many of the nuclides along the predicted path of rapid hydrogen burning, enabling researchers to observe several of the reactions involved in this process. Also, by studying the nuclear properties of these stellar isotopes, scientists will be better able to extrapolate the properties of the nuclides that even the improved facility won't be able to produce.

"This whole process is predicted by calculations, but is not very well grounded in experiment," Olsen says. "We need to establish the nuclear properties of these isotopes to determine how the process of rapid hydrogen burning actually occurs."

#### Expanding nuclear structure studies.

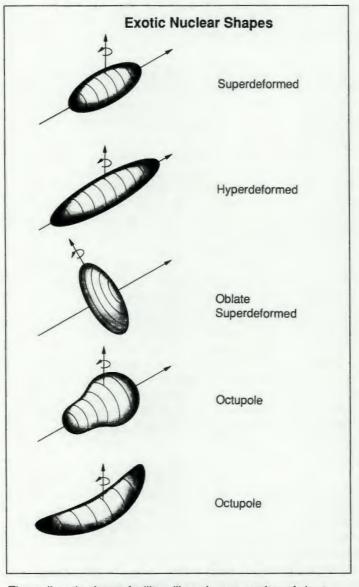
Holifield's new capabilities will also be used to expand its traditional area of endeavor, nuclear structure studies. The enhanced facility will be able to create more than 200 nuclei that could not be produced with stable beams and targets, increasing the number of nuclei that can be produced at the Holifield to about 1600. The new nuclei are concentrated in an unexplored section of the chart of the nuclides and are distributed among the proton-rich isotopes of elements from fluorine to neptunium.

"Our current knowledge of nuclear structure is based on information gained through experimentation with nuclei that can be produced with stable beams and targets," says Garrett. "The use of exotic beams will provide opportunities to answer fundamental questions about nuclear structure and study entirely new phenomena, not observable with current techniques or predicted by current theory."

Proposed areas of nuclear structure research for the upgraded facility include studies of nuclei near the doubly closed shell nucleus, tin-100 (100Sn); heavy nuclei having nearly equal numbers of protons and neutrons; deformed, or "exotic." nuclear shapes; and new regions of nuclear deformation.

<sup>100</sup>Sn is the heaviest possible nucleus with full, or "closed," shells containing equal numbers of protons and neutrons. Nuclei with closed proton

"What we'll be looking at is not the first three minutes of the universe, but the next 16 billion years." "In less than three years . . . we will have an accelerator system that will be unique in the world."



The radioactive beam facility will produce a number of short-lived nuclei in a previously unexplored section of the chart of the nuclides. Theory predicts several of these will have exotic nuclear shapes, including those shown above.

or neutron shells are particularly stable and exhibit other nuclear properties of interest to researchers. Detailed measurements of the properties of nuclides in the area of <sup>100</sup>Sn will test the basic assumptions underlying the widely accepted shell model of nuclear structure.

Nuclei having nearly equal numbers of protons and neutrons play an important role in nuclear structure studies by helping researchers understand the structural changes resulting from variations in neutron number, proton number, and other factors. These nuclei provide both fertile ground for the study of exotic nuclear shapes and a stringent test of model calculations.

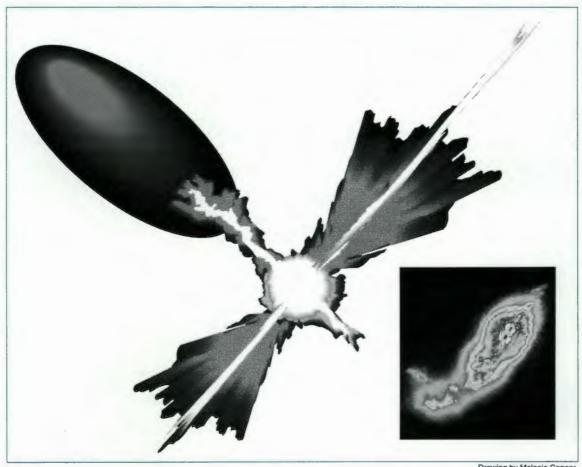
For example, the researchers can use radioactive beams to produce a number of short-lived nuclei which theory predicts will exhibit exotic shapes. These nuclei come in several varieties, including superdeformed (football-shaped), octupole (pear-shaped), and hyperdeformed (cigar-shaped), and their lives are measured in billionths of seconds. Researchers are particularly interested in the hyperdeformed nuclei accessible to the new facility, because they have never before been observed experimentally.

Other experiments involving nuclei with identical or nearly identical numbers of protons and neutrons include tests of widely accepted ideas about the relationship between the weak nuclear force and the electromagnetic force, two of the four forces in the universe. These tests have already been made on lighter nuclei, but the use of radioactive beams will allow them to be performed more accurately on heavier nuclei.

Retooling the Holifield. The

retooling of the Holifield facility was first conceived of several years ago when researchers at ORNL realized that most of the equipment needed for producing radioactive beams at the Holifield was already in place.

Currently, the Holifield's 25 million-volt tandem accelerator is configured to accelerate



Drawing by Melanie Conger

Artist's conception of the binary star system R Aquarii, where rapid hydrogen burning is taking place. Hydrogen is drawn away from the red giant onto the surface of the white dwarf where it detonates in a thermonuclear explosion, causing a jet of proton-rich heavy elements to shoot out into space. This jet is also visible in the inset, a recent Hubble Space Telescope photograph of R Aquarii, sensitive to the light of O18. Used with permission of Francesco Paresce of the Space Telescope Science Institute.

stable, heavy ions. If extra energy is needed, the Oak Ridge Isynchronous Cyclotron (ORIC), which in pre-Holifield days was used to accelerate light ions, serves as a booster after the ions exit the tandem accelerator.

"To produce exotic beams," says Garrett, "this configuration is reversed. The cyclotron slams an intense light-ion beam, made up of protons or helium-3 nuclei, for instance, into a target, resulting in a variety of radioactive collision products. The desired isotope is magnetically separated from the other products, transformed

into negative ions, and accelerated through the tandem as a radioactive beam."

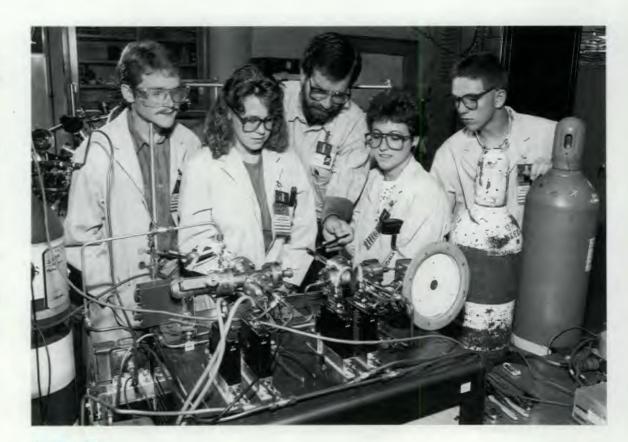
Reconfiguration of the Holifield has already begun and will continue through 1994. The exotic beam facility is expected to go on line early in 1995.

"In less than three years, for the fairly modest cost of about \$3 million," says Holifield Director Russell Robinson, "we will have an accelerator system that will be unique in the world for quite a number of years."—Jim Pearce

### **Educational Activities**

## M&C Division Hosts Appalachian Students and Teachers

Lee Heatherly (center) shows a teacher and three students from four Appalachian states how diamond films are grown at ORNL. He is pointing at a hot filament over which methane gas is passed to form a diamond film. Looking on are, from left, Todd Shrewsbury, a student from West Virginia; Laura Crawford, a student from Tennessee; Joan Wiles, a teacher from Kentucky; and Adam Robertson, a student from Mississippi.



ake several high school students and teachers from schools across
Appalachia, mix in world-renowned materials science researchers, add state-of-the-art technology, and you get a formula for a rewarding educational experience.

Researchers in ORNL's Metals and Ceramics (M&C) Division recently experimented with such a formula to enrich science and math education for students from the Appalachian region.

"The problems in Appalachia began long before these students were born," said Chet Richmond, ORNL's director of science education and external relations. Their states often cannot afford to furnish schools with the facilities and equipment needed to provide the caliber of education critical in today's technological society.

"Because of these educational problems, some of the brightest students in Appalachia often find themselves unfairly disadvantaged when they have to compete with students from other areas of the country for college and career opportunities," Richmond said. "When this happens, financial opportunities are also usually limited, which only reinforces the region's depressed economic cycle."

In 1990, as part of its educational program, DOE signed a memorandum of understanding with the Appalachian Regional Commission (ARC) in an effort to provide badly-needed educational opportunities to the region. One result of this effort was a materials sciences workshop at ORNL for Appalachian students and teachers.

For two weeks, 31 students and 7 teachers selected by the ARC worked with researchers in ORNL's M&C Division. For most of them, it was the first time they had been exposed to science at such a high level.

"I've never seen anything like this," said Paul Terry, a junior at Livingston (Tennessee)
Academy, describing his first impression of working with a scanning electron microscope.
"The first day, it felt like I was watching some science fiction movie." He and two other ARC participants, Marvin Stemple, a science teacher at Calhoun County High School, Grantsville, West Virginia, and Lisa Campbell, a senior at Hurley (Virginia) High School, were using the microscope to examine the surface details of different materials, primarily silicon carbide composites.

Terry said he is grateful for the workshop opportunity. "Most schools in our state have a hard time just finding money for the basics," he said. "Without programs like this, small towns like mine wouldn't know what is going on in the science world."

For most workshop participants, it also was the first time they had heard the term materials science. Adam Robertson, a junior at Falkner (Mississippi) High School, said he wasn't quite sure what to expect when he heard he would be studying materials science at ORNL. "But within a few hours, Lee (Heatherly) helped us understand how materials science affects just about every area of our life, even things like our cars, that we just take for granted," Robertson said. "Everything here is so new to me that it's been a little overwhelming, but it sure beats trying to learn from an outdated science book."

Heatherly, a research associate in ORNL's M&C Division, said he hopes the program will make students aware of the variety of fields and opportunities available to them in science. "I just wish we could reach more of them (students and teachers)," Heatherly said.

In addition to their research, workshop participants studied the issues of recycling, learned about college funding resources, and attended a career fair. But just as important, they got to know other students with whom they had a lot in common.

"It's nice to see there are so many other kids like me—we have a lot of the same goals and dreams. I think most of us realize we may have to work a little harder to get where we want to go," said Christy White, a senior at Ripley (Mississippi) High School, whose goal is to be a doctor. But even though materials science seems far removed from medical science, White said the ORNL workshop had helped her understand the significance of science.

"Life itself is dependent on science," she said. "Everything you see and touch is affected by it. It's an exciting field, and what I've seen here just makes me want to learn more."— Karen Bowdle

## Reactor Experience for UT Students at ORNL

Since the fall of 1991 at ORNL, nuclear engineering students from the University of Tennessee (UT) have been gaining hands-on experience at what is arguably the best shielding research reactor in the western world.

ORNL has entered into an agreement that will open its Tower Shielding Reactor II to senior nuclear engineering students from UT. The reactor is located at the Tower Shielding Facility.

A memorandum of understanding outlines a program that will allow the students to perform startups and shutdowns and to become familiar

Students are briefed on the operations of the Tower Shielding Facility reactor before entering the control room for training.



with aspects of reactor operations, such as equipment lineups, conduct of operations, and compliance issues. The students will perform all operations under direct supervision of ORNL's certified senior reactor operators.

"This type of tangible experience is crucial for students in the nuclear engineering program," said Tom Kerlin, head of UT's Nuclear Engineering Department. "Working with an actual reactor, not just computer simulations, instills in the students a heightened level of respect for a nuclear facility." UT graduate William E. Hill, now an assistant section head for Category-B reactors at ORNL, said the Laboratory is looking forward to providing students this educational experience. "There are so few research reactors available for students now," he said. "We think it's very important to provide these types of opportunities whenever possible."

In 1987, following procedural reviews, a DOE shutdown order for several ORNL reactors eliminated the availability of facilities for student-participation programs at Laboratory reactors. Said Hill, "We're really pleased to get the program started again."

Work at the Tower Shielding Reactor II includes experiments to gauge various materials' abilities to act as a shield against radiation. Currently, a joint Japanese-American shielding program is under way there.—Wayne Scarbrough

## ORNL, TVA, UT Form Joint Institute for Energy and the Environment

In December 1991, ORNL joined the Tennessee Valley Authority (TVA) and the University of Tennessee (UT) in establishing a Joint Institute for Energy and Environment to promote and develop support for cooperative research and educational programs with an emphasis on energy and environmental projects.

The institute will also examine the sociological and economic impacts of such research- and education-related issues as oil

supplies, nuclear energy, ozone depletion, waste

disposal, and water quality.

The Laboratory has worked with TVA and UT on cooperative research and education projects since 1983, but this is the first time these organizations have cooperated on such a broad spectrum of issues.

The agreement is expected to strengthen education, training, and on-the-job experience for UT students in ecology, engineering, biological sciences, and other fields.—Joe Culver

### RE: R&D Updates

### **Bulk Shielding Reactor Shut Down Permanently**

t offered U. S. researchers a unique capability for studying the effects of neutron irradiation on materials at extremely cold temperatures. It provided important information on the ability of shielding to stop radiation. It served as a training facility for budding nuclear engineers. But the life of this 40-year-old reactor facility in Oak Ridge is over.

In September 1991, DOE ordered ORNL to shut down permanently the Bulk Shielding Facility (BSF), which includes the 2-MW Bulk Shielding Reactor (BSR) and the adjacent Pool Critical Assembly (PCA). The reason given was insufficient funding to support reactor operations.

Along with ORNL's other
Category-B reactors—the Tower
Shielding Reactor II (TSR-II), the
Health Physics Research Reactor, and
the Oak Ridge Research Reactor, the
BSF had been shut down by DOE in
March 1987 following the shutdown of
the High Flux Isotope Reactor (HFIR)
because of technical and management
concerns. The TSR-II and the HFIR
were returned to operation in late 1989
and early 1990, respectively, and are
currently in service.

The decision will cancel experiments planned for the Bulk Shielding Reactor's Low-Temperature Neutron Irradiation Facility. Some researchers had counted on using this facility to "freeze in" radiation-induced material defects that normally migrate in samples at ambient temperatures. In this way, they had hoped to understand how radiation alters material properties on almost an atomic level.

The PCA had been used to train generations of nuclear engineers. Officials say it will be particularly missed by the University of Tennessee's Nuclear Engineering Department because it had provided hands-on experience to both the undergraduate and graduate students.

A proposal has been made to DOE to retain use of the PCA, either in the BSR pool or at another



The Bulk Shielding Reactor, now permanently shut down, has served many useful purposes at ORNL for 40 years.

ORNL location. It would be used in support of training and education activities for a broad range of users, including the University of Tennessee, Louisiana State University, Mississippi State University, and Oak Ridge Associated Universities. It would also support DOE mathematics and science education initiatives.

The Bulk Shielding Reactor was originally used as a source for radiation-shielding experiments, from 1951 through 1963. After that, it served as a general-purpose research reactor.

ORNL officials are developing a closure plan. The BSF is expected to be decommissioned in several years at a cost of at least \$2 million.—

Carolyn Krause

### ORNL Model Results Dispute CO<sub>2</sub> Claims

Some scientists led by John Martin of Moss Landing Marine Laboratories in California believe that adding iron to the Antarctic oceans could substantially slow the rise of atmospheric carbon dioxide (CO<sub>2</sub>), which may contribute to global warming. However, results of an ORNL computer model suggest this action would be ineffective.

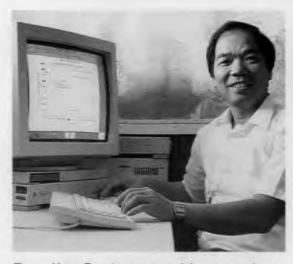
The scientists theorize that the presence of more iron would increase the biological productivity of phytoplankton, or microscopic algae. As a result, the algae would remove more CO<sub>2</sub> from the oceans' surface water, making it possible for the water to pull additional CO<sub>2</sub> from the atmosphere in order to reach thermal dynamic equilibrium.

But ocean models developed by Tsung-Hung Peng of ORNL's Environmental Sciences Division indicate that iron fertilization would not significantly increase CO<sub>2</sub> uptake. These models, which are calibrated to observed radiocarbon concentrations in the world's oceans, indicate that if iron were added to the Antarctic oceans, the subsequent decrease in atmospheric CO<sub>2</sub> would be only about one-third of the amount initially hypothesized.

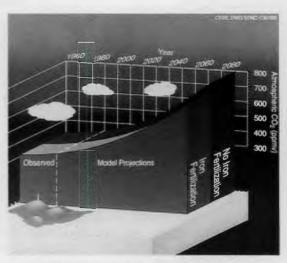
The ORNL models indicate that ocean mixing, the natural circulation of waters, plays a more important role than iron fertilization would in regulating the oceans' absorption of CO<sub>2</sub>.

# Greenhouse Gas Rise Linked to Changes on Land

For the past two decades, deforestation in Rondonia, Brazil, has increased at an unprecedented rate. As a result, less biomass is available to absorb atmospheric carbon dioxide and slow the rising level of this greenhouse gas produced by increased burning of fossil fuels. The large amount of deforestation and the resulting changes in human migration and land-use patterns in the area have been linked to increases in carbon dioxide levels.



Tsung-Hung Peng's ocean models are complex but can be executed quickly on computer workstations.



ORNL's ocean models indicate that if iron were added to the Antarctic oceans, the subsequent decrease in atmospheric CO<sub>2</sub> would be only about one-third of the amount initially hypothesized.

Virginia Dale, an ecologist in ORNL's Environmental Sciences Division, recently visited agricultural areas of Rondonia to gather data on changes in population patterns and land use resulting from deforestation. She and her ORNL colleagues used the data to construct computer simulations that predict both the effects of colonization and ecological changes on carbon dioxide concentrations.

"By tracking the history of each lot and tenant, we can simulate aggregate land-use patterns," Dale says. "Then we look at the results of different scenarios to help determine the best mix of land use and immigration to slow the increase in carbon dioxide levels."

Since the early 1970s, the Brazilian government has constructed roads and encouraged colonization in the Amazon region to reduce overpopulation of coastal cities. Thus, Dale says, road expansion is a reliable indicator of the amount of deforested area.

The vast majority of the farmers who have settled in Rondonia have burned large portions of the lush rain forests and converted the land to crop production and later to pasture as the ground became depleted of nutrients. Because forests contain about 90% of the carbon stored in the earth's vegetation, such burnings release large amounts of carbon dioxide into the atmosphere. "For at least a month each year," Dale says, "the smoke is so thick that the sun is visible only at sunrise and sunset."

Marcos Pedlowski, a Brazilian researcher at Oak Ridge Associated Universities, accompanied Dale for much of the research trip and interviewed 86 local farmers to determine more precisely how they use their land. Only two were managing their farms with agroforestry techniques—cultivating trees for lumber and coffee or planting cacao trees for chocolate while raising a mix of crops. The others still employ slash-and-burn agriculture, which is lowering the fertility of increasing amounts of land.

"Mixing crops and allowing trees to remain and reach a harvestable size," Dale says, "appears to be a much more sustainable strategy in the long run." She added that the development of the computer models, which is supported by the ORNL Director's Research and Development Fund, will be vital in planning future land-use strategies in South America and elsewhere.— Wayne Scarbrough

## DOE Okays ORNL's Corrective Action Plan

Implementation of an action plan to correct 414 deficiencies identified at ORNL during a 1990 Tiger Team assessment is estimated to cost \$740 million.

On November 25, 1991, Secretary of Energy James D. Watkins approved and directed implementation of the "corrective action plan" for ORNL. The plan describes the organizational structure, management systems, and specific responses that are being developed to implement corrective actions and to resolve root causes identified in the Tiger Team assessment. The DOE Oak Ridge Field Office and ORNL prepared the action plan with input from DOE's offices of Energy Research, Nuclear Energy, and Environmental Restoration and Waste Management.

The Tiger Team assessment is part of an overall initiative introduced by Admiral Watkins in June 1989 to strengthen environmental, safety, and health programs at DOE. The Tiger Team identified a total of 414 "findings" during the assessment, conducted from October 22 through November 30, 1990. The findings included 331 safety and health, 70 environmental, and 13 management inadequacies.

Many deficiencies already have been corrected, according to Mike Kuliasha, who headed preparation of the action plan. Corrective actions are being taken in order of priority to address the most serious problems first. ORNL had no category-1 findings that pose an immediate risk to health or the environment. The Tiger Team did make 12 category-2 findings that present a significant risk. Kuliasha said that 10 of the 12 category-2 findings made by the Tiger Team will be corrected by the end of 1992 and that the other two deficiencies in this category will be remedied by 1994.

According to a DOE news release: "In many cases, the planned corrective actions are straightforward and can be readily implemented within funding levels. Because of the need to hire additional people, develop and implement

Number One, 1992 73

oversight procedures and practices, design and construct monitoring equipment and correct the many legacy problems, some corrective actions will require additional funding and years to implement.

The total cost for these efforts is approximately \$740 million. A schedule for accomplishing all corrective actions has been established."

Copies of the ORNL Tiger Team Corrective Action Plan are available for reference at the DOE Headquarters Reading Room in Washington, D.C., and in the Reading Room at the DOE Oak Ridge Field Office.—Carolyn Krause

business reason—it allows them to postpone the need to build expensive new power plants.

Many utilities run programs that promote energy-efficient lighting systems for commercial

buildings, including electronic ballasts, new lamps, better reflectors, and controls. Utilities often work with architects. engineers, and builders to encourage construction of more energyefficient homes and office buildings. And some utilities help pay for the extra cost of energyefficient



### Benefits of Lowering Demand for Electricity

U. S. electric utilities could reduce the projected growth in demand for additional electricity by nearly half by accelerating programs that encourage more efficient use of electrical power. Aggressively implementing such demand-side management programs could cut the nation's electric bills by \$61 billion a year and reduce total carbon dioxide emissions in the United States by 9% by the year 2010.

This is a conclusion of Eric Hirst, a corporate fellow in ORNL's Energy Division, in his report entitled "Possible Effects of Electric Utility Demand-Side Management Programs." He notes that an increasing number of utilities are interested in reducing the demand for their product for a good

appliances, such as refrigerators and water heaters.

Hirst believes these benefits will result assuming that (1) regulatory and other incentives cause the percentage of U. S. utilities offering demand-side programs to grow from 20 to 75% by 2010, (2) those utilities succeed in increasing the percentage of customer participation from 7 to 12% each year, and (3) the savings per customer in the programs increase from 15 to 22%.

According to Hirst, "The potential benefits to be gained are so large that utilities, state regulators, the federal government, and customers should consider expanding demand-side management activities. Such expansion may result from several emierging factors that could influence the regulatory climate."

These factors are (1) the growing interest in integrated resource planning, (2) increased concern about protecting the environment, (3) the trend of giving utilities financial incentives to operate cost-effective demand-side programs, (4) an increasing reliance by utilities on competitive bidding, and (5) the growing recognition of the role utilities can play in overcoming market

barriers to the adoption of conservation measures, such as the compact fluorescent lightbulb.

"Utilities in as many as 20 states use integrated resource planning to choose new supply- and demand-side options," Hirst said. "Among other things, those programs explicitly consider conservation as an alternative to new power plants."

The report observes that electricity generation results in about two-thirds of the sulfur dioxide and one-third of the nitrogen oxide and carbon dioxide emissions in the United States. "In the past, some utilities reduced emissions beyond levels required by federal and state laws to be good corporate citizens," Hirst said. "Now, utilities have another motive for reducing electricity generation to reduce pollution. Because utilities must abide with regulations such as the 1990 Clean Air Act Amendments, pollutants will become more expensive for them and, consequently, for ratepayers."

The report, issued and available from ORNL, also examined the reasons why utilities should encourage their customers to adopt energy-efficiency measures.

"Among the factors that should make utilities want to intervene," Hirst said, "are their interest in improving relationships with customers, technical know-how, and access to large amounts of capital."—Darryl Armstrong

## Promising Results on Cold Neutron Source

Preliminary test results show that ORNL's development of a "cold" neutron source for an advanced research reactor is promising. The source will be operated at extremely low temperatures on the world's most powerful research reactor currently under design.

That reactor, the Advanced Neutron Source (ANS), is being considered for construction at ORNL. The ANS would be designed to meet the

national need for an intense, steady-state source of neutrons for research and would enable the United States to recapture world leadership in neutron-scattering experiments.

A major justification for the ANS is to provide neutrons of very low energy for research in materials science, biology, and fundamental physics. These cold neutrons are produced by passing neutrons from the reactor's core through a moderator, which slows them down by absorbing much of their momentum during collisions with other atoms. The two cold neutron sources that will be located near the core of the ANS will be identical vessels containing liquid deuterium at a temperature of about 20 K.

Deuterium, an isotope of hydrogen, was chosen as the moderator for the ANS cold source because its molecules efficiently slow down the neutrons without absorbing them and because deuterium does not freeze at these low temperatures.

At ORNL tests are being conducted using models of the cold neutron source because this type of moderator, known as a boiling moderator configuration, has never been used at the high heating levels expected in the ANS. Because of the heat from gamma rays produced by the reactor, the temperature of the deuterium will tend to increase. This type of cold source dissipates heat by allowing the deuterium to boil so that its vapor transfers the heat to a heat exchanger located above the cold source vessel. The condensed deuterium flows back to the vessel through a liquid return line.

In recent tests using a model consisting of liquid nitrogen (at a temperature of about 75 K) instead of deuterium and a grid of electric heater wires to simulate the gamma heat, researchers at ORNL have demonstrated stable operation of the cold source at power levels greater than expected in the ANS facility.

Further experiments will be conducted using models that simulate the shape and heating of the ANS cold source even more accurately. A second series of tests using liquid hydrogen or liquid deuterium will be performed.—Wayne Scarbrough

"A major justification for the ANS is to provide neutrons of very low energy for research in materials science, biology, and fundamental physics."

Number One, 1992 75

Todd Halihan, a student at Monmouth College, uses image-processing software to determine the number of bubbles of different sizes in a rectangular column of liquid flow captured by a video camera.



### Bubble Studies for the Cold Neutron Source

By combining video footage of air bubbles in an aquarium-size water tank with image-processing software developed by the federal government, researchers at ORNL are gaining a better understanding of liquid flow patterns and can better calculate the portion of a fluid volume that is vapor.

The findings may lead to the development of an instrument to measure the void fraction (volume of liquid occupied by bubbles) of liquid deuterium in the Cold Neutron Source now being designed for use on the ANS (see the preceding story). If the vapor fraction is too high, neutron-scattering researchers might not have a sufficient number of cold, or low-energy, neutrons for their projects.

Because of the heat from gamma rays produced by the reactor and the energy transferred from the neutrons as they slow down, the temperature of the deuterium will tend to increase. Bubbles will be produced in the liquid deuterium because of the deposition of heat in the Cold Neutron Source. Too many big bubbles could reduce the output of cold neutrons.

"By using free Shareware image-processing software developed by the National Institutes of Health," says Art Ruggles of ORNL's Engineering Technology Division, "we will be able to simulate bubbly flows in liquid deuterium and calculate the number and size of bubbles in a Cold Neutron Source vessel to determine how much deuterium is liquid and how much is vapor.

"By simply using things found in people's homes—an aquarium

made bubbly with rubber hoses, a Macintosh computer, software, and a video camera, we are developing an inexpensive technology for applications on a very expensive device."

Ruggles said he first learned about the software from a friend at Washington University who was using it to study deflections of the human eardrum. Ruggles decided this software, originally designed for medical diagnostic purposes, has applications in thermal hydraulics.

The image-processing software allows
Ruggles and Todd Halihan, a student at
Monmouth College, to determine the number of
bubbles of different sizes in a rectangular
column of liquid flow captured by a video
camera. The direction of travel and the velocity
of the bubbles can also be determined.

Ruggles says the work could be applied to chemical reactors in which heated mixtures of liquid and vapor result in difficult-to-understand patterns of liquid recirculation.—

Carolyn Krause

### : Technical Highlights

## "Fuzzy Logic" Control System Guides Maze-Navigating Robot

new fuzzy logic control system, including custom-designed fuzzy inferencing computer chips and circuit boards, serves as the brain of a mazenavigating robot being tested at ORNL's Center for Engineering Systems Advanced Research (CESAR).

Developed by Francois Pin of the Engineering Physics and Mathematics Division and researchers from the University of North Carolina (UNC), the control system successfully combines the processing power of high-speed computer chips with the efficiency of approximate, or "fuzzy," reasoning.

Using sensors to gather approximate information about its surroundings, the robot can successfully navigate a maze on the basis of inferences it makes about its environment, rather than precise measurements. Pin compares fuzzy logic to his reaction to touching a hot stove. "I don't need to know exactly how hot the stove is," says Pin. "I simply sense that it's hot, and I pull my hand away."

Thanks to the processing power of its fuzzy control system, the robot can also think on the move. "We had hoped that the chip would be able to process 100 inferences per second," says Pin, "about the same level as the human brain." As it turns out, the chip is capable of processing 30,000 inferences per second—far faster than data can be gathered.

Part of fuzzy logic's appeal is that it approximates human decision-making, which is based, largely, on fuzzy or approximate reasoning. "In the field of reasoning there are situations that cannot be characterized by 'yes' or 'no," Pin says. "There are large gray areas where human reasoning is simply approximate."

The theory behind fuzzy logic was developed about 25 years ago by Lotfi Zadeh, a professor of electrical engineering and computer science at the University of California at Berkeley, to provide a mathematical framework for dealing with undefined quantities. Pin has found that the fuzzy approach stands in marked contrast to traditional problem-solving methods in his field.

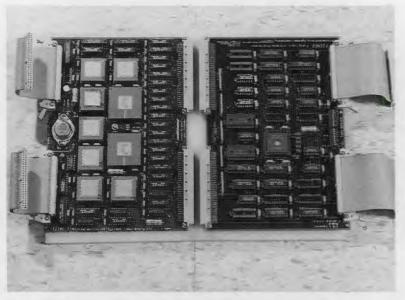
"We have always thought in terms of binary situations—'yes' or 'no' dualities," said Pin. "This is reflected in modern math and computing, which allow very accurate and detailed representations of



Francois Pin removes the seven-chip fuzzy logic control system from its slot on the mobile robotic platform. The cube-shaped objects ringing the platform are acoustic sonar sensors the robot uses to navigate.

Number One, 1992

"Now, instead of thousands of lines of code, we have just 15 rules that control how the robot moves."



The robot's enhanced fuzzy logic control system incorporates seven fuzzy chips that can be reconfigured on-line, allowing multiple stages of reasoning, as well as advanced induction and deduction.

things, and, for many problems we wanted to solve, this approach was very appropriate."

But, eventually, as Pin and other robotics researchers searched for innovative methods of controlling intelligent machines, they decided the level of precision and detail they were achieving was not entirely necessary. This realization led them to investigate several approximate methodologies, from which they settled on fuzzy logic. Fuzzy methodology allows approximate variables like "near" and "far" to be expressed in terms of numbers. Once the variables are quantified, they can be used to develop navigation rules such as, "If the object is far, speed up."

The obvious advantage of using fuzzy control systems is that they can be more cost effective and user friendly than traditional methods of control. "We used to deal with tens of thousands of lines of computer code to describe the process of navigation," said Pin. "We found that, by using fuzzy reasoning, judicious trade-offs could be made among speed, complexity, and accuracy. Now, instead of thousands of lines of code, we have just 15 rules that control how the robot moves."

Another advantage of fuzzy logic is that, because it can deal with and merge tendencies, in addition to "off" and "on" conditions, it generally leads to much smoother controls, as has been demonstrated in subway and airplane control applications.

Fuzzy chips and control systems are already increasing the efficiency of household appliances, subway systems, and automobile transmissions. Even the National Aeronautics and Space Administration (NASA) is looking at the possibility of using fuzzy systems for spacecraft control.

The robot used in fuzzy navigation experiments is a state-of-the-art, omnidirectional wheeled platform developed by Pin and his colleagues. It is ringed by 24 acoustic sonar sensors that allow it to approximate the distance to objects in its environment.

"We used the least accurate sensors we could find to demonstrate the power of fuzzy reasoning," Pin said. "The robot navigates with no problems in an unknown environment on the basis of inaccurate and uncertain data—even when only a few of the sensors can provide data. In the past when one or more sonar sensors failed, the robot was usually disabled, but this is not a problem with the fuzzy system," says Pin. "It's extremely robust in this respect."

To further improve the robot's performance, Pin and his colleagues at UNC have developed an enhanced fuzzy logic control system that incorporates seven fuzzy chips. "As far as I know, this is the only fuzzy control system that uses multiple chips," says Pin, "and it is particularly useful because it can be reconfigured on-line, depending on the application. This feature allows the system's mode of reasoning to be changed at the flip of a switch."

The use of several chips enables the system to perform "cascades," or multiple stages of reasoning, as well as advanced forms of inferencing involving induction and deduction cycles. Based on the promising results of their chip-development activities, Pin and his colleagues at UNC are negotiating with an industrial partner to manufacture and market their fuzzy control systems.

Future plans for Pin and his colleagues include applying their knowledge of fuzzy reasoning to other intelligent behaviors, such as artificial vision. "Conventional artificial vision systems tend to analyze images in great detail before they can characterize what they see," Pin says. This requires a great deal of computational power and processing time. On the other hand, humans can quickly recognize things on the basis of general characteristics. We are investigating using fuzzy logic to extract this type of approximate information from an image that could enable us to directly recognize specific characteristics or objects within the image."

Pin stresses that fuzzy logic is not applicable to all situations, and he and his colleagues have developed a list of criteria to identify situations that could benefit from the application of approximate reasoning. "If we have a system that is well known and quantifiable," says Pin, "we use conventional techniques. But if a system is not completely known or is too complex to be handled quickly enough with conventional techniques, and the measuring techniques or available data are subject to large uncertainties, it may be amenable to solution by fuzzy logic."—Jim Pearce

### Mount St. Helens: Life Rising from the Ashes

When Washington's Mount St. Helens volcano roared back to life in 1980 after lying dormant for more than a century, it did so with a vengeance. The blast decapitated the mountain and raced

down its north face at speeds up to 250 mph, incinerating nearly all signs of life within six miles and scorching trees up to 23 miles away.

Despite its barren appearance, the landscape left in the wake of the eruption provided an ideal natural laboratory for studying the recovery of life in the devastated area.

Virginia Dale of ORNL's Environmental Sciences Division, who has spent the last decade studying the reestablishment of plant life on the debris avalanche northwest of Mount St. Helens, says, despite the destruction it caused, the eruption of Mount St. Helens has taught us some important lessons.

"We've learned something about the resilience of nature," says Dale. "We've also learned that we don't have to *do* something to reestablish vegetation after natural disasters. No one would



By the time research plots were established in 1981 and 1982, at least 20 plant species, including Western hemlock (*Tsuga heterophylla*) seedlings, were growing on the debris avalanche.

"We've learned something about the resilience of nature," says Dale. "We've also learned that we don't have to do something to reestablish vegetation after natural disasters."

Number One, 1992

have predicted that plants on the mountain would recover so quickly."

However, the first reaction of federal and state agencies was to do something about the devastation caused by the eruption. This attitude was fostered, in part, by the extensive property damage caused by recurring mudflows along the Toutle River, east of the mountain. Eventually Congress granted \$1.6 million to address the problem, and a campaign to stabilize the

mudflows by seeding a huge area around the mountain with grasses was begun by the Soil Conservation Service (SCS).

"I was at the International Congress of Systematic and Evolutionary Biology in Vancouver, British Columbia, shortly after the eruption occurred," Dale says. "We were concerned that seeding the area would ruin its potential as a natural laboratory and inhibit the colonization and growth of other species." A

> resolution passed by the group failed to stop the seeding, but it played a role in reducing the size of the seeded area from over 200,000 to only 21,000 acres."

Aerial seeding was used to spread special mixtures of seeds over the target areas. Because adequate supplies of native seeds were not available, the seed supplied by the SCS consisted mainly of "exotic" (mostly European) species of grass and groundcover, selected for their adaptability, rapid germination, suitability as food or cover for wildlife, and ability to "fix" nitrogen in the soil.

Despite these efforts, erosion was not controlled, partly because of the failure of the seeds to take root in the eroded areas and partly because of the nature of the erosion. Much of the erosion occurred when large sections of mud and debris became saturated and slid, or "sloughed off," downhill. "I don't know of anything they could have seeded that area with that could have controlled slough erosion," says Dale.

Her study focused on the revegetation of the debris avalanche on the northwest slope of the mountain, several miles east of the seeded areas. The avalanche was surveyed two months after the eruption and was chosen for its nearly complete lack of vegetation

"Plots with concentrations of introduced species



These photos taken in 1985 (upper) and 1989 (lower) illustrate the change in vegetation cover brought about by the Soil Conservation Service's seeding of exotic grasses.

actually decreased in plant diversity between 1983 and 1989. whereas plots with only native species increased in

diversity."

high

(the eruption covered the area with deposits of mud and debris averaging 45 m thick).

In 1981 and 1982, Dale and her team established 97 250-m<sup>2</sup> research plots on the debris avalanche and found that, despite the eradication of most plant life, widely scattered representatives of at least 20 species were growing in the area.

"These plants apparently grew from pieces of roots or stems that survived the landslide," says Dale. "The soil in the avalanche area has enough nutrients to sustain plant life, but nothing grows very well there."

By 1989, nine years after they were sown on the mudflows, the exotic species of grass and groundcover had been carried by wind or animals to the 11 westernmost plots of Dale's study area, allowing her to study the effect of introduced species on natural revegetation. "The ability of these species to cover an area rapidly is one of the reasons they were selected for the revegetation program," Dale says. "However, on the debris avalanche, they are also associated with poor development of the native species." In fact, plots with high concentrations of introduced species actually decreased in plant diversity between 1983 and 1989, whereas plots with only native species increased in diversity during those six years.

"It could be that seeding with native species would have enhanced the recovery of native trees and herbs," Dale says, "but the SCS had to use the seeds that were available at the time because the money allocated by Congress had to be spent within 6 months—that's not enough time to cultivate a supply of native seeds." To avoid similar problems in the future, the SCS now maintains nurseries of native species to build up their seed reserves.

The use of exotic seeds also had some unforeseen side effects, such as increasing the seed-eating mouse population to 25 times its normal level in some areas. When winter came and the grasses stopped producing seeds, the mice turned to eating the bark around the bases of trees. It is estimated that 55% of the die-off of conifers following the eruption resulted from mouse damage. Eventually predators, including

coyotes, hawks, and eagles, moved into the area, and the mouse population was reduced to a sustainable level.

"The Mount St. Helens eruption was a tremendous opportunity for scientific study," Dale says, "and it was taken advantage of. The main thing we have learned from studying the revegetation of the area is that the natural recovery has been phenomenal, even without human interference," Dale says. "We've found nearly 90 species on the debris avalanche alone."

"Species you'd never expect to see again have survived," says Dale. For instance, before its eruption, Mount St. Helens was home to the pink and purple-flowered *Penstamon cardwellii*, found nowhere else on earth. Today, growing in abundance through the ash on the slopes of the mountain, these delicate wildflowers are a living testament to nature's subtle strength and perseverance.—*Jim Pearce* 

### **Addressing Global Chemical Pollution**

Can the Environmental Protection Agency's (EPA's) current approach to controlling exposure to chemical pollutants significantly reduce the cancer rate in the United States? Would addressing the problem in terms of global chemical pollution be a more effective approach? These questions are addressed by Curtis Travis, director of the Center for Risk Management at ORNL, and Sheri Hester, an information specialist at Integrated Laboratory Systems in Oak Ridge, in their study of global chemical pollution, published in the May 1991 issue of Environmental Science and Technology.

Citing a recent study that found that the \$100 billion spent annually to comply with EPA regulations has resulted in, at best, a 1.3% reduction in cancer deaths, Travis claims that current attempts to appreciably reduce the cancer death rate are failing, not because of a lack of funding but because of a short-sighted approach to regulating environmental pollution.

"Travis claims that current attempts to appreciably reduce the cancer death rate are failing because of a short-sighted approach to regulating environmental pollution."

81

Number One, 1992

"The problem is that current regulatory approaches to environmental pollution do not incorporate ways of dealing with global pollution," says Travis. "Instead the major focus is on protecting the maximally exposed individual. Locally high concentrations of pollutants are decreased, not by destroying the chemicals or decreasing production, but rather by moving them to another environmental medium."

As an example of the problem, Travis points to the practice of reducing stack emissions using scrubbers in which water removes gases and particulates from emissions. "Scrubber water is often flushed into the sewer system and carried to the local waste treatment plant, where up to 99% of the volatiles are released back into the air."

Once chemicals are released into the environment, they seek out the environmental medium (air, water, soil, or biota) in which they are most soluble. For example, benzene is most soluble in air, so people are generally exposed to it through inhalation. On the other hand, because some pesticides and polychlorinated biphenyls (PCBs) are most soluble in organic matter, they are transferred to humans through the food chain.

Atmospheric transport is recognized as the primary mode of global distribution for organic chemicals. Although most organic compounds reside mainly in the soil, small amounts volatilize to the atmosphere and are transported globally. These pollutants enter the food chain through various routes and are then taken up in the predators that feed on the herbivores.

As more is learned about the effects of chemical pollutants on the environment, a consensus is emerging that even trace levels of contamination can have serious environmental consequences. "With increasing regularity, we find chemical contamination in parts of the world previously thought to be pristine," Travis says, giving examples such as the near-toxic levels of PCB exposure experienced by Arctic inhabitants as a result of their consumption of contaminated fish and aquatic mammals. "We maintain that ambient levels of pollution have

risen to the point where human health is being affected on a global scale."

The following chemicals are among the pollutants that humans are exposed to on a regular basis, largely because of atmospheric transport.

PCBs. Until they were banned in 1977, PCBs were widely used as dye solvents, plasticisers, dielectric fluids, and hydraulic fluids. Although virtually all PCB mass is found in soil, volatilization of PCBs from spills, landfills, and other sources makes atmospheric transport the primary mode of PCB distribution.

Dioxins. One of the most potent carcinogens ever evaluated by the EPA, dioxins have been measured in practically all environmental media, including air, soil, meat, milk, fish, vegetation, and human samples. Air transport of TCDD (2,3,7,8-tetrachlorodibenzo-p-dioxin, the most toxic of the dioxins) accounts for 66% of the TCDD in the forage for beef and dairy cattle. As a result, the food chain, particularly meat and dairy products, accounts for 99% of human exposure to TCDD.

Benzene. Benzene is a widely used commercial chemical and a by-product of burning wood, garbage, organic wastes, and cigarettes. It has also been shown to cause cancer in humans. Benzene is found almost exclusively in the air (99%); less than 1% resides in water, soil, and other environmental media. Thus, inhalation is the primary human exposure pathway.

Mercury. The primary man-made sources of mercury are the burning of fossil fuels, mining, manufacturing, and waste incineration. Because of this toxic metal's high volatility and long atmospheric residence time, atmospheric deposition is the major source of global mercury contamination. Evidence of this is found in the increasing number of reports of mercury contamination of fish from remote lakes despite the lack of nearby sources of man-made mercury.

Lead. Primarily found in paint and gasoline, lead is particularly toxic to children and the young of other species. The major cause of lead poisoning in children in the United States is the

"With increasing regularity, we find chemical contamination in parts of the world previously thought to be pristine."

#### Background cancer risk from 11 global pollutants<sup>a</sup>

Chemical and exposure medium	Risk (×10 <sup>-4</sup> )
Indoor air	
Benzene	1
Trichloroethylene	0.15
Tetrachloroethylene	0.12
Carbon tetrachloride	1.2
Formaldehyde	0.65
Xylenes	0.11
Water	
Chloroform	3
Food chain	
Dioxins and furans	2.1
Dieldrin	0.78
EBDCs	3.4
PCBs	1.1
Total lifetime cancer risk	14

<sup>a</sup>Risk estimates are based on current EPA methodologies for estimating cancer risk. Because of uncertainties in these methodologies, the above risk estimates may not represent actual risk to individuals. Source: Haemisegger, E. R.; Jones, A. D.; Teinhardt, F. L. J. Air Pollut. Control Assoc. 1985, 35, 809–15.

ingestion of lead in paint, with the inhalation and ingestion of lead in soil a close second.

Travis raises the question of whether global background cancer risk may be as high as 1 cancer per 1000 people (10<sup>-3</sup>) instead of as low as the generally accepted 1 cancer per 10 million people (10<sup>-7</sup>). According to Travis, "Humans are exposed to hundreds of synthetic organic chemicals every day, but the true extent of human exposure to environmental pollution has never been quantified. Background cancer risk based on measured exposure can account for 1 to 2% of actual annual cancer deaths, which is consistent with other estimates of the contribution of chemical pollution to background cancer rates. However, this figure is far in excess of the generally accepted target range of 10<sup>-7</sup> to 10<sup>-4</sup>."

The high background cancer rate documented in the table above brings into question EPA's regulatory focus on controlling local exposure to large point sources of pollutants. These sources typically have maximum individual risks in the  $10^{-3}$  to  $10^{-4}$  range, but because risk drops off rapidly with distance from the source, the risk to the average individual is typically in the  $10^{-5}$  to  $10^{-7}$  range. The effect of this approach to controlling exposure is to protect the most highly exposed individuals while doing little to reduce the cancer rate in the general population resulting from exposure to chemical pollutants.

"If we do not want to reduce our standard of living, the only way to reduce global chemical pollution is to make our consumption and production processes more efficient and lower the level of production of these toxic chemicals," Travis warns. "The only reasonable solution to global pollution is not increased regulation of isolated point sources, but rather an increased emphasis on waste reduction and material recycling. Until we focus on these issues, we

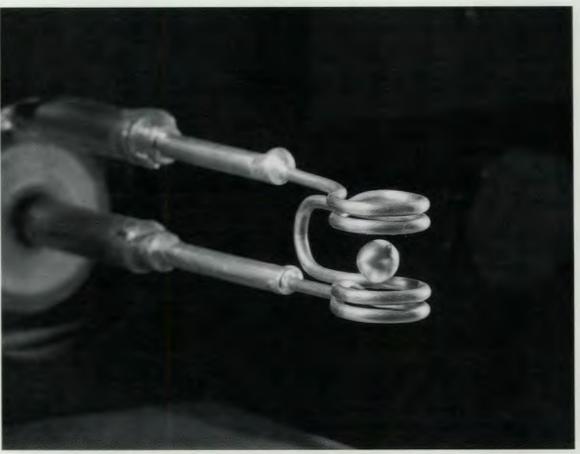
will continue to experience background cancer risk in the 10<sup>-3</sup> range."—*Jim Pearce* 

## Researchers Simulate Space Conditions

Relying on earthbound and airborne experiments, ORNL researchers Dick Fox and Chuck Hahs, both of ORNL's Instrumentation and Controls Division, have worked with the National Aeronautics and Space Administration (NASA) to successfully simulate experimental conditions in space and aboard the space shuttle.

In November 1991, Fox and Hahs approximated the high-vacuum, weightless

"When the undercooled metal finally crystallizes, it does so very rapidly, affecting the crystal structure."



Dick Fox and Chuck Hahs use two high-frequency electromagnetic coils to levitate samples in metallurgical experiments that investigate the effects of undercooling on crystal structure. A third, higher-frequency coil (not shown) is used to gradually heat and cool the sample.

conditions of space when they simultaneously levitated and melted a 5-mm (0.2-in.) niobium sphere in a vacuum. Two electromagnetic coils were used to suspend the sample, and another adjustable coil operating at a higher frequency regulated its heating and cooling. This successful experiment was the latest milestone in an 18-month effort to supply NASA with a simulation of the conditions that will exist during metallurgical experiments both on the space shuttle and on the proposed wake shield, a 4-m (12-ft) experimental platform that will be tethered to the outside of the shuttle.

Experiments mounted on the wake shield will take advantage of the ultrahigh vacuum the shield

will create as it pushes aside trace gases, such as hydrogen, helium, and oxygen (10<sup>-14</sup> torr H, 10<sup>-18</sup> torr He, 10<sup>-35</sup> torr O). On the earth, 10<sup>-11</sup> torr is considered an ultrahigh vacuum.

Undercooling studies and other metallurgical experiments will also be conducted aboard the space shuttle. Undercooling is the process of gradually cooling molten metal to temperatures below its melting point. When the undercooled metal finally crystallizes, it does so very rapidly, affecting the crystal structure. "Using the adjustable electromagnetic heating coil," says Fox, "we can gradually reduce the temperature of a sample to achieve undercooling. If we could cause the metal to undercool enough, it might

never recrystallize, and, instead, form an amorphous metal glass."

Fox and Hahs were first approached by representatives from NASA's Marshall Space Flight Center in Huntsville, Alabama, about the project.

"They were interested in melting and recrystallizing niobium in space," says Fox. "And they wanted to know if we could do something on the ground that would resemble those conditions." They were interested in niobium primarily because its high melting point would provide a rigorous test of the system's heating capabilities and because it undercools severely.

Because of the space and power constraints of the space shuttle, Fox and Hahs had to downsize their hardware. The normal furnaces being used in laboratories are about the size of an office desk and operate on 220 volts of alternating current. "Dick has reduced the furnace to about the size of a cigarette box," says Hahs. "That, combined with a high-efficiency radiofrequency generator, allows us to use 28 volts of direct current from the shuttle to run the experiment."

Although Hahs and Fox proved in November that they could melt levitated niobium in a vacuum on the ground, one factor was still hampering their simulation—gravity. This problem was overcome in December when Hahs accompanied the experimental apparatus on a flight of NASA's specially modified KC135A transport plane, the Weightless Wonder.

Diving repeatedly from an altitude of 11,600 m (38,000 ft) to 6100 m (20,000 ft), the Weightless Wonder (also known as the Vomit Comet) traced a parabolic path in the sky every 90 seconds, providing 20 seconds of near-weightlessness for researchers on every descent. During the flight, Hahs successfully tested the system's levitation capabilities in microgravity by levitating spheres of gold, silver, lead, niobium, and aluminum.

In November 1992, Hahs and Fox plan to conduct a test of the entire system on the Weightless Wonder by both levitating and melting niobium in microgravity.—Jim Pearce



NASA's
Weightless
Wonder provided
ORNL researchers
with the
microgravity
environment
necessary to
simulate
conditions in earth
orbit.

#### : Technology Transfer

## **President Bush Visits ORNL for Signing of Coors CRADA**

President George Bush (center), applauds Coors president, Joseph Coors, Jr., seated left, and Alvin Trivelpiece, ORNL director, as they sign a CRADA. Looking on from left is Secretary of **Energy James** Watkins. At right is Secretary of **Education Lamar** Alexander.



n February 19, 1992, President George Bush visited ORNL to witness the signing of a \$3.6 million, three-year cooperative research and development agreement (CRADA) between the Laboratory and Coors Technical Ceramics Company. The agreement, which was signed by Joseph Coors, Jr., president of Coors (based in Golden, Colorado), and ORNL Director Alvin Trivelpiece, will create 85 jobs and may lead to precisely shaped ceramic parts for multiple uses, including the highly efficient and durable high-temperature engines of the future.

"This agreement," the president told 800 ORNL employees, "combines in one place the resources of government with the energy and

inventiveness of private enterprise, and you're pointing our country toward the next American century." He added that the future of U. S. competitiveness in the world marketplace depends on research and development. "I'm talking about something you all know a lot about."

A CRADA is a partnership agreement that enables national laboratories and U.S. industrial firms to combine their resources for developing commercially attractive technology. The goal may be achieved by sharing personnel, facilities, services, equipment, or other resources. CRADAs have been made possible by the National Competitiveness Technology Act of 1989.

President Bush is only the second U. S. president to visit ORNL (unless you count

Zachary Taylor, whose remains were analyzed for arsenic at ORNL in 1991). The first president to visit ORNL was President Jimmy Carter in 1978.

President Bush, who had just won the New Hampshire Republican primary election, delivered his message in front of the High Temperature Materials Laboratory (HTML), which he toured. He cited this CRADA, the 26th signed by Energy Systems, and 675 other public-private agreements as examples of recent successes in overcoming obstacles to sharing government technology with private industry.

President Bush called the HTML "a world-class advanced materials testing facility" and said it "will be working with American industry to take the world lead in making precision ceramic parts. We're in a race with other nations in this multimillion dollar market, and we will get there first with the best product, thanks to the hard work of the people right here and the imagination of your scientists."

The president said that ORNL and Coors researchers would "attack one of the obstacles to wider use of durable, efficient, and lightweight ceramic parts—machining ceramics without destroying their desirable qualities." The collaborative work, which will involve staff members of the Oak Ridge Y-12 Plant, will take place largely in the new Ceramic Manufacturability Center in the HTML.

The president thanked Coors for presenting him with a ceramic golf putter. "If this doesn't help," he said. "I'll use it as a hammer." Also present at the ceremony were U. S. Secretary of Energy Admiral James Watkins; Education Secretary Lamar Alexander (former Tennessee governor and president of the University of Tennessee); and Tennessee Representatives James Quillen, Don Sundquist, and John Duncan.

The ORNL-Coors agreement is the first of several CRADAs to be entered into under a new cooperative program for precision machining of cost-effective ceramic components. This CRADA will combine ORNL's materials expertise with the technical capabilities of the Y-12 Plant in

precision machining and inspection of ceramic parts.

Under the new program approved by DOE on February 5, a new Ceramic Manufacturability Center will be located in the HTML. The new center's staff will include ORNL experts in characterizing materials and Y-12 Plant staff members who have skills in precision machining developed for manufacturing nuclear weapons components. Working in research partnerships with American companies, they will develop new ways to precision manufacture and machine advanced structural ceramics and other hard materials more efficiently and economically than is possible using current industrial practices.

Five major U.S. structural ceramic companies have agreed to conduct manufacturing research in this center under CRADA arrangements. Another company, a major supplier of coordinate-measuring machines, has agreed to provide a state-of-the-art system in the center as part of another CRADA agreement.

According to the CRADA abstract, Coors is interested in improving its control over the quality of ceramic processes and products by developing fabrication and testing techniques that are better than the standard ones. The goal is to evaluate the high-strength aluminum oxide tubes fabricated by Coors to determine how much material defects affect tube strength. The expected results of the work are better methods for manufacturing and inspecting these tubes and a data base that helps researchers determine how to improve processes to produce tubes having the most desired mechanical and material characteristics.

The Ceramic Manufacturability Center is the result of over a year's efforts by Vic Tennery and Ray Johnson, both of ORNL; Fred Jones, Bill Barkman, and Tom Morris, all of the Y-12 Plant; and Warren Siemens of the Office of Technology Transfer of Martin Marietta Energy Systems, Inc. The new center, which will initially occupy four laboratory modules and several offices in the HTML, will house some machines transferred from the Y-12 facility, new machines donated

"President
Bush called
the HTML
"a worldclass
advanced
materials
testing
facility."

"Lauf initiated the development of a furnace that uses the same type of microwavegenerating equipment employed by U.S. armed forces to jam Iragi radar during the Persian Gulf War"

under CRADA agreements by U. S. machine tool companies, and some instruments from HTML laboratories.

According to Siemens, "The Ceramic Manufacturability Center represents a significant program combining the expertise and skills of ORNL and the Y-12 Plant and having substantial long-range benefits. It will provide the scientific base and proof-of-principle development for reliable and cost-effective machining of ceramics. Full prototype evaluation of the experimental technologies will be accomplished in the planned Manufacturing Technology Deployment Center at the Y-12 Plant."

### New Microwave Furnace Eliminates Hot Spots

If you cook with microwave ovens much, you know they have a problem with thermal gradients—hot spots. This is usually most apparent when, after you've had two perfectly normal bites of casserole, the third bite parboils your tongue and peels the skin from the roof of your mouth.

This characteristic lack of uniformity in microwave heating also concerns materials researchers, such as Bob Lauf of ORNL's Metals and Ceramics Division. He and other ORNL researchers use single-frequency microwave furnaces to increase density, strength, and structural uniformity in a wide range of ceramic products. Their success depends, to a great extent, on being able to heat objects rapidly and uniformly. When uneven heating occurs, internal stresses develop that can cause objects to weaken or even shatter.

To overcome this problem, Lauf initiated the development of a furnace that produces not just one frequency, but a range of microwave frequencies, using the same type of microwave-generating equipment employed by U.S. armed forces to jam Iraqi radar during the Persian Gulf

War. The development involved the exchange of technology in a CRADA between ORNL and Microwave Laboratories, Inc. (MLI), a military contractor in Raleigh, North Carolina.

"Using conventional, single-frequency microwave techniques, you can approach the problem of hot spots in one of two ways, and neither one completely solves the problem," says Lauf. "One way is to physically disrupt the microwaves as they enter the furnace, scattering them more evenly around the furnace cavity. Another approach is to combine a large furnace cavity with high-frequency microwaves. Because high-frequency microwaves have short wavelengths, there are no single, large standing waves—waves that intersect the object being heated at a relatively limited number of points. The result is fewer hot spots. Unfortunately, these techniques only lessen the severity of the problem; they don't eliminate it."

To avoid thermal gradients altogether, Lauf and others considered building a variable frequency furnace. This type of device could achieve highly uniform heating by "sweeping the frequency"—varying the frequency of the microwaves back and forth across a given range, from thousands to millions of times per second. A variable furnace would also allow researchers to experiment with a range of microwave frequencies to determine if one yields optimum results for a particular material.

Lauf asked Don Bible of the Instrumentation and Controls Division about the possibility of making a mechanically adjustable gyrotron—the device used to generate microwaves in some single-frequency furnaces. "The problem is that these high-vacuum, high-voltage tubes would be a nightmare to build," Lauf says. "Instead, Bible suggested using a traveling wave tube to amplify the output of an adjustable, low-power microwave generator."

Finding a traveling wave tube that was both powerful and robust enough to use in a microwave furnace turned out to be a challenge. Lauf and Bible found that traveling wave tubes having from 10 to 50 W of power are used both in satellites and in the ground stations that communicate with them. Higher-power tubes, in the range of 1 kW

and above, have been used by the U.S. armed forces since the beginning of the war in Vietnam to jam enemy radar with microwave noise.

After checking with all the major radar and microwave manufacturers, Lauf and Bible were referred to MLI, a manufacturer of traveling wave tubes for radar jamming applications. It turns out that MLI is the only U.S. company that makes tubes having the power, bandwidth, and heat transfer properties that can be adapted for use in a microwave furnace.

"Most microwave tubes are connected to

antennas that radiate power into free space," Lauf says. "If they were connected to a closed cavity, they would quickly burn out. MLI's tubes are designed to handle reflected power, like that encountered in a microwave furnace."

With the end of the cold war, MLI's chief executive concluded that radar jamming would not be the growth industry of the 1990s, so he became interested in entering the microwave furnace business. "He said they could provide us with the tube we needed, help us engineer the system, and help design the power supply," Lauf says. "He wanted to manufacture whole systems and sell them to laboratories, and ORNL wanted someone to license this technology. From a technology transfer point of view, it's a success story in the making."

The furnace, the only device of its kind in the world, has been up and running since October 1, 1991, with funding from Defense Programs at the Y-12 Plant. "The system worked great the first time they turned it on, thanks to Don Bible's expertise with high-power microwave



Carl Everleigh, Jr., of Microwave Laboratories, Inc.: Bob Lauf of **ORNL's Metals** and Ceramics Division: and Don Bible of the Instrumentation and Controls Division pooled their talents to turn a piece of hightech military hardware into a state-of-the-art research tool.

equipment," says Lauf. "Right now it's an experimental tool. We're looking at every ceramic specimen we can get our hands on to see how they respond to different frequencies."

The furnace is now capable of generating microwaves in a range from 4 to 8 GHz; however, money set aside by DOE's Office of Energy Research to help researchers enter CRADAs with industrial partners will be used to upgrade the furnace to accommodate higher-frequency microwaves. At the same time, MLI will modify their 8- to 16-GHz tube for use in the furnace, giving it an effective range of from 4 to 16 GHz.

Eventually, the furnace will be used by Defense Programs to sinter boron carbide. This chemical compound is of particular interest to researchers because its light weight and high hardness make it ideal for use in the development of ceramic armor for military vehicles and for various nuclear applications. It is also expected to be useful in the manufacture of cutting tools and abrasives.

"Boron carbide is difficult to sinter using conventional microwave techniques," Lauf says.

Jack Young (right) of ORNL's Analytical Chemistry Division, and Gleb Mamantov (left), head of UT's Chemistry Department, check the laser setup as Dow Chemical president George Shier looks on. Photograph by Kelly Scott Walli of The Oak Ridger.



"We can achieve a reasonably high density using sintering aids, like free carbon, but it's hard to find a sintering aid that doesn't degrade the properties we wanted to obtain in the first place. Using the variable furnace, we hope to create high-density boron carbide without sintering aids."

Although the furnace is currently being used to process ceramics, a number of other applications for this technology have been suggested. As a research tool for industry, the furnace could be used to find the best frequency for a particular industrial application; then a full-scale, fixed-frequency industrial furnace could be built to process large quantities of material. Other suggested applications include using microwaves to energize plasmas over a range of energies to observe their changing properties, deposit thin films more uniformly, and more effectively

sterilize medical equipment or contaminated waste.—Jim Pearce

# UT, Dow Chemical, and ORNL in CRADA

Researchers from ORNL, the University of Tennessee (UT), and Dow Chemical Company are combining their expertise to help Dow produce magnesium more efficiently.

The collaboration is based on the development and use of on-line sensors placed in the electrolytic cells that are part of Dow's magnesium production process at Freeport, Texas. The sensors will determine the concentration of magnesium in the cells, which annually produce millions of pounds of the silver-white, lightweight metallic element. Magnesium alloys are used in numerous consumer products, including beverage cans, computer parts, and cars.

Energy Systems is administering the project under a CRADA. DOE is contributing half of the project's cost through the Office of Industrial Technology, Conservation, and Renewable Energy.

The partnership will be based on a collaborative effort among Jack Young of ORNL's Analytical Chemistry Division; Gleb Mamantov, head of the Department of Chemistry at UT, and Ken Claus of Dow Chemical Company.

The sensor technology, which is in the developmental stage, could help Dow and other metals manufacturers reduce energy costs and improve production efficiency. Benchmark research and development work on the new technology will take place at ORNL and UT. Commercial-scale development and testing will follow at Dow's Freeport facility.

"We believe this project could strengthen the position of major U.S. metals suppliers such as Dow in a highly competitive global market," says William W. Carpenter, Energy Systems vice president for Technology Transfer.

According to George Shier, Dow Chemical president, the efficient production of magnesium is vital to Dow, the largest producer of magnesium in the world. "Those benefits go right down the line," Shier adds. "The automobile industry is a perfect example. Because of its light weight and strength, magnesium alloy is being used more and more in automobiles where less weight means greater fuel economy."

Magnesium and magnesium alloys also are used in beverage cans, computer parts, and a number of iron and steel applications.

Successful collaboration on this project could lead to application of the technology to other energy-intensive processes such as aluminum production.

### **CRADA on Precision Optics**

Energy Systems and United Technologies
Optical Systems (UTOS) have begun a CRADA
that will allow them to jointly develop optimum
processes for producing complex mirror surfaces.
These lightweight mirrors made of silicon-clad,
high-strength silicon carbide are typical of the
optical components used in advanced defense
weapons and satellite systems.

The work will be performed at ORNL's Optics Manufacturing Operation Development and Integration Laboratories (Optics MODIL). There, single-point diamond turning machines, which can cut metal at the surface at precise angles, will be used to determine the best process for manufacturing silicon-clad mirrors having the desired optical properties. Arthur C. Miller, a project manager in Optics MODIL, said one goal of the work is to produce a silicon-clad curved mirror, finished under optimum conditions, whose curvature is within 100 millionths of a centimeter of the design specifications.

UTOS is a pioneer in optical and electro-optical technology and a leading supplier of specialized, high-performance and laser components and related systems.—Karen Bowdle

#### Check Valve Technology Licensed

The technology for checking on check valves in nuclear reactors to improve their operational safety has been licensed to a company founded by the technology's creator.

Two nonintrusive methods of monitoring check valves have been licensed to Valvision Inc., a Cambridge, Massachusetts, company founded by David Eissenberg, a former ORNL engineer and co-inventor of the technology.

Check valves are used extensively in nuclear plant safety systems to prevent the water flow in pipes from moving in the wrong direction. The failure of several check valves at the San Onofre Nuclear Generating Station, which led to a stable cold shutdown of the plant in late 1985, prompted ORNL researchers to develop the valvemonitoring technology.

Whether a valve is open or shut can be monitored by external alternating-current and direct-current magnet methods developed by Don Casada, Howard Haynes, and Eissenberg in ORNL's Engineering Technology Division. The check valve's position can be indicated by an emitted magnetic signature.

Although used primarily in the nuclear power industry, check-valve monitoring technology has the potential for use in other industrial settings such as steam plants.

### Rights to Raman Spectral Library Granted

Commercial rights to a technology developed by the Y-12 Plant to help scientists more easily identify unknown compounds has been granted by Energy Systems to two companies.

Information and data on inorganic compounds and polymers will be provided by the Y-12 Plant's Raman Spectra Library to the Fiveash Data Management Co., in Ft. Atkinson, Wisconsin. The information will be available in digital form as electronic copies.

An exclusive license has also been awarded to the Texas Engineering Experiment Station in College Station, Texas, for a hard copy, or bookform, listing of Raman spectral data.

The Raman spectral data catalog is a listing of unique "fingerprints" created when compounds undergo Raman spectral analysis. These

fingerprints are unique wave-form patterns displayed on a computer screen or in a printout. An unknown compound can be identified by matching its pattern with a corresponding pattern in the Raman spectral data catalog.

Before the Fiveash agreement, Raman spectra libraries were available only in a hard copy format. As a result of the agreement, high-quality spectra of more than 300 organic, polymer, and inorganic materials are available to help scientists using Raman spectroscopy.

William Costa, president of Fiveash Data Management, said his company would make Raman spectroscopy "viable for a growing number of industrial problem solvers and innovators, while helping the technology emerge into a more useful tool for sophisticated companies examining polymers and inorganic materials."

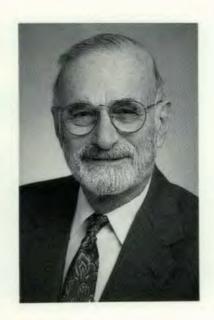
Doyle Hembree and Norm Smyrl, analytical development staff members with the Y-12 Plant's Quality Services Division, compiled the Raman spectra data base. Hembree said the data base should be "very useful to Raman spectroscopists involved in all areas of analytical work, particularly researchers working in private industry and in government laboratories."

In a Raman experiment, a laser beam is focused on a sample. A small quantity of radiation then is scattered at different frequencies. These shifted frequencies reveal the structure of the molecules responsible for the scattering.

The Raman effect—part of the light-scattering phenomenon causing the sky to appear blue—was first observed experimentally in 1928 by Sir C.V. Raman, who was awarded the Nobel Prize for his discovery. In 1960, the invention of the laser enabled scientists to generate intense radiation at a single frequency to make Raman scattering more easily observable.

Energy Systems has initiated some 54 licensing agreements with industrial companies since establishing its technology transfer program in 1985. Five licenses were granted to industry in 1991.

### Farewell to Our Consulting Editor



Alex Zucker—acting director of ORNL in 1988, an ORNL associate director for nearly 20 years (first for the physical sciences, then for the nuclear technologies), and a Laboratory employee for 42 years—has left ORNL physically but not

spiritually. In April 1992 he moved to the Oak Ridge Y-12 Plant, where he is offering his considerable expertise on ORNL research to Martin Marietta Energy Systems, Inc., as special advisor to its president, Clyde Hopkins.

He made his mark on ORNL in many ways. As a physicist, he and his colleagues conducted pioneering research in nuclear physics in the early 1950s at ORNL's 63-inch cyclotron, which he built. There they observed 20 new nuclear reactions, such as the fusion of nitrogen nuclei and the formation of the heavier nuclei of fluorine, sodium, and aluminum by bombarding oxygen and carbon targets with beams of nitrogen nuclei. The results of their nitrogen fusion studies eased the fear that detonation of a hydrogen bomb might set the earth's atmosphere on fire.

As a manager, he was instrumental in bringing many ORNL projects to fruition, usually helping them over formidable hurdles. Among the most notable are the Holifield Heavy Ion Research Facility, the High Temperature Materials Laboratory, and the Advanced Neutron Source (which has reached the design stage and would be ORNL's 15th research reactor).

A native of Yugoslavia, he received his B.A. degree in physics from the University of Vermont and his M.S. and Ph.D. degrees in physics from Yale University. He came to ORNL in 1950 and spent his first 20 years here conducting nuclear physics experiments and studying reaction mechanisms and the scattering of heavy ions and protons.

During much of his career, he has had an impact on American science as well as ORNL research directions. From 1970 to 1972, he was executive director of the Environmental Studies Board of the National Academy of Sciences/National Academy of Engineering. He has been a member of the editorial advisory board of *Science* magazine. He is chairman of the American Society of Mechanical Engineers National Laboratory Technology Transfer Committee. He is a fellow of the American Physical Society and the American Association for the Advancement of Science.

Since 1975 Alex Zucker has been the consulting editor for the ORNL Review, but he will be unable to continue in this role in his new position. The Review staff will miss him as our consulting editor; he has been a fine mentor, an excellent source of article ideas, and a good friend. He reviewed the magazine articles carefully, praised the good ones, weeded out the politically unwise statements, and sent back the less readable ones for rewriting. He has greatly influenced the quality of the articles in the Review as well as the quality of research at ORNL.—Carolyn Krause, Review editor

### OAK RIDGE NATIONAL LABORATORY REVIEW P.O. Box 2008, Oak Ridge, Tennessee 37831-6144

U.S. Postage
PAID
BULK RATE
Oak Ridge, Tenn.
Permit No. 70



#### **Next Issue**

Do the eyes have it—
the ability to influence
reactor, robot, and
computer control?
ORNL's improvements
of eyegaze
measurement
technology could lead to
fascinating applications.