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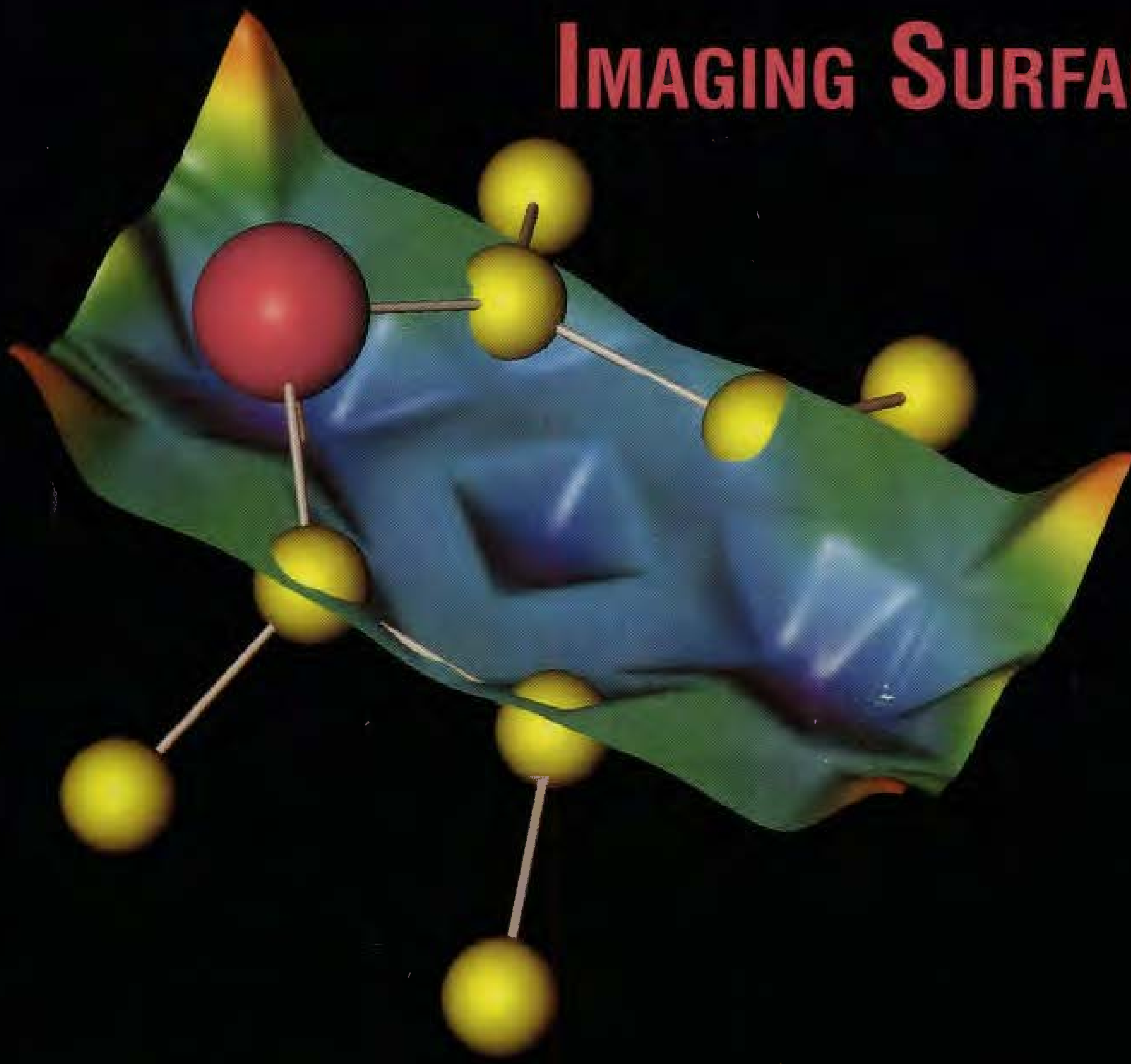
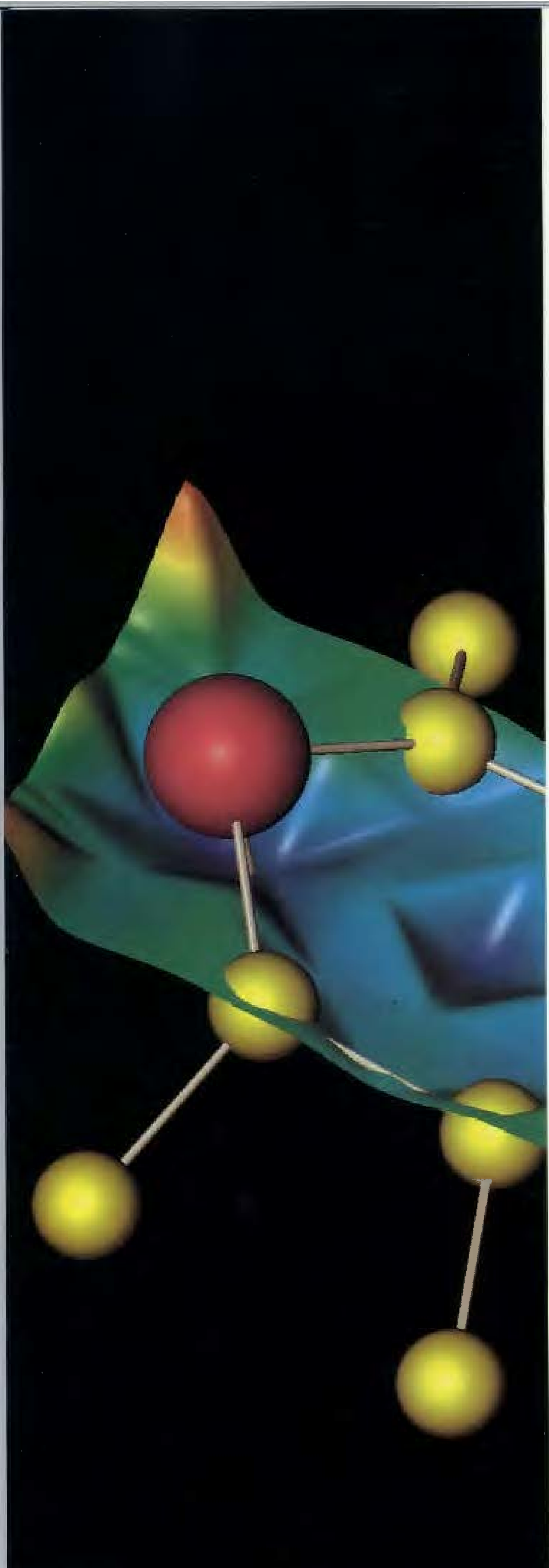
Imaging Surfaces



ORNL's Magic Bullets

Tumor-Fighting Genes



ON THE COVER

This colorful map of calculated electron energies on a reconstructed silicon surface shows the preferred binding sites for a germanium atom (red ball). Germanium prefers the low-energy regions, shown in blue, rather than the high-energy regions, shown as multi-colored mountain peaks. The yellow balls are silicon atoms. This theoretical model by physicist Victor Milman was suggested by Steve Pennycook and Dave Jesson's imaging data (see p. 60). The data and the calculations may contribute to the growth of silicon-germanium films that can conduct light for use in advanced semiconductor devices. Milman constructed the cover visualization from calculations using the new Intel Paragon XP/S 35 supercomputer at ORNL. The high-resolution print of the computer image was made by Ross Toedte of the Computing and Telecommunications Services' Visualization Laboratory of Martin Marietta Energy Systems, Inc. (See articles in "Technical Highlights" on pages 60 and 62.)

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REVIEW

Volume 26
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FEATURES

DEPARTMENTS

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in the physical, chemical, material, and life sciences; in fusion, fission, and fossil energy; and in energy conservation and other energy-related technologies.

Reinventing Ceramic Production

By Carolyn Krause

Ceramic materials can take the heat, but repeated stresses will do them in because they are inherently brittle. When subjected to one too many stresses, ceramics will crack or even shatter, like Humpty Dumpty falling off the wall. The problem lies in tiny flaws that undermine the strength of ceramics. Voids or particles of the wrong size or shape that don't quite fit together can be the Achilles' heel of a ceramic, setting it up for eventual failure. The solution lies in the close packing of the particles that make up the material. Controlling the sizes and shapes of the particles that become the building blocks of ceramics is an essential first step toward developing highly reliable ceramics for energy applications.

Three ORNL engineers have developed a device that may help industry reinvent ceramic production. Called the electric dispersion reactor (EDR), the device produces ultrafine precursor ceramic particles of desired shapes and distribution of sizes. Such control could eliminate the tiny flaws that eventually grow into cracks in normally brittle ceramics, especially those containing multiple components. In addition, such control could eliminate the problem of misaligned grains, which limits the amount of electrical current that bulk superconducting ceramics can carry. Thus, this approach could improve the electrical current-carrying capacity of high-temperature superconducting materials.

In June 1992, a patent was issued to Michael Harris, Timothy C. Scott, and Charles H. Byers, all of ORNL's Chemical Technology Division, for the EDR. For this invention the three researchers were honored with an Inventors Award during the May 1993 Awards Night of Martin Marietta Energy Systems, Inc.

The EDR offers several advantages over the two conventionally used techniques—oil-water emulsion and spray pyrolysis—for making fine ceramic powders in the micron to submicron regime (a micron is a millionth of a meter). The EDR works well in converting aqueous metal salt solutions and metal alkoxides to hydrous metal oxides, oxygen-containing compounds dissolved in water. It has been used to produce silica, alumina, zirconia, titania, and the precursor powder for yttrium-barium-copper oxide, a high-temperature superconducting ceramic.

The EDR combines the features of homogeneous precipitation and the emulsion phase contactor, an invention of Scott, Robert M. Wham, and Byers that uses electric fields to improve the efficiency of solvent extraction—a separation method widely used by industry for recovering chemicals.

In solvent extraction, a substance is transferred from one liquid phase by dissolving it into a second one that does not mix with the first liquid. The movement of a substance from one liquid to another is called mass transfer. To increase the rate of mass transfer, conventional solvent-extraction systems agitate the mixture using mechanical mixers to increase the interfacial area by the formation of liquid drops. Considerable energy is required to agitate and mix both phases.

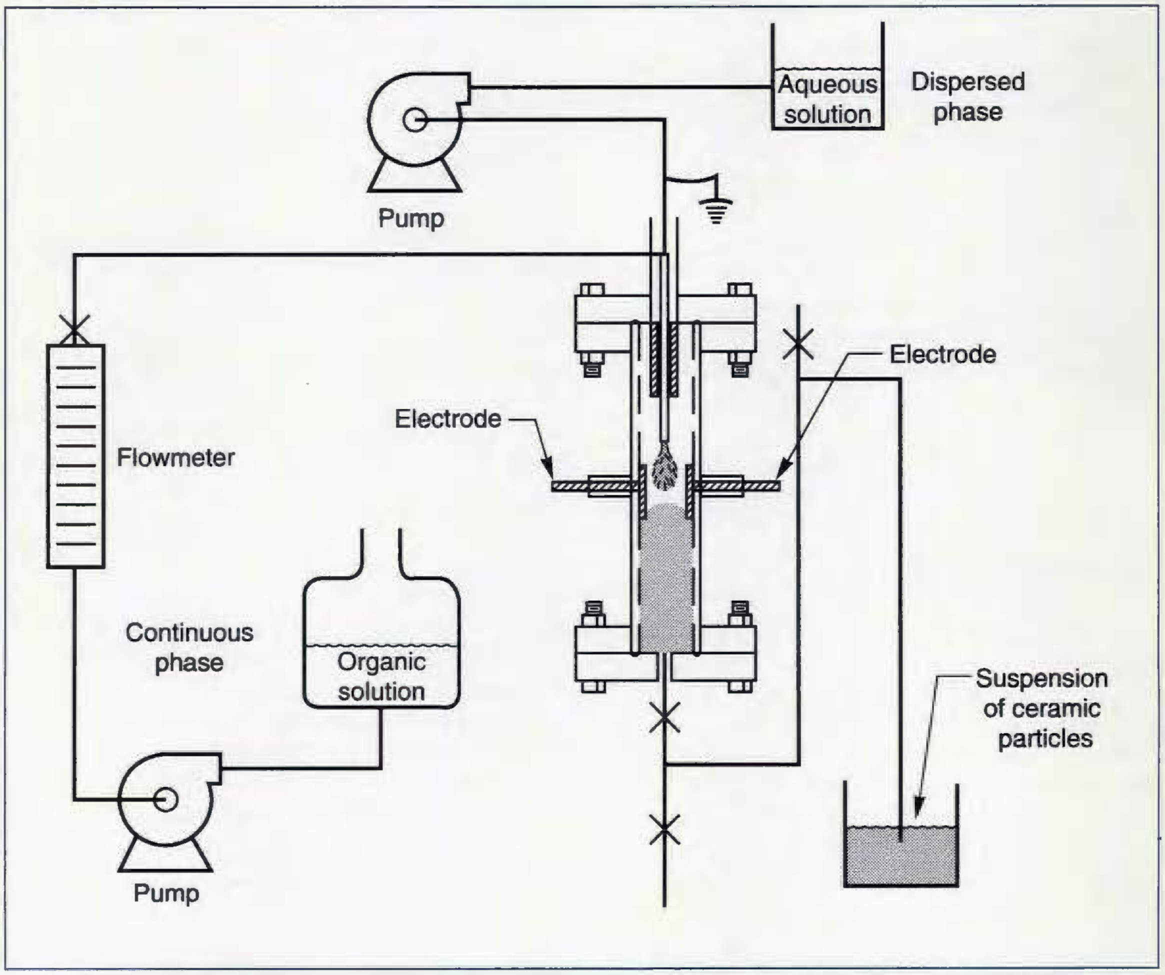
By subjecting the liquid mixture to high-intensity electric fields in the emulsion phase contactor, Scott and Wham obtained mass transfer rates 100 times greater than those achieved by mechanical systems. The increase in mass transfer was a result of a decrease in the size of the liquid drops, making possible an increased interfacial area. The ORNL system is also energy efficient, using 1% of the energy required by a mechanically agitated system. Because of its higher efficiency, the recovery method can be carried out in vessels one-tenth the size of those used in conventional solvent extractors. In 1990 the ORNL technology was licensed to Analytical Bio-Chemistry Laboratories of Columbia, Missouri, and National Tank Company of Tulsa, Oklahoma.

Three ORNL engineers have developed a device that produces ultrafine precursor ceramic particles of desired shapes and distribution of sizes.

While Scott and Wham were developing the emulsion phase contactor, Harris was conducting research on homogeneous precipitation and particle growth. Homogeneous precipitation is the separation of a solid substance from a solution through a chemical or physical change. Under controlled conditions, the product is insoluble crystalline or amorphous particles that have a uniform size, shape, structure, and chemical composition.

Harris was studying particle production because his predecessor, Dave Williams, under the direction of Byers, was interested in measuring the viscosity of organic solvents at high temperatures. To accomplish this, he laced the liquids with ~0.1-micron-size ceramic "seed" particles because they are rigid enough to withstand high temperatures. Because the ways that laser light shone on particles in a solution may scatter can be related to the Brownian motion

Mike Harris checks the newly designed electrode that generates an electric field in the electric dispersion reactor he helped develop. The compact device produces ultrafine precursor ceramic particles.

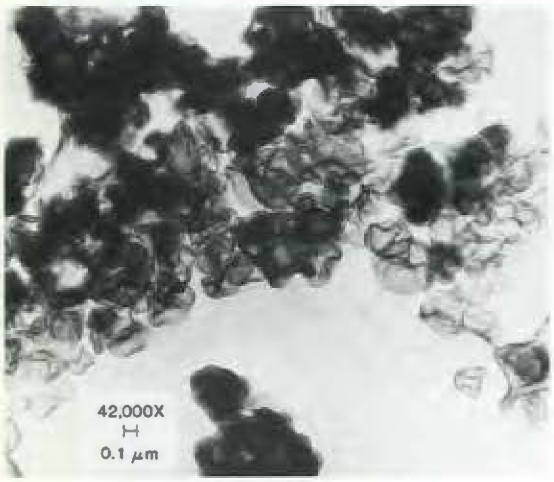


In the electric dispersion reactor, ceramic precursor powders are synthesized by dissolving metal oxides in a water solution. This aqueous phase, which is sprayed into the EDR through a nozzle, is dispersed by the electric field to form tiny droplets. The ammonia in the organic solution of the continuous phase in the reactor diffuses into the aqueous droplets from the dispersed phase, causing the three metal oxides in the droplets to precipitate as fine powders.

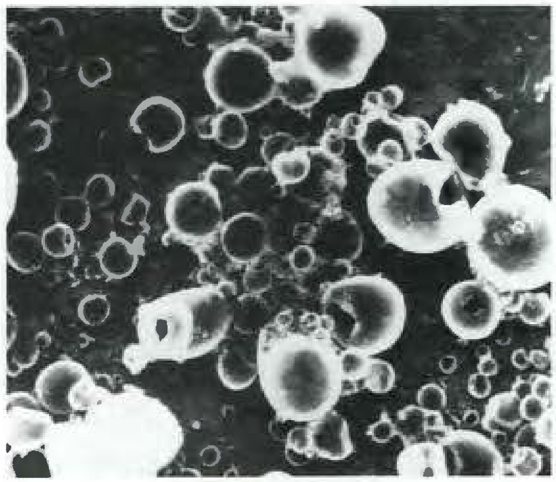
of the particles, the technique could be used to measure liquid viscosity if the particle size is known. The technique can also measure particle size if the liquid viscosity is known. Hence, Williams and Byers later wanted to use dynamic light scattering to investigate the earliest possible stages of particle formation and growth. After the departure of Williams, Byers asked Harris to develop homogeneous precipitation techniques to generate silicon oxide (silica) and other metal oxide particles as small as possible and to study how they grow. Because well-defined powders are crucial to the development of advanced ceramics, this was a promising area of research.

Chemistry in a Drop

The homogeneous precipitation technique was used to easily form well-defined ultrafine powders of metal oxides containing one or two components. However, multicomponent metal oxide particles are difficult to synthesize by this technique. Thus, it became necessary to use physicochemical techniques to form ultrafine



Silica particles produced in the electric dispersion reactor have been dubbed "porous prunes." They are made by precipitating silica during hydrolysis of tetraethylorthosilicate on the surface of the water-ammonia droplets and then drying them.



These "PacMan particles," so named for the holes on their surfaces, are formed by precipitation of hydrous aluminum oxide inside droplets during the transport of ammonia from the continuous to the dispersed phase.

multicomponent metal oxide particles. In such techniques, particle size is determined by localization of the precipitation reactions in "microreactors" such as micron-size droplets.

While developing the electrically driven emulsion phase contactor, Scott and co-workers determined that micron-size droplets were formed during dispersion of aqueous drops (e.g., water) into an insulating organic phase (e.g., ammonia) by intense-pulsed direct-current electric fields. After reading some publications coauthored by Scott and after discussing matters with Byers and Scott, Harris suggested that the micron-size droplets serve as microreactors for the localized precipitation of metal salts and metal alkoxides. Thus, the electric dispersion reactor was conceived.

"In the EDR electrical stresses accumulate at the interface between the aqueous and organic solutions and atomize the aqueous phase into droplets at the spray nozzle," Harris says. "The result is a very fine mist. We can make particles of different sizes and shapes by changing the location and concentrations of the reactants on the droplets and by changing the intensity of the electric field."

Using the EDR, Harris and his colleagues have made particles of several different shapes (morphologies) as well as sizes. One particle type, dubbed the "porous prune," is made by precipitating silica during hydrolysis of tetraethylorthosilicate on the surface of the water-ammonia droplets and then drying them. Another particle, called a "PacMan particle" because of the hole on its surface, is formed by precipitation of hydrous aluminum oxide in droplets during transport of ammonia from the continuous to the dispersed phase.

EDR and Industry

The EDR is valuable for producing high-quality precursor ceramic powders for research purposes and possibly industrial production of ceramics. Very fine ceramic powders of known size, shape, structure, and chemical composition could be the basis for fracture-resistant ceramics. "The smaller the particles, the more you can control the microstructure and the less likely that the material will crack," Harris says. "In the EDR, we should be able to produce ceramic particles of a desired size or size distribution,

We can make particles of different sizes and shapes by changing the location and concentrations of the reactants on the droplets and by changing the intensity of the electric field.

They showed that the EDR can produce a large enough quantity of material to suggest that it could be scaled up for industrial production.

These particles produced in the electric dispersion reactor contain hydrous oxides of yttrium, barium, and copper. When sintered, they form high-temperature superconducting material.

whatever is needed to achieve an optimum packing density."

In January 1993 Harris and his associates achieved a milestone. By making 100 grams of zirconia powder in the EDR's largest production run, they showed that the EDR can produce a large enough quantity of material to suggest that it could be scaled up for industrial production. This production run was made possible by funding from the Department of Energy's Office of Basic Energy Sciences, Advanced Energy Projects, which has supported development of the EDR.

As a result of this success, Harris is trying to attract industrial interest from potential customers such as Du Pont, Dow Corning, and PPG. The group may also have a chance to work with Rohm and Haas and Dow Corning as part of the cooperative research and development agreements (CRADAs) involving use of the emulsion phase contactor and the EDR.

Harris is also collaborating with researchers in ORNL's Chemical Technology and Metals and Ceramics divisions. The precursor superconductor powder that Harris produces is of interest to Terry Lindemer of the Chemical Technology Division because of the ability to produce gram quantities of homogeneous powders in the EDR. Harris makes the precursor powder by dissolving yttrium nitrate, barium nitrate, and cuprate chloride in a water solution. This aqueous phase, which is sprayed into the EDR through a nozzle, is dispersed by the electric field to form tiny droplets. The ammonium in the continuous phase present in the reactor diffuses into the aqueous droplets, where it causes the three metal oxides to precipitate as fine powders containing yttrium (Y), barium (Ba), and copper (Cu). These powders will be sintered by Lindemer to produce yttrium-barium-copper (Y-Ba-Cu, or 1-2-3) superconductivity material. The main challenge for the EDR researchers is the formation of particles smaller than 0.1 micron.

Harris thinks that the ceramic industry should be attracted by the EDR's advantages over two competitive powder-producing techniques. One is spray pyrolysis, a generic term to describe a wide range of processes that generate ceramic particles directly from atomized precursor solutions or sols in a gas phase at elevated temperatures. The other is the water-oil emulsion technique in which mechanical agitation is used to form micron-size drops that serve as microreactors. In this case, Harris says, considerable energy is used to "beat" the fluid into micron-size particles, which are made even smaller by use of surfactants (detergentlike substances that reduce surface tension) that later must be removed.

EDR's Advantages

According to Harris, the EDR offers these advantages over the conventional techniques:

- It will potentially use about one-tenth as much energy as the water-oil emulsion technique because no stirring mechanism is required. Only a small amount of electricity is needed to spray the aqueous phase from the nozzle and create a field to disperse it. (ORNL researchers will do an economic analysis in 1994 to calculate the precise energy savings of using the EDR instead of conventional techniques.)
- Surfactants are not needed.
- No moving parts are used, so much less maintenance is required.

- Because soft agglomerates are formed in the EDR, it offers a potentially higher yield than spray pyrolysis.
- Ceramic processing in the EDR is dust-free because it is contained in a slurry phase; thus, it will present reduced adverse health impacts because no breathable particles will be released into the air.
- The solvent will be recycled through a continuous flow scheme, minimizing discharge of waste products.
- By connecting modular units in a series, the EDR can be scaled up more readily than spray pyrolysis.

Does the EDR have any disadvantages? "Some products might require a conductive continuous phase," says Harris. "In the EDR the continuous phase must be a nonconductive or insulating fluid. A conductive fluid would be heated up by current flow, thus wasting energy."

Warren Sisson, who helped assemble and improve the design of the electric dispersion reactor, examines the device's product stream.

Improving the EDR

Harris says he and his colleagues are considering using small amounts of a surfactant to reduce particle size and the energy needed to disperse droplets. A surfactant would lower the surface tension at the interface between the aqueous metal oxide and inorganic liquids, thus decreasing the energy required to atomize the aqueous phase.

To further enhance EDR performance, Harris and his associates are also trying to improve the spray nozzle design. "Osman Basaran, a group leader in the Chemical Technology Division, and I have done theoretical calculations to enhance nozzle design, and our results have been submitted for publication in the *Journal of Interfacial Science*," Harris says.

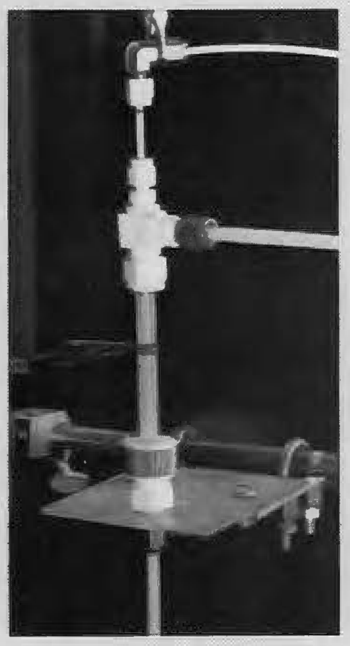
He explains that the effects of an electric field on droplets was first studied systematically by Zeleny in 1915. He was interested in understanding mechanisms of charge separation in thunderclouds and its effects on the shapes and instabilities of soap bubbles.

Harris says that it has long been known that droplets accumulate charges on their surfaces, causing them to deform in an applied electric field. "We study the point at which a static drop becomes unstable in an electric field. We found that the energy required to cause a droplet to break apart into a spray decreases as nozzle length increases up to a point. Utilization of a particular nozzle-electrode geometry could result in a more efficient use of electrical energy."

As industry searches for a fracture-resistant ceramic for energy applications, ORNL's electric dispersion reactor may be the key to reinventing the ceramic manufacturing process to make more durable and efficient products.

Michael Harris: Why He Chose Chemical Engineering and ORNL

In 1976, when Mike Harris was a high school senior in Mound Bayou, Mississippi, he knew virtually nothing about ceramics, superconductors, or Oak Ridge. What he did know for certain was that he loved chemistry and disliked English.



Seventeen years later, Harris has been recognized by Martin Marietta Energy Systems, Inc., for an invention at Oak Ridge National Laboratory that produces fine ceramic powders. These are useful for making high-temperature superconducting material and other products requiring a finely controlled microstructure. Ironically, this researcher who hated English has even won a Best Paper Award from the American Institute of Chemical Engineers.

Harris' dislike of English was so strong that it even affected his choice of a major at Mississippi State University in Starkville, Mississippi.

"During my senior year in high school," he says, "I thought of going into chemistry because my best subjects were science and math. One of the subjects I liked least was English. A recruiter came from Mississippi State and talked about chemical engineering. I learned from the recruiter that majoring in chemistry at Mississippi State required two years of English and a chemical engineering major required only one semester of English. So I said that's the one for me. I majored in chemical engineering, and I loved it."

Harris says that at least five professors at Mississippi State provided motivation, gave him advice, and encouraged him. One professor sent him a Christmas card urging him to "continue to broaden my sphere of perspective." He also was encouraged by his co-op experiences at the U.S. Environmental Protection Agency in Athens, Georgia.

In 1981 Harris earned his B.S. degree in chemical engineering from Mississippi State and searched for a job. He interviewed for positions with Dow Chemical, Exxon, Proctor and Gamble, Mobil, Eastman Chemical, and numerous other companies.

Why did he end up working for ORNL? "I didn't know anything about Oak Ridge when it was suggested that I interview here," he says. "It was my last interview. I had pretty much decided when I came here that I was going to work for Eastman Chemical. I met with Dr. Chuck Scott and several of his co-workers. They told me about the educational opportunities as well as the type of research I'd be doing. I saw this as a perfect place for doing interesting research and working on an advanced degree. So I decided that, in terms of what I wanted, Oak Ridge was ideal for me."

"I decided that, in terms of what I wanted, Oak Ridge was ideal for me."

Harris joined ORNL in 1981. He studied chemical engineering at the University of Tennessee at Knoxville, earning an M.S. degree in 1987 and a Ph.D. degree in May 1992.

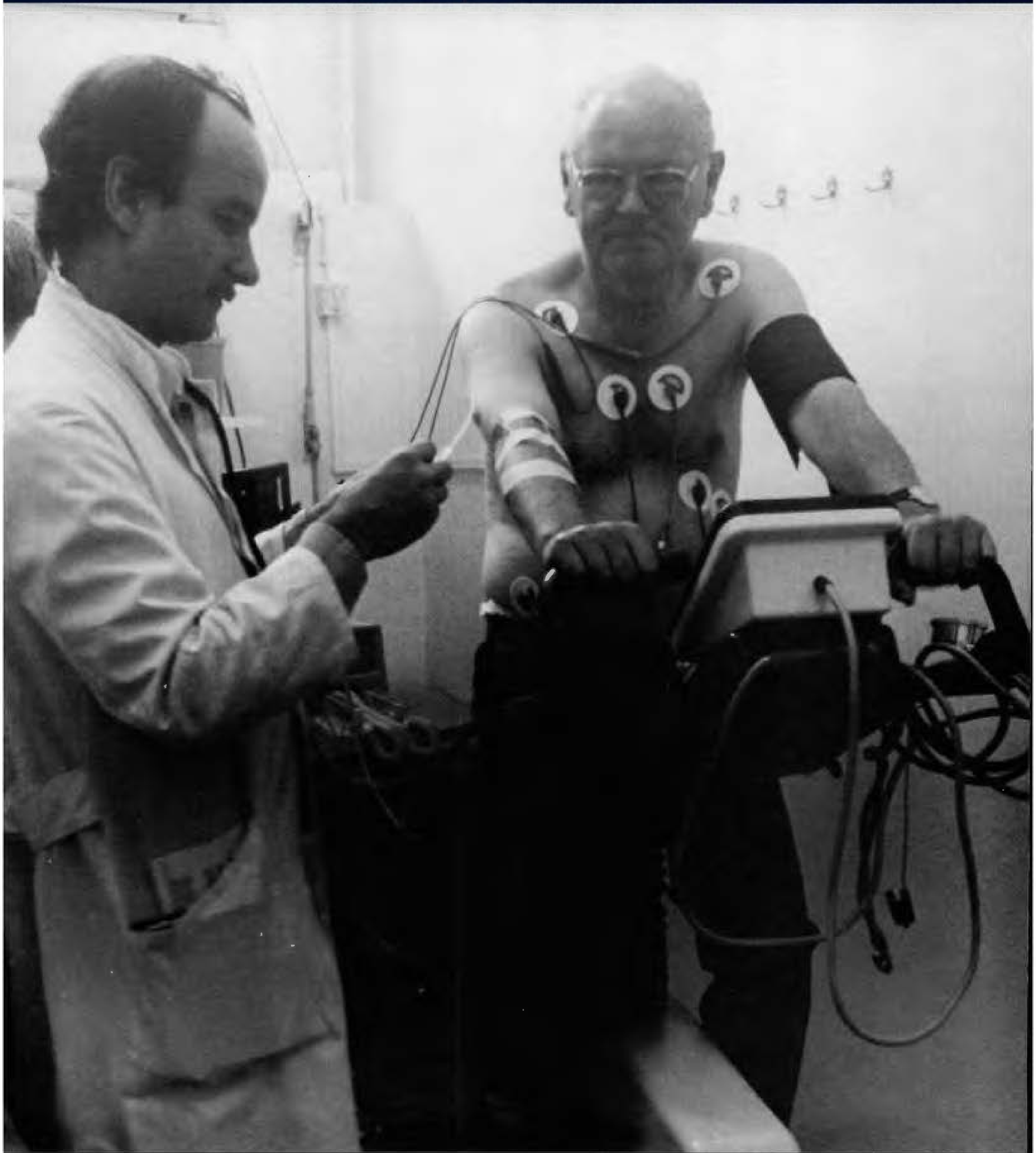
Since 1981 Harris has been author or coauthor of 22 scientific publications and has written a doctoral dissertation entitled "Ultrafine Powder Synthesis by Homogeneous Precipitation and Electrodispersion." Because he has written numerous papers, he now appreciates and respects English as a discipline.

Mike Harris has come a long way since his days in Mound Bayou. He knows a lot about ceramics, he appreciates Oak Ridge, and he is constantly broadening his "sphere of perspective" in the boundless arena of scientific research and technological development.

—Carolyn Krause

ORNL's Magic Bullets: On Target for Health

By Jim Pearce



Magic bullets. That's how we've come to know a group of chemical compounds that have an uncanny ability to home in on particular targets within the body. Their "magic" is provided by chemically attached radioactive isotopes, labels made of small quantities of radioactive material that enable physicians to obtain detailed images of internal organs, deliver doses of radiation to specific destinations, and trace the movement of medications—all without picking up a scalpel.

In recent years, a barrage of magic bullets has been fired from laboratories around the country, but because of their long and involved development process, relatively few have been tested in human patients—fewer still have found commercial applications. Despite these odds, the researchers of ORNL's Nuclear Medicine Group have gained reputations as sharpshooters, thanks to four new magic bullets now in clinical testing—a radiolabeled antibody that targets colon cancer cells, a test agent for pancreas problems, and imaging agents for monitoring blood flow in the heart and detecting early signs of heart disease. A fifth agent that promises to help track the changes in brain chemistry resulting from Alzheimer's and related diseases is undergoing preclinical studies.

Aiming for a Killer

Colorectal cancer is expected to claim 57,000 lives this year in the United States, making it among the most deadly forms of the disease. This grim distinction places it high on the "hit lists" of scientists who work to make magic bullets ever more effective. One of the obstacles facing these researchers is the need for radiolabeled compounds that not only do the diagnostic or therapeutic job they were designed for, but also are easy and convenient to use.

A new radioisotope generator system developed at ORNL promises to make the versatile radioisotope, rhenium-188, readily available for the treatment of colon cancer and arthritis for weeks at a time. "Rhenium-188 is expected to have several applications," says Russ Knapp, head of ORNL's Nuclear Medicine Group. "It can be attached to therapeutic agents and used as a tracer to monitor their movements through the body, or it can deliver a dose of radiation to shrink or kill an inoperable tumor. It may also be attached to small ceramic particles and injected into patients' abdominal cavities to treat uterine cancer. Members of the group who have made important contributions to the development of this generator system include Al Callahan, Ed Lisic, Saed Mirzadeh, and Arnold Beets.

In addition, the rhenium isotope can be used to treat rheumatoid arthritis in knees and other, fluid-filled joints. In this treatment the isotope is bonded to compounds that are injected into the fluid of the joint; the energy released as the rhenium decays helps relieve the painful swelling and inflammation of joint membranes. Similar applications have been suggested for reducing the pain associated with bone cancer.

The grapefruit-size rhenium-188 generator system has two advantages over systems that produce other therapeutic radionuclides. First, rhenium-188's parent isotope, tungsten-188, which is produced at ORNL's High Flux Isotope Reactor, has a half-life of 69.5 days. So, it takes about 10 weeks for half of the tungsten-188 to change or "decay" into rhenium-188. The tungsten's gradual decay provides a constant supply of rhenium for several weeks—making it much more convenient to use than most other radioisotopes. In addition, as it decays, the rhenium isotope produces photons, short bursts of energy in the form of light, which allow its distribution to be monitored with the photon-sensitive cameras that are already widely used for imaging in health-care facilities.

Working with David Goldenberg and his colleagues at the Center for Molecular Medicine and Immunology at the University of New Jersey, researchers have developed a quick and easy procedure for chemically linking rhenium-188 to an antibody that homes in on colon cancer cells. This combination, known as an immunoconjugate, delivers a precisely targeted dose of radiation to colorectal tumors. Although the half-life of radioactive rhenium is only 16.9 hours, the radiation it releases can penetrate nearly a centimeter into tumor tissue, suggesting this technique could be useful for treating larger tumors.

Initial studies in a group of 12 patients with tumors that had not responded to other treatments demonstrated the immunoconjugate's knack for concentrating in colorectal cancer

"Magic bullets" enable physicians to trace the movement of medication or obtain detailed images of internal organs—all without picking up a scalpel.

Despite the long and difficult process of developing "magic bullets" and getting them approved for testing in humans, four new ORNL-developed compounds are now involved in clinical studies, and one is undergoing preclinical testing. Here a patient exercises while being given ORNL's iodine-123-labeled heart-imaging agent. *(Courtesy, J. Kropp, M.D., and H.J. Biersack, M.D., et at., Clinic for Nuclear Medicine, University of Bonn, Germany.)*

The rhenium-188–labeled antibody homes in on colon cancer cells, delivering a precisely targeted dose of radiation.

The bright area just to the upper right of center shows a rhenium-188–labeled antibody concentrating in a colon cancer that has spread to the patient's bone. *(Courtesy of D. M. Goldenberg, M.D., et al., Center for Molecular Medicine and Biology, Newark, New Jersey.)*

cells. Full-scale clinical trials for the compound are scheduled to begin in the near future.

Targeting Pancreatic Disease

The inability to digest fat has been recognized for years as an indication of problems with the pancreas or upper intestinal tract. Using another magic bullet, Knapp and his German colleagues have developed the first effective, easy-to-administer test to diagnose this condition. The new urine test measures the ability of the pancreas to break down radiolabeled fat contained in a sugar cube swallowed by the patient.

The pancreas is a gland located behind the stomach that secretes both insulin, a hormone that enables the body to absorb sugar, and enzymes that help digest food, including fat. The role of the pancreas in digestion begins after food is eaten and partially digested in the stomach. When food enters the upper intestinal tract, it stimulates the pancreas to secrete its digestive enzymes. Most fat can't be absorbed by the small intestine. It must first be broken apart by digestive enzymes, then absorbed by intestinal cells, and finally reassembled and transported to the liver and other tissues for storage or use.

The failure of the pancreas to produce enough of these enzymes often signals serious problems, such as pancreatic cancer or inflammation of the pancreas.

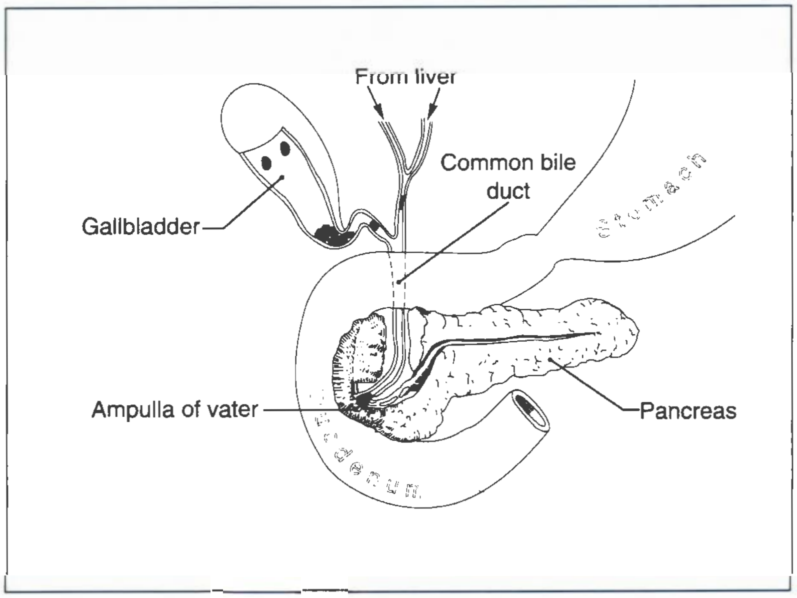
Traditional tests for measuring the performance of the fat-digesting enzymes produced by the pancreas are impractical and unpleasant because they usually require a chemical analysis of fecal samples to determine how much fat has passed through the digestive system without being absorbed.

Over the years, researchers studying alternatives to traditional techniques began to experiment with oral doses of oils or fats tagged with radioactive iodine-131. Once a fat or oil molecule was digested, the radioactive tag—still attached to a portion of the original fat or oil molecule—was released into the blood or urine.

Analysis of the radioactive contents of the blood was eventually discontinued because of purity and stability problems with the radioactive fat test agent and the agent's tendency to lose its radioactive tag in the body. There was also disagreement over the correlation between levels of radioactivity in the blood and the amount of fat in fecal samples. Early urine tests were also abandoned because digestion of the fats and oils used in these tests did not produce enough radioactive by-products in the urine for analysis.

Recently, ORNL's Nuclear Medicine Group has overcome the problems that plagued earlier research efforts and developed a test that produces enough radioactive by-products in the urine to provide a direct measure of the metabolism of fat by pancreatic enzymes. This technique, which has been proven successful in both animal tests and initial human studies, was designed by Knapp while he was conducting research as a Senior American Scientist of the Alexander von Humboldt Foundation at the University of Bonn in Germany.

"We asked ourselves whether the problem was with the concept of what should be measured or with the chemical structure of the radiolabeled fat that was used," says Knapp. "We decided that, if we could synthesize a fat whose radiolabeled by-products would probably be excreted in the urine, we could develop an effective test." While in Bonn, Knapp synthesized a new triglyceride fat containing the iodine-131–labeled fatty acid residue. This radiolabeled test agent is stable, can be stored for several weeks, and most importantly, its radiolabeled component is released in the urine. The amount of radioactivity in urine samples is then analyzed and compared to the amount administered to determine the rate at which the fatty acid residue is being metabolized by the pancreas.



The pancreas (right) produces enzymes that help the body break down fat. Failure to produce enough of these enzymes often signals serious problems, such as pancreatic cancer or inflammation of the pancreas.

Initial studies in laboratory rats were conducted at ORNL with an iodine-125–labeled compound by Nuclear Medicine Group members Kathleen Ambrose, Al Callahan, Carla Lambert, and Dan McPherson. The iodine-125 tag has a longer half-life than iodine-131 (60 days versus 8), making it more convenient to use in animal experiments. The results of these studies were very promising—18.9% of the radioactivity from the orally administered test agent was released in the urine during the first 24 hours.

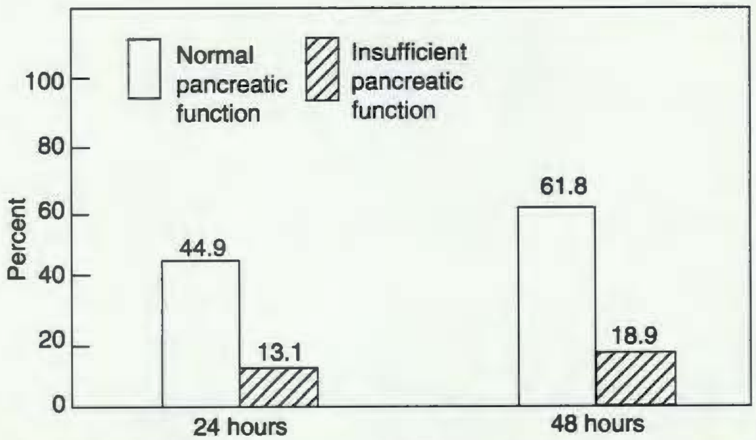
Knapp then developed a test procedure and synthesized the iodine-131–labeled agent for initial tests in humans conducted by Joachim Kropp, M.D., at the Clinic for Nuclear Medicine in Bonn. Of the 23 individuals participating, 20 had normal pancreatic function and 3 had previously documented pancreatic insufficiency. The results of these studies showed that participants with normal function released an average of 61.8% of the iodine-131 in their urine after 48 hours. The patients with impaired function released only 18.9%—significantly less than the control group.

These preliminary results demonstrate that this technique provides a simple test for pancreatic insufficiency. "This approach is not as direct as a typical nuclear medicine imaging procedure, such as imaging a tumor," says Ambrose, "but it gives indirect proof of pancreatic disease or intestinal absorption problems. Low excretion levels identify individuals who need to undergo further testing."

Over the next year, Knapp and his collaborators Joachim Kropp and Hans Biersack, both of the University of Bonn, plan to gather more extensive data from a larger group of control patients and also from several different groups of patients with various other types of gastrointestinal disease.

Tracing Blood Flow in the Heart

Heart function tests are administered to thousands of Americans each year. These tests are of critical importance in diagnosing and treating both congenital defects and diseases of the heart.



In the first round of clinical tests, Kropp found that patients with no pancreas problems released 61.8% of the iodine-131–labeled test agent in the first 48 hours. Patients with impaired pancreas function released only 18.9%, demonstrating that this technique provides a simple, effective test for pancreatic insufficiency.

The isotope's short half-life enables tests to be repeated almost immediately to monitor the effects of exercise and drug therapy on the heart.

In a typical heart function test, a photon-emitting isotope is injected into the patient's bloodstream and a photon-sensitive camera then captures an image of blood flow through the heart's chambers and within the heart muscle itself.

One of ORNL's contributions to cardiac imaging has been the development of a generator system for producing iridium-191*m*. This ephemeral test agent is the product of the decay of osmium-191, which has a 15-day half-life and is produced at ORNL's High Flux Isotope Reactor. Because iridium-191*m* has a half-life of less than 5 seconds and emits photons, it provides a safe, fast method of obtaining high-quality cardiac images. In fact, the isotope's short half-life enables tests to be repeated almost immediately to monitor the effects of exercise and drug therapy on the heart's pumping efficiency. In European tests, the iridium generator has been successfully used in evaluating heart performance in more than 200 patients.

Applications of the generator technology for producing the short-lived isotope are currently being discussed with groups with the expertise and specialized instrumentation needed to handle iridium-191*m*.

Spotting Early Signs of Heart Disease

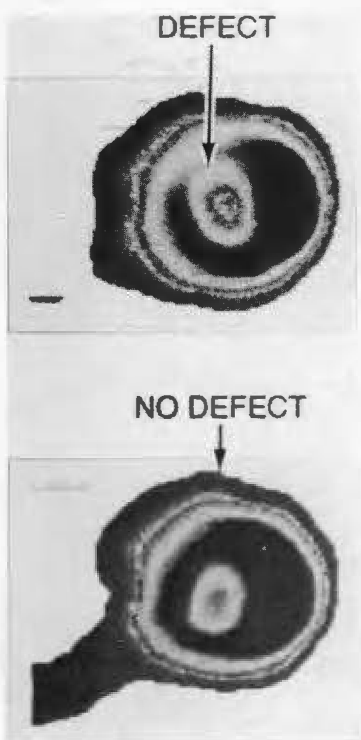
In their early stages, several cardiac disorders, such as hypertensive heart disease, may have none of the symptoms traditionally associated with heart trouble—clogged arteries, restricted blood flow, or oxygen-deprived heart muscle. What they do have, ORNL researchers have determined, is a habit of altering the way affected areas of the heart muscle metabolize and absorb fatty acids. To detect these subtle changes, ORNL researchers developed a blood-borne fatty acid tagged with radioactive iodine-123, which emits photons as it decays.

The usual first step in deciding whether a problem with fatty acid metabolism exists is to use a radioisotope to produce an image of blood flow to the patient's heart muscle through the coronary arteries. If blood flow is normal, the radiolabeled fatty acids are administered to the patient. An uneven distribution of these fatty acids throughout the heart, as detected by a photon-sensitive camera, suggests that the ability of some areas of the heart muscle to metabolize fatty acids is impaired, perhaps as a result of the early stages of heart disease. The image may also enable a physician to determine which regions of a damaged heart muscle could be salvaged through treatment.

The clearest indication that the ORNL-developed agent has helped shed new light on the subtleties of cardiac metabolism is its worldwide acceptance. Studies of iodine-123 are in progress at several European clinics and at

ORNL's iridium-191*m* system provides a fast, safe method of imaging the heart. (*Courtesy, Medical Department, Cyclotron Research Center, University of Liege, Belgium.*)

Uneven distribution of fatty acids may signal the early stages of heart disease.



Using fatty acids tagged with radioactive iodine-123 gives researchers insights into subtle changes in the heart that may mark the early stages of disease. The top image shows an area of decreased concentration of the radiolabeled compound following exercise. After rest, the bottom image shows the concentration has increased, indicating the patient is a good candidate for corrective surgery or other treatment. *(Courtesy, J. Kropp, M.D., and H.J. Biersack, M.D., et al., Clinic for Nuclear Medicine, University of Bonn, Germany.)*

Brookhaven National Laboratory. The agent has already won approval from the Japanese Food and Drug Administration and is being marketed in the Far East by Nihon Medi-Physics Co., Inc., under the name Cardiodine™. Studies of more than 600 patients at 30 Japanese institutions were completed before the agent was approved for use.

Need more evidence? Two symposia recently held in Japan, the Third International Symposium on Radioiodinated Free Fatty Acids in Cardiac Imaging and the Thirteenth New Town Conference on Nuclear Cardiology, had a single focus—the clinical use of ORNL's iodine-123–labeled fatty acids as a gauge of the heart's metabolism.

Tracking Communication in the Brain

Alzheimer's disease, Parkinson's disease, and many other neurological disorders are characterized by abnormalities in the central nervous system. For example, normal brain cells have many receptors that receive chemical messages from other cells; in contrast, the brain cells of Alzheimer's patients often possess fewer receptors or many of their receptors are "turned off."

Other brain-centered disorders involve the message-carrying chemical compounds that interact with receptors, known as neurotransmitters. A neurotransmitter of critical importance to normal brain function is dopamine. Its absence in the brains of patients with Parkinson's disease leads to a debilitating loss of muscle control; on the other hand, high levels of dopamine are often associated with schizophrenic behavior.

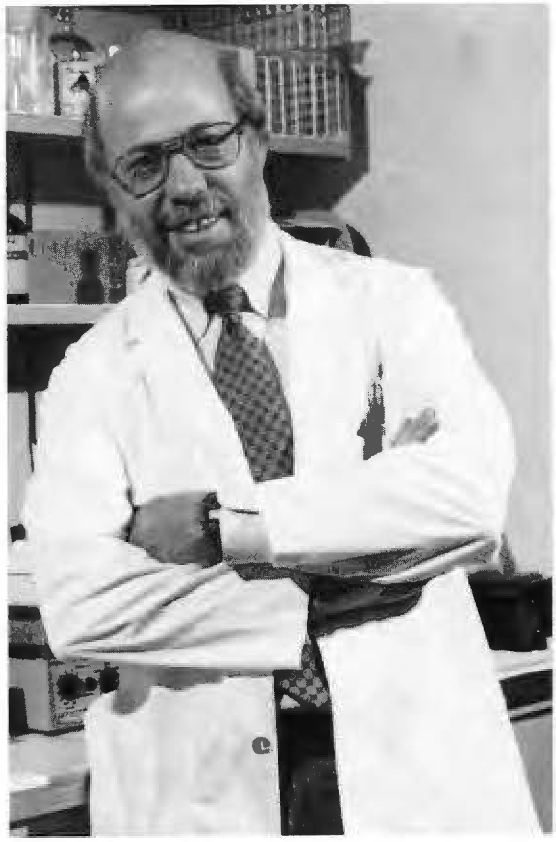
To aid in the diagnosis and treatment of these disorders, Dan McPherson is leading an effort in ORNL's Nuclear Medicine Group to develop new radiopharmaceutical agents that attach themselves chemically to the receptors involved in neurological diseases, such as Alzheimer's. Researchers have developed a simple method of producing large quantities of an iodine-123–labeled imaging agent, designated IQNP.

Because iodine-123 produces photons as it decays, its concentration and activity in the brain can be determined using photosensitive imaging techniques. A fluorine-18–labeled version of INQP is also on the drawing board and should be available in the next few months. The advantage of using fluorine-18 as a radioactive tag for

By attaching itself to neuroreceptors in the brain, the INQP imaging agent enables researchers to note changes in the number and activity of receptors. The bright areas of this cross section of a normal rat brain are receptor-rich regions where INQP has concentrated. *(Courtesy, P. Som, D.V.M., Medical Department, BNL.)*

INQP is that it emits positrons as it decays and, therefore, can be used in conjunction with higher-resolution positron emission tomography (PET) imaging systems.

Use of these agents will help researchers track changes in the concentration and activity of receptors and neurotransmitters in the brain. These changes mark the onset and progress of Alzheimer's and similar diseases of the brain. Initial studies in rats have demonstrated that INQP concentrates almost exclusively in the receptor-rich areas of rat brains. Further tests of INQP in primates are planned as a prelude to seeking approval for testing in human patients.



Russ Knapp and the Nuclear Medicine Group's sharpshooters hit their targets with enviable consistency.

The magic bullets developed by ORNL are finding their targets with enviable consistency.

Summing Up

From the brain to the heart to the pancreas, the magic bullets developed by ORNL's Nuclear Medicine Group are finding their targets with enviable consistency. The care with which the group chooses its targets and takes aim has resulted in the development of a series of magic bullets that have shown promise in patient studies. As a result, they are now making their way into the commercial market as agents for diagnosis and treatment of a wide range of diseases.

Tumor-Fighting Genes and Chemical Health Risks

By Carolyn Krause

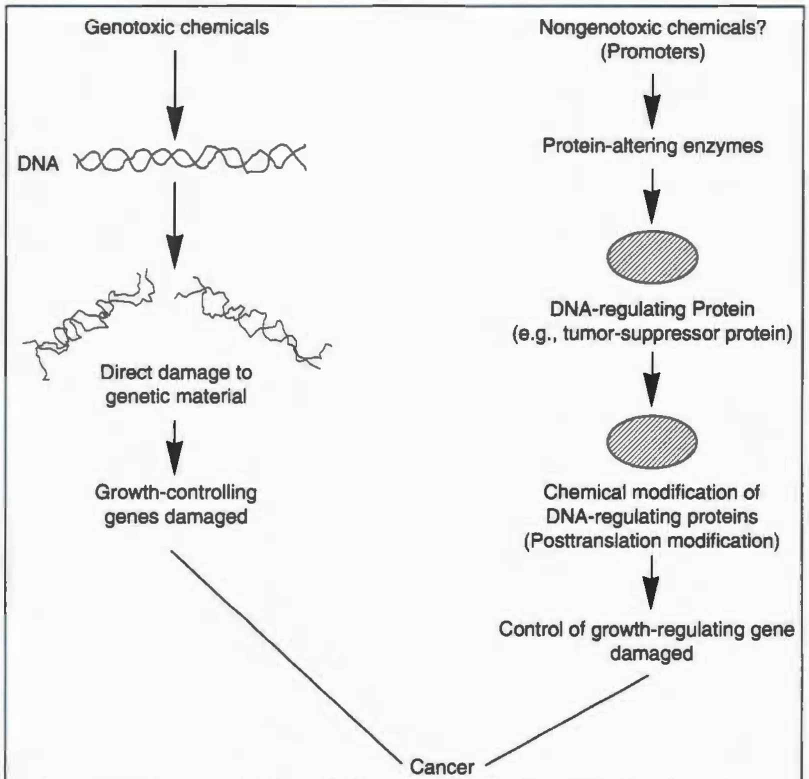
Hazardous waste is a mixed bag. Many chemicals present at hazardous waste sites may not be very hazardous to human health. As a result, the cancer-causing potential of hazardous waste can vary from one site to the next. Determining the precise health risk at different waste sites is the first step in identifying the particularly dangerous sites that should be cleaned up first. It can also identify the sites that do not require immediate cleanup, potentially saving millions of dollars.

Using the techniques of molecular biology, ORNL researchers are developing new ways to evaluate the health risks of potentially hazardous chemicals. Examples of such chemicals are benzene in gasoline and perchloroethylene, a degreasing agent that ends up in landfills. The new methods potentially can be used to identify cancer-causing chemicals and to stop cancers by restoring normal growth patterns to cancer cells.

The tumor-suppressor gene, called wildtype p53, is responsible for production of the p53 protein, which is present in trace amounts in normal human cells. The p53 protein has the ability to stop cells from growing. Mutation or deletion of the p53 tumor-suppressor gene is now recognized as an almost universal step in the abnormal cellular growth process called cancer. Mounting evidence indicates that tumors caused by certain viruses result from inactivation by the virus of the antigrowth properties of the p53 protein.

Loss of tumor-suppressor genes by inheritance is thought to make some individuals predisposed to development of cancer. For example, individuals who have lost both copies of the tumor-suppressing retinoblastoma gene develop cancer of the eye. Similarly, it is thought that some women who lack or have a damaged p53 tumor-suppressor gene are predisposed to breast cancer. It is now possible to test breast cells to determine if copies of the p53 gene are lost or mutated. Such a screening test can help physicians identify those women at increased risk of developing breast cancer.

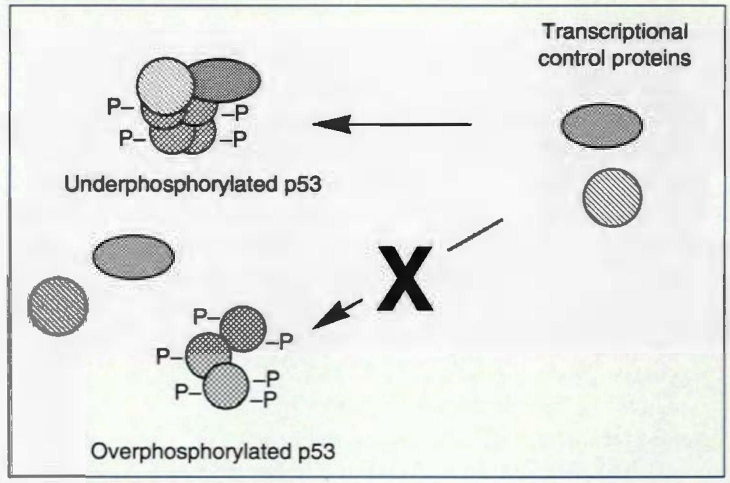
Exposure to certain toxic chemicals or radiation can result in the eventual appearance of a mutated p53 gene in cells. Detection of mutant protein or a loss of p53 function in suppressing cell growth may serve as a good biomarker indicating that a person or animal is at greater risk of developing cancer. However, it is likely that cells that contain a mutated p53 gene are rare events hidden in a background of a large number of normal cells. Therefore, detection of these cells requires the new molecular biology techniques that have the highest level of sensitivity. Even more sensitive and specific techniques may have to be designed to



Genotoxic chemicals directly damage genetic material, or DNA. Most known or suspected chemical carcinogens appear not to damage DNA. How these chemicals stimulate uncontrolled growth is unknown. These nongenotoxic carcinogens may act by adversely modifying proteins that control reading of the genetic code. As a result, genes that control growth may fail to function or growth-stimulating genes may run out of control.

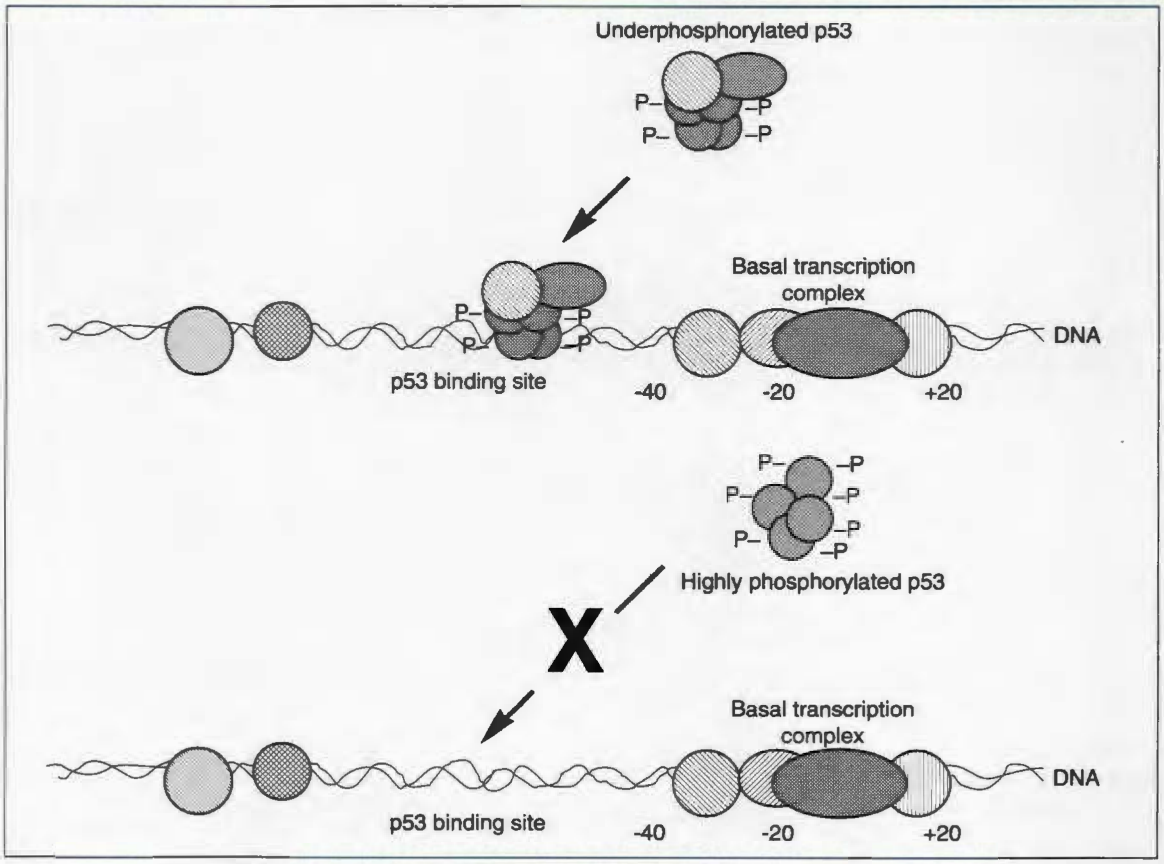
ORNL researchers are developing new ways to evaluate the health risks of potentially hazardous chemicals.

Craig Dees prepares to evaluate clones of the human p53 tumor-suppressor gene to determine the ones to be incorporated in a human tumor cell used to study the effect of chemicals on the p53 protein. The genetically engineered human tumor cells now produce very high levels of p53. The tumor cells will be treated with chemical carcinogens important in energy use or production to determine if they increase the phosphorylation of the p53 gene product, possibly causing it to stimulate rather than suppress cell growth.



Extra phosphate on the p53 tumor-suppressor protein interferes with the protein's ability to form working complexes with itself and other proteins. These complexes are required to properly regulate cell growth.

ORNL researchers would especially like to clarify the human health risks, if any, of exposure to cancer-causing chemicals or radiation at very low levels.



Extra phosphate on tumor-suppressor proteins also alters the ability of the tumor-suppressor protein to bind to specific binding sites in the genetic code. Extra phosphate could alter the ability of p53 and other tumor-suppressor proteins to turn on the genes that shut off cell growth. Highly phosphorylated p53 may also not be able to bind to DNA sequences that turn off other genes. In this way, p53 protein modified by phosphate loses its ability to control cell growth, causing cells to become cancerous.

detect genetic events that are responsible for cancer before disease begins.

Craig Dees, a molecular virologist in ORNL's Health Sciences Research Division (HSRD), and Curtis C. Travis, director of the Laboratory's Center for Risk Management, are trying to design new methods for analyzing the health risks to humans using molecular biology techniques. Because of the central and near-universal role of the p53 gene in the induction of cancer, their research has focused on determining whether suppressor genes are damaged by exposure to chemicals or radiation produced through energy use or production. By better understanding the genetic events responsible for cancer, they hope to identify new biomarkers to predict human health risks.

These ORNL researchers would especially like to clarify the human health risks, if any, of exposure to cancer-causing chemicals or radiation at very low levels. "This topic is a very controversial subject in the scientific and lay community at this time," Dees says. "Bruce Ames, one of the most prominent designers of a test to detect chemical carcinogens, recently published an article in *Science* magazine in which he argues that our current testing methods are identifying chemicals as hazardous to humans even though they are carcinogens only in laboratory rodents. In addressing the low-level exposure issue, Ames essentially stated that it is not realistic to worry about low-level chemical exposures that are below the background level of naturally occurring sources like foods. I side with Ames, but other investigators think differently."

Treated with chemical	-	-	+	++	+++	+++ +	++++ ++
Untreated	+	+					
Lane	1	2	3	4	5	6	7

Dees and Travis genetically engineered rat liver cells to produce the human p53 protein and then grew them in a medium that contained radioactive phosphate. Cells were treated with a chemical promoter that increases cell growth. The amount of radioactive phosphate found on the p53 tumor-suppressor protein was analyzed using an antibody to p53 to precipitate the protein from the cell extracts. The proteins were then separated using an electric field (gel electrophoresis). The amount of radioactive phosphate on the p53 protein was determined by exposing X-ray film. Lane 1 shows that very little radioactive phosphate is found on p53 protein taken from cells that were not treated with the growth-stimulating chemical. As the amount of chemical given to the cells is increased, the amount of phosphate on the p53 is clearly increased, as shown by the increasingly darker bands in Lanes 2 through 7.

"In addition to the problems of determining human health risks based on exposure of laboratory animals," Travis says, "a large number of chemicals suspected to be carcinogens, like perchloroethylene, have not been shown to directly damage genetic material. It is important to determine how these chemicals cause cancer."

"Do they really pose any real health risk to humans?" Dees asks. "Maybe they put at risk only certain individuals with inherited genetic defects in growth-stimulating genes or growth-suppressing genes like p53? The answer to these suppositions lies in a better understanding of the molecular alterations that are responsible for causing a cell to suddenly grow uncontrollably. This knowledge may help us rationally design new molecular biology–based assays to identify these individuals before problems start."

For example, the normal p53 protein is known to have phosphate chemically bound to it. The processes of adding or removing phosphate from proteins is known to be a mechanism through which cells regulate protein function; these processes are called phosphorylation and dephosphorylation. Dees and Travis hypothesize that some chemicals found in hazardous waste may cause cancer not by inflicting damage directly on genetic material but rather by altering the function of proteins that control cell growth.

"One way this might work," says Dees, "would be to adversely affect the phosphorylation of key regulatory proteins like p53 that are involved in regulating growth."

For many years it has been known that some chemicals activate a specific enzyme called protein kinase C, which puts phosphate on proteins. However, no one has been able to fully explain how this effect of chemicals on protein kinase C caused loss of the genetic control of cell growth.

At a 1992 information meeting of HSRD, Dees and Travis presented the first evidence that chemicals such as benzene and perchloroethylene change the phosphorylation levels of two tumor suppressor gene products (p53 and rb105), possibly causing them to stimulate rather than suppress cell proliferation. Several other laboratories have recently confirmed the original observations of Dees and Travis.

"The ultimate goal is to be able to identify specific individuals who are at increased risk."

"Presumably," Dees says, "chemical alteration of tumor-suppressor gene products contributes to the process by which these chemicals cause cells to grow at abnormally high rates. It may now be possible to screen chemical carcinogens by examining their effects on the tumor-suppressor gene products."

The almost universal occurrence of damage to p53 genes in cancer cells now provides a target for analyzing the effects of chemical carcinogens.

"We hope to be able to answer some of the pressing questions on the health effects of low-level exposure to chemicals and clarify the human health risks," says Dees. "The ultimate goal is to be able to identify specific individuals who are at increased risk and perhaps to genetically reengineer them with normal tumor-suppressor genes to ensure that they have the proper growth controls to inhibit the formation of cancer cells."

Observing the effects of various chemicals on tumor-suppressor genes could be a sensitive way of measuring the ability of these substances to cause cancer. It could help regulators make better sense of the mixed bag of hazardous waste. ■

Tumor-Suppressor Genes and the AIDS Virus

Craig Dees examines a bottle of broth used to grow bacteria for amplifying production of the human or mouse p53 gene.

Among the 50,000 to 100,000 genes enabling humans to function and reproduce are the genetic "switches" that regulate growth. Some of these switches "turn on" cell division and others turn it off, thus permitting individual organs to grow to the right size but no larger. The "oncogenes" stimulate cell proliferation and the "tumor-suppressor genes," or anti-oncogenes, shut down the process.

At ORNL researcher Craig Dees has become curious about the effects of a tumor-suppressor gene on the human immunodeficiency virus (HIV) that causes the acquired immuno-deficiency syndrome (AIDS).

In 1992 Dees and biologist Steve Foster, formerly with ORNL, showed that the ability of the AIDS virus to reproduce itself can be blocked by a gene product that suppresses the growth of cancerous tumors.

Dees and Foster demonstrated that the p53 tumor-suppressor gene can shut down, or "down regulate," the AIDS virus. For their research, they used a crippled AIDS virus that is unable to cause the deadly disease because it lacks genetic material that is normally "read" to produce the components of the AIDS virus.

The ORNL scientists found that the p53 protein may bind to part of the AIDS virus controller region, apparently interfering with its ability to stimulate production of genetic messages.

"The ability of the controller region of the AIDS virus to strongly stimulate genetic message production," says Dees, "helps the virus reproduce itself so very effectively." Thus, he added, interference with this process by p53 proteins might slow or stop duplication of the deadly virus.

Dees presented his results at the November 26, 1992, annual meeting of the Council of Animal Research Workers of America in Chicago, during a November 10, 1992, seminar at the University of Wisconsin–Madison, and at the 1993 AIDS symposium at Palm Springs, California.

The ORNL findings, Dees says, could have favorable implications for treating AIDS patients and people testing positive for HIV. "One remote possibility," he notes, "would be to remove a patient's bone marrow, genetically engineer the cells to produce large amounts of p53 protein, which might keep the AIDS virus under control, and reinfuse the treated marrow back into the patients. A more practical implication is that this new knowledge on how the virus controls itself could lead to development of new drugs to treat AIDS patients."

The ORNL scientists' original goal was to develop a new assay to screen chemicals for carcinogenicity. They theorized that many chemicals that stimulate uncontrolled cell growth may act by adversely affecting transcription, the process by which the genetic code is read and transcribed into a chemical message made of ribonucleic acid, known as messenger RNA. Messenger RNAs are read and translated into proteins that are used in the biochemical

"The AIDS virus has a very simple task, which is to make a large number of copies of itself."

Boosting Production of Tumor-Suppressor Protein

It is impossible to obtain usable amounts of p53 protein from human cells because the protein is present at such low levels and for such a short time (only 15 to 20 minutes after it is made). Fortunately, genetic engineering techniques make it possible to produce large amounts of human or animal proteins, such as p53, in bacteria or insect cells.

Lois Miller, formerly of ORNL's Biology Division and now at the University of Georgia, uses insect cells for protein production. She inserts the mouse p53 gene into an insect virus called *Baculovirus* and infects insect cells with the virus, causing them to make high levels of the p53 protein. The protein is then purified using anti-p53 antibodies in a process called immunoaffinity chromatography. These large amounts of p53 protein can then be used to study the cancer process.

machinery or structural components of the cell.

Little is known about the complicated process of transcribing the genetic code into messages. The p53 protein is thought to be involved in this complex process. Viruses such as HIV insert themselves into the human genetic material and use the host cells' transcription machinery to duplicate themselves. The parts of the AIDS virus involved in stimulating transcription are many times more powerful than those found in a human cell.

"ORNL scientists began using the AIDS virus' transcription system to study the effects of chemical carcinogens on transcriptional control."

"The AIDS virus has a very simple task, which is to make a large number of copies of itself," Dees says. "In the process of making more virus, the AIDS virus damages the human immune system, and other viruses, bacteria, or parasites combine to destroy our ability to defend ourselves. The virus apparently reproduces itself easily as a result of the powerful ability of its controller region to strongly stimulate transcription."

Because the transcriptional mechanisms of the AIDS virus are so potent, the ORNL scientists began using the AIDS virus' transcription system to study the effects of chemical carcinogens on transcriptional control, especially when the AIDS virus is combined with the p53 gene product. In the process, they discovered the ability of the p53 protein to limit transcription by the AIDS virus.

"Our current evidence," says Dees, "suggests that the p53 protein recognizes a specific genetic sequence within transcription-controlling regions of certain human genes and the AIDS virus. We think that p53 interacts with other cellular and perhaps viral proteins that bind to the controlling regions, turning down production of genetic messages.

"We also think that p53 acts in concert with other cellular transcription-controlling proteins to physically change the structure of the DNA, thereby making it less available to be transcribed. It seems that the key to curing AIDS is better understanding the molecular process of viral transcription and then rationally designing new drugs to suppress HIV transcription. Alternatively, we may be able to genetically engineer into the human immune system the ability to control the AIDS virus."

Tumor-Suppressor Genes and Cancer Treatment

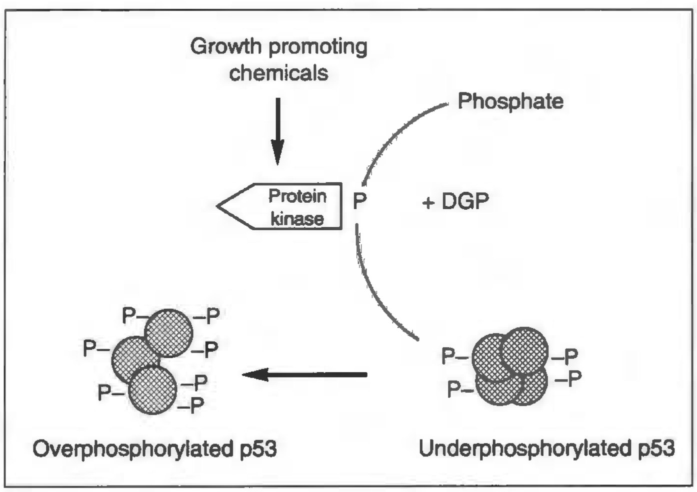
Could new treatments for cancer result from research into the function of tumor-suppressor genes? ORNL scientist Craig Dees thinks so. "It's possible to genetically reengineer tumor cells using tumor-suppressor genes so that the normal growth pattern is restored," Dees states. "Here at ORNL, we have done it with rat liver epithelial cells, and other laboratories have been successful using human colon and lung cancer cells. We have also been the first to genetically repair a cell line that had been transformed into tumor cells by a retrovirus that is closely related to the two viruses that cause human T-cell leukemia and AIDS."

In a recent development, Dees conducted an experiment using nude mice. Because nude mice are defective in their ability to reject tumors or transplants of cells from humans or other animals, they can be used to study the effects of antitumor genetic engineering methods. Tumor cells from rat liver or tumor cells formed from normal cells by a retrovirus were injected under the skin of the nude mice. A genetic element, called a plasmid, engineered to contain the human p53 tumor-suppressor gene was injected weekly in each mouse at the site of the tumor cells.

After several weeks Dees found that tumors in treated animals were much smaller than the large tumors found in untreated mice. This difference in tumor size is attributed to insertion of the human p53 tumor suppressor gene into the tumor cells.

"These results are intriguing," Dees says, "because this is the first time that a genetic engineering method has been shown to slow the growth of tumors caused by cells made cancerous by an AIDS-like virus. Secondly, even though liver cancer is less common in humans than other cancers, it almost always results in death only a few months after it is diagnosed. The results suggest that perhaps the method for genetic reengineering of tumor cells employing a tumor-suppressor gene could be used as a cancer treatment for a highly fatal liver cancer as well as tumors caused by certain viruses."

"The results suggest that perhaps the method for genetic reengineering of tumor cells employing a tumor-suppressor gene could be used as a cancer treatment for a highly fatal liver cancer."



The function of proteins that regulate genetic material is often modified by the amount of phosphate chemically attached to them. Phosphate is placed on proteins by enzymes called protein kinases. Dees and Travis have shown that chemicals that contribute to cancer stimulate a protein kinase to put extra phosphate on tumor-suppressor proteins, possibly making it more likely to stimulate than suppress cell proliferation.

Strategies for Radwaste Management

By Charles W. Forsberg

The production of electricity by any technology produces waste: coal burning creates ash and air pollution, solar-cell wastes contain hazardous heavy metals such as arsenic and cadmium, and nuclear power generates radioactive wastes. Protecting the environment requires careful control of all of these wastes. Radioactive wastes are also a by-product of defense activities, research, medical applications, and industrial production. ORNL has long engaged in development of new technology to ensure safe and environmentally benign disposal of these wastes.

The basis of radioactive waste management is simple. Because radioactive materials become less radioactive over time, the way to safely dispose of radioactive materials is to store them until they become nonradioactive. Different radioactive materials have different half-lives, so their storage times are different. For example, cobalt-60, a radioactive isotope used to sterilize medical equipment and treat cancer, has a five-year half-life. Thus, a pound of radioactive cobalt-60 five years later would decay to a half pound. Every five years the quantity is reduced in half. A rule of thumb is that, after 10 half-lives have passed, the material is essentially no longer radioactive. In contrast, chemical wastes, such as dioxin, can be destroyed by incineration, and toxic heavy-metal wastes, such as lead and arsenic, remain toxic forever and require other waste management technologies to isolate them from the environment.

Very short-lived radioactive wastes are disposed of by storing them in buildings until they are nonradioactive. For example, hospitals use radioactive molybdenum-99/technetium-99*m* to diagnose diseases and injuries of the brain, liver, and other organs. Because this material has a half-life of three days, hospitals can store molybdenum-99 radioactive wastes for a month until they become nonradioactive. Longer-lived radioactive wastes containing cobalt-60 and similar radioactive materials must be isolated from the environment for approximately 100 years. Such materials are called low-level waste (LLW) and typically become relatively nonhazardous within a century or less. High-level waste (HLW), including spent fuel from power reactors, contains radioactive materials that must be isolated for thousands of years.

Disposal Technologies

The major goal of radioactive waste disposal is to isolate waste materials from groundwater and air until the radioactivity has decayed away. The basic approach is to convert waste to solids that do not readily dissolve in water, put these insoluble solids in sealed waterproof containers, and store the containers away from moving water. For LLW a well-built structure can store the waste. For HLW, the waste must be buried hundreds of meters underground to ensure its isolation from people for thousands of years. In nature, toxic ore deposits, such as lead, arsenic, and cadmium, which have toxicities similar to HLW in a disposal site, do not poison people because the ores are isolated deep underground. Thus, similar underground isolation is planned for disposal of HLW.

ORNL is involved in developing improved methods of LLW and HLW isolation, including engineered waste storage. Michael Gilliam of ORNL's Chemical Technology Division (CTD) is working to devise better wasteforms to solidify liquid LLW. Better methods to predict and demonstrate the long-term performance of waste disposal sites are being developed by researchers in the Environmental Sciences Division. Larry Shappert of CTD and others are testing waste packages to ensure their ability to both store wastes and survive accidents during waste transportation.

On the Oak Ridge Reservation, the staff of the Waste Management and Remedial Action Division is demonstrating tumulus disposal of LLW—a method of storing wastes for more than 100 years until they become nonhazardous. In a tumulus, the solidified waste is confined in concrete packages that are placed on a special concrete pad and covered with layers of different materials to prevent the flow of rainwater through the wastes (see the series of photographs throughout this article).

Finally, research is under way at ORNL on advanced disposal options for spent fuel and HLW. Two options are island repositories and waste destruction.

The island repository is a good example of advanced exploratory research—work I have been involved in—to find environments for hazardous wastes where natural forces isolate the wastes

ORNL has long engaged in development of new technology to ensure safe and environmentally benign disposal of these wastes.

A concrete box (left) has been transferred from the truck by crane onto the pad of the engineered storage "tumulus" facility at ORNL for isolating low-level radioactive waste.

The concrete box holding radioactive waste is filled with cement to further immobilize the material.

from humans. The idea is to place the waste 500 meters under the ocean floor in manmade tunnels accessible by mineshaft on a temporary manmade island. After the repository is filled, the tunnels are backfilled and sealed, and the temporary island is removed. It has several potential advantages.

- No groundwater flow. Waste disposal sites fail when groundwater runs downhill through a disposal site, dissolves hazardous material, and carries it to the environment by a spring or well water. Under most of the ocean floor, groundwater does not flow because there is no place for it to flow to and no pumping of underground water occurs. With no water movement, wastes cannot escape.

- On-land disposal sites can fail because of climate changes or accidental human intrusion. The ocean floor is not exposed to climatic changes. Any future human intrusion after removal of the manmade island would require a very large effort by a large, sophisticated organization that would recognize a hazardous disposal site and know what to do if it accidentally entered such a site.

- The region below the ocean floor has chemically reducing conditions that make most waste insoluble, whereas chemical conditions on land vary.

Added research will be required to confirm the advantages of this disposal option. ORNL is also examining more futuristic options, such as destruction of long-lived radioactive materials using nuclear reactors and accelerators (see sidebar by Gordon Michaels on p. 32).

How Dangerous Is Radioactive Waste?

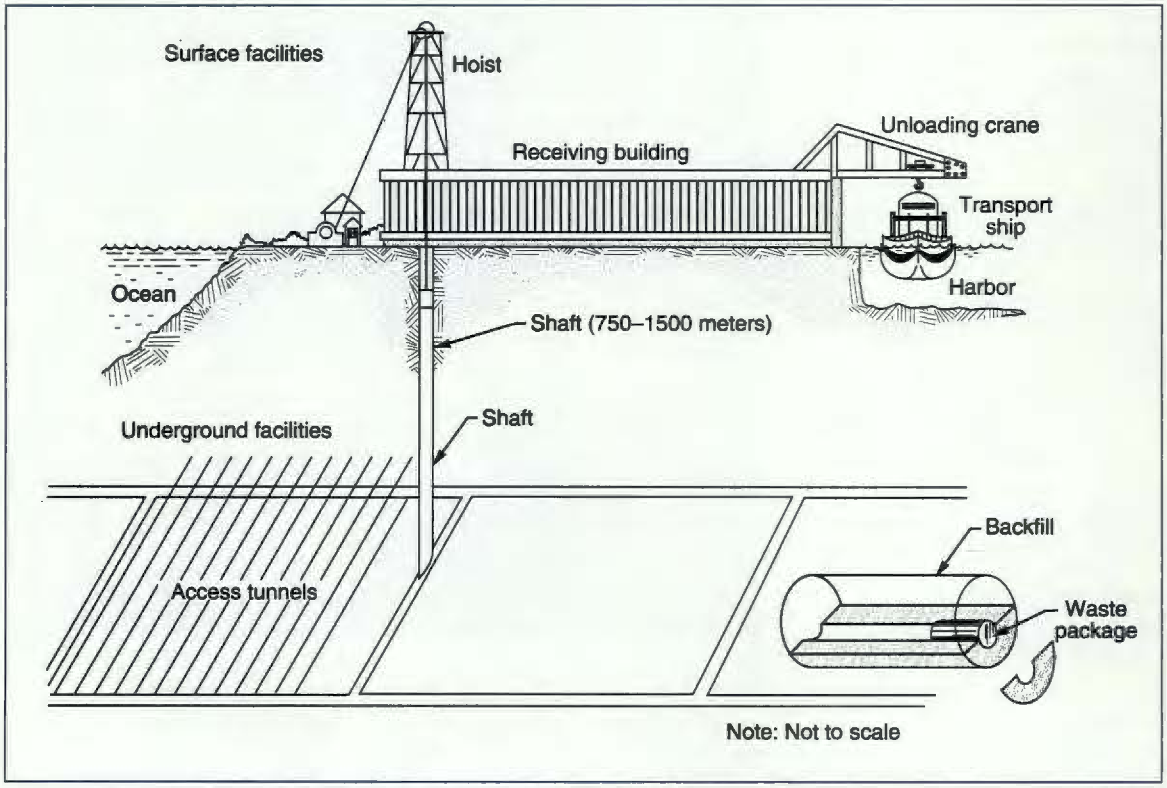
Several characteristics of radioactive wastes are often misunderstood.

- **It is widely thought that all radioactive waste is highly hazardous to human health.** This assumption is not true. ORNL inventories and projects quantities of all types of radioactive wastes for the U.S. government. Analyses, like those done by CTD's Jerry Klein, show that almost all radioactive waste by volume is LLW, but spent fuel and other forms of HLW contain at least 99% of the radioactivity. Radioactive waste is like any other hazardous waste type—its hazard varies from very toxic (HLW) to some types of LLW that are almost as nontoxic as household garbage.

- **HLW and spent nuclear fuels are highly toxic because they are concentrated.** True. This concentration has an advantage. A large nuclear power plant that generates electricity for a half million people produces approximately 25 tons of spent fuel annually. An equivalent coal plant produces 10 million tons annually of air pollutants, potentially hazardous ash, and other wastes. Because spent nuclear fuel is concentrated, large sums of money can be spent per ton to ensure it is carefully disposed of without significantly increasing the cost of electricity. Thus, environmental pollution from properly operated nuclear power plants is low. The large volumes of coal plant emissions make economic pollution control more difficult.
- **Many people believe that disposal sites for radioactive wastes are highly dangerous.** In reality, the risks are low for properly disposed of radioactive wastes, and these wastes pose no risk of large-scale accidents. Human experience with lead shows why. Lead poisoning of children has

The tumulus facility comprises stacks of waste boxes on a concrete pad. The boxes are then covered with more concrete, plastic liners, and soil to keep water away. At top is Solid Waste Storage Area Number 6.

The first pad of the tumulus facility is full, and its waste boxes are covered with a plastic sheet. The second pad is rapidly filling up with concrete boxes containing low-level radioactive waste from ORNL.



Design of a subseabed geological waste repository with access through a temporary man-made island. It is proposed that radioactive waste be isolated under the ocean floor.

been a major health concern—particularly for children living near freeways. Much of the lead came from leaded gasoline burned in cars. Because of the health problems, leaded gasoline is now banned. Similarly, we have banned use of lead pipes for carrying drinking water because lead can dissolve in the water over time. Lead in car batteries is still acceptable because it does not pose major health risks. The danger occurs when the hazardous material is a liquid, easily dissolves in water, or generates very small airborne particles—in this case, gasoline vaporizes the lead and spreads it through air or water. For the same reasons, the past problems of radioactive wastes have been confined to liquid wastes or wastes that are easily dissolved in water. Radioactive materials, after solidification, packaging, and proper disposal, present small risks because no big energy source is available to spread the material in the environment.

Institutional Barriers

The institutional problems in selecting disposal sites are often greater than the technical challenges. Early ignorance, the rush of World War II, and Cold War priorities resulted in a legacy of neglect that is only now being addressed. The Cold War increased the fear of radioactivity. Our national policy was to prevent war by deterrence. This tactic required a potential enemy to fear our nuclear weapons; but in scaring enemies, we scared ourselves. The distinction among low risks from solidified wastes, somewhat larger risks of wastes in liquid form (weapons production sites), and the very large, real dangers of radioactive materials in air (nuclear weapons) was a fine point lost in scaring our enemies. The complexity of waste management and the legacy of past wastes have created real barriers to siting future facilities.

Our society is also becoming more open and more accepting of an environmental ethic. These desirable changes create new challenges for waste management. Historically, society sited unwanted but needed facilities by building them on the wrong side of the tracks. From the caveman until recently, the waste management philosophy has been "dilution is the solution to pollution." Our goal today—containing radioactive and hazardous waste to isolate it from the environment—requires waste management facilities that were not needed when it was acceptable to dump waste in the river or discharge it up the smokestack. Our changing goals require both new technologies and new institutional arrangements to site facilities in an open, publicly accepted manner. ORNL economists, sociologists, and political scientists are actively investigating how these issues can be resolved. Education is part of the solution, but equally important are mechanisms (such as voluntary siting of facilities and community involvement) to develop trust between local communities and operators of waste disposal sites.

All forms of energy generation produce wastes—from the toxic metals used to build solar cells to the radioactive wastes from nuclear power plants. Whether this waste is a risk to mankind depends upon the care we take for proper disposal. Just as the end of the Cold War has brought about the need for industrial restructuring from military to civilian applications, ORNL's development of radioactive waste management technologies allows the Laboratory to address waste problems that are a legacy of the Cold War. These efforts enable the Laboratory to better safeguard the environment and reduce costs as it continues to meet the nation's needs in the post–Cold War era.

Biographical Sketch

Charles Forsberg joined the research staff of ORNL's Chemical Technology Division in 1975. He holds a B.S. degree in chemical engineering from the University of Minnesota and a Ph.D. degree in nuclear engineering from the Massachusetts Institute of Technology. Forsberg has managed several programs to develop passive and inherent safety systems for nuclear and chemical production and waste management facilities. He is a member of the DOE High-Level Waste Tank Advisory Panel. He is the author of more than 60 publications and has several patents.

Partitioning and Transmutation: Making Wastes Nonradioactive

The word transmutation originates from the never-realized goal of ancient alchemists to transform, or transmute, the base metals into gold. Today scientists seek ways to transmute radioactive waste into nonradioactive elements, thereby eliminating the radiological hazards and waste disposal problems.

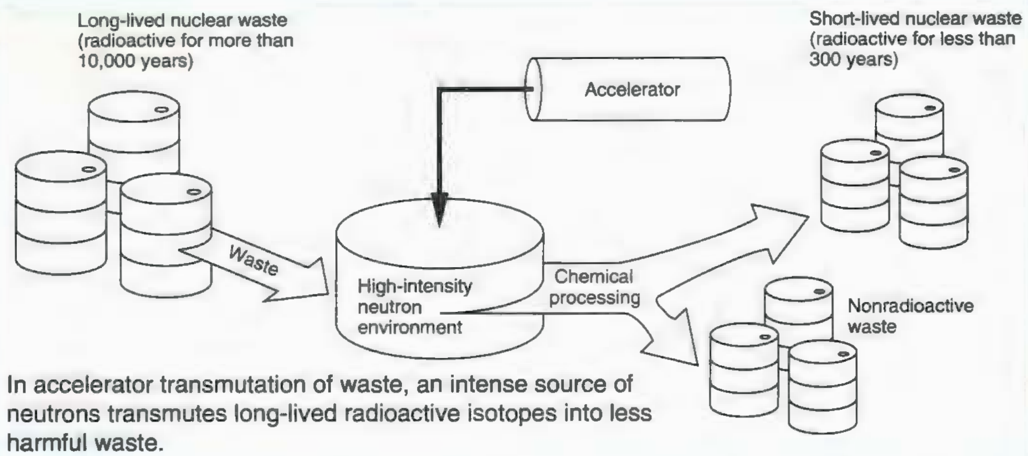
An example of two radioactive isotopes that can be transmuted into less hazardous forms are technetium-99 and iodine-129. Both of these isotopes are very long-lived and require disposal strategies that will isolate them from the environment for long periods of time. Both iodine and technetium are considered difficult to isolate because they dissolve readily in groundwater and move easily throughout the ecosystem. Irradiation of the long-lived technetium-99 isotope by neutrons will cause it to absorb a neutron and become technetium-100, which undergoes complete radioactive decay into stable ruthenium within minutes. Similarly, the iodine-129 isotope can be transformed by neutron absorption into stable xenon isotopes.

"Interest at ORNL has turned inward to see whether partitioning and transmutation offer any near-term advantages for management of some of our own radioactive wastes."

Another class of radioactive wastes that can be transmuted into less hazardous forms are the actinide elements, particularly the isotopes of plutonium, neptunium, americium, and curium. When irradiated with neutrons in a nuclear reactor, these isotopes can be made to undergo nuclear fission, destroying the original actinide isotope and producing a spectrum of radioactive and nonradioactive fission products. Isotopes of plutonium and other actinides tend to be long-lived with half-lives of many thousands of years, whereas radioactive fission products tend to be shorter-lived (most with half-lives of 30 years or less). From a waste management viewpoint, transmutation of actinides eliminates a long-term radioactive hazard while producing a shorter-term radioactive hazard instead.

A challenging aspect of this waste management strategy is the required waste partitioning. Just as household wastes must be partitioned into categories, such as paper, glass, and aluminum, before they are recycled, radioactive waste must also be sorted before being recycled back into nuclear reactors.

One particularly challenging partitioning task involves the actinide



In accelerator transmutation of waste, an intense source of neutrons transmutes long-lived radioactive isotopes into less harmful waste.

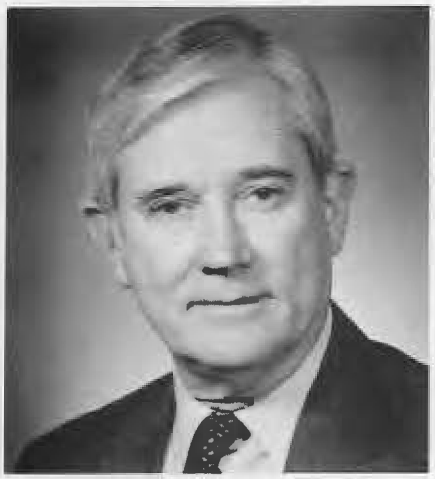
and lanthanide (rare earth) elements. Actinide and lanthanide elements are chemically similar and, thus, very difficult to separate efficiently. Most lanthanide isotopes are nonradioactive, and the few radioactive lanthanide isotopes are long-lived, so there is little incentive to invest neutrons in transforming them into stable elements. However, lanthanide elements tend to absorb neutrons efficiently (they are so-called neutron poisons) and will prevent the efficient transmutation of americium and curium if they are intermixed. Improved methods of separating lanthanides from actinides are needed to reach the goal of actinide transmutation.

The largest program at ORNL focusing on partitioning and transmutation is investigating methods for accelerator transmutation of wastes (ATW). Conceived by scientists at Los Alamos National Laboratory, ATW uses a linear accelerator system to produce neutrons for transmutation of excess weapons plutonium and other radioactive DOE wastes, such as technetium-99 and iodine-129. Activity at ORNL is centered on developing chemical separations technology, including processes for performing actinide-lanthanide separations, and on studying, designing, and ultimately testing the reactorlike flow loops in which the transmutation occurs.

A second program is developing technology for using a nuclear reactor to transmute the actinides in spent nuclear fuel from light-water reactors (LWRs). This program offers an alternative to direct disposal of LWR fuel in geological repositories. ORNL researchers are developing techniques for the front-end processing of LWR fuel to prepare it for introduction into the chemical partitioning system and are examining wasteform technologies for immobilizing some of the unique waste streams produced during the partitioning process. Additionally, we have performed several studies to characterize the benefits and disadvantages of recycling spent nuclear fuel.

Recently, interest at ORNL has turned inward to see whether partitioning and transmutation offer any near-term advantages for management of some of our own radioactive wastes. Transmutation of highly radioactive europium isotope wastes (currently stored at ORNL solid waste area groups) into nonradioactive gadolinium isotopes appears to be practical and is being studied further. These europium wastes pose the dominant health risk to the public in certain environmental scenarios, and their elimination might be beneficial to the Laboratory. As proposed, the transmutation device would be the High Flux Isotope Reactor or the proposed Advanced Neutron Source. The physical and chemical partitioning of the radioactive europium from nonradioactive europium and gadolinium represents a key technology that must be developed for this task.

Ultimately, the potential of partitioning and transmutation to waste management is this: If a radioactive waste stream no longer exists, then it poses no radiological hazard. More than anything else, this simple fact has spurred the recent resurgence of interest in partitioning-transmutation technology.—*Gordon E. Michaels, Chemical Technology Division*


Alvin Trivelpiece


Charles Baker


Lynn Boatner

Gordon Fee, former director of ORNL's Engineering Technology Division, has been named president of Martin Marietta Energy Systems, Inc., replacing **Clyde Hopkins,** who has been appointed president of Martin Marietta Corporation's Energy Group.

Alvin W. Trivelpiece has been elected to the National Academy of Engineering.

Bill Appleton has been named head of the Advanced Neutron Source Task Force.

Charles C. Baker has been named U.S. "Home Team" leader of the multinational effort to complete design of the International Thermonuclear Experimental Reactor (ITER).

Lynn A. Boatner and **James M. Corum** have been named corporate fellows by Martin Marietta Energy Systems, Inc.

Ward Plummer and **Kenneth Kliewer** have been named University of Tennessee–ORNL Distinguished Scientists.

Barry A. Berven has been appointed director of ORNL's Health Sciences Research Division.

John Sheffield has been elected a fellow of the American Nuclear Society.

John C. Miller and **James R. Thompson** have been elected fellows of the American Physical Society.

Curtis C. Travis has been elected a fellow of the Society for Risk Analysis.

Barbara Walton has been appointed to the faculty of the University of North Carolina, Chapel Hill, at the rank of adjunct professor. She has also been appointed to the Science Advisory Committee for the Center for Ecological Health Research at the University of California, Davis.

Rich Leggett has received a two-year appointment to the National Council on Radiation Protection and Measurements' Committee on Dosimetry and Metabolism of Radionuclides.

The **Radiochemical Development Facility,** Building 3019, has been designated a nuclear historic landmark by the American Nuclear Society.

Bill G. Eads, director of the Instrumentation and Controls Division, has been temporarily assigned to be chief science and technology advisor to the Tennessee Department of Economic and Community Development. **D. W. McDonald** has been appointed acting division director in his absence.

Frances E. Sharples has been named to the American Association for the Advancement of Science's Committee on Science, Engineering, and Public Policy.

The **Environmental Sciences Division** has received a certificate from the Secretary of Energy in recognition of its exemplary service and outstanding dedication to increasing educational excellence in science and to achieving the national education goals of America 2000.

Margaret B. Emmett has been named chair of the Radiation Protection and Shielding Division of the American Nuclear Society for 1992–93.

Lawrence W. Barnthouse has been selected to serve as an editor of *Environmental Toxicology and Chemistry*.

Jerry L. Hammontree has been appointed director of the Plant and Equipment Division. He succeeds **George W. Oliphant,** who has retired.

Allen G. Croff has been named chairman of the Nuclear Development Committee of the Organization of Economic Cooperation and Development of the Nuclear Energy Agency.

Patricia S. Hu has been named to two committees and one task force on the National Research Council's Transportation Research Board.

James Kahn has been named an international collaborator at the Environmental Science Center of the University of Amazonas.

Philip Childs and **Kenneth E. Wilkes** have received a 1992 "Best of What's New" Award from *Popular Science* magazine.

Kimiko O. Bowman has been named to the Disability and Employment Concerns Standing Committee of the President's Committee on Employment of People with Disabilities.

Judson P. Jones has been named a charter member of the Institute of Electrical and Electronics Engineers (IEEE) Technical Committee on Mobile Robots of the IEEE Robotics and Automation Society

Gary T. Alley has been named guest editor of *1992 Nuclear Science Symposia,* published by the IEEE.

D. Kip Soloman has been awarded the 1992 Alumni Gold Award by the University of Waterloo, Ontario, Canada.

Steven H. Stow has been appointed Executive Committee Member-at-Large for the American Geological Institute.

Monica G. Turner has been appointed to a three-year term on the National Science Foundation's Ecosystem Panel.

John Caughman has been named to the board of directors of the Tennessee Valley Chapter of the American Vacuum Society.

James E. Turner has received the Distinguished Scientific Achievement Award from the Health Physics Society.

Phillip W. King has received a Chapter Service Award from the Energy Systems Chapter of the National Management Association.

Carolyn Krause has received a Distinguished Chapter Service Award from the Society for Technical Communication for her services to the society's East Tennessee Chapter.

Jean C. Thorpe has been named to the Radiation Protection Training Special Interest Group Steering Committee of DOE's Training Resources and Data Exchange (TRADE).

Ida Lee has been named to the board of the Tennessee Valley Chapter of the American Vacuum Society.

Katie U. Vandergriff has completed her Leadership Development Initiative Program Internship, which was sponsored by the American Society of Mechanical Engineers.

Dan Lubben has been named to the board of the Tennessee Valley Chapter of the American Vacuum Society.

Stephen J. Pennycook has received the Presidential Heinrich Award from the Microbeam Analysis Society. He also was awarded the 1992 Materials Research Society Medal.

J. Michael Ramsey has been named to the Editorial Advisory Board of the journal *Analytical Chemistry.*

Lynn A. Boatner, Stan A. David, R. A. Steele, and **J. M. Vitek** received a second-place award in the Crystal Photo Competition at the 10th International Conference on Crystal Growth.

Lynn A. Boatner, Brian C. Chakoumakos, and **Allison Baldwin** received a first-place award in the International Metallographic Contest sponsored by ASM International and the International Metallographic Society.

Thomas A. Fontaine has been appointed chairman of the Surface Hydrology Technical Working Group of the American Water Resources Association.

James Corum

Ward Plummer

Kenneth Kliewer

Barry Berven

Frances Sharples

Margaret Emmett

Robin L. Graham has been selected to be a peer reviewer for the Hydrocarb Program of the Global Warming Branch of the EPA Air and Energy Engineering Research Laboratory.

Michael Ramsey has been appointed to a three-year term on the Editorial Advisory Board of the journal *Analytical Chemistry.*

Dora F. Pedraza has been granted the title of professor in residence at the Department of Metallurgy at the University of Connecticut.

Allen G. Croff has been elected a deputy program chair and program chair-elect for the International High-Level Waste Management Symposium, sponsored by DOE, the American Society of Civil Engineers, the American Nuclear Society, and the University of Nevada at Las Vegas.

Robert D. Hatcher, Jr., has been elected president of the Geological Society of America.

Oak Ridge National Laboratory has been designated part of the World Data Center system by the National Academy of Sciences. The World Data Center-A for Atmospheric Trace Gases will be part of the Environmental Sciences Division and will acquire, process, and distribute data from studies of trace gases and their role in global climate change.

T. R. Curlee will head the newly formed Energy and Global Change Analysis Section of the Energy Division.

Richard J. Norby has received the Environmental Sciences Division 1992 Scientific Achievement Award for his research on the physiological ecology of forest trees and the effects of pollutants on plants.

Jacqueline M. Grebmeier has been asked to serve on the National Science Foundation's Arctic System Sciences Ocean-Atmospheric-Ice Interactions Science Steering Committee.

Lynn A. Kszos has been appointed to the Ecology Committee of the Water Environment Federation.

Dianne D. Gates has been selected to participate in the National Urban League's Black Executive Exchange Program as a visiting professor for 1993.

George N. Miller has been selected to lead the Measurement and Controls Engineering Section in the Instrumentation and Controls Division.

Andrew A. Francis and **Sylvia S. Talmage** have been certified as diplomates of the American Board of Toxicology, Inc.

Paul S. Rohwer has been appointed associate division director of the Health Sciences Research Division.

Richard E. Swaja has been named head of the Assessment Technology Section of the Health Sciences Research Division.

Barbara G. Ashdown has been appointed director of the Energy Systems Chapter of the National Management Association.

Richard K. Genung has been elected vice president of the Energy Systems Chapter of the National Management Association.

Lola M. Roseberry has received a Distinguished Service Award from the East Tennessee Chapter of the Amercian Society for Information Science.

Several ORNL publications won awards in the Public Relations Society of America's 1992 Competition. In internal publications, one or two colors, **William H. Cabage** received a third-place award. In external publications, annual reports, **Judy H. Campbell, Walter S. Koncinski,** and **Robert A. Eldridge** received second-place awards. In external publications, brochures, one or two colors, **Betty Martin, Melanie D. Conger, Larry H. Bohanan, M. W. Darnell,** and **Edward Aebischer** received third-place awards. In external publications, three or more colors, **Wanda G. Jackson, Robert A. Eldridge, Linda Jeffers,** and **Berta S. Swain** won first-place awards.

E. Kaye Johnson has been named 1992 Outstanding Engineering Technology Advisory Committee Member by Pellissippi State Technical Community College.

Calvin E. Pepper has received the Distinguished Member Award from the American Welding Society and has been named chairman of the society's Qualification and Certification Committee.

Robert M. Wham, L. Kevin Felker, Walter Bond, Dennis E. Benker, R. G. Stacy, Fred R. Chattin, and **Rodney W. Brewer** have received a DOE Waste Minimization Award for their work on the Off Gas Caustic Scrubber System Evaluation.

David R. Mullins has been elected president of the Tennessee Valley Chapter of the American Vacuum Society

Thomas J. Wilbanks has been elected chairman of the U.S. National Committee for the International Geographic Union.

Al Geist and **Jack J. Dongarra** have received the Best Heterogeneous Computing Distribution Award in the Heterogeneous Computing Challenge at Supercomputing Conference '92.

Wilbert D. Minter has been elected vice president of the National League of Cities–National Black Caucus/Local Elected Officials.

Virginia H. Dale has been named to the U.S. Environmental Protection Agency's Science Advisory Board.

Robin L. Graham has been named chairperson of the Center for Forest Environmental Studies' Technical Steering Committee and has also been selected to serve on the review panel of the U.S. Department of Agriculture's Forest/Rangeland/Crop Ecosystem Competitive Grants Panel.

Anne M. Hoylman, N. T. Edwards, and **Barbara T. Walton** have received the Society of Environmental Toxicology and Chemistry's Best Student Poster Award.

Robert I. Van Hook received a Certificate for Commitment to Education from former U.S. Secretary of Energy James Watkins.

Richard B. Gammage and **Barry Berven** are co-editors of the book *Hazardous Waste Site Investigations: Toward Better Decisions.*

Robert E. Uhrig has received the Glenn Murphy Award for Outstanding Teaching in Nuclear Engineering from the American Society for Engineering Education.

Robert J. Lauf has received an Award for Excellence in Technology Transfer from the Federal Laboratory Consortium.

Donna S. Griffith, Marilyn A. Brown, Teresa McGeorge, Louise B. Dunlap, Amanda Renshaw, and **Yvonne Horton** have received Tribute to Women Awards from the Knoxville YWCA.

Steve DeGangi has been named director of the Energy Systems Chapter of the National Management Association.

James S. Bogard has been named to the Laboratory Accreditation Policy Committee of the Health Physics Society.

Jennifer D. Taylor has been named to the Human Resources Issues Special Interest Group Steering Committee of DOE's Training Resources and Data Exchange (TRADE).

Robert Hatcher

Patricia Hu

Kimiko Bowman

Michael Ramsey

T. R. Curlee

Thomas Wilbanks

H. Chet Thornton, Jr., has received an Environmental Award from the Inventors Clubs of America for his work on the Cl_2EAN OUT Project to remove chlorine from wastewater.

Sybil T. Wyatt and **Cindy S. Robinson** have received an Honorable Mention award in the National Association of Government Communicators' 1992 Blue Pencil Awards competition.

Carl A. Burtis, Wayne Johnson, and **William Walker** have received an Advanced Technology Award from the Inventors Clubs of America for developing the blood rotor.

George E. Wrenn, Jr., Cressie E. Holcombe, Jr., and **John Lewis, Jr.,** have received an Advanced Technology Award from the Inventors Clubs of America for their work on ZZX-4200 Thermal insulation structures.

Alston E. Hodge has been appointed manager of the Capital Assets Planning Department of the Office of Planning and Management. He succeeds **Steve McNeany** who has taken a position in the Engineering Technology Division.

Colin West, project director for the Advanced Neutron Source proposed for ORNL, has been named an editor of the *Journal of Neutron Research,* a new international publication.

John McCarthy has received the 1992 American Geophysical Union Editors' Citation for Excellence in Refereeing Technical Papers.

N. E. Korte has been appointed to serve on two committees of the Arizona/Nevada Academy of Science, the High School Grant-In-Aid Committee, and the Outstanding Science Teacher Award Committee.

The following ORNL researchers were honored for receiving patents for their innovative developments: **Raymond E. Garvey** (first patent), **Edmund T. Grostick** (first patent), **Jack Watson, Vinod K. Sikka, Quirinus G. Grindstaff, Robert L. Shepard, Theron V. Blalock, Michael Roberts** (first patent), **Lonnie C. Maxey** (first patent), **Charles W. Forsberg, Harold D. Kimrey, Jr., Mark A. Janney, Mattison K. Ferber, Chain T. Liu, Cressie E. Holcombe, Norman L. Dykes, Roeland Feenstra, Lynn A. Boatner, Roger W. Anderson, Wayne Neff** (first patent), **Robert Hawsey, Milton Bailey, Carlos E. Bamberger, Michael T. Harris, Timothy C. Scott, Charles Byers, Louis K. Mansur** (first patent), **Eal H. Lee** (first patent), **Lawrence S. Hawk, Joe H. Turner** (first patent), **Mark A. Janney** (fifth patent), **Ogbemi O. Omatete, Stephanie A. McElhaney** (first patent), **Martin Bauer, Marion M. Chiles** (first patent), **Cressie E. Holcombe, Norman L. Dykes, Djula Eres** (first patent), **Douglas H. Lowndes** (first patent), **Hyoun-Ee Kim** (first patent), **Arthur Moorhead** (fifth patent), **Carl A. Burtis, Wayne Johnson,** and **William Walker** (fifth patent).

Six senior managers at ORNL were recognized for their leadership and commitment to ORNL Equal Employment Opportunity/Affirmative Action goals: **Richard Genung, Amanda Renshaw, Shirley Shugart, David Reichle, Hal Glovier,** and **Bob Van Hook.**

J. E. Nyquist, W. E. Doll, R. K. Davis, and **R. A. Hopkins** won an award for the best paper at the 1992 Symposium for the Application of Geophysics to Environmental and Engineering Problems.

Liane B. Russell has received the 1993 Environmental Mutagen Society Award for her research contributions in environmental mutagenesis.

Monica G. Turner served on the Terrestrial Ecology Technical Panel of the National Aeronautics and Space Administration.

Isidor Sauers has been elected a senior member of the Institute of Electrical and Electronics Engineers.

Marcy Espergen has been asked to serve on the Mesa State College committee organizing this year's "Expanding Your Horizons" conference, which is designed to increase awareness of career opportunities for women in mathematics and science.

Energy Systems entries received three awards in the 1993 International Technical Publications Competition of the Society for Technical Communication (STC). **Jim Pearce, Carolyn Krause, Mike Aaron,** and **Vickie Conner** received an award of distinction in the category of trade/news articles for "Covering All the Bases: ORNL Probes the Human Genome," which appeared in the *ORNL Review;* **Daniel Schaffer** and **David J. Feldman** received an award of merit in the category of whole periodicals for *Forum for Applied Research and Public Policy;* and **Martha Stewart** and **Brendlyn D. Faison** received an award of achievement in the category of scholarly/professional articles for "The Chemistry of Low-Rank Coal and Its Relationship to the Biochemical Mechanisms of Coal Biotransformation," which appeared in the book *Microbial Transformations of Low-Ranked Coals.*

Numerous ORNL publications won awards in the Technical Publications and Art Competition sponsored by STC's East Tennessee Chapter. In newsletters, an award of merit was given to **Bill Cabage, Ralph W. Sharpe,** and the **Office of Planning and Management;** in newsletters, award of achievement, **Frederick M. O'Hara, Jr., Frederick W. Stoss,** and **Marvin Dickerson;** in organization manuals, award of merit, **Mickie McBee** and **Judy E. Kibbe;** award of achievement, **Laura J. Morris, Gay Marie Logsdon,** and **Balie M. Ross;** in house organs, award of excellence, **Carolyn Krause, Jim Pearce,** and **Vickie Conner;** award of achievement, **Judy M. Wyrick, Gloria M. Caton,** and the **Ceramic Technology Project Staff;** award of achievement, **Gloria Caton, Tim G. Elledge,** and **Marilyn Langston;** in periodic activity reports, award of excellence, **Edward L. Hillsman, Deborah P. Stevens,** the **Publications Division,** and **Martin Marietta Energy Systems, Inc.;** in periodic activity reports, award of merit, **Amanda Renshaw, Walter Koncinski, Jr.,** and **Elizabeth S. Martin;** award of merit, **Anne Adamson, Judy M. Wyrick,** and **Denise Casey;** in whole periodicals, award of excellence, **Daniel Schaffer** and **David Feldman;** in whole periodicals, award of achievement, **Marvel D. Burtis, Robert M. Cushman,** and **Frederick W. Stoss;** award of achievement, **Linda M. Houlberg, G. Todd Hawkins,** and **Marti S. Salk;** in scholarly/professional articles, award of distinction, **Martha Stewart** and **Brendlyn D. Faison;** award of excellence, **Donna R. Reichle** and **Brendlyn D. Faison;** award of achievement, **Patrick J. Mulholland** and **Curtis R. Olsen;** award of achievement, **Janet M. Strong-Gunderson, Richard E. Lee, Jr.,** and **Marcia R. Lee;** in trade/news articles. award of distinction, **Jim Pearce, Carolyn Krause, Mike Aaron,** and **Vickie Conner;** award of excellence,


Colin West


Liane B. Russell


Robert J. Lauf

Carolyn Krause, Mike Aaron, and **Vickie Conner;** award of merit, **Charles C. Coutant;** award of merit, **Carolyn Krause, Mike Aaron,** and **Vickie Conner;** award of achievement, **Jim Pearce, Carolyn Krause,** and **Vickie Conner;** in books, award of excellence, **S. Marshall Adams, C. T. Hackney,** and **W. H. Martin;** award of merit, **Donald L. DeAngelis** and **Louis Gross;** award of achievement, **Denise Casey, Judy M. Wyrick,** and the **Human Genome Management Information Staff;** in technical reports, award of merit, **Pete Lotts, Gordon Michaels,** and **Kathryn H. King-Jones;** award of merit, **Thomas A. Boden, Robert J. Sepanski,** and **Frederick W. Stoss;** in mechanical illustration, line art, black and white, award of excellence, **Mark Robbins** and **David Cottrell;** award of excellence, **Mark Robbins** and **David Cottrell;** in interpretive illustration, line art, color, award of achievement, **Dami Rich** and **Mitchell Williamson;** in design graphics, covers, color, excellence, **Elizabeth Martin;** in design graphics, posters, award of distinction, **Vickie Conner,** the **ORNL Values Committee,** and the **ORNL Health Division;** award of merit, **Vickie Conner** and the **ORNL Values Committee;** in design graphics, presentations, award of achievement, **Jamie Payne** and **Donna Griffith;** in design graphics, exhibits/displays, award of merit, **Richard Booker, Mitchell Williamson,** and **Dami Rich.**

On Letting Computers Make Decisions

By Alan Solomon

Human decision making is traditionally intuitive and based largely on experience and expertise. Normally, this process requires both qualitative and numerical data, but in the end, intuitive feelings about a dilemma lead to the decision. Many theories try to explore the nature of this intuitive process, but at this point all we know is that it normally works!

At first glance, computer decision making is much simpler to understand, because it is based wholly on numerical criteria. When should a stock be sold? When the current price falls below a particular value. When is a contaminated soil site undergoing remediation considered clean? When all the sensors at the site report levels of contaminant below a certain critical value. When should an alarm system go off? When the temperature exceeds a certain value. However, the stock decline may be a result of a general decline in prices; the recorded sensor values, although low, may result from seepage of hazardous material to the bottom of the aquifer from whence it will slowly pollute the water in the future; and the temperature may have been sensed exactly when someone was lighting a cigar. Generally speaking, making a computer "smart" is a nontrivial task because we must be able to foresee such possibilities as the need to account for other stock prices, dense contaminants, and cigar smoking and somehow make the computer take these factors into account.

Automated decision making is a process of determining and carrying out an act in response to a given input; the determination is made among many responses to inputs that may vary substantially. The actual input will normally be a string of numbers. The key component of such a process is the mathematical algorithm that must determine what to do in response to the input. Some common problems facing the algorithm writer are the following:

a. How do we measure the input string to determine our response?
b. How do we determine whether the chosen response corresponds to what we intuitively wish to happen?
c. How do we take noise and uncertainty into account?
d. How do we make use of other possibly non-numerical and sometimes subjective information in our decision-making process?
e. How do we take into account contradictory sensory input and still reach a decision on what to do?

The first problem is related to the classic question, "How big is big?" It suggests the need to define a size estimate or "norm" for our inputs.

The solution to problem b is often the most difficult to determine. Commonly, automated decision systems are developed to meet problems arising in emergencies, for which actual tests are not possible (e.g., explosions or fires). To address this point, detailed simulations of the system of interest must be combined, if possible, with extensive human input.

Automated decision making is a process of determining and carrying out an act in response to a given input.

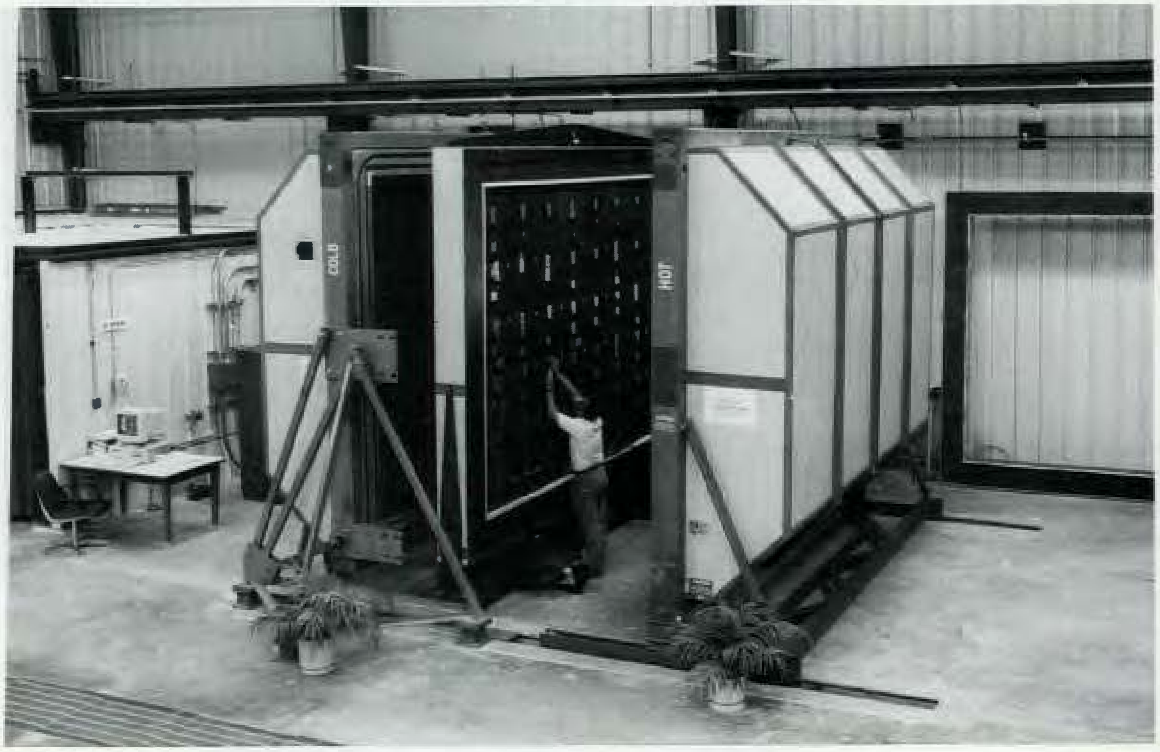
The noise and uncertainty of problem c are constant companions to all systems. The combined effect of all things that are either of unknown form or origin or arise from known effects can be regarded as noise. It is generally treated by tools of probability. Uncertainty refers to varying degrees of belief about various features of a process. For example, given a variety of sensors for measuring temperature at a point, measurement by one sensor may be believed more accurate than that by another. The actual belief can be assigned using the tools of fuzzy analysis in which numerical estimates of belief are blended with our expertise.

Problems d and e are probably the key difficulties of artificial intelligence today. To deal with d, we develop "expert systems" in which the rules to be followed, such as when to sell stocks, are implemented in accordance with the advice of an expert in the field. Problem e arises when two experts give opposing opinions about what is going on or what policy is to be followed. Although criteria abound for reaching decisions based on multiple sources of information, the area is still at the stage of basic research and trial.

Considering the exponential growth of computing power, it seems certain that number and logic "crunching" will be less of a source of computing difficulties. But it is equally clear that, as we turn to the computer to make decisions in real time, we will have little choice but to confront the problems raised here and to develop new mathematical tools to deal with them.

ORNL's Building Envelope Research Center: Fighting the Other Cold War

Our job is to work with private industry to make building components more energy-efficient.



Research engineer Andre Desjarlais adjusts a sensor mounted on a wall section in BERC's Rotatable Climate Simulator. The simulator can determine the effect of a range of weather conditions on the insulating abilities of walls, floors, doors, and windows.

Is the Cold War really over? Well, yes and no.

Centuries before Nikita Khruschev's pounding shoe became a tool of international diplomacy and a symbol of the icy staredown between the United States and the Soviet Union, another kind of cold war was being waged—every winter, by people trying to build shelters that would keep the cold out and the heat in.

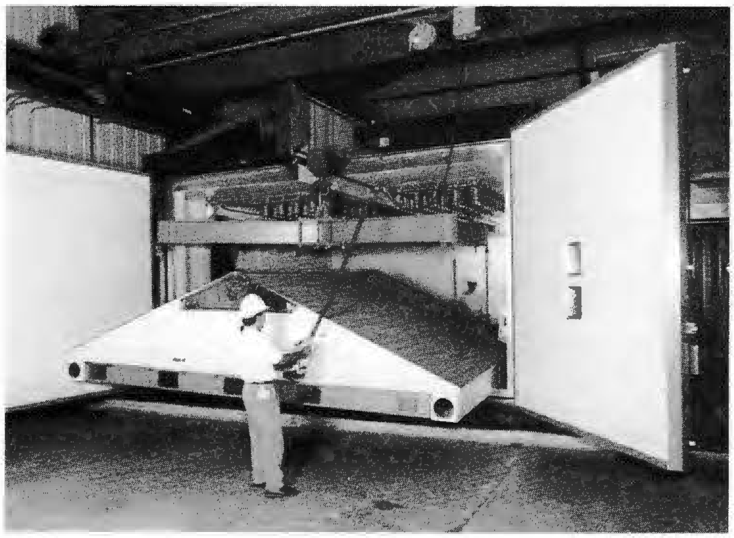
At ORNL's Building Envelope Research Center (BERC), modern-day cold warriors carry on the struggle using high-tech analytical tools. Formerly known as the Roof Research Center, BERC is the result of a cooperative effort between government agencies and private industry to develop more efficient and environmentally friendly techniques for constructing both residential and commercial buildings.

The center's new, vise-like Rotatable Climate Simulator clearly illustrates the center's research mission. Stenciled letters identify one side as HOT and the other as COLD. In between is a removable wall section, studded with temperature sensors. Determining how well walls and other building components keep the HOT side hot and the COLD side cold is the primary focus of research at the center.

As the center's name implies, BERC scientists study building envelopes—foundations, walls, windows, and roofs. "Our job," says BERC director Jeff Christian, "is to work with private industry to make building components more energy efficient. Our vision is to be the world's foremost center of excellence in the development of globally competitive building envelope technologies—already, a third of our staff is made up of visiting researchers, from both the United States and abroad."

BERC's research efforts are concentrated around four specially designed test facilities.

Large-Scale Climate Simulator (LSCS). The performance of a roof system depends on a number of factors, including temperature, humidity, and exposure to the sun. Rather than sitting on a roof until the right weather came along, BERC researchers developed the LSCS. This test facility allows roof systems up to 4 meters (13 feet) square to be exposed to any combination of temperature, moisture, or sun conditions on earth.



Factors that affect roof performance—temperature, humidity, and exposure to the sun—can all be simulated in BERC's Large-Scale Climate Simulator.

If changes can be made in overhead insulation, overall heat loss through residential ceilings in cold climates could be reduced by as much as 20%.

Using the LSCS, ORNL researchers working with Energy Saving Solutions, Inc., a private insulation manufacturer, determined that, under cold winter conditions, up to 50% of the heat loss through attics insulated with some types of low-density, loose-fill fiberglass is a result of convection—warm air circulating through the insulation.

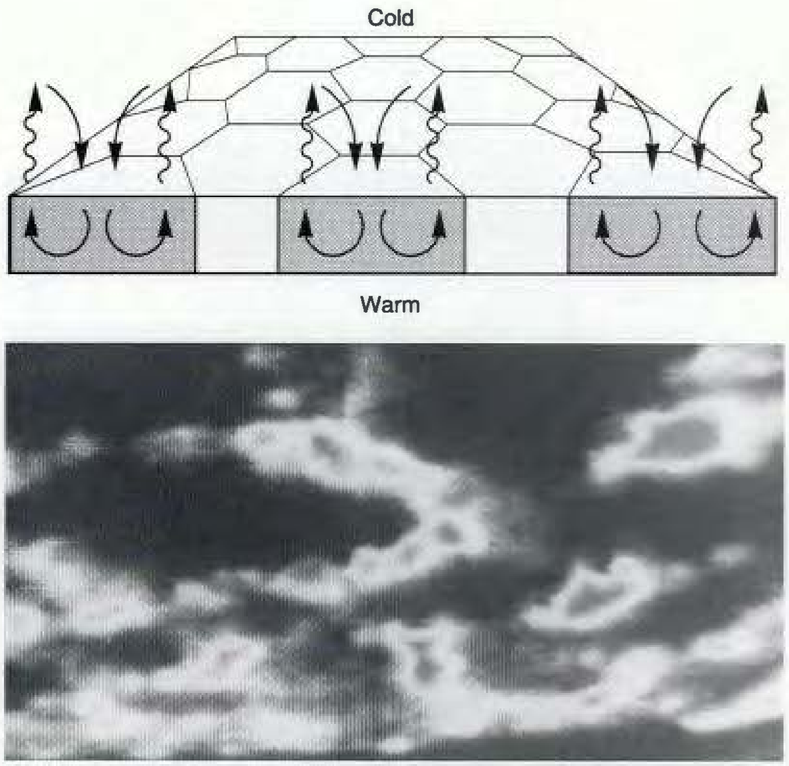
Researchers confirmed the presence of this convection cycle by analyzing infrared photographs of the top surface of various types of attic insulation. Infrared photos of low-density, loose-fill fiberglass attic insulation showed a pattern of six-sided hot and cold areas that is characteristic of convection heat loss. This evidence, combined with direct measurements of ceiling heat loss in the LSCS, led researchers to question the effectiveness of some common types of blown-in fiberglass insulation in very cold weather.

To help solve this problem, BERC worked with Energy Saving Solutions to evaluate the effectiveness of different insulation covering systems designed to reduce convection-related heat losses. Building on this research, Energy Saving Solutions developed a way of wrapping fiberglass batts in plastic bags that can be laid on top of existing insulation. The bags are designed to "breathe," allowing moisture to pass through the insulation while eliminating nearly all heat losses caused by convection.

Researchers estimate that, if changes can be made in overhead insulation to completely eliminate convection, overall heat loss through residential ceilings in cold climates could be reduced by as much as 20%. These findings have already had an effect on state building codes. Recently, Minnesota authorities beefed up their code to require that manufacturer claims of insulation performance hold up even in the coldest expected weather. This collaborative effort earned BERC a 1992 "Best of What's New" award from *Popular Science* for significant achievement in science and technology, one of only ten in the building products category.

The unique capabilities of the LSCS have also enabled researchers to determine that small amounts of moisture trapped in the insulation of flat, commercial-type roofs like those found on many schools, factories, and shopping malls, can seriously damage their performance. "Trapped moisture is a big problem with flat roofs," says Christian. "That's why we are developing a guidebook to help building owners decide

Environmentally friendly foam insulation manufactured without ozone-destroying CFCs is one of many products being tested at the center.



Using the Large-scale Climate Simulator, researchers determined that convection—warm air circulating through insulation—can account for up to 50% of attic heat loss under cold winter conditions. The diagram (above) and infrared photograph (below) of the top surface of attic insulation show a pattern of six-sided hot and cold areas that is typical of convection heat loss.

whether to replace or re-cover their roofs." The decision to replace old roofs can be further complicated by growing restrictions on disposal of used roofing materials, particularly those containing asbestos.

Currently, the facility is being used to test the moisture absorbency and drying rates of five different commercially available roof sections, with the goal of developing faster-drying, more durable roofing material. "The key to solving this problem," Christian says, "is to provide a way for water vapor to exit the roof."

To help improve the performance of flat roofs, ORNL and Dow Corning, Inc., are collaborating to demonstrate reroofing techniques that trap little or no moisture. Experimental roofing systems will be installed on the ORNL cafeteria and on Building 2518 later this year. Heat transfer data will be collected before and after the roofs are installed to measure their effect on the energy efficiency of the buildings.

Roof Thermal Research Apparatus (RTRA). For lower-cost field testing of flat roofing sections, BERC researchers rely on the RTRA. This climate-controlled facility actually serves three purposes. Its removable roofing sections allow roof system samples as small as 1.2 meters (4 feet) square to be tested, and the facility's walls are equipped with four test frames for studying the thermal performance of exterior, aboveground masonry walls. Two test areas for study of slab-on-grade, or ground-level, foundation insulation are also available.

Data on up to 14 test systems can be collected simultaneously at the facility and can be integrated with data from the complete weather station at the site.

The RTRA roof is now being used to determine the long-term performance of coatings designed to save energy by keeping the surface of the roof cooler than a typical black roof by reflecting sunlight rather than absorbing it.

Envelope Systems Research Apparatus (ESRA). The construction and operation of the ESRA is a result of unprecedented cooperative research and development agreements (CRADAs) among DOE, the Environmental Protection Agency, and several private companies. The information gathered from this joint effort has been so rewarding for its industrial partners that they recently extended their participation in the project for three more years and doubled their financial support of the facility.

Like the RTRA, the larger ESRA can be used for both roof and foundation studies. Up to 40 different roof sections can be tested at once on this facility. Its current roof is made up of several common roofing systems that are insulated with experimental polyisocyanurate foam. This common type of insulation is usually manufactured using chlorofluorocarbons (CFCs), chemicals that also break down the protective layer of ozone in the earth's stratosphere, but the experimental materials are CFC-free. Research being conducted at ESRA on this new insulation will thoroughly document its performance, contributing to the successful marketing of this more environmentally acceptable product.

Because the facility's foundation is covered with "designer dirt," soil with uniform and known properties, it is ideal for conducting studies of heat and humidity transfer from residential or small commercial foundations to the surrounding soil. Results of this research are being used to validate the computer models used to develop the national building code standards for foundation insulation. Several builder handbooks have also been developed from these models.

Andre Desjarlais can choose from a range of weather conditions when programming the Rotatable Climate Simulator.

BERC has been active in development of the standard for energy-efficient design of new low-rise residential buildings.

Rotatable Climate Simulator (RCS). Donated to ORNL by Dow Chemical Corporation, the RCS is the newest addition to BERC's cold-war arsenal and has been upgraded by BERC researchers to provide state-of-the-art analyses of walls, floors, doors, and windows. "Getting the RCS operational required assembling a large in-house team from four ORNL divisions, including Instrumentation and Controls, Plant and Equipment, Engineering, and Energy," says Christian. "This experience was good for building the cooperation and internal teamwork that will be needed to maintain and extend this facility's capacity."

The RCS can accommodate wall, floor, or roof sections up to 4 meters by 3 meters (13 feet by 10 feet), including masonry walls, and it can simulate almost any combination of temperature, air pressure, and wind. It also meets or exceeds American Society for Testing and Materials requirements for this kind of test facility.

Christian predicts that, within the next few years, manufacturers will be required to include thermal performance rating labels on windows, doors, skylights, and, eventually, prefabricated wall sections. "As more and more engineered building components come on the market," he adds, "we have to position ourselves to be a major player in the area of factory-produced housing."

The center is already playing a major role in many areas. For example, BERC has been active in development of the American Society of Heating and Refrigeration Engineers' standard for energy-efficient design of new low-rise residential buildings. When completed, this standard will replace an earlier version that has been adopted in 45 of the 50 states.

Most recently, BERC researchers and their counterparts in the Energy Division have launched a new cold-war offensive by establishing the Building Technology Center. Expected to begin operations later this year, the center will be made up of BERC and several Energy Division groups that are developing and implementing state-of-the-art heating and cooling technologies for new and existing buildings.
—Jim Pearce

Take the OREN Exit to the Information Highway

The Oak Ridge Educational Network opens a world of information resources to students and teachers.

OREN helps schools tap into the Internet, a global network of data bases, libraries, and electronic mail services.

Thanks to the marriage of fiber-optic cable and state-of-the-art computer technology, the nation's "information highway" is beginning to take shape. As a result, data bases and other educational resources that were once available only to a select few are increasingly accessible to anyone with a phone line and a personal computer.

Still, getting out on the highway and driving can be pretty daunting. Most of what you hear about the information highway is pretty heady stuff—university researchers trading data with scientists at national laboratories and pint-size computer wizards using supercomputers to plot the orbits of the moons of Jupiter. You can just imagine these guys tooling down the information highway in their Ferraris. That's great for them, but what about the regular folks who want to get out on the highway in their Chevettes and Pintos?

That's where the Oak Ridge Educational Network, or OREN, comes in. OREN helps schools use old or donated computer equipment to tap into a part of the highway called the Internet, an international network of data bases, libraries, and electronic mail services, without running up a Ferrari-sized tab. "There are other programs that aim at high-performance computing or at schools with established programs and lots of equipment," says OREN administrator, John Wooten, a physicist in ORNL's Office of Science and External Relations. "We aim at schools in the counties around Oak Ridge that need basic access to information. We help them set up a network with whatever computers they have to start with. We also give advice on wiring, networks, software, and electronic communication standards, so they can expand their system when they're ready."

Richard Hicks introduces students to the nCube computer. The Adventures in Supercomputing program enables students to access ORNL's computing resources from their schools through the Internet.

Laboratory research and development programs benefit as well from the increased visibility offered by the network.

Once the system is installed, both students and teachers discover there is a world of electronic information literally at their fingertips. Students mostly use the system to explore. There are all sorts of things on the Internet—health and science information, movie reviews, college catalogs. "The age of the student has a lot to do with what they are drawn to," Wooten says. "Once the kids get used to the system, they begin thinking how things could work better and some of them get interested in programming. We encourage that and try to locate local mentors to support and encourage their interests."

Teachers often use the system to communicate with scientists and other teachers across the country and throughout the world to locate materials for their classrooms. The ability to do this kind of research on-line helps these teachers make the most out of limited resources. Complete courses are available on-line from the National Aeronautics and Space Administration, the Library of Congress, and the U.S. Department of Education, among others.

This no-frills approach to computing has gained more than 1200 users among resource-hungry students and educators alike. "We try to recruit people to become agents of change in their classes and schools," says Wooten. "Then they go and get others involved."

OREN users aren't the only beneficiaries of the network. Laboratory research and development programs benefit as well from the increased visibility offered by the network. "As people begin to use the indexing services on the network," says Wooten, "they begin to use ORNL resources. We have a lot of resources available for distribution that the public isn't aware of."

For example, ORNL, along with Vanderbilt University and Argonne National Laboratory are developing the "Ask a Scientist" program, which

OREN has also been asked by the National Academy of Sciences to provide network access for all of the Presidential Awardees—outstanding teachers from all 50 states.

allows teachers or students to use the network to request information on things like the effects of global warming. When a request is received, a researcher at the Laboratory or one of the other institutions provides an answer via the network.

Similarly, ORNL's Engineering Physics and Mathematics Division offers a service called Netlib. Netlib is a data base of mathematical routines students and teachers can access through the network to perform a variety of time-consuming functions, such as inverting a matrix. This service has been around for years but has become much more popular since it has been accessible through the Internet.

OREN has also been asked by the National Academy of Sciences to provide network access for all of the Presidential Awardees—outstanding teachers from all 50 states. OREN will provide these educators with a way to interact with their peers nationwide and share some of their award-winning insights.

Wooten sees OREN as a winning proposition for ORNL, its community, and the system's users. "It allows the Lab to be both a good citizen and a source of information," he says. "One of the functions of a national laboratory is to support and inform the community around it," he says. "If you don't get the word out, you're not doing a lot of good."—*Jim Pearce*

"Adventures in Supercomputing" Program Takes Off

Six Tennessee high schools will participate in DOE's "Adventures in Supercomputing" (AiS) program at ORNL. Twenty-five high schools from across the state applied for spots in the two-year-old program, which is offered by ORNL, Ames Laboratory, and Sandia National Laboratories.

Today, many public schools still have little or no access to computers. The AiS program provides students with first-rate computing systems and networks at no cost to the school.

Each selected school will receive a free, open-ended DOE loan of four Apple Macintosh computers, software tools, a color printer, curriculum materials, and continuing support from technical consultants. Students will have access to federal laboratory supercomputers through the Internet communications network. This service, program coordinators say, will encourage development of essential skills for high-tech research in the future.

"Increasingly, science is advanced by use of computer simulations and other computational science techniques," says Richard Hicks, AiS coordinator for ORNL. Because computer models can save considerable time and money and are inherently safe, they benefit nearly every branch of science.

Barbara Summers, who teaches chemistry, calculus, and computer programming at Central High School in Wartburg, said AiS has revitalized her students' interest in math and science. "It has literally been a springboard for taking our school into the world of high technology. Before we got into the program, we didn't have many kids with a driving interest in math and science. Now, the computer lab is full constantly," she said. Her students' research projects range from design of better materials for spacecraft to environmental cleanup technologies.

In June, a team of two teachers from each selected Tennessee high school attended a two-and-a-half-week summer institute at ORNL, where they were shown how to set up their classroom workstations and were trained in programming, networking, and the basic concepts of high-performance computing.

Selection of schools is based on their ability to fulfill the program's goal of reaching women, minority, and disadvantaged students and to provide two highly motivated teachers. "This program," Hicks says, "not only addresses the issue of improving overall technical literacy but also seeks to expand the pool of students who seriously consider scientific careers."

Summers says she's convinced the program is already steering students in that direction. "Our school doesn't start until 8:45, but we have kids showing up at 7:30 just to get on the computers," she said.

"It's so exciting to see where we are now, compared with where we were before the program started here."—*Wayne Scarbrough and Karen Bowdle*

RE: R&D Updates

Unearthing Buckyballs

The first evidence that fullerenes occur naturally on the earth came to light when researchers examined a sample of shiny black rock from Russia.

Bob Hettich uses a soccer ball to illustrate the unusual structure of buckyballs. The small vials below the ball contain meteorite samples Hettich has analyzed in search of these puzzling carbon clusters.

At first they were considered laboratory-created freaks. Then some of them turned up in outer space. Now they're being sent to ORNL from the frozen reaches of northern Russia. What's going on here?

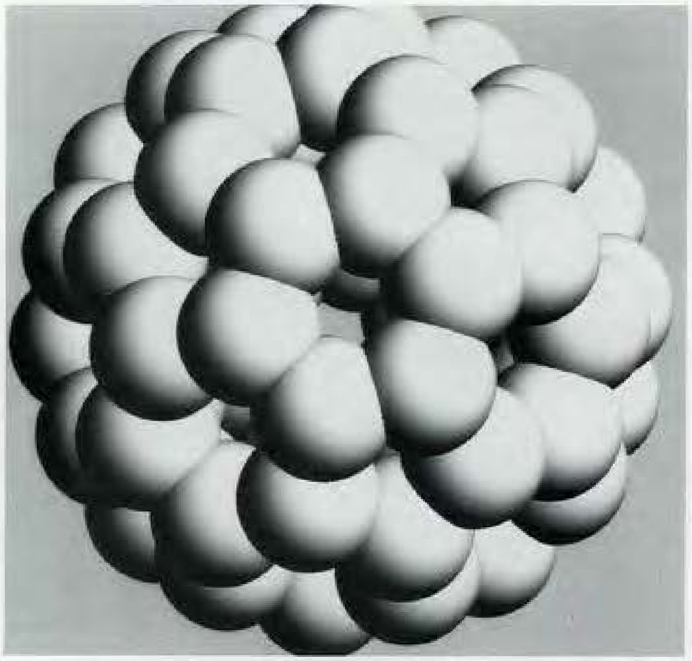
ORNL's Bob Hettich was on the case. He analyzed. He checked. He double checked. His conclusion? "Buckyballs. Definitely buckyballs."

These enigmatic clusters of carbon atoms have been puzzling scientists since 1985 when they were discovered in a research laboratory among the by-products of laser-vaporized graphite. Their hollow spherical structure, reminiscent of the geodesic domes of eccentric architect Buckminster Fuller, earned them the names "buckyballs" and "fullerenes."

Qualities, such as their unique structure, heat resistance, and electrical conductivity, have fueled speculation about their possible applications in high-temperature lubricants, microfilters, more efficient semiconductors, and manufacturing processes.

To learn more about buckyballs and how they are formed, researchers began to look for naturally occurring fullerenes, particularly on the earth. The first evidence that fullerenes occur naturally on the earth came to light when Arizona State University researchers Semeon Tsipursky and Peter Buseck examined a sample of shiny

Hettich's analysis confirmed the presence of fullerenes in the rock.



Researchers have found that buckyballs can occur as roughly spherical clusters of from 20 to over 500 carbon atoms.

black rock, known as shungite, from northeastern Russia. Shungite is a rare, carbon-rich variety of rock believed to have been formed between 600 million and 4 billion years ago, although *how* it was formed is debatable. Electron microscopy of the shungite samples revealed a pattern of white circles with black centers—similar to micrographs Tsipursky had seen of laboratory-produced fullerenes.

To confirm their suspicions, Buseck and Tsipursky sent a trace of powdered rock between two glass slides to Bob Hettich of ORNL's Analytical Chemistry Division for examination by mass spectroscopy, a technique that sorts molecules by weight and electric charge. Hettich had previously worked with Buseck to analyze samples from both meteorites and terrestrial rocks for evidence of fullerenes, but they had found none. The shungite sample was different, however; Hettich's analysis confirmed the presence of fullerenes in the rock.

"We wanted to make sure we were looking at only what was in the sample and not distorting it in any way," says Hettich. So, he conducted two separate analyses of the sample. In the initial analysis, he used a pulsed laser to vaporize and ionize the sample, preparing it for analysis by mass spectroscopy. Hettich also analyzed carbon samples known not to contain fullerenes to ensure that none were being created by the laser vaporization process itself. The initial analysis confirmed the presence of both C_{60} and C_{70}, two common fullerenes, in the shungite sample.

To dispel any lingering doubt, Hettich repeated the analysis without a laser, this time using a 400°C stainless steel probe to vaporize the sample and introduce it into the mass spectrometer for ionization. This technique, known as thermal desorption, cannot create fullerenes in fullerene-free graphite material, yet it yielded identical results, confirming the presence of the two types of buckyballs in the sample.

When Buseck and Tsipursky told Hettich that the rock had come from Russia and not a meteorite, he was somewhat surprised. "In the laboratory," says Hettich, "fullerenes are created in an atmosphere of inert gases, like helium, because common diatomic gases, like nitrogen and oxygen inhibit fullerene growth. This is why fullerenes are not found in ordinary soot, like that in household fireplaces. It seemed more likely to find naturally occurring fullerenes in meteorites, where interaction with these gases would be less of a problem."

The discovery of fullerenes in the shungite sample has provided some hard information for buckyball hunters who have been working mostly on educated guesses and speculation. "We've been working with Peter Buseck for quite a while analyzing various samples, but until now we hadn't found any fullerenes," Hettich notes, "This discovery helps us redefine where to look." More recently, C_{60} and C_{70} have also been found in a sample of glassy rock from the mountains of Colorado. Known as a fulgurite, this type of rock structure is formed when lightning strikes the ground. Busek, Tsipursky, and Hettich speculated in a 1992 paper that lightning strikes could provide conditions that are favorable for the formation of buckyballs.

The shungite fullerenes are notable not only for their earthly origin, but also because they may have been formed as solids—most laboratory-created fullerenes are grown in the gas phase. "This is the first example of solid-phase fullerene growth," says Hettich, "It has raised a lot of questions about how the rock was formed, how old it is, and how its composition may have changed over time. Because the shungite sample may be volcanic in origin, you can imagine conditions, like those in a volcano, that would be hot enough to form fullerenes and, at the same time, have little or no oxygen or nitrogen present. But right now, no one is sure exactly how these fullerenes were produced."

"This kind of discovery raises more questions than it answers," says Hettich, "but that's not necessarily a bad thing."—*Jim Pearce*

Sizing Up Fullerenes—*"SANS Doute"*

"Sans doute!" a confident Frenchman might say—"without a doubt!" But in the brand new world of fullerenes, this sort of certainty is sometimes in short supply. Much of the uncertainty surrounding these newly discovered carbon clusters stems from their size—you could line up 25 million C_{60} molecules on a ruler before passing the inch mark.

So, although tools like mass spectrometers can be used to distinguish heavier fullerenes from lighter ones—separating C_{120} from C_{180}, for instance—researchers still have trouble answering some of the most basic questions about them. How big are they? Are they shaped like spheres, dumbbells, or what? How and where do other atoms bond to their inner and outer surfaces?

Using a time-tested analysis technique of small-angle neutron scattering, appropriately labeled SANS, a team of researchers from ORNL's Biology, Chemical Technology, Health Sciences Research, and Solid State divisions is working to dispel some of the mystery surrounding fullerenes, including how they interact and bond with other elements and with each other.

The preferred method of studying the structure of most materials is crystallography. This technique enables researchers to pinpoint the location of every atom in a sample. "Even though C_{60} has been crystallized, this is not always possible with other materials," says Stephen Henderson of ORNL's Biology Division. "Other techniques, like SANS, are more accessible, though they give less structural information." SANS requires only that the material be dissolved, rather than crystallized; then scattered neutrons are counted for several hours and the data are analyzed.

The SANS research facility, located at ORNL's High Flux Isotope Reactor, is operated by George Wignall of the Solid State Division. There, dissolved fullerene samples are placed in the path of a neutron beam. As the beam passes through the sample, neutrons are deflected, or scattered, by carbon molecules in the solvent. This scattering is recorded by a detector, providing a two-dimensional pattern, or "signature," for the material, which can then be analyzed to determine the size and shape of the dissolved molecules. (See the back cover of this issue for a SANS-eye view of a solution of C_{60} molecules.)

"The greatest significance of using SANS to analyze fullerenes is its ability to discern shapes," says Bob Haufler, a postdoctoral fellow in the Health Sciences Research Division (HSRD). "This is clearly fertile ground for new chemistry. I think it will be especially helpful in situations where atoms of hydrogen or metals are attached to the inside of the fullerenes." "It's also interesting to see how the fullerenes interact with the solvents," says Kathleen Affholter of the Solid State Division, "to see if polymers are forming, for example."

The SANS facility "sees" objects in its neutron beam by keeping track of the neutrons the objects scatter. This scattering varies with the square of an object's volume, so when its diameter decreases by half, it scatters only one-quarter as many neutrons. As a result, the smallest fullerenes are near the lower limit of what the SANS can see—a factor in the past reluctance of researchers to use SANS in this type of research.

Much of the uncertainty surrounding these newly discovered carbon clusters is due to their size.

"The greatest significance of using SANS to analyze fullerenes is its ability to discern shapes."

Even though the outcome was in doubt, Wignall encouraged Affholter and others to pursue the project because the potential scientific payoff was so high. "If it hadn't been for George," Affholter says, "the project wouldn't have started in the first place." When Affholter introduced the idea of using the SANS facility for fullerene studies to Bob Compton of HSRD, he said his group was making some C_{120} and C_{180} molecules and they didn't know what they looked like—whether they were dumbbell-shaped or just bigger versions of the more or less round C_{60} and C_{70} balls. "We decided to look at the C_{60} and C_{70} balls first," says Affholter, "because they were available and their sizes and shapes were already known."

Because of the relatively small sizes of these fullerenes, the researchers sought to optimize several factors in the experiments. First, the distance the neutron beam traveled through the fullerene solution was increased from a typical 2 mm to 20 mm, increasing the likelihood of interactions between the fullerenes and the neutron beam. "As a result," says Henderson, "we got incredibly good statistics after an hour or so. Often, for solution work, differences are hard to see even after 10 hours of counting."

Second, the fullerenes were dissolved in a solvent that is relatively transparent to neutrons to maximize the contrast between the two. "A visual analogy," says Henderson, "would be observing blue balls in a transparent solvent, rather than in a blue solvent." Fortunately, the solvent that provided the best contrast also dissolved C_{60} and C_{70} most effectively, again putting more molecules in the path of the beam.

The team hopes to expand its work to include further explorations of the basic chemistry of buckyballs, including imaging fullerenes that have been combined with other elements, such as hydrogen, fluorine, and various metals. They expect to be able to determine how many and where these "piggyback" atoms are attached to the inner and outer surfaces of the fullerenes. They also expect to be able to produce and analyze larger fullerenes.

"It is difficult to get this kind of information from other techniques," Henderson says. "We also expect to be able to see whether these additional atoms have expanded the structure of the fullerenes. The actual mechanics and chemistry of adding other atoms to these molecules helps us understand how they react and combine with other elements. It could be that these materials—hydrogenated fullerenes, for instance—are better starting points for making other products."

"This project was an excellent example of cooperation among four research divisions," says Affholter. "Everybody had something to add to the project. Everybody talked and pulled together to make it work." The success of this group bodes well for the future of the informal collaboration. "We've gotten together to determine what we want to do next," Affholter says. "We like doing this kind of work, and if we don't do it, people at other labs will."

Sans doute!

Evaluating Stealthier Submarine Designs

Now that the "new world order" left in the wake of the Cold War has had a couple years to take shape, several trends are clear. One is that, despite predictions of a new prosperity and a peace dividend, conflicts, both ancient and new, continue to make the world a very dangerous place. Another more disturbing trend is that unfamiliar variables must be figured into the world's balance of power—an equation that had remained relatively unchanged for four decades.

Far from causing peace to break out across the world, the end of the Cold War and the collapse of the Soviet Union have actually *increased* the number of nations with access to sophisticated military hardware. In addition, the economic instability that accelerated the Communist bloc's demise continues unabated in its successor states, pressuring some of them to offer high-tech armaments to any government that can afford them.

Among the weapons finding their way into the burgeoning international arms market are submarines. For example, last November *The New York Times* reported deployment of a U.S. nuclear submarine in the Persian Gulf following Russia's

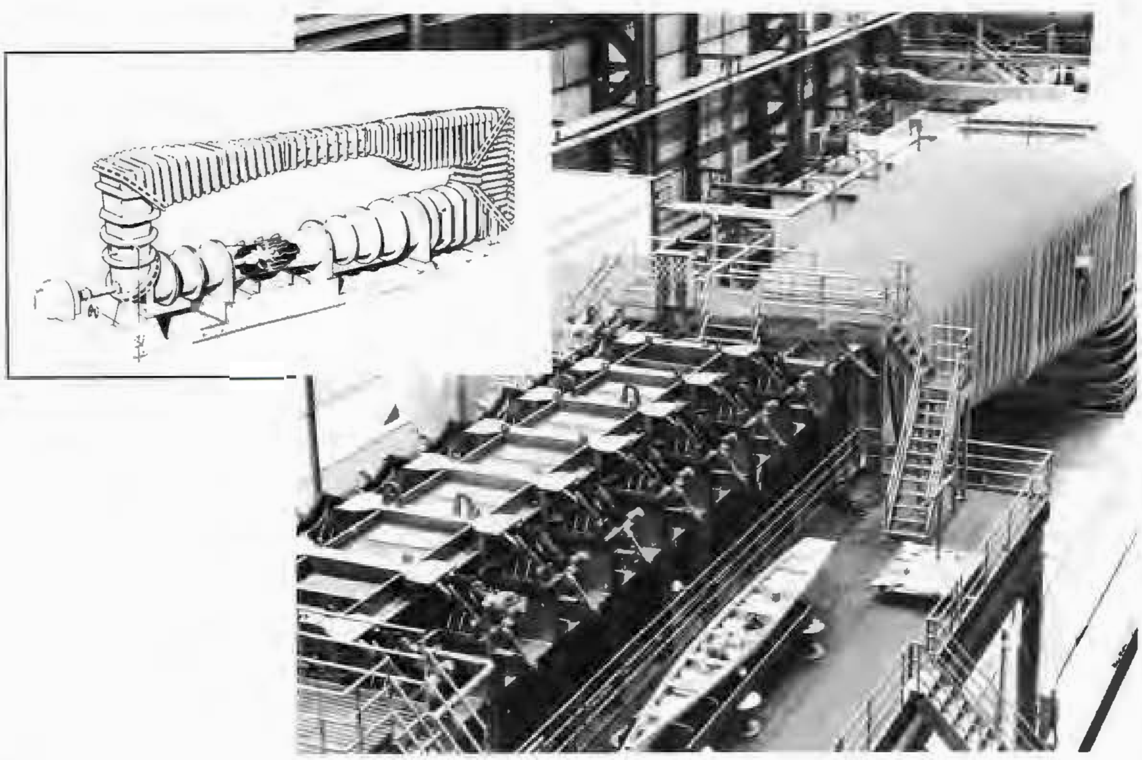
$600 million sale of three submarines to Iran. The deal went through despite U.S. objections, with the former Soviet republic citing its obligation to fill arms contracts and its need for hard cash.

The U.S. submarine deployment, ostensibly conducted to check out the sonic properties of the Gulf, highlights the importance of acoustic stealth to effective submarine operations. The obvious advantage a submarine has over a surface ship is its ability to travel, conduct surveillance, or initiate an attack without attracting the attention of other vessels. However, in recent years the technology used to detect sound underwater has improved dramatically, rendering older, noisier subs ineffective for many tasks and putting a premium on developing new "silent-running" ships.

Designing a submarine that can evade a state-of-the-art acoustic dragnet is no small trick, especially given the immense size of these ships. The pride of the U.S. fleet, the 171-meter-long (560-foot-long) Ohio class vessels, displace nearly 19,000 tons of seawater. Their counterparts in the former Soviet navy are the 171-meter-long Typhoon-class ships. These seagoing behemoths displace 25,500 tons of water, making them, by far, the largest underwater vessels ever built.

To ensure that U.S. submarines maintain the upper hand in these underwater games of cat and mouse, the U.S. Navy, with help from ORNL, has constructed the Large Cavitation Channel (LCC), the world's largest pressurized water tunnel, in Memphis, Tennessee.

The facility is named after the primary cause of submarine noise, cavitation. Cavitation occurs when a submarine's movement through the water creates air bubbles. When these bubbles collapse, they make noise—noise that may be detected by other vessels in the area.



U.S. Navy/David Taylor Research Center

To ensure that America's submarines maintain the upper hand in underwater games of cat and mouse, the U.S. Navy, with help from ORNL, has constructed the Large Cavitation Channel, the world's largest pressurized water tunnel.

Researchers use state-of-the-art computer to eavesdrop on the most minute sonic ripples emanating from scaled-down submarines.

The LCC provides a 91-meter-long (300-foot-long) model ocean that enables researchers to simulate underwater conditions like pressure, temperature, and current flow to test low-cavitation hull designs and other low-noise components in a realistic environment.

Because the LCC is located on dry ground, researchers can use state-of-the-art computers and acoustic sensing technology to eavesdrop on the most minute sonic ripples emanating from scaled-down submarines and components during underwater operations. The LCC's sophisticated instrumentation is largely a result of work done over the past seven years by ORNL's Real-Time Computing Systems Group working with researchers at the Navy's David Taylor Research Center in Bethesda, Maryland, and the Naval Sea Systems Command.

The product of this long-term joint effort is the Large Cavitation Channel Data Acquisition and Analysis System (LCCDAAS). By incorporating instrumentation that can be electronically steered to look at all aspects of a propeller, hull, or other component, this system is 5 times more sensitive than any other noise-detection facility and focuses on noises in three dimensions, instead of one or two. This capability allows researchers to more effectively isolate unwanted noises in the components being tested.

The method of noise detection and isolation used by the LCCDAAS is called beamforming. Beamforming is a way of combining individual sensor data to enhance the signal-to-noise ratio for noise levels below that of the background noise in the ocean or test facility. Beamforming also enables researchers to determine where the noise is coming from.

The beamformers use 95 sensors, or hydrophones, in four frequency bands, from 1250 Hz to 20 kHz, covering four octaves of sound. A single hydrophone would pick up noise from all directions, but by using an array of hydrophones, beamforming "aims" the array at the target and keeps extraneous noise to a minimum.

When a beamformer is operating in a large body of water, the distance between the beamformer and its target is much larger than the distance between hydrophones, so the sound waves reaching the hydrophones are assumed to be traveling in the same plane—arriving simultaneously at all of the sensors when the array is steered broadside to the target. In reality, sound waves are spherical, but for closely spaced hydrophones at a great distance from the target, the difference is negligible. When the target is much closer to the hydrophone array, as close as 2 meters (6 feet) in the LCC facility, the sound waves reach different hydrophones at different times, and the computer must make instantaneous time-delay adjustments to determine the source of the sound.

To accomplish this feat in real time, the system's sensors funnel 4.6 million measurements each second to a bank of eight computers operating in parallel. The system can beamform 45 acoustic data channels simultaneously as well as monitor 128 facility-related sensors measuring parameters such as water temperature, pressure, and acidity level. This amount of computational firepower produces an instantaneous acoustic analysis of each component being tested. The computer system then integrates acoustic data with the facility measurements to give researchers a picture of the environmental conditions being simulated as the data are gathered.

In a time when both national security and government spending often dominate the news, the LCCDAAS is proving to be doubly beneficial. Not only do the data the system produces translate into stealthier submarines with greater versatility and effectiveness, but they also streamline the design process and help avoid cost overruns by enabling designers to correct potential problems on scaled-down hulls and other components before they go into production.

Future plans for the system include expanding capabilities at the LCCDAAS to decrease analysis time and possibly developing a more compact, shipboard version of the system to monitor experiments at sea. In the meantime, the LCCDAAS is helping ensure that U.S. forces can keep both a low profile and a watchful eye on things as the new world order evolves.
—Jim Pearce

Data Base Compiled on Forest Growth in CO_2-Enriched Air

If the atmospheric concentration of carbon dioxide (CO_2) were doubled, the total biomass of young tree seedlings apparently would increase by about one-third, based on the results of 58 controlled exposure studies. Averaged across forest species, this increase in biomass would be evenly allocated to leaves, stems, and roots, especially fine roots.

These tentative conclusions are based on data collected by Stan Wullschleger and Rich Norby, both of ORNL's Environmental Sciences Division. They are compiling the first data base on the capacity of forest trees of different species to sequester carbon in a future world whose atmosphere is enriched in CO_2.

The ORNL data base should help clarify the growth responses of 73 forest tree species to elevated concentrations of atmospheric CO_2. Extensive data bases have already been compiled to address the growth responses of agricultural crops to increased atmospheric CO_2 concentrations.

Once completed, this data base will make it possible to determine whether growth responses to experimental CO_2 enrichment vary according to climate and whether CO_2-induced increases in biomass above and below the ground are likely to be limited by nutrient and water availability, which may be linked to global warming. Information from this data base will be evaluated within the context of global carbon models to assess future global change scenarios.
—*Carolyn Krause*

Sea-Level Rise Threatens Coastal Species Habitats

Habitats of threatened and endangered birds, turtles, alligators, and fish in South Carolina may be vulnerable to a rise in sea level that could result from global warming, according to ORNL research.

Tammy White and Richard Daniels, both of the Environmental Sciences Division, identified nine species whose habitats are at risk to a sea-level rise that could result from glacial melting.

"The habitat of the nationally endangered Bachman's warbler will be most affected by sea-level rise," White says. "This finding is significant because the species is near extinction in South Carolina.

"The continued existence of nesting habitat is essential for the survival and reestablishment of these species. The threat to the species of a potential climate warming is not considered by the Endangered Species Act of 1973. This act, which defines methods for identifying and protecting threatened and endangered species, assumes that the climate remains stable."

In this analysis, White and Daniels considered geophysical factors such as elevation, land erodibility and subsidence, shoreline retreat, and the energies of high waves and tides. They correlated a coastal vulnerability index—calculated values indicating the relative vulnerabilities of coastlines to inundation and erosion as a result of sea-level rise—with the habitats of the threatened and endangered species.

The species and percent of habitat at risk were found to be Bachman's warbler, 67%; red-cockaded woodpecker, brown pelican, and bald eagle, 50%; loggerhead sea turtle and wood stork, 40%; American alligator and piping plover, 35%; and shortnose sturgeon, 14%. Except for the shortnose sturgeon, these species nest along the coastline.—*Carolyn Krause*

If the atmospheric concentration of CO_2 were doubled, the total biomass of young tree seedlings would increase by one-third.

Informatics and the Human Genome

Even in this age of information, "informatics" is not a household word. Nevertheless, it is the linchpin of what may prove to be one of science's greatest feats—deciphering the human genome.

Individual laboratories at ORNL are microcosms of global efforts now under way to understand the estimated 100,000 human genes

"The habitat of the nationally endangered Bachman's warbler will be most affected by sea-level rise."

Biologist Richard Mural and computer scientist Ed Uberbacher are helping to unravel the mystery of human genetics by combining their specialties in the new field of informatics.

"A tremendous volume of biological data is being generated in hundreds of labs, all of which work a little differently. They each tend to log information in a somewhat customized manner," Mural said.

To benefit mutually, he explained, researchers need to be able to create, access, and exchange research data across the country or around the world. Facilitating this information flow is the essence of informatics.

The final outcome of genome data is a message composed of four letters—A, T, C, and G—that represent the individual chemical bases that form strands of DNA. Their order along the DNA strand defines the genes that encode life's essential proteins.

that make up the genome and encode our very beings. As the mystery unravels, reams of data with many loose ends will have to be dealt with.

"Informatics is an emerging field that will help tie it all together," Ed Uberbacher, informatics group leader in ORNL's Engineering Physics and Mathematics Division, said. "It's an area that has combined biological and computer sciences to support many of the research activities of the Human Genome Project," he said.

In part, the ORNL informatics effort will allow researchers studying animal chromosomes, such as mouse chromosomes, to quickly access and identify corresponding pieces of human DNA. Often, gene abnormalities in mice are strikingly similar to those in humans.

Uberbacher shares responsibility for development of informatics in ORNL's human genome program with the Biology Division's Richard Mural, who says a vigorous fusion of computational and biological sciences is critical to genome work.

But this four-base code's apparent simplicity can be deceiving; spanning the entire genome, it is roughly three billion characters long. That's enough to fill a 200,000-page telephone directory. To recite it completely would require some 26 years of round-the-clock oration.

"A primary goal of the Human Genome Project is to chart the genome in its entirety. This makes for an immense cataloging task, even by today's high-tech standards," Mural said. And the goal of informatics is not simply to catalog and compare this sequence but to apply computer-based methods to learn about its function and importance in human terms.

The ORNL informatics team has three immediate priorities, Uberbacher said. First, it will provide genome scientists an "electronic laboratory notebook" that will keep track of laboratory data that are generated daily and that will ease data entry, tracking, and information exchange. Second, it will construct and make available to the worldwide genome community an accessible, comprehensive data base for ORNL's gene-mapping efforts (in which scientists determine the location of specific genes along strands of DNA). And third, it will implement a variety of analytical "tools" to help researchers access gene-mapping data bases and sequence data to query about a specific base sequence, gene location, or other information about genome function.—*Wayne Scarbrough*

Miniplant Helps Evaluate Wastewater Treatment Methods

In recent years, DOE has strengthened its efforts to clean up hazardous waste resulting from past operations and to greatly reduce the amount of new waste produced at its facilities nationwide.

As part of the efforts, chemical engineers at ORNL have designed a unique facility to monitor and evaluate methods of treating wastewater. The work is being funded by DOE's Office of Environmental Restoration and Waste Management.

Called the Wastewater Treatment Test Facility (WTTF), it was designed to be a scaled-down, combined version of two elaborate wastewater treatment systems at ORNL—the Process Waste Treatment Plant and the Nonradiological Wastewater Treatment Plant.

"It was made to simulate, on a small scale, the operations at both plants," said Cliff Brown, a section head in ORNL's Chemical Technology Division.

The test facility is an aluminum trailer that has been outfitted as a high-tech laboratory. Inside, small stainless-steel tanks and tall plastic columns filled with carbon chips and purifying resins treat samples of wastewater to remove contaminants.

The first phase of treatment in the laboratory simulates the Process Waste Treatment Plant. In the small stainless-steel tanks, calcium, magnesium, and other minerals are separated out to soften the water, and any radioactive contaminants, such as cesium-137 and strontium-90, are removed by a purifying resin.

Then begins a second round of purification, imitating operations at the Nonradiological Wastewater Treatment Plant.

In a process called air stripping, wastewater is pumped to the top of clear plastic columns and allowed to trickle down through about 3 meters (10 feet) of packing material that resembles chips of seashells. This approach increases the water's surface area, making it easier for organics, such as toluene and xylene, to move out of the water and into a flow of air that is continually pumped up through the columns, which reach from floor to ceiling. The air, which carries and disperses the chemicals in a more environmentally safe manner than does water, is then siphoned away through an exhaust system. (If large amounts of contaminants were being stripped, the air from the columns would undergo additional treatment before being discharged to the outside.) To further ensure purification, the water is filtered again, this time through a column filled with chips of activated carbon. Such filtration removes large organic molecules and any mercury that may be present.

Chemical engineers at ORNL have designed a unique facility to monitor and evaluate methods of treating wastewater.

The step-by-step treatment precisely mimics the operations in the two full-scale facilities. "But because of its operating scale, the pilot-plant testing is much less expensive and greatly reduces risks to the environment," Brown said.

The wastewater most recently tested at the pilot plant came from ORNL's Solid Waste Storage Area Number 6 (SWSA-6), which is scheduled to be closed by Martin Marietta Energy Systems' Environmental Restoration organization. During closure, full-scale wastewater treatment will be necessary, and plans are to use the Process and Nonradiological plants for that purpose.

"The pilot plant worked just great in testing the SWSA-6 samples," said Tim Kent, principal investigator at the test facility. He said the tests answered one of the most important questions about closure of the storage area: whether the two full-scale plants could treat the wastewater without producing mixed waste, a combination of wastes that are regulated individually as "hazardous" or "radioactive."

"Mixed waste poses the biggest challenge, both from a regulatory and a disposal standpoint," Kent said. "We were really pleased to find that treating

We were really pleased to find that treating the SWSA-6 wastewater with existing methods did not produce any mixed waste.

Tim Kent inspects purification columns used to remove hazardous materials from wastewater at the Wastewater Treatment Test Facility. This laboratory-in-a-trailer enables researchers to test and refine treatment techniques on a small scale before beginning full-scale operations.

the SWSA-6 wastewater with our existing methods did not produce any mixed waste."

The new test facility is transportable and has a system design that can be altered for various studies without a major expenditure. Thus, it could be useful to other sites involved with waste treatment. It will be used extensively in the future to evaluate treatment of other cleanup-related waste streams and to perform process improvement studies for the ORNL liquid-waste treatment plants.—*Wayne Scarbrough*

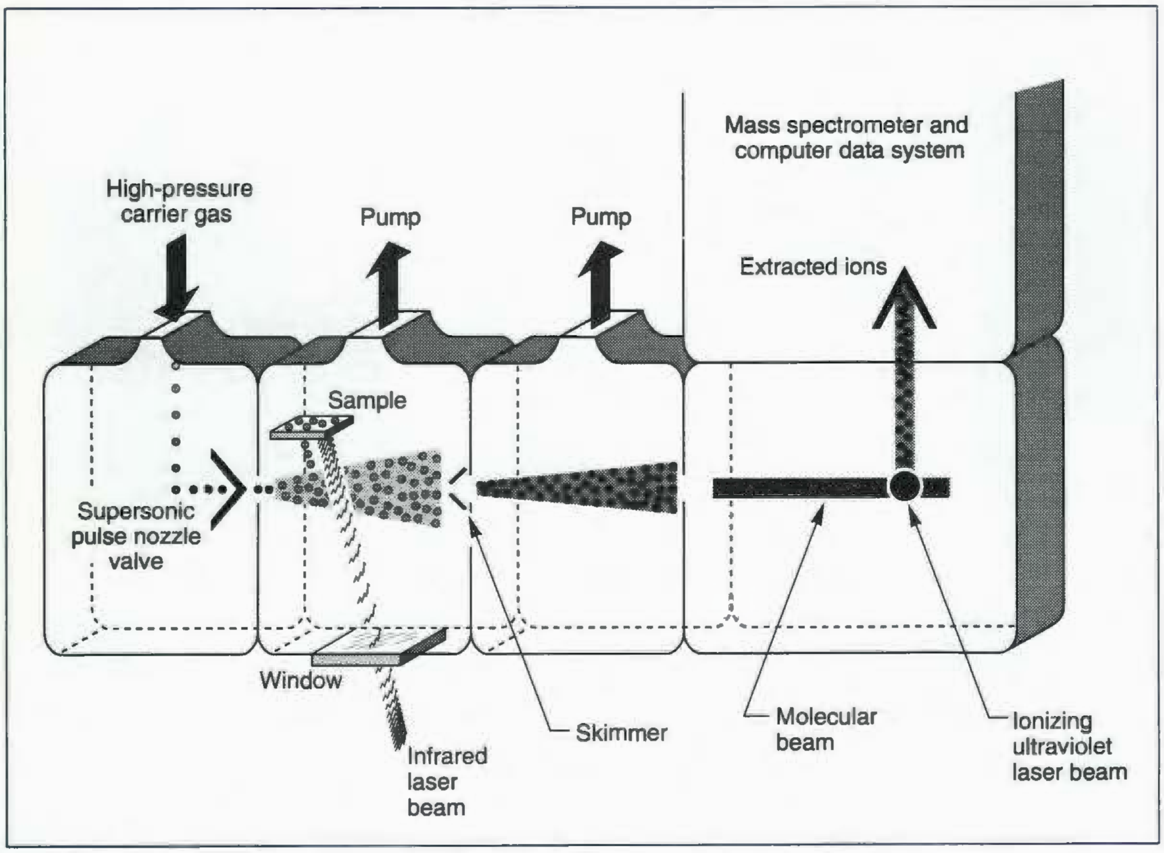
Lasers Accelerate DNA Sequencing

Among the keys to unraveling the mysteries of the human genome is developing a fast and accurate method of sequencing the chemical bases that make up segments of DNA. With this in mind, C. H. Chen and his co-workers in the Health Sciences Research Division's (HSRD's) Photophysics Group have succeeded in using laser mass spectrometry to measure the masses of DNA molecules up to 130 bases long. They have also been able to measure 130-base-long positively and negatively charged ions of DNA molecules using a similar laser technique.

In this procedure, DNA bases are added to a small molecule, known as a primer, which is labeled with an organometallic compound. 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. When the masses of these progressively longer segments are measured, the sequence of their DNA bases can be determined.

In the course of their research, the HSRD research team found that some of the ions they created were stable for as little as 100 microseconds. To analyze these ions before they became unstable, HSRD researchers employed a time-of-flight (TOF) mass spectrometer. Unlike Fourier transform mass spectrometers, which require samples to be confined in a magnetic field for several milliseconds, TOF mass spectrometers can accommodate shorter-lived, "metastable" ion samples, resulting in more complete and accurate data. Also, while traditional mass spectrometry techniques can detect only ionized DNA molecules (those with positive or negative charges) the TOF method can also detect neutral, or chargeless, molecules.

Using this high-speed analysis system, the HASRD team hopes to develop a fast-sequencing laser spectrometry system within the next three years.



Chen's system uses a laser to vaporize fragile DNA molecules and then ionizes them using a weak ultraviolet or laser beam. Finally, the ionized molecules are channeled into a high-resolution mass spectrometer where their masses and sequences are determined.

ORNL-Modified Electron Microscope Directly Images Atoms in Materials

Steve Pennycook will obtain some of the sharpest direct images of atoms in a material using the new 300-kilovolt scanning transmission electron microscope built by VG Microscopes of England and installed at ORNL's Solid State Division. Because it is designed to apply Pennycook's "Z contrast imaging" technique, the microscope has one of the world's highest resolutions.

Gazing at orderly rows of green PacMan-like images on a computer screen, Steve Pennycook can "see" individual columns of silicon atoms and the holes between them. In other materials, he can see defects one millionth the thickness of a human hair.

Pennycook, a scientist in ORNL's Solid State Division, does not have X-ray vision. Instead he has "electron vision"—he uses a powerful electron microscope designed to apply his "Z-contrast imaging" technique to give the sharpest direct images yet of atoms in a solid.

"We now have the ability to use the electron microscope to simply photograph the arrangements of atoms inside materials," says Pennycook. "Our system is more economical than conventional microscopes and provides images that are much easier to interpret."

A 300-kilovolt scanning transmission electron microscope (STEM) built by VG Microscopes of England has been installed at ORNL's Solid State

Division. It is being prepared for operation later this year. Earlier tests of it in England indicated that it can see, or resolve, features as small as 1.3 angstroms. It will complement ORNL's 100-kilovolt STEM, which can image atoms 2.2 angstroms apart. A unit of measure, an angstrom is one ten-billionth of a meter and about one millionth of the diameter of a human hair.

Once in operation, the ORNL microscope should have higher resolution than the 1-million-volt Atomic Resolution Microscope at DOE's Lawrence Berkeley Laboratory, a conventional electron microscope that can resolve individual atoms that are only 1.6 angstroms apart. A 1.3 million volt microscope being built by a Japanese company has achieved 1-angstrom resolution, "but the images produced by these conventional instruments generally cannot be directly interpreted by the eye," Pennycook says.

"The key advantage of the Z-contrast images is that we can interpret them by eye," he adds. "In other words, unexpected structures are immediately apparent."

Furthermore, using special computer programs developed for radio astronomy, Pennycook believes the new ORNL microscope "can break the 1-angstrom barrier" and achieve a resolution on the order of 0.8 angstrom.

Using the 300-kilovolt microscope, Pennycook says, ORNL researchers and collaborators should be able to see copper atoms in high-temperature superconducting material made of oxides of yttrium, barium, and copper. With the 100-kilovolt microscope, scientists can see only the wider-spaced columns of yttrium and barium atoms, which have higher atomic numbers (heavier nuclei based on numbers of protons).

"We should also be able to better observe interfaces—the ways that different crystalline grains of materials come together at grain boundaries," Pennycook says. "Examples are metals, ceramics, semiconductors, and superconductors. This information on grain boundaries is important for many applications of high-tech materials. Examples are increasing electron speed in semiconductors and compact electronic devices and improving the ability of high-temperature superconductors to carry electrical current."

The ORNL method for achieving ultrahigh resolution costs about $2 million, roughly 10% of the cost of building and operating a conventional microscope having equivalent resolution. The conventional approach requires a large building and a team of operators to run and maintain the microscope. The ORNL approach requires only one operator and a normal-size room.

Pennycook says that the interpretation of atomic images is improved by his use of a ring-shaped detector, which picks up electrons scattered through large angles (like foul balls in a baseball game) rather than those moving through the central hole (like balls hit "up the middle" in rapid succession).

"The number of electrons scattered by the sample is directly related to the composition," Pennycook says. "Because atoms of higher atomic number, or Z, scatter more electrons, they produce a brighter image. We call this technique Z-contrast imaging because, although atoms are always white in the image, the heavier an atom is, the whiter it appears."

The 300-kilovolt microscope has higher resolution than the 100-kilovolt one because its higher accelerating voltage produces electrons of a shorter wavelength. The smaller the wavelength and the more tightly the electron beam can be focused, the sharper the image. Pennycook plans to extend the range of materials he images to include more complex semiconducting and superconducting materials and metals and ceramics.—*Carolyn Krause*

Chemical Analysis on Atomic Level Achieved

Unknown elements and the ways they link up to each other in materials can now be identified at the atomic level using a microscope technique developed at ORNL. This approach, described in the November 9, 1993, issue of *Nature*, could lead to more effective high-temperature superconducting materials for energy-saving applications.

ORNL studies have revealed the first clear link between structure and oxygen content in a high-temperature super-conductor.

Atomic resolution chemical analysis, a major long-term goal of analytical electron microscopy, has recently been achieved in ORNL's Solid State Division by Steve Pennycook and his colleague Nigel Browning. Using Pennycook's successful Z-contrast technique for imaging the atomic-scale structure of materials in a direct manner, scientists now use a scanning transmission electron microscope to analyze the chemical composition of a material at the atomic level. In this way, they can identify atoms of unknown elements and determine the details of their chemical bonding.

The Z-contrast image itself has chemical sensitivity in that the higher the atomic number, the brighter the image of that atomic column. However, the image cannot by itself reveal the identity of unknown chemical species.

"The Z-contrast technique's great advantage is that it provides a unique image of the atomic structure that can be interpreted directly," Pennycook says. "Even with a completely unexpected structure, the location of the heavier atomic columns can be seen directly."

Because the Z-contrast image uses only those electrons scattered through large angles, the rest of the electrons may be analyzed by an electron spectrometer. It measures the energy the electrons give up to the specimen they pass through.

This technique, called electron energy loss spectroscopy (EELS), can identify unknown chemical species from the fingerprint of energy loss. In addition, the fine structure on the loss peaks in the electron energy spectrum can be used to determine the number and directions of chemical bonds between neighboring atoms.

One of the challenges of microscopy is to determine the oxygen content in grain boundaries—areas where different crystalline grains of a solid come together—of high-temperature superconducting material made of oxides of yttrium, barium, and copper ($YBa_2Cu_3O_x$).

According to Pennycook, "If there is enough oxygen in the grain boundaries, the material may act as a superconductor, but if there is not enough, it is an insulator." Chemically speaking, the material is superconducting if its formula is $YBa_2Cu_3O_7$, but it is an insulator if its formula is $YBa_2Cu_3O_6$. This subtle difference in oxygen content can be determined by the EELS combined with Z-contrast imaging.

ORNL studies have so far revealed the first clear link between structure and oxygen content. Pennycook and Browning have observed one particular type of grain boundary that has no oxygen deficiency.

"This is a particularly exciting observation," he says, "because of the importance of correlating local structure with local superconducting properties. It will greatly assist our scientific understanding of the effect of defects on superconducting properties and may lead to significant technological advances and applications.

For his research Pennycook received the 1992 Materials Research Society Medal and several Department of Energy materials science awards. *—Carolyn Krause*

First codes run on 512 nodes

Challenge is a key word at ORNL's Center for Computational Sciences. For a year its computer experts struggled to get ORNL's new Intel Paragon XP/S 35 running effectively. ORNL's earlier Paragon machine—the XP/S 5, which has 66 processors, or nodes—had been working soon after the Intel Corporation shipped it to ORNL for testing. But the newer machine was beset by problems largely because of the complications in extending to 512 nodes.

The challenge was recently met by running two large ORNL-developed codes on 512 nodes. Both codes were developed under the Materials Grand Challenge Project of the Partnership in Computational Science (PICS) consortium. The Materials PICS includes ORNL, Brookhaven National Laboratory, and Ames Laboratory.

Grand challenges are huge problems requiring numerous calculations to progress toward a solution. Parallel computers like the Intel Paragon machines have numerous nodes that make calculations simultaneously. They are called supercomputers because if, each node is assigned a small part of a huge problem, the supercomputer can provide solutions in a few hours, whereas previously weeks or even months were required.

The first code to be run on the XP/S 35 was developed by Bill Shelton of the Engineering Physics and Mathematics Division and Malcolm Stock and Yang Wang, both of the Metals and Ceramics Division. This code calculates the physical properties of disordered materials, such as metallic alloys as well as intermetallic and ceramic compounds, on the basis of a fundamental view of the electron "glue" that holds together the atomic nuclei in matter. The code is useful both for understanding physical properties of disordered materials such as electrical resistivity and for predicting the temperatures, pressures, and other conditions under which elements will mix as well as the types of ordered and disordered compounds these elements will form. Such information is critical to the design of new alloy systems and development of new theories.

Another code developed at ORNL under the Materials Grand Challenge Project calculates densities of electrons and surface energies to identify the preferred binding sites for a single germanium atom on a reconstructed silicon surface. The code was developed by Victor Milman, now of the Solid State Division (SSD), and a team of researchers at Cambridge University in England after electron microscope images made by Dave Jesson of SSD suggested that a germanium atom could exchange positions with a silicon atom on a surface. The images were obtained using Steve Pennycook's Z-contrast technique described on p. 60. A colorful visualization of these calculations appears on the front cover of this issue of the *Review*.

"Because experimental information on germanium diffusion on the silicon surface is indirect," says Milman,"theoretical modeling is the only way to understand this interaction between germanium and silicon atoms. This large first-principles calculation is possible only due to the availability of the massively parallel computers."

Such calculations combined with information from Pennycook's Z-contrast electron microscope images (see previous highlights) may lead to an understanding at the atomic level of how to grow light-conducting silicon-germanium films. Such "optically active" silicon-germanium films would revolutionize the manufacture of advanced semiconductor devices that incorporate light-wave guides. These devices will increase the speed of information flow because light signals are faster than electrical currents. Wave guides for compact disk players and other uses are currently made of gallium arsenide. Because gallium arsenide is more expensive than silicon and involves the use of the toxic metal arsenic, silicon-germanium films could better meet the need of the computer, communications, and entertainment industries for faster and cheaper semiconductor devices.

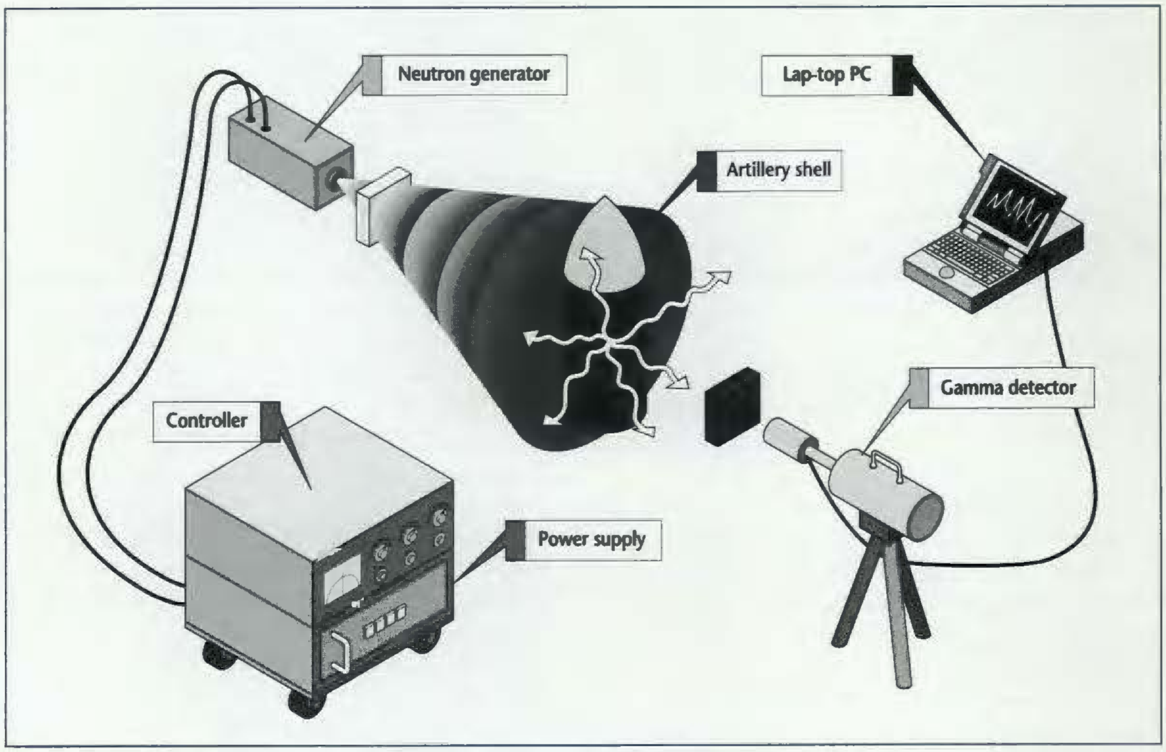
These materials challenges will more likely be met if ORNL succeeds at the challenges of operating a new class of parallel machines with an increasing number of nodes. ORNL in 1994 will be testing an XP/S 75 (1024 nodes) and an XP/S 150 (2048 nodes). Won't it be grand to run ORNL codes on more and more nodes?
—Carolyn Krause

From Waste to Warheads: New Uses for Neutron Interrogation Technology

The system promises to provide a fast and reliable method of differentiating between chemical and conventional weapons.

For the past decade, researchers at ORNL's Waste Examination and Assay Facility (WEAF) have been using neutron interrogation technology to determine or verify the contents of drums of radioactive waste. A spin-off of this process, known as the Pulsed Interrogation Neutron Gamma system, or PING, is demonstrating the versatility of neutron interrogation as an analytical tool.

In recent years, PING has been adapted by ORNL researchers for potential use in airport security systems and is now being billed as a tool for discriminating between chemical and conventional warheads; verifying the absence of high explosives in nuclear warheads; and monitoring the sulfur, energy, and trace-element content of coal.



The Pulsed Interrogation Neutron Gamma system, which is based on technology for analyzing the contents of drums of radioactive waste, has been adapted to distinguish between chemical and conventional warheads and verify the absence of high explosives in nuclear warheads.

If all goes well with the new neutron generator, the PING system may soon add arms control verification to its diverse list of capabilities.

"Components of the PING system have been used for waste characterization work at the site for years," says Fred Schultz, a researcher in ORNL's Waste Management and Remedial Actions Division, who developed PING, along with George Vourvopoulos of Western Kentucky University. "Now we're applying waste assay techniques to entirely new fields."

The PING system can nondestructively analyze a sealed container, such as a warhead or artillery shell, and detect common constituents of both conventional explosives and chemical warfare agents. As a result, the system promises to provide a fast and reliable method of differentiating between chemical and conventional weapons. This capability gives PING the potential to be used for such activities as monitoring arms control agreements and enforcing provisions of treaties that limit conventional or chemical military capabilities, such as the current treaty between the United Nations and Iraq.

The theory behind the PING system is that materials can be distinguished from each other by determining their chemical profiles, that is, which elements are present and their relative concentrations.

PING is capable of detecting carbon, nitrogen, and oxygen, components of conventional explosives, as well as sulfur, chlorine, fluorine, and phosphorus, common constituents of chemical weapons. The system's ability not only to detect the presence of these elements but also to determine their proportions makes it possible for PING to discriminate between various classes of conventional or chemical weapons, such as nerve gas and mustard gas.

The system uses a pulsed neutron generator to bombard samples with bursts of neutrons. The elemental and, under certain circumstances, chemical, composition of the samples is determined by an analysis of several waves of gamma rays resulting from collisions between neutrons and atoms in the sample. These collisions cause atoms of different elements to emit gamma rays of characteristic energies, allowing researchers to determine which elements are present in the sample.

Samples are bombarded with two kinds of neutrons, fast neutrons and thermalized neutrons. The neutron generator produces "fast," or high-energy neutrons in pulses of about 10 microseconds with gaps of approximately 90 microseconds between pulses. At the end of each pulse, some of these neutrons pass through a neutron moderator, which slows them down, creating "thermalized" neutrons.

Within the first few microseconds after a neutron pulse begins, interactions between fast neutrons and carbon and oxygen atoms, if any are present, produce gamma rays of 4.44 and 6.13 million electron volts (MeV), respectively. In the gaps between pulses, the thermalized neutrons interact with nitrogen, sulfur, and chlorine atoms to produce characteristic gamma rays of 10.828, 5.42, and 6.11 MeV, respectively.

After every few hundred pulses, a gap of several microseconds allows the detection of gamma rays from oxygen, fluorine, and phosphorus nuclei (at energies of 6.13, 1.357, and 1.779 MeV, respectively), which have become radioactive through interactions with fast neutrons. This longer gap is necessary for the detection of fluorine and phosphorus because they emit relatively low-energy gamma rays, which are obscured by high-energy gamma rays emitted by other elements during the system's normal cycle.

The neutron generator currently used with the PING system requires 24 minutes to produce enough gamma rays to analyze a sample. A larger generator could cut this time to two minutes or less. Schultz and other ORNL researchers are working with commercial firms to develop a generator for use with the system. They are also working with a group of French researchers to borrow a suitable generator.

"We've proven the principles of the system," says Schultz. "We've collected gamma-ray data on each of the elements separately; now we have to do it all at once with either real or simulated explosives. When we get a larger neutron generator, we can begin doing this kind of work."

If all goes well with the new neutron generator, the PING system may soon add arms control verification to its diverse list of capabilities.
—Jim Pearce

New Probe Detects Trace Pollutants in Groundwater

To determine whether groundwater has been cleaned up or whether a pollution problem is developing, methods for spotting trace amounts of groundwater contamination at waste sites are needed. Such detection technology may be field tested soon in Oak Ridge.

One highly sensitive technique for detecting and identifying trace contaminants in groundwater is being developed at ORNL. The technique has the potential of being a million times more sensitive than current detection methods.

The high-tech probe, which combines a computer, laser, optical fibers, and a power supply, is called a spectroelectrochemical sensor. It is being developed by Eric Wachter, John Storey, Bob Shelton, and Tye Barber, all of the Measurement Systems Research Group (under Richard Gammage) in the Health Sciences Research Division.

Field tests of this groundwater monitoring technique were conducted in September 1993 at the Paducah Gaseous Diffusion Plant, where concentrations of the groundwater contaminant trichloroethylene (TCE) are already well documented. TCE is a potential carcinogen commonly used for removing grease from metals and for dry cleaning clothes. According to Wachter, the technique enabled direct detection of TCE in groundwater at levels as low as 150 parts per million.

Besides TCE, the technique could be used to detect other common groundwater pollutants, such as other chlorinated hydrocarbons, aromatic

John Storey checks the krypton laser that is critical to the operation of the ORNL-developed spectroelectrochemical sensor for detecting and measuring groundwater pollutants.

hydrocarbons, cyanide, nitrates, sulfates, and transuranic elements. It might also be adapted for detection and measurement of trace levels of drugs in body fluids, contaminants in food and water, and nicotine from secondhand smoke.

According to Wachter, with this new technique, virtually any groundwater contaminant can be broken down into a substance that is easy to analyze. This transformation is accomplished by passing an electrical current through a metal electrode in the probe, which is immersed in contaminated groundwater.

Contaminants in contact with the electrode will undergo a chemical change, called an electrochemical reaction. The products of this reaction can be detected and their concentrations measured using spectroscopy—thus the name spectroelectrochemical sensor.

Determining the identity and concentration of the electrochemical product indicates which and how much of a contaminant is present. This information is obtained by shining a laser light down an optical fiber onto the electrochemical product on the metal surface. Interaction of the light with the product's molecules results in emission of light known as surface-enhanced Raman scattering (SERS). The frequencies and intensities of the SERS light indicate the identity and concentration of the target material.

In the ORNL sensor, the SERS light is carried by optical fibers back to an optical spectrometer on the ground. A computer takes data on the light, identifies the detected groundwater contaminant, and calculates its concentration.

In the electrochemical reaction in the ORNL sensor, TCE is broken down into silver chloride and an organic derivative, which emit SERS light when excited by the laser. However, Wachter says, ORNL researchers hope to improve the detection sensitivity for TCE by chemically converting the contaminant's breakdown products to colored products that emit even more light when excited by a laser. To accomplish this goal, they are collaborating with Mike Angel of Lawrence Livermore Laboratory (who will become a faculty member at the University of South Carolina in the fall of 1993). He has used chemical reagents to make colored products from TCE, which should exhibit "surface-enhanced resonance Raman scattering."

"This approach," says Wachter, "may work better on TCE and some other contaminants that do not interact strongly with metal surfaces. It should greatly increase our detection sensitivity and the range of contaminants that can be detected."

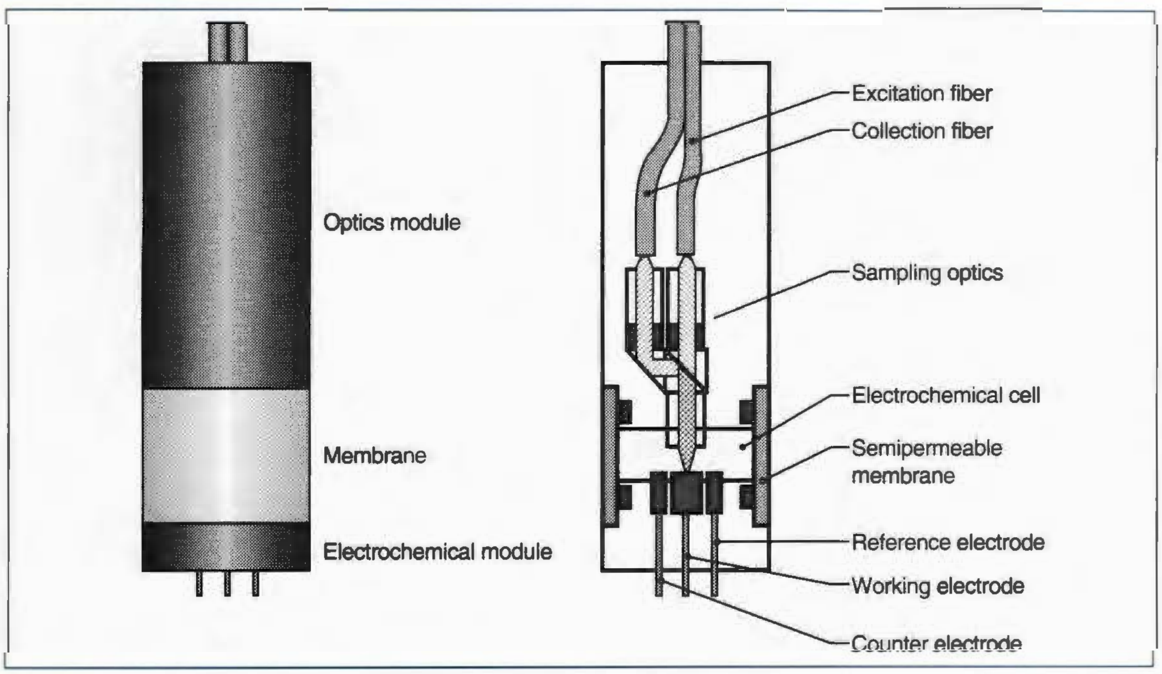
The ORNL group will work with Angel to develop ways to immobilize chemicals for making colored products on the metal surface and to replenish their supplies continuously. Angel is expected to work at ORNL during the summer of 1994.

Wachter says that the current optical probe for groundwater is about 1 inch in diameter but the goal is 0.5 inch. He adds that the equipment aboveground—personal computer, optical spectrometer, and helium-neon or diode lasers—take up a "few cubic feet and could easily fit into the back of a van."

SERS was discovered by Martin Fleishmann of cold fusion fame and later explained by Rick Van Dyne of Northwestern University. A mechanism for SERS involves the surface plasmon, whose existence was predicted by Rufus Ritchie of ORNL's Health Sciences Research Division.

The work is sponsored by the Department of Energy, Office of Research and Development, Waste Management Operations Research and Development Division.—*Carolyn Krause*

Closeup of the laser beam and the spectroelectrochemical sensor.



Schematic of ORNL's modular spectroelectrochemical sensor showing optical fibers, electrodes, and the cell in which the electrochemical reaction takes place.

Cooperative Agreement for Automated Film Deposition by Laser

ORNL laser expert Douglas Mashburn conceived of a computer-controlled system for depositing multilayer structures, such as superconducting films, by pulsed laser deposition. Neocera and ORNL cooperatively developed the concept into a Neocera business opportunity.

ORNL's High Temperature Superconductivity Technology Center can boast its first commercial product—a software-driven, pulsed-laser system for depositing superconducting films of a desired composition and thickness. Called the Automated Multilayer Deposition Accessory (AMDA), the system was developed in collaboration with Neocera, Inc., of College Park, Maryland, through a cooperative agreement.

Robert Hawsey, center director, said, "This is a perfect example of technology transfer—a collaborative project in which two organizations shared their resources, combined their innovative ideas, and developed the technology, resulting in a product that will be useful for basic and applied research, as well as manufacturing."

Douglas Mashburn, a researcher with ORNL's Engineering Technology Division who formerly worked in the Applied Technology and Solid State divisions, came up with a new concept in 1987 while investigating better ways to deposit superconducting films. He conceived a computer-controlled system for conveniently predetermining the exact ratios of different materials making up the film deposited by pulsed laser ablation. The concept makes possible abrupt composition changes for growing superlattices as well as the gradual changes needed for a graded alloy. Precision is maintained by sensing deviations in process conditions, such as laser pulse energy, window fogging, and target wear, and correcting for them in their early stages (feedback compensation). A laser arrangement he devised in 1990 greatly reduces uneven target erosion, making it easier to maintain the desired composition during long runs. The concepts are applicable to a wide range of solid materials.

Neocera president T. Venkatesan, who pioneered the use of pulsed laser deposition for high-temperature superconductors before founding the company, recognized that these concepts were nearly ideal for multilayer deposition, one of Neocera's primary business interests. Together, Neocera and ORNL developed the concept into a business opportunity.

AMDA is compatible with laser deposition systems manufactured by Neocera and other suppliers. It includes a copyrighted, menu-driven software program that enables researchers to specify the number of layers in a film, the composition and thickness of each layer, the frequency of the laser light "boiling" off atoms of material to be deposited in each layer, and the deposition rate. The deposition system controls the positions of the various targets and triggers the laser to create films as thick as 1000 atoms automatically.

Without such a product, researchers typically specify the material for each layer by manually rotating a carousel to expose the appropriate target and then control the thickness by turning the laser beam on and off while keeping time with a stopwatch.

AMDA will be useful for basic and applied research in superconductors, semiconductors, magnetic materials, and optical materials. Neocera has tested the product extensively in the company's program to develop electronic devices from high-temperature superconductors. These devices are multilayer structures made from superconductors, dielectrics, buffer layers, passivation materials, and electrical contact pads. Neocera recently announced their first commercial sale of an AMDA to a European customer.

AMDA can control superconducting layers as thin as a single unit cell (12 angstroms). Its fine thickness control allows researchers to fabricate devices with reproducible properties. It can also automate and control deposition of superlattices—artificial materials created by laying down very thin layers of two or more materials in sequence.

AMDA's hardware components include a motor to move six targets through the laser beam and a plug-in board for an IBM PC/AT computer. The software enables the user to define a layer as a thickness of a given material depositied at a specific rate. Information on a selected sequence of layers can be stored on a disk and recalled for future use, thereby ensuring reproducibility from run to run.

Superconducting Wire Technology Licensed

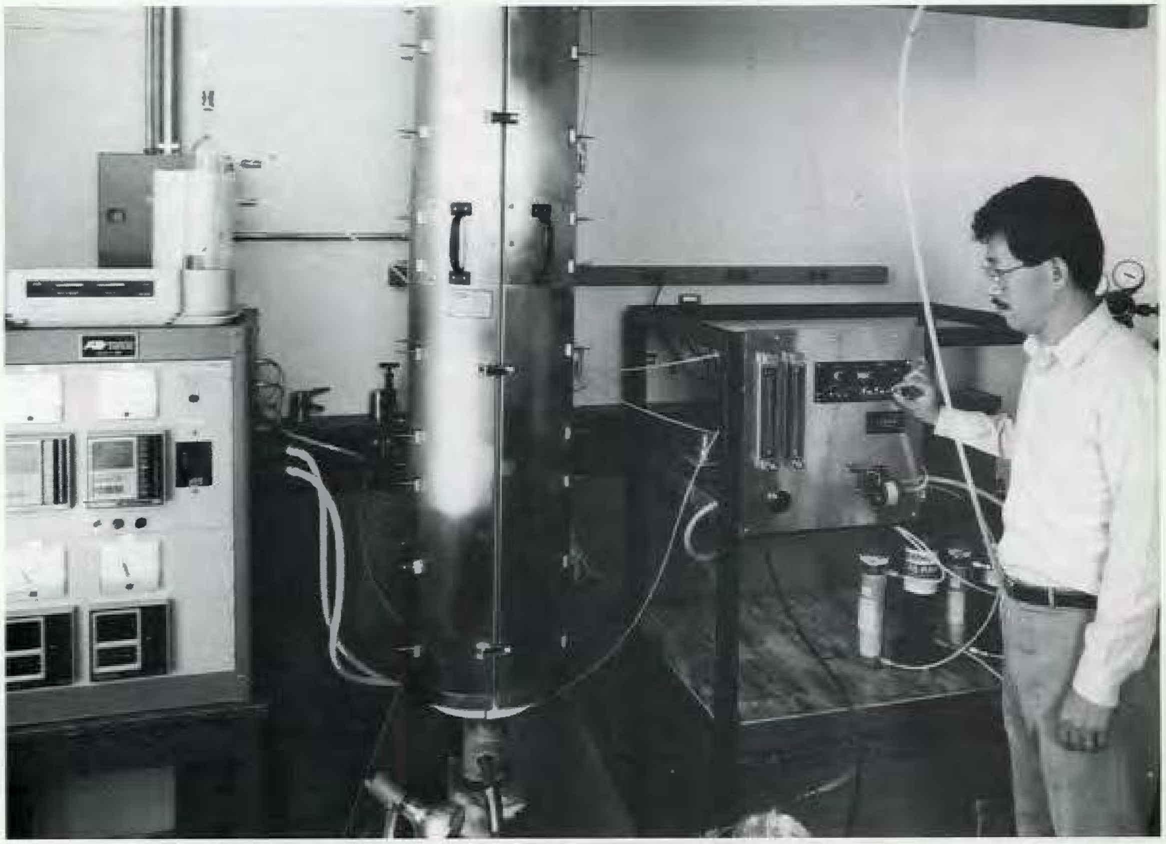
The first license of a superconducting wire manufacturing technology developed at ORNL has been issued. Energy Systems has signed a license agreement to commercialize the technology with Superconductive Components, Inc. (SCI), a Columbus, Ohio, firm. A superconductor is a rare material that conducts electricity without the energy-wasting resistance typical of copper and other common electrical materials.

ORNL researchers Don Kroeger and Jorulf Brynestad and ORNL consultant Huey Hsu have developed a process for producing superconducting powder precursors of BSCCO material, which contains bismuth, strontium, calcium, copper, and oxygen. The product is an oxide metal powder that can be doped with lead to improve its properties.

According to Kroeger, "The process can produce lead-doped powders without measurable lead loss. The distribution of the particle sizes is narrow, from 0.1 to 1.0 micron. The grain size within a particle is very fine. And the chemical homogeneity from grain to grain is good."

The process is scaleable to high powder production rates. SCI will further develop the process to produce powders for sales and for use in bearings, current leads, superconducting wire, and magnetic levitation demonstrations.

Edward R. Funk, president of SCI, says, "The licensing of the ORNL BSCCO process completes



Huey Hsu, an ORNL consultant, adjusts the flow rate for the gas-carrying aerosol droplets in a tube furnace used for aerosol pyrolysis. The product of the process is bismuth-strontium-calcium-copper oxide (BSCCO) powder doped with lead for high-temperature superconducting wires.

our line of high-quality superconductive powders. The ORNL process is an important technological advance in tailoring the BSCCO powder for specific applications."

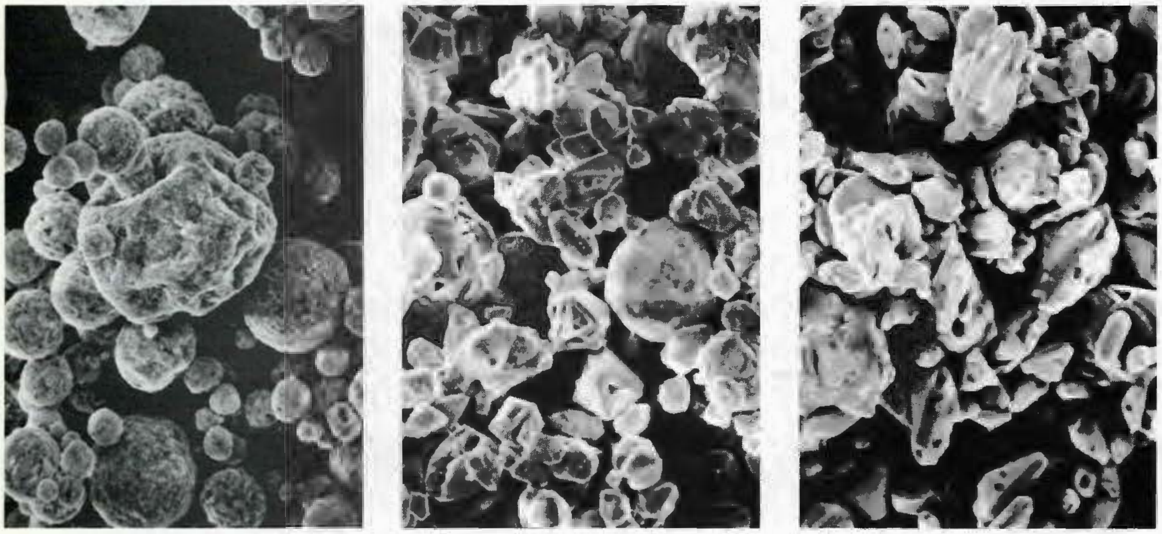
According to Robert Hawsey, director of ORNL's High Temperature Superconductivity Technology Center, "The commercialization of this process will benefit American industry as a whole. The increased quality and availability of the BSCCO powders may make possible large-scale products."

Examples are bulk electrical conductors for magnetic levitation and propulsion of high-speed trains and for superconductive magnetic energy storage devices. These devices promise to make wind and solar power economical by efficient, clean storage of energy for use when needed rather than when produced.

The ORNL process was developed with funding from DOE's Office of Energy Management.
—Carolyn Krause

Ultralight Shielding for Electromagnetic Interference Licensed

ORNL researchers have developed extremely lightweight shielding to protect electronic components in automobiles, aircraft, and spacecraft from stray electromagnetic signals that can cause equipment confusion or failure. Such shielding could also protect people from the electromagnetic fields of cellular phones and other electronic devices. The electromagnetic interference (EMI)



Electron micrographs of BSCCO powders doped with lead produced at ORNL by aerosol decomposition. Notice the changes in powder shapes as the aerosol pyrolysis temperature increases.

shielding technology has been licensed by Energy Systems to Sigma Electromagnetic Shielding Technologies, Inc., headed by Victor Rivas of Nebraska and recently relocated to Oak Ridge.

Rivas had been making lightweight shielding by sandwiching iron foil and carbon cloth in epoxy. The carbon cloth gives structure to the shield, and the iron prevents electromagnetic signals from penetrating equipment by absorbing and conducting them to the ground. His goal has been to make EMI shielding as efficient and light as possible for automobiles, aircraft, and spacecraft to reduce its adverse impact on fuel efficiency. Other applications could include communications satellites, electronically guided weapons, and electronic components within a room or enclosure.

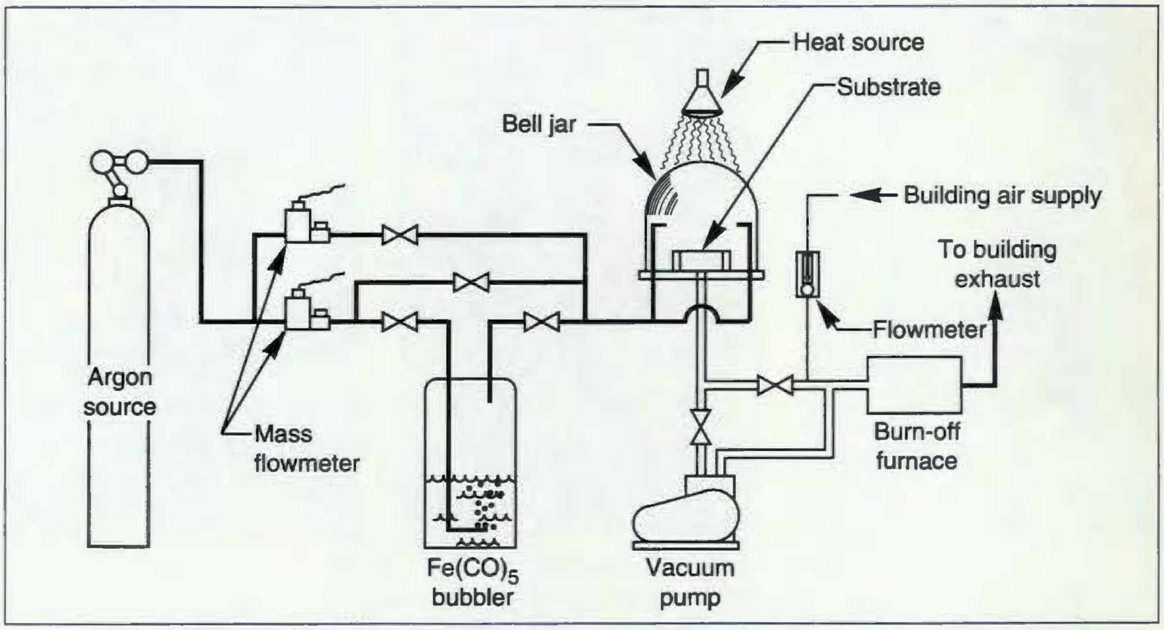
Jim Weir of ORNL's Metals and Ceramics (M&C) Division learned of Rivas's work in December 1990 at a National Aeronautics and Space Administration conference. Weir suggested that ORNL has the capabilities to develop shielding of even lower weights. So he asked David Stinton of the M&C Division to pursue development of an ultralight shielding that uses the minimum amount of iron needed.

Stinton and Millicent Clark found that ultralight shielding could be made by depositing iron on carbon cloth using a low-temperature process called chemical vapor deposition. In this process, the carbon cloth is heated to around 200°C using sunlamps. Vapors of a heated liquid, iron pentacarbonyl [$Fe(CO)_5$], are carried by argon gas into the chamber containing the heated carbon cloth.

If the temperature is right, a layer of iron as thin as 0.1 to 2 microns is evenly deposited on the fibers in the cloth, and the carbon monoxide in the compound is drawn out of the chamber. If the temperature is too high, carbon will also deposit on the cloth, resulting in a poor shield. Stinton and his colleagues are experimenting to determine the best temperatures for obtaining desired thicknesses and purity of the iron layers.

Stinton says that researchers in ORNL's Instrumentation and Controls Division are working with him to determine the shielding capabilities of carbon-iron composites of different thicknesses. They place a source of electromagnetic radiation on one side of the ultralight EMI shield and measure the amount of radiation that actually gets through the shield.

"It is important that the deposited iron is stable, or else it will rust and lose its ability to conduct stray electromagnetic signals to the ground," Stinton says. "If the iron is dense and



Iron coatings can be deposited at low temperatures to make lightweight shielding for electronic parts.

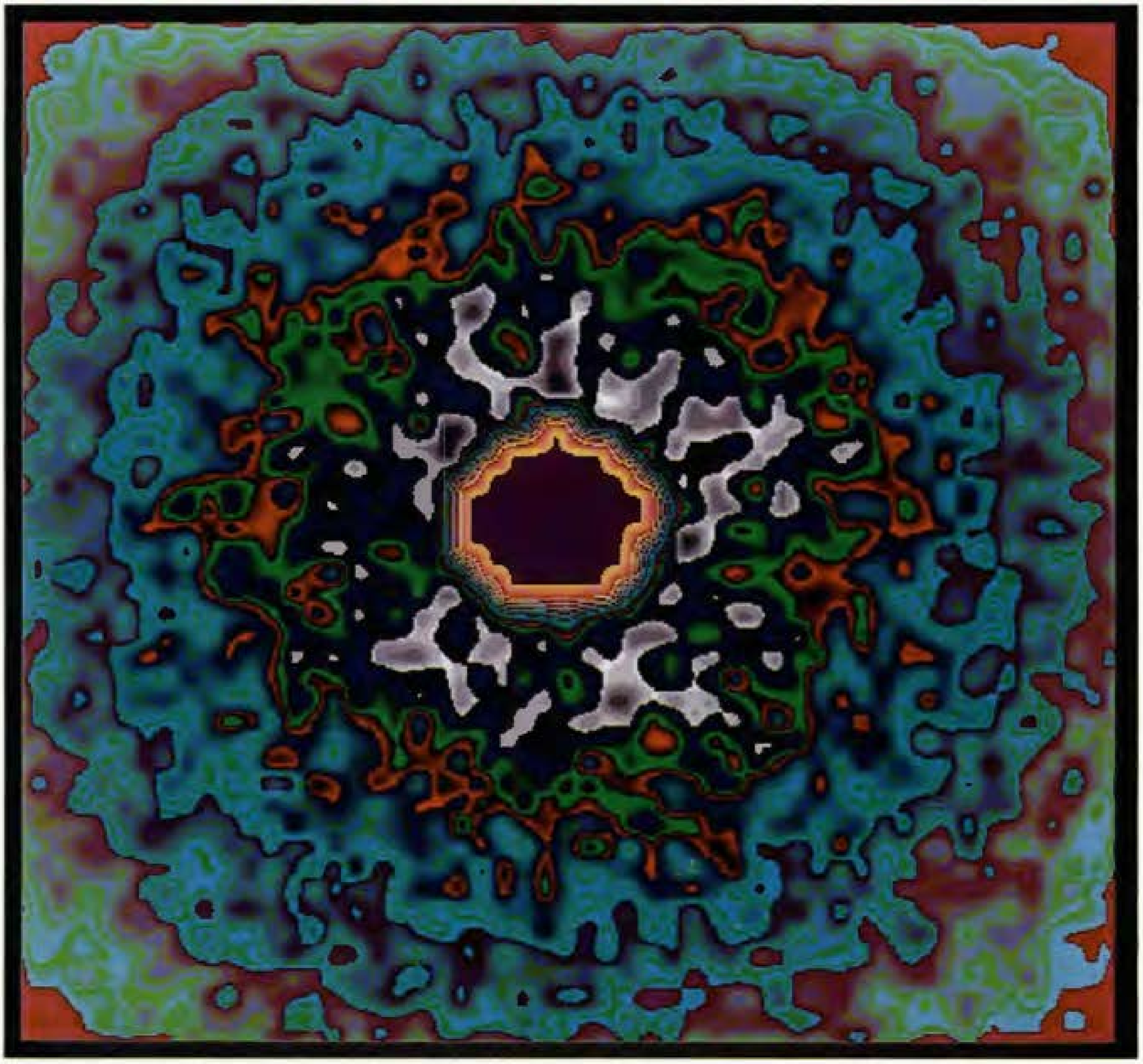
not porous, it will not oxidize and it will stay magnetic. If it's unstable, it will lose its magnetism."

As soon as he obtains financing and organizes a management team, Rivas plans to produce prototype ultralight EMI shielding at the Valley Park incubator building operated by the city of Oak Ridge. Sigma will manufacture multiple layers of iron-coated carbon cloth or iron-coated fiberglass (which is less expensive than carbon cloth) and glue these layers together to make a rigid epoxy composite. Then the company will develop commercial shielding products for multiple applications.—*Carolyn Krause*

NEXT ISSUE

ORNL conducts assessments and other studies associated with licensing hydropower projects. Issues involved in developing U.S. hydropower resources are explored.

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



ORNL researchers are using the Lab's Small Angle Neutron Scattering facility to image clusters of carbon molecules known as fullerenes. The pattern produced by passing a neutron beam through a solution of fullerenes enables researchers to determine the size and shape of the molecules. This particular pattern was produced by a solution of C_{60} molecules. See articles on pages 49 and 51.