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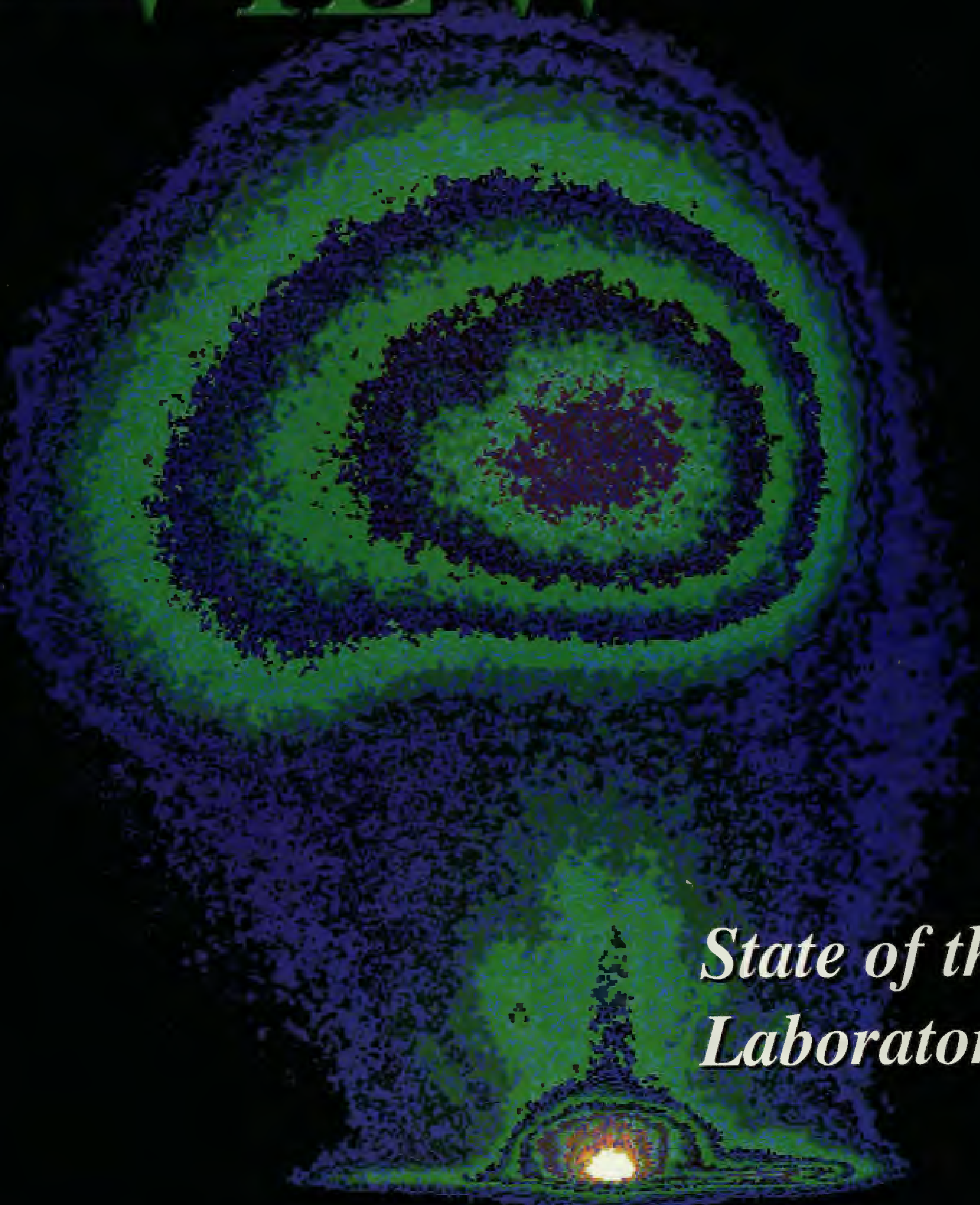
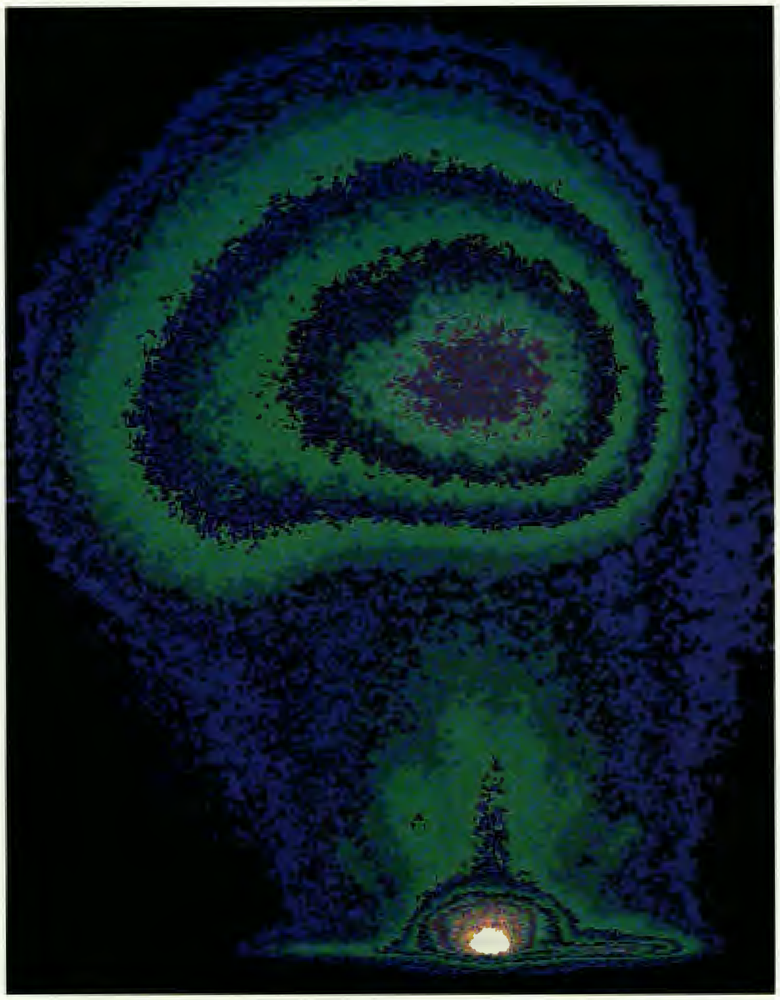
Oak Ridge National Laboratory REVIEW

Vol. 30, Nos. 1 & 2, 1997



State of the Laboratory



COVER CAPTION

Ultrafast (5-nanosecond) photographs of luminescent carbon plasmas reveal how laser-vaporizing graphite in a vacuum can synthesize thin films of amorphous diamond, a transparent, ultrahard form of pure carbon (see pp. 56-58). The energetic ball of carbon ions revealed in the false color image is traveling at 4,000,000 centimeters per second. This energy helps transform ordinary graphite into amorphous diamond when the material is collected to form a thin film at room temperature. It is one of ORNL's many research highlights in 1996 that are presented in this State of the Laboratory issue. The gated intensified CCD-array photography was performed by David B. Geohegan and Alex A. Puretzky in ORNL's Solid State Division. The cover was designed by Allison Baldwin, graphic artist in ORNL's Computing, Information, and Networking Division.

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in energy production and end-use technologies; biological and environmental science and technology; advanced materials synthesis, processing, and characterization; and the physical sciences including neutron-based science and technology.

REVIEW

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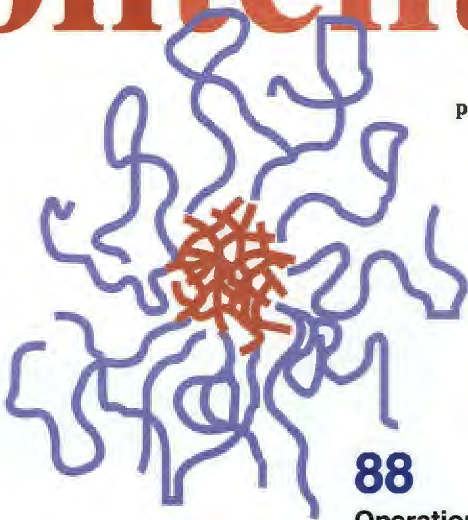
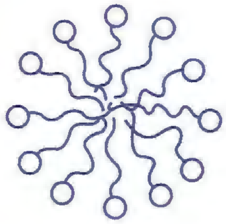

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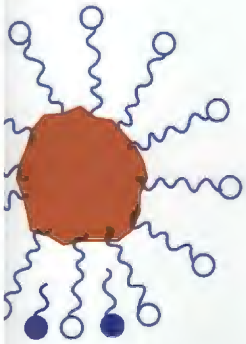

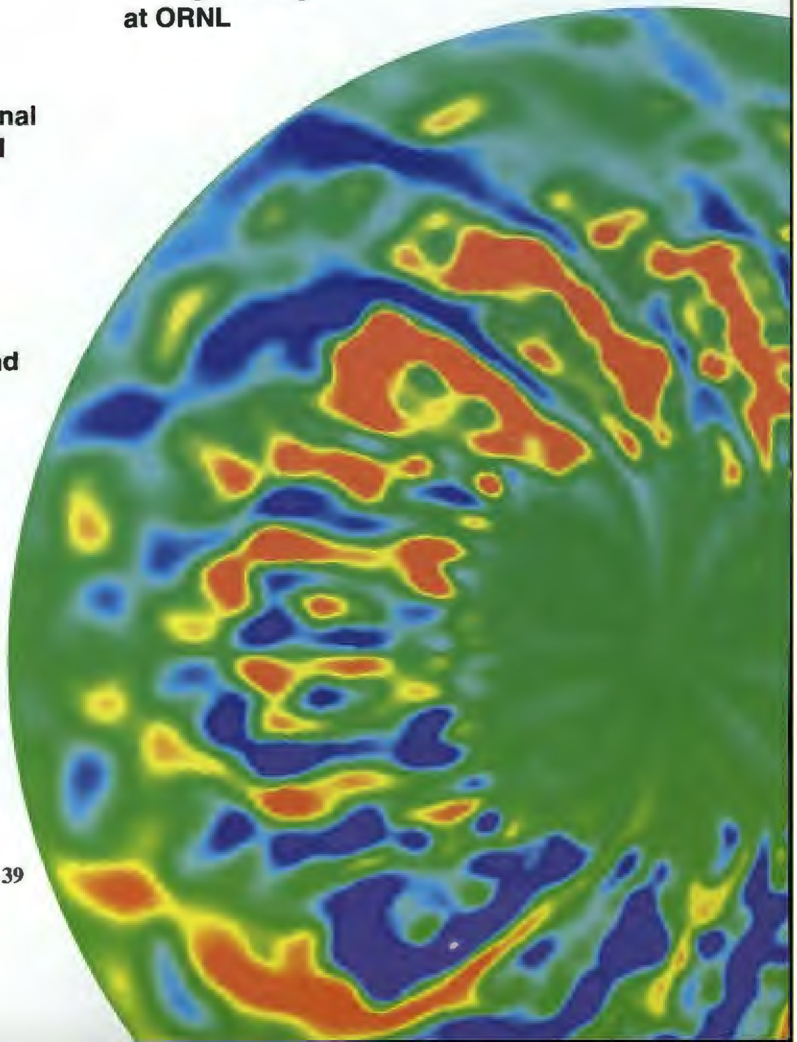

ORNL led experiments that showed how to reduce turbulence—and accompanying heat losses—in a fusion energy device by properly operating it.

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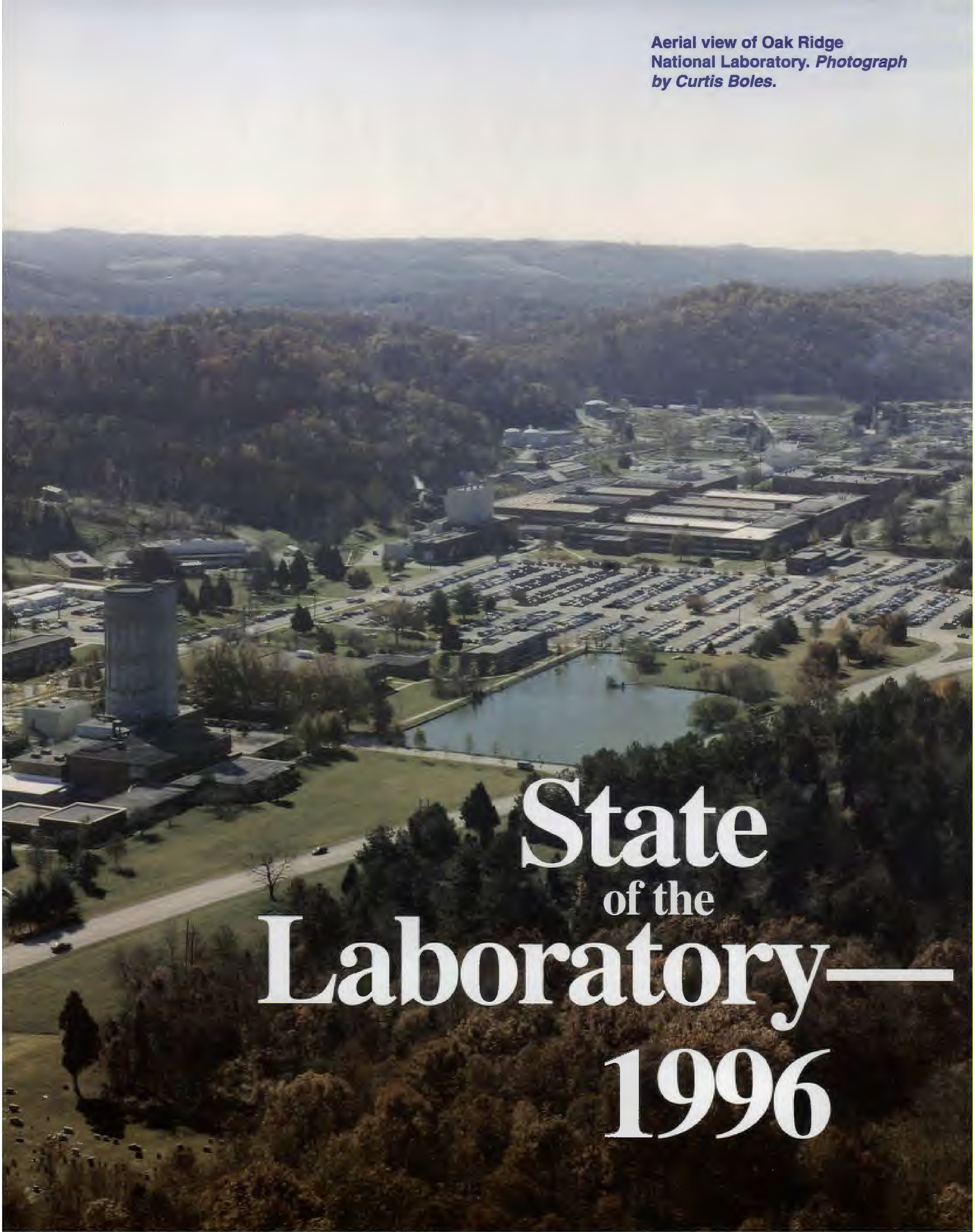


Aerial view of Oak Ridge National Laboratory. *Photograph by Curtis Boles.*

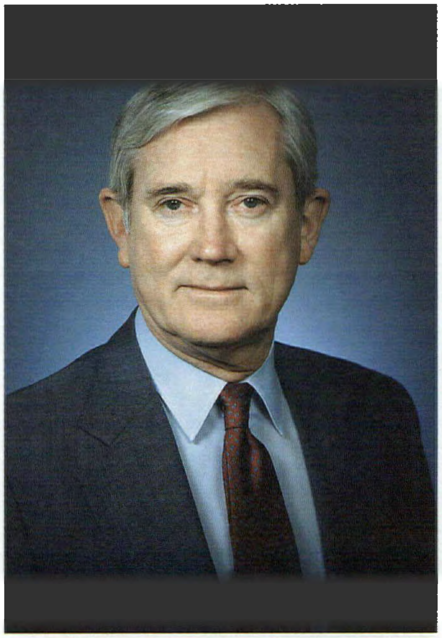
State of the Laboratory—1996

In my State of the Laboratory address last year, I didn't talk about the scientific, technical, and managerial accomplishments of the preceding year. I didn't make any predictions about what might happen in the forthcoming year. I am glad that I didn't, because I would have been wrong again. To avoid being wrong next year, I am not going to make any foolish predictions this year either.

In an ideal world, our Showcase Lectures should keep you up to date on many of the scientific and technical accomplishments inside the Laboratory. Our Distinguished Lecture series should provide some thought-provoking challenges for you to consider. Our new publication, *Ridgelines*, should keep you up to date on changes in management structure and personnel, both here and at Energy Systems. Our World Wide Web pages, such as *ORNL Today* and the *ORNL Review*, now contain a great deal of information about what is going on around here. But this is not an ideal world. I know as well as you that these sources of information don't provide the depth of communication that we should have. This talk will not cure our communication problem. Even so, I hope that what I do say will remind you of the circumstances in which we find ourselves and that my remarks might suggest some things that you might do to improve our situation.

Last year I organized my remarks around three themes: "The Way We Were," "The Way We Are," and "The Way We Need To Be." In commenting on the way we need to be, I listed ten items that I feel are imperative to our long-term survival as a national laboratory. I will not repeat them here today. I hope that you remember them in spirit if not in detail. They were published in *Lab Notes* and the *ORNL Review*, and are still listed on our Web server (http://www.ornl.gov/ORNLReview/rev29-12/text/state95.htm). It is interesting to me that, since last year's talk, no one has said that any of the items on my list of imperatives were unrealistic or inappropriate. In preparing for my remarks today, I reviewed that list. In light of many things that have happened this last year, I believe that a couple of items need to be added to that list.

First, we must collectively and aggressively defend Oak Ridge National Laboratory against those forces that would seek to diminish or destroy it. Second, we must become politically more sophisticated and active on a national, state, and local level.



Alvin Trivelpiece suggests to ORNL employees some ways of defending the Laboratory against internal and external threats to its continued existence. *Photograph by Curtis Boles.*

Editor's note—ORNL Director Alvin W. Trivelpiece delivered his annual State of the Laboratory address to employees and visitors on June 12, 1997, in Eugene P. Wigner Auditorium, Oak Ridge National Laboratory.

Need To Defend Against Threats

In some sense, these thoughts are embedded in the list that I cited last year, but the emphasis is quite different. The shift in emphasis is from passive to active. To be sure, we must continue to be excellent scientists, engineers, managers, crafts workers, and support staff. But unfortunately, it has become progressively clearer that such characteristics, while still necessary, are never sufficient.

A review of the history of ORNL reveals that over the years it has faced several serious threats that might have caused its demise as a great research and development institution. Effective defensive efforts, a little offense, and a little luck have prevented that outcome. If you doubt this, I suggest that you read Alvin Weinberg's book, *The First Nuclear Era: The Life and Times of a Technological Fixer.*

Most of the past threats against the Lab were the result of outside forces. In some cases these were simple matters of regional rivalry or competition. Today, the threats to the continued existence of ORNL are as strong as they ever were. To be sure, these threats are more subtle and insidious, and they are not all external, but these threats are real. There are many ways to destroy or diminish a great institution like ORNL. Loss of a sense of purpose, or loss of dedication to uncompromising standards of excellence—either is a sure way to decay slowly over time so that recovery is not possible. Inattention to small and seemingly innocuous changes that have long-term consequences can lead to irreversible circumstances. (Speaking of slow decay reminds me I need to jog a little more frequently.)

The belief that we are an island and that events beyond our shores have no influence on us is foolish. In some cases, threats come from the unintended consequences of otherwise well-intentioned acts. For example, while I was director of the Office of Energy Research, I established a guideline of about 20% for the level of work-for-others activities at the labs. My intention was to give the lab

We must collectively and aggressively defend ORNL against those forces that would seek to diminish or destroy it.

Linda Horton makes a point about ORNL's materials research to U.S. Senators Pete Domenici (right) of New Mexico and Bill Frist of Tennessee. *Photo by Jim Richmond.*

directors the ability to prevent inappropriate work from dominating proper lab activities. I had no intention that it should become a control point for use by federal employees to regulate laboratory functions. What is worse, it didn't even prevent excessive levels of inappropriate work, as I had hoped. Silly me. I didn't even solve the original problem. We still do sometimes take in work that is not consistent with the functions and missions of a national laboratory. We need to find a better way to deal with this issue.

Need for a Plan

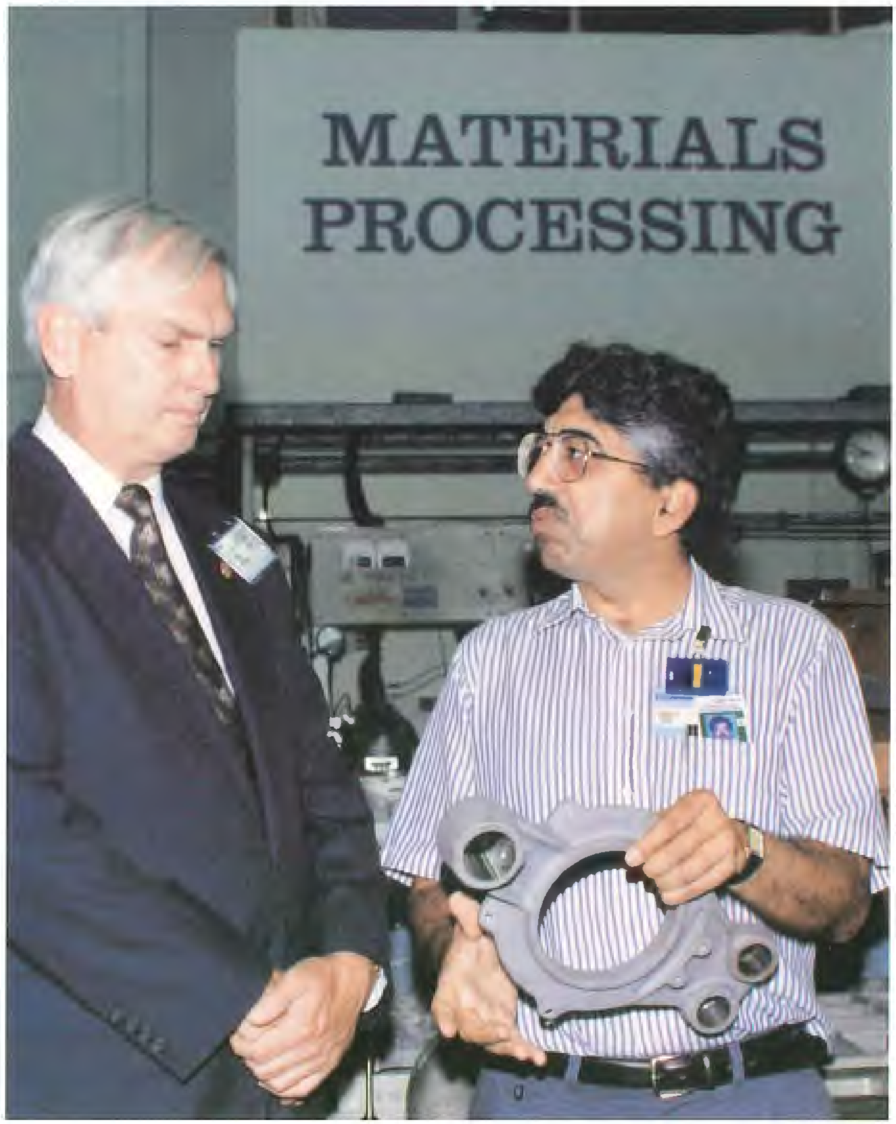
To fend off these threats, we need a strategic plan that does not merely seek to perpetuate the status quo. Rather, we need a plan that defines a challenging future, one that stretches us to perform in a manner consistent with our heritage and traditions. We should not allow ORNL to expire from creeping mediocrity or a self-inflicted, bungling bureaucracy. Developing such a plan is no easy matter. We have developed several plans in the past and we will continue to develop them in the future, as well. They haven't been easy to carry out. The problem is that in our environment, such plans cannot be more than a near-term guideline. The Advanced Neutron Source was a key element in more than one of our strategic plans. We had to adjust our planning to accommodate the reality that it was not going to be built. This doesn't mean that we should stop planning but, rather, that we have to have realistic expectations about what strategic plans can accomplish as tools.

Other threats to our continued existence come from the increased competition for shrinking federal support for research and development. This is, in part, a result of the end of the Cold War. In addition, each congressional session has spawned proposals to abolish the Department of Energy, to establish the equivalent of base-closing commissions for the national labs, to change lab missions in ways that would gut the excellence of the labs, and to transfer some of the labs to other agencies. None of these threats are easy to deal with, but they are understandable, and they are out in the open. The debate that they have generated is probably healthy, even though it makes us a bit uncomfortable. We should not be exempted from the debate on how to perform our jobs better and at less cost to the taxpayer. In fact, we should welcome such debate—if we truly believe that we can compete against anyone in the world in certain areas of basic and applied research and development.

Need To Communicate Value of Our Work

Some of the threats to our existence come from our own failure to explain to the public what we do here and why it is important to the economic well-being of this region and our nation. Remember, the Cold War is over, and we have no inherent right to expect the taxpayers to support us. We must earn their support by making sure that they

We must become politically more sophisticated and active on a national, state, and local level.



U.S. Representative Jimmy Duncan of Tennessee's 2nd District and ORNL's Vinod Sikka discuss materials processing. *Photograph by Curtis Boles.*

perceive that the work we do here is valuable to them. This is not easy, and I do not want to leave you with the impression that an occasional talk at a service club, or even a Community Day, will fix this. But such events do help, and it is important for you to get involved in such activities.

Some of the threats come from proposals to locate activities at ORNL that are not appropriate for this national laboratory. Agreeing to such proposals is difficult to resist, because in some cases it might lead to the short-term gain of a few jobs, but in the long run it would severely diminish the functionality of the Lab or its potential to seize future opportunities of great significance.

Other threats to our continued existence come from the increased competition for shrinking federal support for research and development.

Ernie Moniz, then of the White House's Office of Science and Technology Policy, was a major participant in the December 1996 dedication of ORNL's Holifield Radioactive Ion Beam Facility. ***Photograph by Curtis Boles.***

Some of the threats to us come from our own lack of political sophistication. The word "political" is the one with a small "p." It means understanding the process by which government programs get created. It also means understanding the relationship between various political entities that have influence over our well-being. I know, from various ORNL leadership development courses that I have been involved in over the past eight years, that too many of you don't have a clue about where our funding comes from or how we get it. This is not acceptable.

More of you need to have a better understanding of the process, even if you do not directly receive or compete for the money. You need to better understand some of the debates and issues of our times, because they do influence what we do. I know that many of you are raising families or work long hours here, and you correctly ask, "How do I find the time to do more?" I don't know. But let me remind you that surveys to identify national priorities consistently fail to mention science and technology. This is in spite of the fact that science and technology are the engines of our economy. So it might be appropriate to find a little time to tell your friends or neighbors what we do and why ORNL is important to them, and to our nation. Remember, the national lab that you save might be your own.

Defending ourselves against any of these threats is not straightforward or simple, and in some cases it may not even be possible. But in the words of Dylan Thomas: "Do not go gentle into that good night, Old age should burn and rave at close of day; Rage, rage against the dying of the light." We should not go gentle into that good night. We are not at the end of our days. But, we do need to become more aggressive in our own defense.

Reengineering as a Defense

Our first line of active defense is the reengineering effort that we have undertaken. Let me remind you that it was less than two years ago, on August 15, 1995, that it was announced that we would be managed by a new company. This announcement set us on a path that has been both difficult and rewarding. Between August 15, 1995, and January 1, 1996, the Lockheed Martin Energy Research Corporation was established, a new contract with the Department of Energy was written, and management of the Lab was transferred to the new company. Since then we have been about the business of improving the operations of the Lab. This is serious business! It has required the dedicated efforts of many of you here today. It will require even more effort on your part in the future. I know that some of you are impatient and frustrated that it has not gone faster or, in some cases, hasn't gone in a direction that you believe it should. Fantastic! Continued impatience and frustration are good signs. They mean that you still care.

What I worry about is not impatience and frustration, but ignorance and apathy. There is an old joke about the fellow who was asked what he thought about ignorance and apathy. He replied that he didn't know and he didn't care. Well, I do know and I do care. I hope that you do take the time to know and that you do care. Ignorance and apathy are real threats. If you don't know and you don't care, who will? After all, you are the assets of this institution. ORNL continues to provide many of you with opportunities to work on projects that are interesting and challenging. This privilege carries with it the burden of giving good value to the taxpayers who fund our work and to their agents, our elected and appointed officials in various branches of government.

Having said this, our reengineering efforts are going well. Not as fast as some of us might wish, but realistically, they are going well.

Remember, the national lab that you save might be your own.

ORNL Director Alvin Trivelpiece and former Laboratory directors Alvin Weinberg and Herman Postma show the National Medal of Science plaque awarded years ago to the late Eugene P. Wigner, a former ORNL research director. Wigner's widow gave the plaque to ORNL, and it now graces a wall in Wigner Auditorium, which was dedicated in 1996. *Photo by Curtis Boles.*

Some of the threats to our existence come from our own failure to explain to the public what we do here and why it is important to our region and nation.

The main objective of the reengineering effort is to enable us to perform our jobs better. One of the major concerns expressed about the national labs is that we cost too much. In one sense, this is a subjective judgment about what constitutes productivity in our kind of knowledge business. This judgment might be wrong because it does not take into account the quality of the work. Unfortunately, we cannot defend ourselves against charges that we cost too much because we cannot simply and accurately track our costs with a suitable cost accounting system. Correcting this is not a simple matter, nor will it be cheap, but an appropriate system will pay for itself in a short time. With the recent progress on acquiring the software for the SAP system and the hardware platform to run it, we are on our way to having the tools we need. This Delta project, as it is now known, is the linchpin of our reengineering efforts. Without such a new system, it is not clear that we can meet any of our other reengineering goals or our commitments to the Department of Energy on cost savings. We now have some 80 duplicative accounting systems at ORNL. This makes it impossible to understand where costs could be reduced. If we cannot accurately understand our internal circumstances, how can we hope to prove that we are a cost-effective alternative to another lab, a university, or industry? The new system will eliminate those separate systems and permit us to understand our costs. This new system is essential to our survival.

Trivelpiece bids farewell to Bob Van Hook, ORNL deputy director who left the Laboratory in the fall of 1996 to prepare to become president of Lockheed Martin Energy Systems. *Photograph by Curtis Boles.*

Reengineering human resources is no less important. I have said many times that our principal enduring assets are the talents and skills of the individuals who make up ORNL. We need to have a personnel system that is fair to all and competitive on a national and international basis. We need a system that pays for performance and not simply for duration of employment. We need a system that will make it easy to recruit and retain a next generation of scientists and engineers to carry out the programs of the future. I am pleased that the human resources team is doing an excellent job. You can see just what they've accomplished on the reengineering home page.

The reengineering team charged with improving the ability of the scientific and technical staff to get their work done faster, better, and at less cost to the taxpayer looked at the role of the Plant and Equipment Division. This team has developed a set of agreements that speak to improved productivity and recognize the degree to which everyone at ORNL plays a key role in its ability to survive. This is a unique agreement, and all the parties are to be congratulated. Again, the national laboratory that you save may be your own. The other reengineering projects are making good progress and will lead to improvements in our operations in due course.

What should we do about the threats to ORNL?

- Keep up the good work and don't get distracted by some of the extraneous activities. Keeping up our scientific and technical productivity during these uncertain times is one of our best defenses.

- Write letters to your sponsors and tell them that you really appreciate the hard work they do to defend the programs from which you derive your support. Write your contact at a site or operations office with the same message.

- Make sure that you let everyone you can know that ORNL is alive and kicking.

Many of you already do this through your scientific and technical societies. I hope that the rest of you make sure that the word gets out to your friends and neighbors in the area about what we do here and why it is important to the economy of the region. Talk to reporters and the press in the language they use to communicate with their readers. That is, please avoid your usual dedication to technobabble.

Need To Train New Leaders

Another line of defense has to do with training the next generation of leaders for ORNL. In that regard, ORNL Deputy Director Richard Genung has proposed that we start a program called Leadership ORNL. This program would be similar to Leadership Oak Ridge and Leadership Knoxville. It will take a selected group of employees through a several-month sequence, a few hours at a time, to review various programs and functions of ORNL. This program will conclude with the final week of our existing Leadership Development Program. This is a great idea, and Richard has graciously agreed to lead the effort to develop the Leadership ORNL program.

Secretary of Energy Peña visited ORNL on May 30, 1997. His visit lasted only one hour. As a result we weren't able to show him very much. I hope that he comes back so that we can show him more. But, even though his stay was brief, I don't think it could have gone any better. Sometimes it seems as though we don't believe our visitors have a good understanding of what we do unless we show them everything. Having had many marathon briefings inflicted on me, I can attest that this strategy doesn't work. Those of you who didn't get to personally tell Secretary Peña what

Doug Lowndes (right), ORNL corporate fellow, discusses advances in pulsed-laser deposition with Charles Townes, Nobel Prize-winning inventor of the maser who was a Distinguished Lecturer in 1996 at ORNL. Looking on is ORNL's Ben Larson. *Photograph by Curtis Boles.*

you do should rest assured that each of your colleagues who did get to brief him did an outstanding job.

Our Initiatives

Just prior to coming to Oak Ridge, Secretary Peña gave the keynote address at the Knoxville Summit. In his talk he said that he supported going forward with the National Spallation Neutron Source (NSNS) and that he looked forward to seeing it in operation at ORNL. I could say a lot more about this initiative, but that remark by the Secretary was about as good as it can get. On June 23, 1997, a team of about 60 scientists and engineers came to ORNL to conduct a review of the Conceptual Design Report for the NSNS. The objective of the review was to determine if the proposed approach will work technically, if the facility can be built as proposed, and if it can be finished within the proposed cost envelope. The NSNS is the best example of a collaborative project involving several Department of Energy laboratories that I have ever seen. Brookhaven, Berkeley, Argonne, and Los Alamos national laboratories are partners with ORNL in this project. We all hope that the $23 million requested by the Department for FY 1998 gets approved by the Congress. Even though we have a justifiable right to be optimistic, you should remember that there are always strong forces that try to stop projects like the NSNS. This is another area where the collective and aggressive defense of ORNL is essential. Anyone that believes that once a project is approved it is secure forever should examine the history of the Superconducting Super Collider.

I wish that some of our other initiatives were in as good shape as the NSNS. We do not have a solution to our problem of improving our Mouse House. This will be the focus of some increased attention during the next year.

We are still working to acquire a multi-teraflops massively parallel supercomputer. I am optimistic that we will eventually be successful in some measure, but the path to success is not clear at the moment.

The Knoxville Summit also saw the establishment of a joint University of Tennessee and ORNL transportation research center. This is off to a good start.

The Knoxville Summit saw the establishment of a joint University of Tennessee and ORNL transportation research center.

Jeff Christian of ORNL's Buildings Technology Center provides an overview on the Laboratory's energy-efficiency research to Oak Ridge City Manager Bo McDaniel (left) and Parker Hardy, president of the Oak Ridge Chamber of Commerce.

On the disquieting side, the selection of a Management and Integration contractor to run the Environmental Management programs at the former Oak Ridge K-25 Site (now called the East Tennessee Technology Park) is likely to result in a reduction in force at the Laboratory. The magnitude and timing are still only estimates, but eventually we will have to deal with some loss of work that had been done by ORNL staff.

In general, the state of the

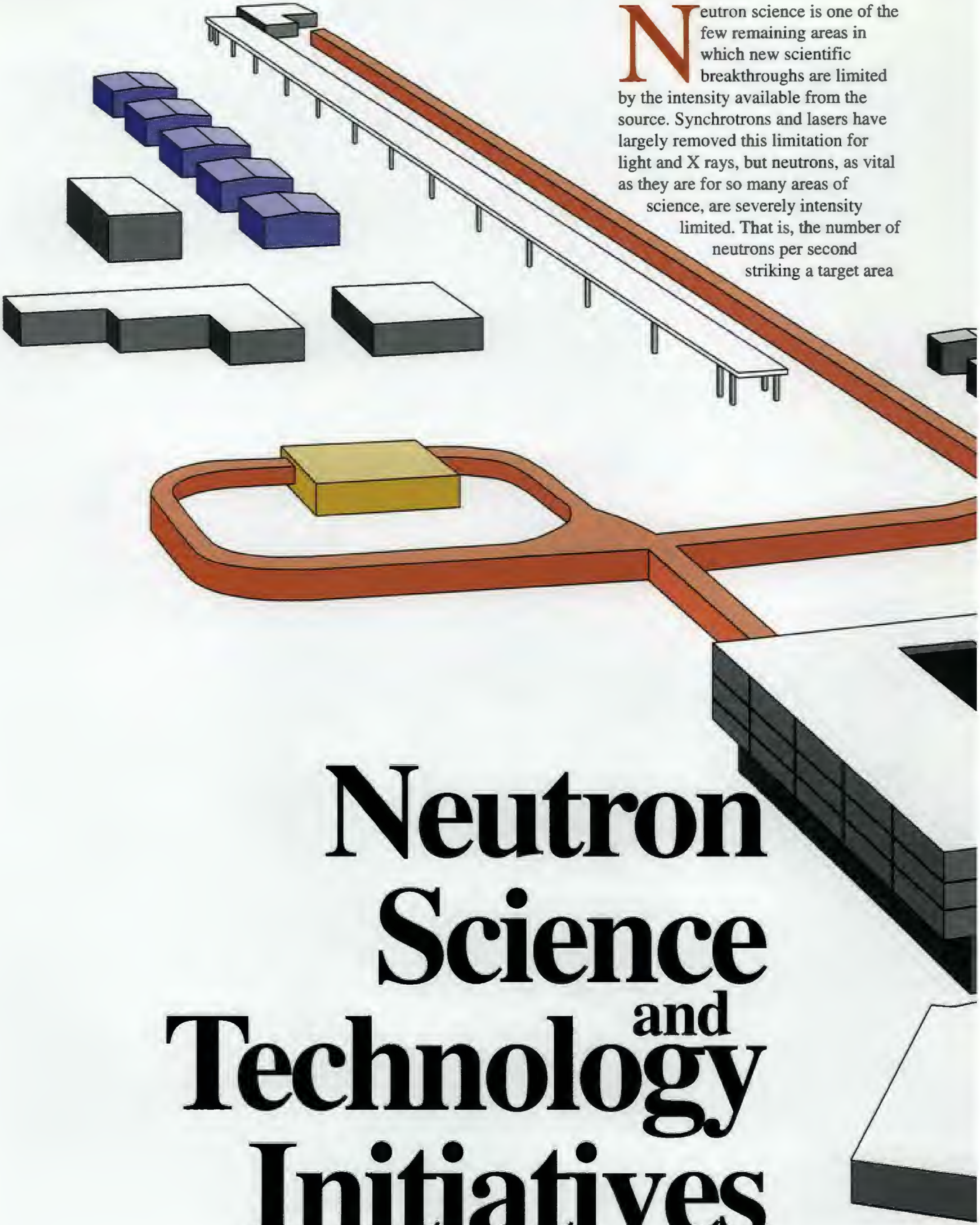
The NSNS is the best example of a collaborative project involving several DOE laboratories that I have ever seen.

Laboratory could be better, but when I look at the circumstances that many other research and development institutions are facing, I can only conclude that we are pretty well off. I am also optimistic about the generally positive climate for the support for research and development by this administration and Congress. I can only hope that future budgets reflect the positive statements recognizing the value of research and development.

In my remarks this year, I haven't singled out any individual for praise or recognition. This is deliberate. I wouldn't know how to do so without mentioning several hundred people. The list would include reengineering teams, transition teams, those of you who were presented with awards and honors, etc. You know who you are. Without you we wouldn't be making progress on any of our scientific and technical initiatives, or on our reengineering efforts, or on program development, or on any of the other projects that will contribute to our survival. It was a deliberate decision to involve as many of you as possible in the transition and reengineering teams. I am glad that we did. It is working well. Each of you has a debt to your fellow workers for what they are doing for you. I hope that as this year unfolds we can continue to make progress toward solving the many problems and challenges that we face. I am proud of what you have accomplished this year.

Last year I closed with a quote from Sir Isaac Newton about how he had seen further because he had stood on the shoulders of giants. This year I am going to close by telling you that the future of ORNL now rests on our shoulders. You must now become the giants for the next generation. This means that there is a lot of hard work yet to do. Let's get on with it. **ornl**

Liane B. Russell, Lockheed Martin corporate fellow, shows a Mouse House resident to U.S. Representative Bart Gordon of Tennessee's 6th District.



Neutron Science and Technology Initiatives

Neutron science is one of the few remaining areas in which new scientific breakthroughs are limited by the intensity available from the source. Synchrotrons and lasers have largely removed this limitation for light and X rays, but neutrons, as vital as they are for so many areas of science, are severely intensity limited. That is, the number of neutrons per second striking a target area of a sample should be significantly increased to obtain the finely detailed information on physical and biological materials that will be needed.

Although the United States pioneered in the development and use of early neutron sources, the Europeans and Japanese have capitalized on this early experience and developed newer sources that have been the best in the world for the past 15 to 20 years. In the meantime, the research uses and practical applications of neutron sources have exploded in science and industry. The need for a brighter source of neutrons in the United States is urgent, and because it will take at least six to ten years to design and construct such a source, it is essential to start now to meet the nation's future needs in neutron science.

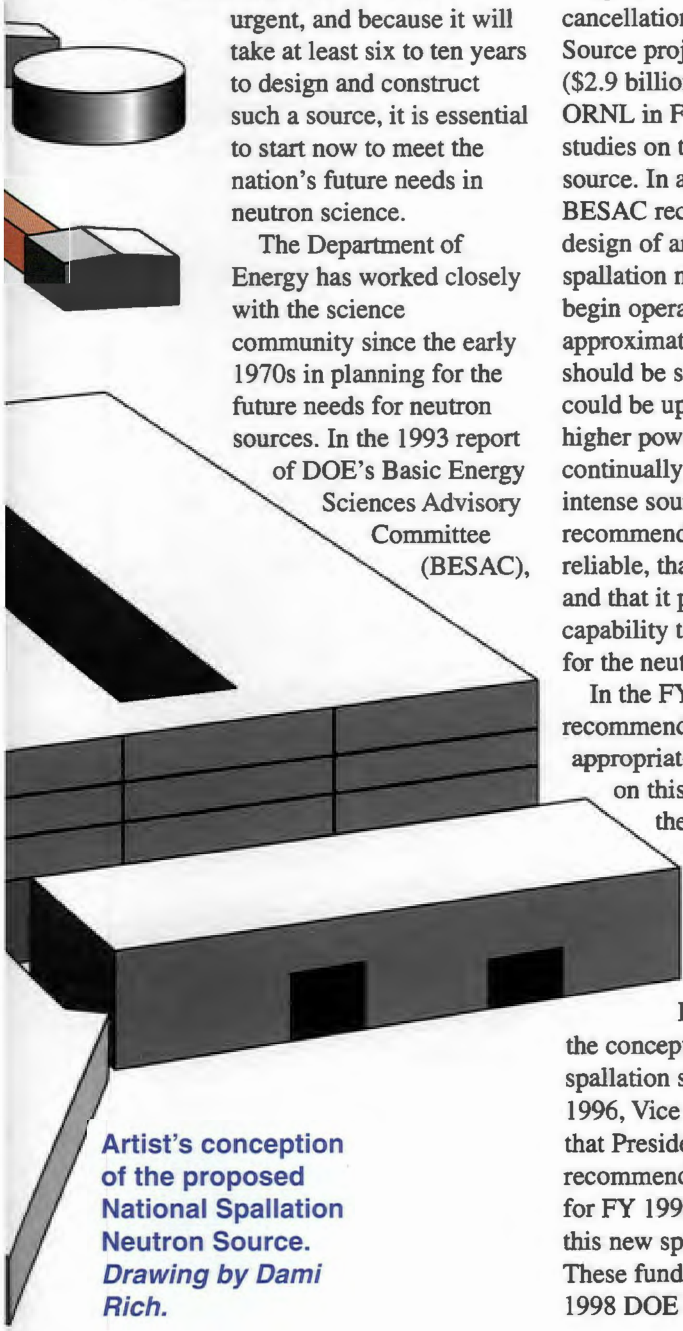
The Department of Energy has worked closely with the science community since the early 1970s in planning for the future needs for neutron sources. In the 1993 report of DOE's Basic Energy Sciences Advisory Committee (BESAC), *Neutron Sources for America's Future,* the scientific community strongly recommended to DOE the construction of the Advanced Neutron Source (a new steady-state reactor) and a complementary spallation neutron source. The report eloquently summarized the broad uses of and future opportunities for neutrons in science and technology. In the 1996 budget, DOE recommended cancellation of the Advanced Neutron Source project because of the cost ($2.9 billion) and provided $500,000 to ORNL in FY 1995 for initial scoping studies on the spallation neutron source. In a reassessment of priorities, BESAC recommended in 1996 the design of an accelerator-based spallation neutron source that could begin operation at a beam power of approximately 1 megawatt. The design should be sufficiently flexible that it could be upgraded to significantly higher powers in the future to meet the continually growing needs for an intense source. The report also recommended that the source be highly reliable, that it have high availability, and that it possess the inherent design capability to provide future capabilities for the neutron user community.

In the FY 1996 budget, DOE recommended and Congress appropriated $8 million to begin work on this new source. DOE directed the funds to ORNL to initiate research and development (R&D) and a conceptual design. The department has since provided an additional $8 million in the FY 1997 budget to complete the conceptual design for the new spallation source. On September 6, 1996, Vice President Gore announced that President Clinton would recommend $23 million to Congress for FY 1998 to accelerate design of this new spallation neutron source. These funds have been included in the 1998 DOE budget requests, and DOE's Office of Energy Research has designated neutron science as a top priority for FY 1998.

Spallation Source Collaboration

To complete the design of the proposed $1.33 billion neutron source, ORNL has organized a collaborative design effort called the National Spallation Neutron Source (NSNS) project, which involves ORNL, Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL), and Los Alamos National Laboratory (LANL). Other laboratories, U.S. industrial firms, and universities are already involved in the conceptual design, and more will join as the project matures.

This truly collaborative design effort is a relatively new approach to designing and constructing a major DOE project. Although ORNL has responsibility for coordinating the design and construction and will ultimately operate the NSNS, the other participating laboratories are totally responsible for designing, constructing, and delivering their parts of the system for the final facility. The project focuses on the strengths of the individual DOE national laboratories and avoids costly duplication of expertise and subsequent downsizing by the lead laboratory when the project is finished. This collaborative approach was taken to gain access to the best technical expertise available, to initiate a conceptual design process that made the most efficient use of DOE manpower and resources, to incorporate results of a number of previous feasibility studies conducted by the collaborating laboratories, and to consolidate community consensus. In addition, memoranda of understanding have been signed with the European Spallation Source and



Artist's conception of the proposed National Spallation Neutron Source. ***Drawing by Dami Rich.***

The U.S. urgently needs a brighter source of neutrons to make possible scientific breakthroughs that could significantly benefit the nation.

several European laboratories that will allow access to research results and technology developments that could further leverage the NSNS design effort. Similar cooperative technology-sharing arrangements have been initiated with laboratories in Japan, as well.

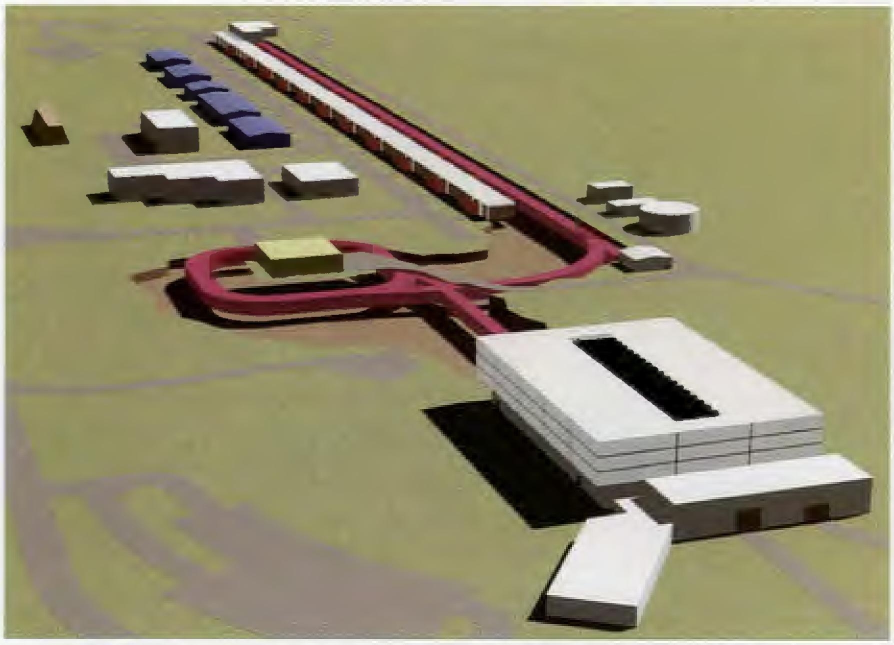
The NSNS Design

The reference design proposed for the NSNS consists of a high-energy linear accelerator (linac) injecting negative hydrogen ions from an ion source into an accumulator ring that produces short bursts of protons at extremely high energies and power levels. These proton pulses will be directed onto a heavy metal target, which will be a container of liquid mercury. In the spallation process, protons interact with and heat the mercury nuclei, which then release neutrons. The free neutrons will be moderated and guided through beam lines to areas containing special instruments. There the neutrons can be used in a wide variety of experiments.

BNL, LANL, and LBNL are responsible for the accelerator system design, which will be coordinated by an accelerator design group at ORNL. LBNL is responsible for the ion source and front-end system that produces the hydrogen ion beams. LANL is responsible for the linac, which accelerates this beam to energies of 1 billion electron volts (GeV). BNL is responsible for the accelerator ring, which bunches and intensifies the ion beam into proton pulses of about 1 microsecond in duration and then delivers these pulses onto the heavy metal target to produce the neutron beams. ORNL is responsible for the coordination, installation, and operation of the new source; for project management; conventional construction; design and construction of the liquid mercury target; and—with ANL—the experimental facilities and instruments that will be used by the neutron science community.

The goal of the NSNS is to complete the conceptual design in time for a construction line item request to DOE for FY 1999. The conceptual design of the NSNS will take three years to complete, and assuming a 1999 construction start, it should be in operation by the year 2005. The completed facility will occupy a site of approximately 110 acres. The NSNS will produce the highest-flux, pulsed, neutron beams in the world for neutron scattering. The NSNS is designed to make future upgrades to higher powers extremely cost effective, so that the United States should be able to stay at the forefront of neutron science for many years to come.

The NSNS will attract 1000 to 2000 scientists and engineers each year from U.S. universities, industries, government laboratories, and other nations.



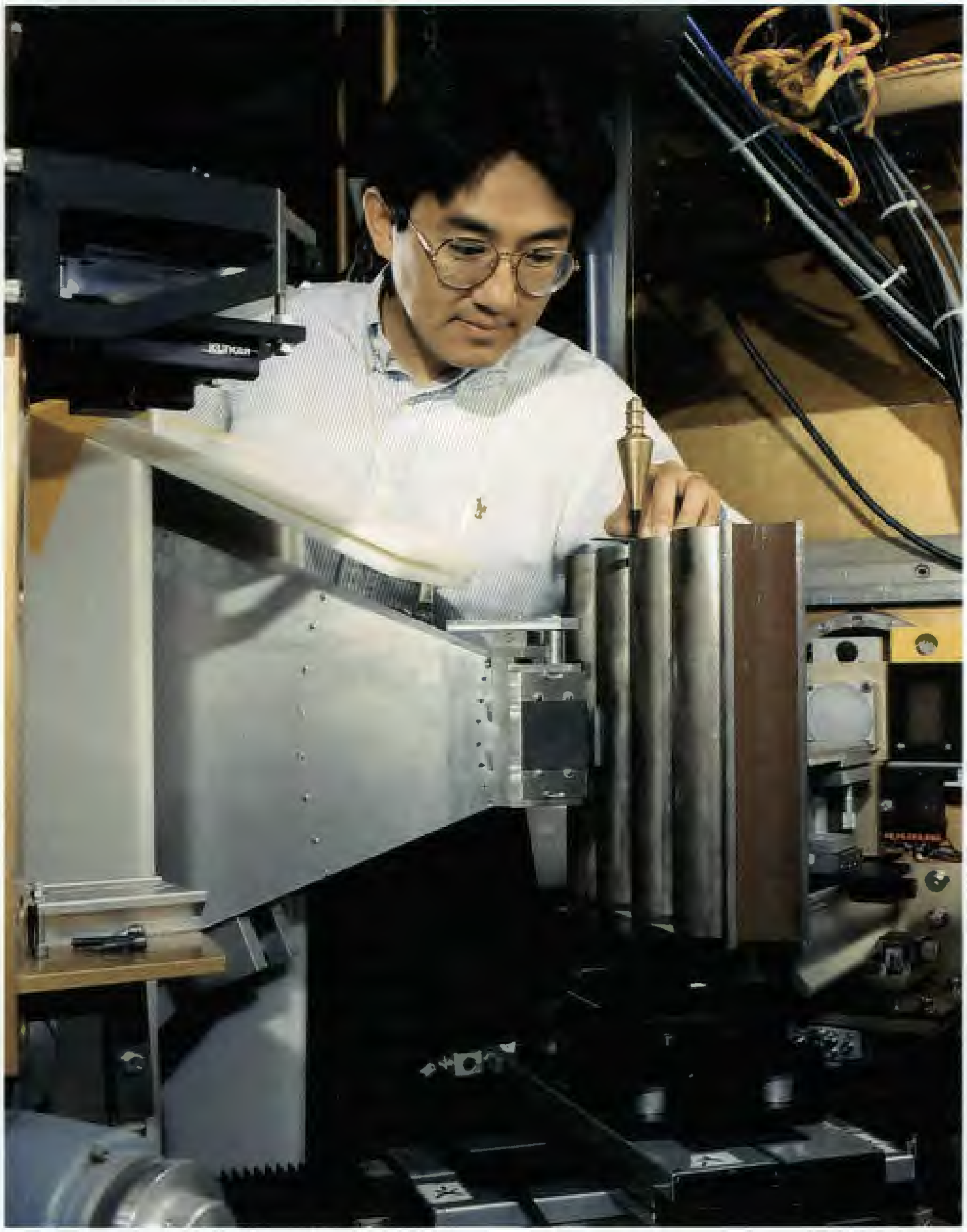
The Joint Institute for Neutron Sciences will provide meeting facilities, offices, laboratories, and housing for researchers throughout the world.

Joint Institute for Neutron Sciences

It is estimated that the NSNS will attract 1000 to 2000 researchers each year from U.S. universities, industries, government laboratories, and other nations. The governor of Tennessee has committed $8 million for ORNL and the University of Tennessee (UT) to construct a Joint Institute for Neutron Sciences (JINS). Funds were included in the state of Tennessee's FY 1996 budget to begin design of the JINS. This facility will enhance the utility of the NSNS and ORNL's High Flux Isotope Reactor by providing meeting facilities, offices, laboratories, a communication center, and housing for scientists and engineers from universities, industries, and the international community. It will also be a focus for expanding neutron science R&D with UT, other regional universities, and industrial collaborators. It will serve as an interface and economic-development gateway for outside access to ORNL facilities.

Now that the intensity of activities to restore U.S. leadership in neutron science has picked up, we hope to stay on the path to many new scientific breakthroughs.—*Bill Appleton, director of the National Spallation Neutron Source.* ornl

Aiming for the Next Level: Upgrades for the High Flux Isotope Reactor



Xun-Li Wang examines a composite steam tube panel used in a chemical recovery boiler in a paper mill. The panel is placed between a beam of neutrons (that will be produced at right when the High Flux Isotope Reactor resumes operation) and a detector-array (left). Neutron scattering from the panel will help scientists determine residual stresses in the tubes caused by the welding process. The goal of this research is to find ways to manufacture tube panels with lower residual stresses and with improved resistance to cracking. Cracking in steam tubes allows water to contact hot chemicals and possibly cause a deadly, economically devastating boiler explosion. *Photograph by Curtis Boles.*

ORNL's High Flux Isotope Reactor (HFIR), which provides the highest thermal neutron flux in the world, is a national resource that has missions in four important areas: radioisotope production, neutron scattering research, neutron activation analysis, and irradiation testing of materials. To perform these important missions even better, modernization of the HFIR is a must.

The reactor was originally designed primarily to produce the transplutonium isotopes—elements that do not occur naturally on earth, beyond plutonium in the periodic table of elements. However, over time, the neutron scattering mission has grown in scientific and economic importance—providing, for example, much of our knowledge about the molecular and magnetic structure and behavior of the new high-temperature superconductors. The package of upgrades (some already under way) would enhance our capabilities in all four areas, but the biggest impact would be on neutron scattering.

One enhancement proposed is a return to the original 100-megawatt (MW) design power level instead of the 85-MW level that has been used since 1989. This change will benefit all missions, because the neutron production rate, which is proportional to reactor power, will be increased by nearly 20%. Likewise, modernizing instrumentation and electrical equipment and replacing certain other components of the reactor system will reduce maintenance downtime, making more operating time, and hence more neutrons, available for all users.

Neutron Scattering Improvements

For neutron scattering, a cold source will be installed in one of the reactor's four beam tubes. The source will be an aluminum chamber of very cold hydrogen, at a temperature of only 20 K (about –420°F and –253°C). At this temperature, the hydrogen molecules move fairly slowly, so neutrons that enter the chamber are slowed down by collisions with those molecules. These very slow neutrons have a larger wavelength than the faster ones, so cold neutrons are more useful for studying large molecules, including big polymer chains (plastics) and biological structures (e.g., proteins). The best cold neutron beams in the world are those at the Institut Laue-Langevin (ILL) in France, but with higher power at the HFIR (85–100 MW vs 59 MW at ILL) and new cold source design concepts, our cold beams will be as bright or brighter. Although space limitations mean that we will have fewer beams and instruments, the ones we do have will be world beaters.

The second change will be to install larger beam tubes for neutron scattering and to put neutron guides at an existing beam port called HB-2. Neutron guides work exactly like fiber-optic guides—they are rectangular conduits, typically about 5 × 18 centimeters (2 × 7 inches), whose inside surfaces are coated with a layer or, for greater effectiveness, multiple layers of a material (e.g., nickel) that will reflect neutrons that strike the surface at a glancing angle. Thus, the guides can bring neutrons from close to the reactor, in a series of ricochets, to a distant instrument with little loss of neutrons. This is important for two reasons: first, there isn't enough room close to the reactor for many big instruments. Second, close to the reactor is considerable background radiation, including gammas and fast neutrons, that tend to swamp the small signals scientists are looking for. However, the guides reflect only fairly slow neutrons, so this undesirable background radiation escapes through the wall of the guide, where it can be absorbed by shielding, before reaching the experimental sample and the detector at the far end. These guides will provide additional spaces for instruments in the HFIR beam room. Eventually, we hope to extend the guides outward from the reactor into a new "guide hall" where up to nine additional neutron scattering instruments could be placed.

The HFIR already has the most intense beams of thermal neutrons (those that have slowed down to the equivalent of room temperature or so) in the world. The enlarged beam tubes and guides will make them brighter still and, by increasing the number of beams and instruments, will also raise the number of users that can be accommodated.

Neutron Activation Analysis Upgrades

Neutron activation analysis (NAA) is a sensitive, quick technique for determining the elemental composition, including trace elements, in a sample (such as contaminated soil in a small box). In general, the sample is inserted in the reactor for a predetermined, usually short, period: The intense neutron bombardment will make many of the elements radioactive. The elements can be identified by detecting the characteristic signatures in the emitted artificial radioactivity. An important example is the analysis of samples from the floodplain of East Fork Poplar Creek in Oak Ridge for environmental pollutants such as mercury. The upgrade proposal includes more, and larger, facilities that will allow improved access to the reactor so that measurements of more irradiated NAA samples can be taken.

Isotope Production

The HFIR, because of its very high neutron flux, is able to produce radioisotopes of very high specific activity. Some are needed for diagnostic and therapeutic medical applications (including treatments for patients having ovarian or prostate cancer). Other isotopes find industrial applications, for example, iridium-192, which is used as a source of gamma rays for the radiographic inspection of welds. The upgrade proposals include additional irradiation positions and an improved neutron spectrum for isotope production.

Materials Testing Capabilities

The development of new fusion and fission reactor systems depends on the development and testing of materials that can retain their strength, ductility, and shape, among other characteristics, even under intense radiation. Because of its high flux and versatility, the HFIR is the preferred reactor to conduct these materials tests. We propose to provide improved capabilities for handling and dismantling the test capsules.

Because neutrons are now so important to so many fields of science and engineering, the upgrade program has been carefully planned to minimize the time the HFIR will be out of service. It is planned that much of the new equipment will be installed during a planned outage of HFIR, expected to begin in 1999 to replace a large beryllium neutron reflector, an essential part of the reactor.

The HFIR is a research reactor whose operations are essential to the nation. It provides some of the world's best capabilities for isotope production, neutron scattering, NAA, and materials irradiation testing. The planned upgrades will make the world's highest-flux research reactor even better.—*Colin D. West, director of the Neutron Sciences Program Office at ORNL.* **ornl**

Functional Genomics Research

Human genome research worldwide is now shifting into its next phase of completing the sequence of chemical bases in the entire human genome. Within the next decade, the Department of Energy's Joint Genome Institute and the other genome centers will have discovered, mapped, and sequenced all of the genes that define humanity. This knowledge will undoubtedly change the nature of biological research in the "post-genome era." Using the sequence gene mapping information from the genome program, molecular geneticists will be able to begin tackling problems in biological research that were previously impossible to define or solve. For the first time in human

Monica Justice shows mutant beige mice, which are models for the human disease Chediak-Higashi Syndrome, to U.S. Representative Jimmy Duncan of Tennessee's 2nd District (right) and Rick Woychik, then director of ORNL's Functional Genomics Program, who briefed the congressman on ORNL's capabilities in relating genes to body functions. *Photograph by Curtis Boles.*

history, scientists will have the tools that will help them begin to understand, at the molecular level, how complex networks of genes are involved in human disorders, ranging from birth defects to physical and mental illnesses in the adult.

An important focus of research in the post-genome era will be a study of how genes function within the body. Biologists have been studying gene function for many years, but most of their research has been slow, very costly, and directed at single genes. Access to the powerful reagents from the genome program will change all of this. In the post-genome era, among other things, it will be possible to (1) perform gene function experiments on a genome-wide scale, hence the name functional genomics; (2) study large numbers of genes, perhaps all of them, at the same time; and (3) begin to study the large numbers of functional partnerships that genes establish with other genes. The understanding of these genetic relationships will provide an enormous insight into how genes participate in human health and well-being.

Many different approaches can be taken to studying gene function. One of the most useful ways to gain insight into the function of a gene is to turn the gene off or change its normal pattern of expression through genetic mutagenesis. For example, when a gene is not functioning normally and an individual carrying that mutant gene develops a certain form of cancer, the cancerous function can be assigned to that gene. In fact, this approach has enabled scientists to identify the genes associated with major diseases in humans, such as Huntington's disease, cystic fibrosis, and breast cancer.

Because gene mutagenesis is such a useful way of studying gene function, it would be useful to generate new gene mutations on a genome-wide scale. For obvious reasons this cannot be done in humans. Therefore, genome researchers are turning to model organisms like the mouse. The mouse is anatomically and physiologically similar to humans in many important ways. Mice, for example, develop a kind of obesity and adult-onset diabetes that are very similar to conditions in humans. Mice can be afflicted with many other "human" diseases such as polycystic kidney disease, which is one of the major causes of kidney problems in the human population. The most compelling reason to use the mouse as a model organism is that, in many instances, a mutation in a mouse gene that is the counterpart of a major human disease gene can cause essentially the same disease in mice as that observed in humans. In these instances, the mutant mice are exceptionally appropriate models of human disease. Also, unlike other model organisms, mice have a relatively short generation time. Considering that the gestational period for the mouse is about three weeks, the time to sexual maturity is another three weeks, and each pregnant mouse has about ten offspring, one breeding pair of mice can give rise to tens of thousands of mice in just a matter of months. Mice can also be bred in such a way that all the offspring are essentially twins of each other, which is an important consideration for many genetic experiments.

ORNL scientists are preparing to investigate, at the molecular level, how complex networks of genes are involved in human disorders.

ORNL's unique heritage in radiation biology puts it in a strong position to conduct large-scale mutagenesis experiments in the mouse. Based on the extensive work in mouse genetics research by Liane and Bill Russell over the last several decades, the Mammalian Genetics Section in the Life Sciences Division has the knowledge, resources, and experience to perform mouse mutagenesis on a scale that is unparalleled at most other institutions. ORNL operates one of the world's largest experimental colonies of mice for research purposes. In the facility dubbed the "mouse house," hundreds of mutant lines of mice are being maintained by trained geneticists. Many of these mutants develop specific forms of disease that model conditions in humans. For example, several different mutations have been identified that give mice a genetic predisposition to becoming fat. One of these "fat" genes has been identified at the molecular level at ORNL (for more details, see the highlight on p. 26). The human counterpart for this gene has also been identified, and, as is true for most genes in humans and mice, the human gene encodes a protein that is remarkably similar to that encoded by the mouse gene (see figure on next page). By cloning the mouse gene and analyzing a mouse mutant line, it was possible to assign an obesity function to a gene on the human DNA.

In FY 1997, through its Laboratory Directed Research and Development Program, ORNL launched a focus area in functional genomics that will be supported by internal funding for the next three years. This new initiative will enhance the Laboratory's capabilities in support of the DOE mission in determining gene functions. The functional genomics initiative will build on our expertise in mouse mutagenesis and will incorporate many other capabilities at ORNL, including protein chemistry, structural biology, instrumentation, robotics, automation, and computer science. The interdisciplinary nature of this new program will allow the mouse mutagenesis capabilities to be expanded to genome-wide proportions.

Through this exploratory research funding, ORNL is positioning itself ultimately to form a core functional genomics effort dedicated to the large-scale generation, characterization, molecular analysis, and distribution of new mutations in the mouse. To reach this goal, it will be necessary to achieve a major increase in the rate at which new heritable mutations can be generated and screened for disease traits that are caused by single and/or multigenic mutations. To map and quickly identify these new mutations, researchers will need to develop new strategies for high-throughput analyses of DNA fragments that are markers for specific sites on the genome. New approaches in molecular biology and instrumentation must be generated for the purpose of differentiating wild-type from mutagenized genes and to detect changes in gene expression in mutant lines of mice. Innovative approaches must be developed for cataloging this new information, and new user-friendly tools must be generated for disseminating this information to the rest of the world.

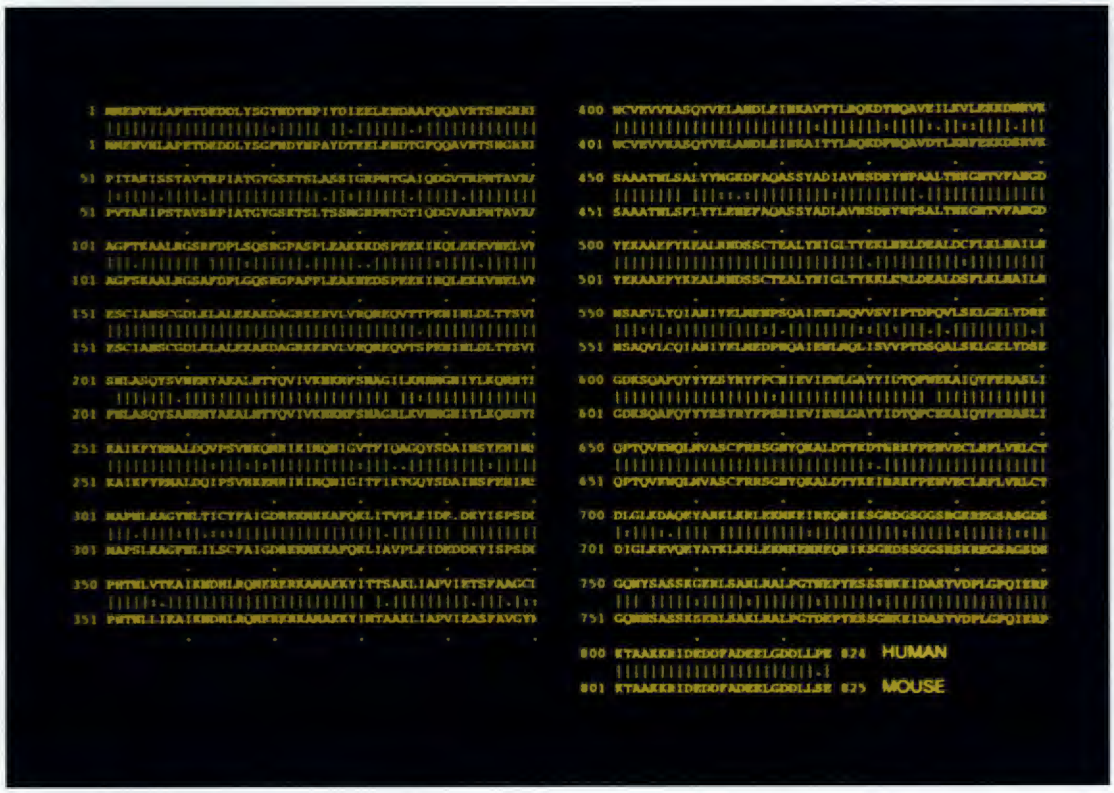
Over this past year, this new program began to take shape. Our researchers worked on a variety of projects, such as the development of (1) innovative approaches for conducting mouse mutagenesis experiments that have the potential to be applied on a genome-wide scale; (2) novel, high-throughput techniques using mass spectrometry to detect specific kinds of new mutations in mouse chromosomes; and (3) new functional genomics applications for ORNL's award-winning "lab on a chip" for detecting genome-wide molecular markers that are generated by the polymerase chain reaction. They also worked on expanding research on new miniaturized devices, called genosensors, that can be applied to the simultaneous analysis of hundreds and even thousands of genes from mutant mice. ORNL's microfluidics and imaging capabilities are crucial to the success of this research.

We are also working to build a robotics capability for the functional genomics infrastructure at ORNL. To keep all of the data that are being generated from this collective effort organized and to help bring about a new user-friendly interface for this research to the outside world, ORNL investigators are developing innovative bioinformatics capabilities that use the Laboratory's unique computing capabilities.

Collectively the programs that were funded in FY 1997 are allowing the functional genomics effort to take the shape of a program that is highly compatible with the established goals. Projects that will be funded in the next three-year program will build on the accomplishments of the first year will incorporate more of our capabilities in molecular biology, biochemistry, instrumentation, and automation. The willingness and ability of ORNL researchers to conduct interdisciplinary research increase the likelihood that our functional genomics program will be successful.

Research in functional genomics will help us continue our tradition of success in the biological sciences, thereby serving the needs of DOE and our society. It will also facilitate expanded outreach and partnerships with industry and academia. In the past, the multidisciplinary achievements at ORNL, which bridge basic and applied research, have been honored by two Enrico Fermi Awards from DOE and more than a dozen memberships in the National Academy of Sciences. The new functional genomics effort should help provide ORNL with improved opportunities for making exciting new discoveries in the post-genome era that will greatly expand our knowledge of how genes function. Using this information, scientists will be able to develop drugs and other therapies to improve human health.—*Rick Woychik, former director of ORNL's Functional Genomics Program.* **ornl**

Knowledge of gene function may lead to new therapeutic drugs.



A comparison of the types and order of DNA bases in human and mouse genes shows a striking similarity.

High-Performance Computing: Maintaining a Leadership Pace

The confluence of ever-accelerating scientific expectations and technical innovation is dramatically extending the limits of computational power. Indeed, "limit" may be an inappropriate word here. Machines now running exceed a teraflops (1 trillion FLoating point OPerations per Second, or 1 TF), 10-TF machines are being planned, and the path to petaflops (1000 TF) is being defined. So, given the remarkable rate of change in the computing realm, we must talk in terms of current technological capabilities, as well as near-term design objectives with a well-defined time horizon in describing computational capabilities. It is clear, though, that planning for machines in the range of 5 to 10 TF in the 1998–1999 time frame is an appropriate target; this is the target for which we are aiming.

The Center for Computational Sciences (CCS) at ORNL has been one of the world's leaders in computational power over the last several years. However, contracts in place for systems at DOE Defense Programs (DP) laboratories (Los Alamos National Laboratory and Lawrence Livermore National Laboratory) provide for systems extending to 3 TF, or well beyond the roughly 200 gigaflops (GF, or billion flops) in the CCS. The applications emphasis for these DP machines is assurance of the reliability of the U.S. nuclear stockpile in an era of no weapons testing, which basically defines DOE's Accelerated Strategic Computing Initiative (ASCI).

Computation, modeling, and simulation requirements for the DOE Energy Research (ER) community also extend into the multiple-TF realm. Providing a substantial component of this computational capability and establishing routine TF-level distributed computing are the foci of this ORNL initiative. Given the striking accomplishments of the CCS in bringing its Intel Paragons to very high levels of productivity by

- connecting the two largest CCS Paragons over high-speed asynchronous transfer mode (ATM) OC-12 networks to provide a machine with peak performance near 200 GF and

- taking the distributed computing lead with Sandia National Laboratories (SNL) by solving huge problems through linking the Paragons at the two sites over ATM networks,

the CCS clearly represents the development environment required to bring a multiple-TF machine to optimal effectiveness for an extensive range of ER applications. This last point is of prime importance because the ER requirements extend across a very wide spectrum.

Materials Science

A striking array of challenges awaits TF-level machines. Meaningful modeling of mechanical behavior becomes possible, including static and dynamic properties of dislocations and dislocation arrays, radiation effects, and complex phenomena such as stress-corrosion cracking. Further, proper modeling of mechanical behavior can lead to structural integrity and an understanding of aging far surpassing current levels. Multiple-component-alloy design studies with the objective of maximizing strength-to-weight ratios will be key to achieving fuel efficiency goals for automobiles. Investigations of the performance of these alloys in simulated harsh environments will lead to alloys providing improved longevity and safety when operating in such environments and will also extend the range of operating conditions for many systems. Modeling of computer processor and memory chips with ever-decreasing feature sizes will require highly sophisticated semiconductor models incorporating accurate thermodynamic capabilities to deal properly with heat generation and dissipation strategies.

Computational Chemistry

A multi-TF system will greatly aid computational chemists in meeting the challenge of accurately describing structure and interactions in nucleic acids (DNA and RNA) and in understanding the interactions between these molecules and proteins. Successes here will have very significant implications for biology and medicine. It is likely that an understanding of the complexities of protein folding can emerge from computational studies with adequate power. We anticipate dramatic advances in characterizing catalytic mechanisms in problems such as the photoinduced transformation in bacteriorhodopson and key electron and proton transfer steps in photosynthesis. Detailed models for catalysis in complex structures such as zeolites will be computationally manageable. Very powerful systems will make it possible to investigate in detail the subtle chemistry that occurs in our atmosphere and in the earth's ozone shield.

Computational Fluid Dynamics

Computational fluid dynamics simulations usually involve flow coupled to processes such as chemical reactions. Frequently there are great disparities in temporal and spatial scales that demand powerful computational resources for simulations of high accuracy. Compressible fluid flow is of fundamental importance in a wide variety of contexts—wakes and boundary layers of aircraft, missiles, and projectiles in flight; mixing regions of air and combustible material in reactive flows; environmental fluid dynamics of atmospheric storms; and mixing in rivers and estuaries. More accurate models requiring TF computing are needed here as they are for the design of superior spark-ignition and compression-ignition (diesel) engines.

Quantum Chromodynamics (QCD)

QCD is widely accepted as the fundamental description of the strong interactions of elementary particle

A possible layout of the computer cabinets for a 5-teraflops massively parallel computer. Such a machine will be able to perform 5 trillion arithmetic calculations per second. By comparison, the Intel Paragon XP/S 150 at ORNL can perform 150 billion arithmetic calculations per second.

physics. Much of the experimental work carried out at DOE's high-energy and nuclear physics laboratories is aimed at probing this theory; it has seminal implications for understanding the development of our universe. In principle, this theory should allow the calculation of some of the most fundamental quantities in nature. In practice, it has proven extremely difficult to extract many of the predictions of QCD. Currently, the only promising avenue for doing so is through large-scale numerical simulations. A multi-TF system should enable definitive first-principles calculations of the mass spectrum of strongly interacting particles such as neutrons and protons and of their observable physical properties. Another computational target is an understanding of the phase transition from ordinary matter to the suggested quark-gluon plasma state of matter. This state of matter, where particles like protons disintegrate into their quark and gluon constituents, is predicted to occur under conditions of extraordinarily high energy, in other words, extraordinarily high temperatures. The Relativistic Heavy Ion Collider, a powerful accelerator soon to come on line at Brookhaven National Laboratory, will help scientists search for evidence of the quark-gluon plasma; computational modeling will be needed to complement this search.

Geosciences

A multi-TF system would enable highly accurate three-dimensional simulations of earthquakes in specific geographic locales. In addition to providing an expanding database and concomitant extended understanding of these phenomena, the simulations would provide ground motion information to assist architects and engineers in designing buildings capable of withstanding these motions.

The complex nature of subsurface biological, physical, and chemical processes has, in the last decade, prompted extensive development of computer models to simulate and predict the fate of environmentally toxic materials in one of the most valuable resources of this nation—groundwater. The addition of valid bio-physicochemical processes to current models of this highly heterogeneous system necessitates computational systems in the TF range. Such systems will enable the incorporation of scientifically validated subsurface flow and transport processes in multiphase fluids and fractured geological formations and promote the inclusion of phenomena such as in-situ bioremediation and molecular-level geochemical kinetics. Perhaps even more significant are the large-scale water resources management strategies that we would be able to establish given TF-level computing. Risk assessment and decision analysis could be carried out for a time scale sufficiently long to provide scientifically sound and technologically plausible solutions, thereby providing invaluable support for those making environmental and safety decisions where financial realities compel priority setting.

Global Climate Change

Substantial strides have been made in modeling the oceans and the atmosphere. However, additions of land mass details and polar ice together with improved resolution require TF capabilities. Having accurate models is extremely important for the future because the effects of pollution, greenhouse gases, and other atmosphere constituents, if improperly analyzed and interpreted, can lead to technical and political decisions that can have seriously deleterious consequences for the planet.

In all of these application areas, and more that could be included, important problems already identified require computational power in the range of 5 to 10 TF and even more for some areas. Processing power is but one factor in the specification of the requisite balanced system. For a 5-TF system, additional requirements include

- computer memory—5 terabytes
- data storage capacity—7 petabytes
- input-output (I/O) capacity—200 gigabits/s

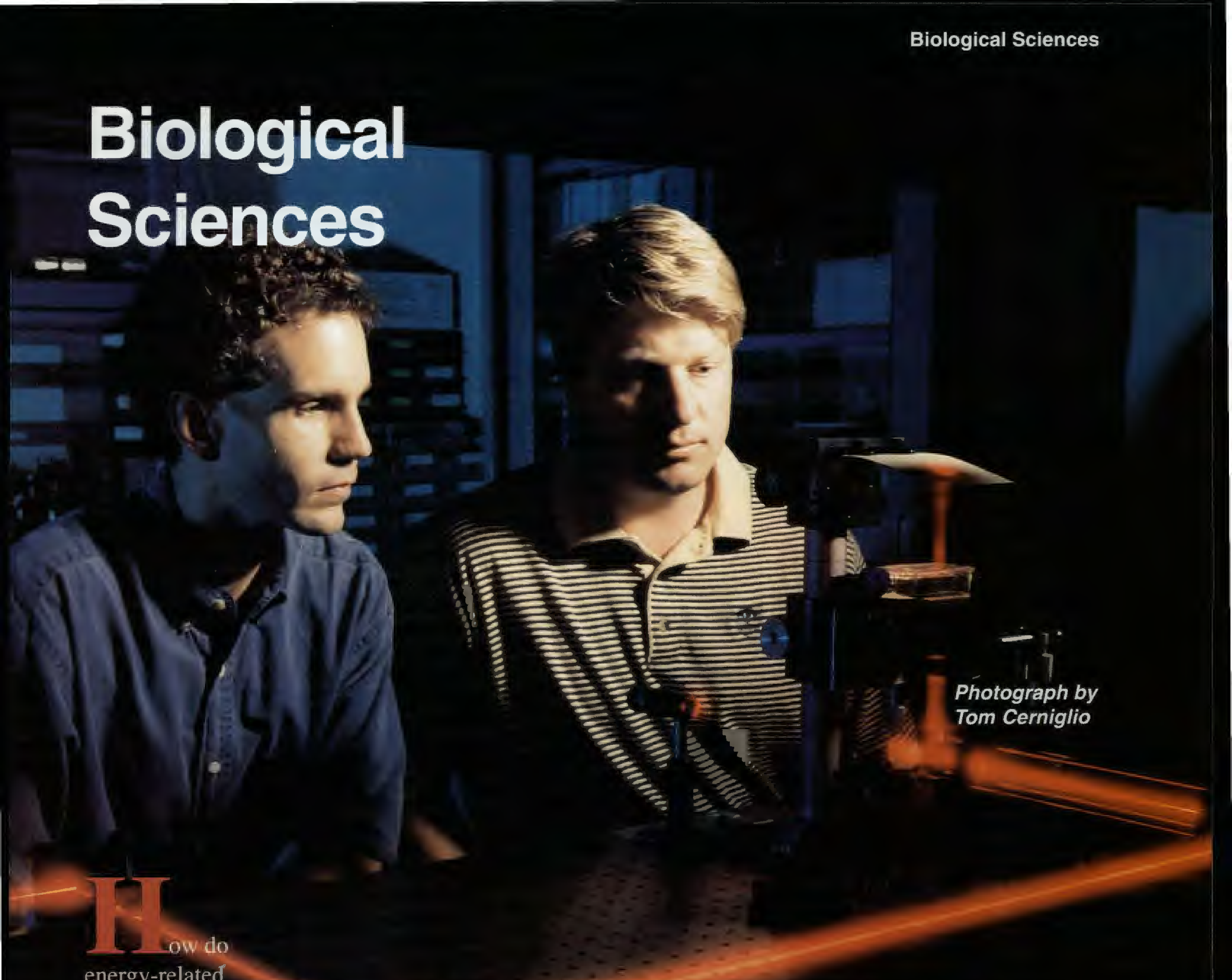
Further, the CCS partnership with SNL has shown the way to solving problems of extraordinary size and complexity through linking supercomputers over high-speed networks. To extend this strategy into the multiple-TF regime, an essential expectation in our view, will require networks operating in the range of 10 gigabits/sec, roughly OC-192 requirements.

The extension of computational capabilities into the range described here does require a very high degree of sensitivity to the tenets of scalability. To illustrate the scope of the proposed system, we show on p. 21 a possible layout of the computer cabinets for a 5-TF machine.

Hardware does not a 5-TF computer make. Software challenges abound. Operating systems, I/O software, communications software and protocols, visualization systems, and network interfaces, together with applications software, must all work together with the hardware in solving problems. Indeed, it is here in the software realm that many of the most difficult scalability issues will emerge.

It is obvious that there are major challenges in designing, developing, and ensuring near-optimum performance from a system in the 5-TF range. However, the contributions this system would provide to the ER science/technology programs and to meeting ever-expanding expectations of these programs demand that these challenges be faced. Furthermore, the partnership between ORNL and SNL that has brought distributed computing to unprecedented levels of capability should be encouraged to extend these capabilities into the TF realm. With the Intel Teraflops machine now being assembled at SNL (the design goal is 1.8 TF) and the proposed TF-level machine at ORNL, this extension is assured.—*Kenneth L. Kliewer, director of the Center for Computational Sciences at ORNL.* ornl

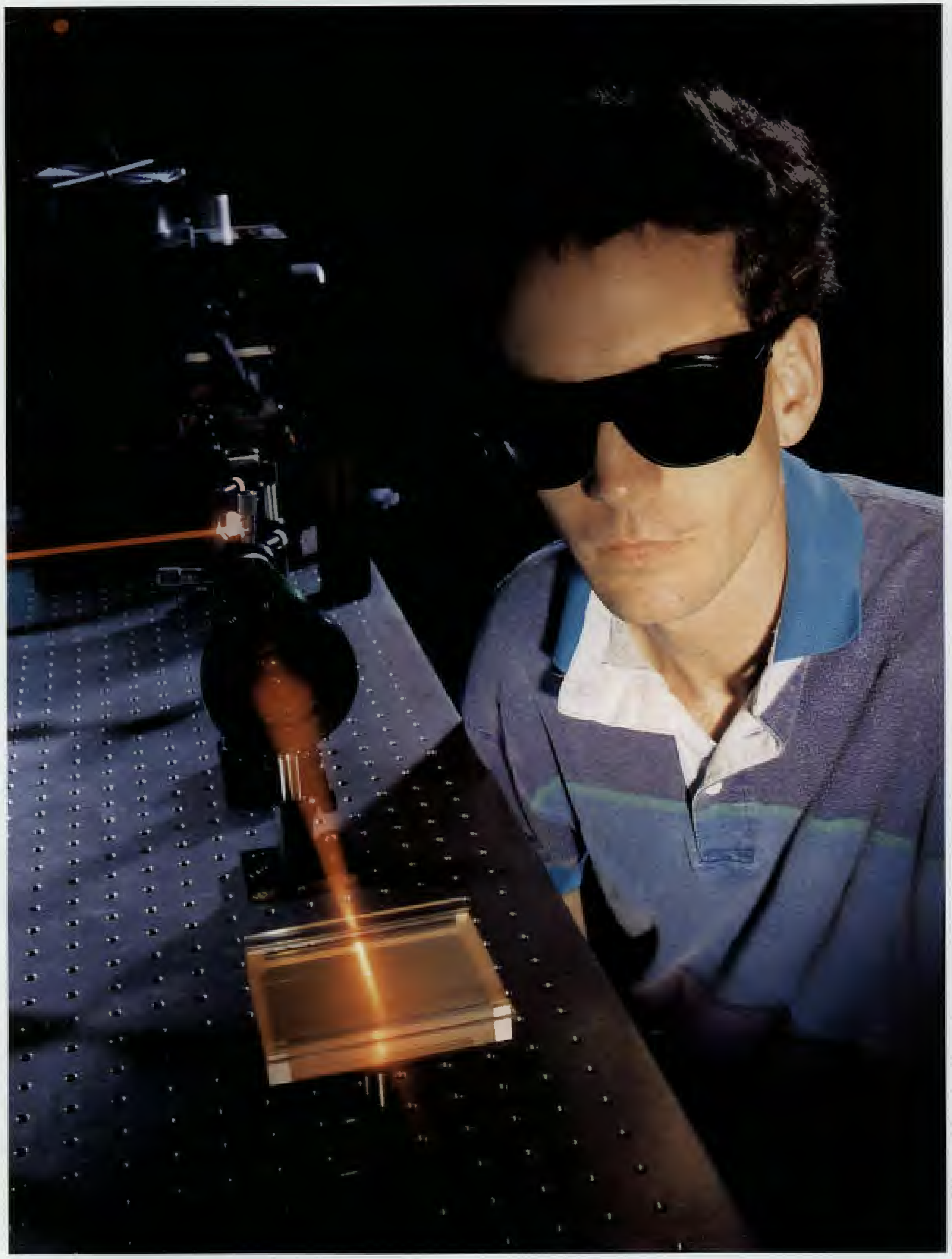
Biological Sciences



Photograph by Tom Cerniglio

How do energy-related physical and chemical agents—ranging from radiation to fossil fuel pollutants—interact with living organisms and the environment? Can we reduce the risk to human health from exposure to hazardous materials and radionuclides? As we learn where genes sit on chromosomes and how their chemical building blocks are arranged, can we also find out what these genes do? Can we decipher the molecular basis of protein as well as gene function? Can we treat cancer and other diseases using our isotopes and technologies such as the laser? ❦ These are some of the questions being addressed by researchers in ORNL's Biological and Environmental Research Program, under the sponsorship of the DOE-Energy Research, Office of Biological and Environmental Research (OBER). Our program, which covers a diverse range of basic and applied studies, is one of the broadest biological and environmental multidisciplinary research programs in the nation. ❦ Our biology research calls for expertise in mammalian genetics, molecular genetics, protein engineering, cell biology, carcinogenesis, macromolecular structure, mutagenesis, and risk assessment. We are developing competencies in new areas such as functional genomics and computational biology. For this work, we use our existing facilities such as the Mouse House with its 92,000 mutant mice and the Intel Paragon supercomputers. ❦ We don't keep the answers to our questions—the products of our work—to ourselves. We are proud of our successes in transferring OBER-funded research findings and technological developments to the private sector and the R&D awards we have won.

New Breast Cancer Treatment Proposed



ORNL chemist Eric Wachter is part of a team that is testing the medical uses for this two-photon, near-infrared laser. The light from this laser can target and damage cancer cells by activating an ingested drug that concentrates in them. This two-photon laser technique, which has great potential for curing breast cancer, has been licensed to a local company called Photogen. *Photograph by Tom Cerniglio.*

For many breast cancer patients, today's treatment options can be a nightmare. They must face possible removal of one or both breasts by a surgeon. And they may have to endure side effects from chemotherapy or radiation treatments used to kill cancer cells on the loose.

A new treatment for early breast cancer may soon be at hand. ORNL has developed a treatment approach that shows promise in destroying breast tumors without surgery or side effects. This kinder, gentler therapy for breast cancer combines laser light and currently available drugs in a minimally invasive technique that awaits in-vivo testing by Photogen, a local company to which this technology has been licensed.

When fully developed, the technique will use a focused beam of near-infrared laser light that passes harmlessly through skin and delivers photons in a one-two punch to the target. The beam of light, two photons at a time, is absorbed by the targeted tumor, activating an ingested pharmaceutical agent that is taken up by rapidly proliferating cells like those found in cancerous tumors. The activated agent kills the cancer cells, either by disabling their DNA or destroying their cell walls.

Pinpoint activation of the pharmaceutical agent is confined to a

A new breast cancer treatment concept shows promise in destroying breast tumors without surgery or side effects.

tightly controlled area as a result of the unique physics of the photoactivation process, called simultaneous two-photon excitation. In contrast, other commonly used optical excitation processes can cause undesirable activation, even at low intensities, and can produce damage over far wider areas than is desired.

The laser light can be focused deep within the tumor, and the drug is activated only in this focus. Therefore, in contrast to conventional radiation or chemotherapy, only tumor tissue is affected. Normal tissue is unaffected outside the focus of the beam—even as the light enters and leaves the body.

We have already demonstrated that the technique can selectively kill *Salmonella* bacteria and human breast cancer cells. The ability of the technique to focus deep within tissue has been shown in a tumor that was removed from a mouse with breast cancer.

A drug that could be safely used with this laser method is 8-MOP, a derivative of psoralen, which has been approved by the Food and Drug Administration for treatment of a number of diseases, including skin cancer and psoriasis. The 8-MOP and other psoralen derivatives are normally activated using ultraviolet light. As a consequence of the low penetration of UV light through skin, such agents are currently only effective for topical applications and treatment of near-surface lesions. Because our simultaneous two-photon excitation process uses near-infrared light (which, unlike ultraviolet light, can penetrate deeply into tissue), drugs like 8-MOP will become useful for treatment of subsurface lesions, such as breast cancer.

We believe that the majority of photoactive pharmaceutical agents will work well with the new activation method. As a result, the technique may be used someday to treat many other diseases, including cancers of the skin and liver, possibly spelling an end to some people's bad dreams.

The research was supported by ORNL's Laboratory Directed Research and Development Program.

Radioactive Antibody Targets Tumor Blood Vessels

If a radioisotope could be delivered specifically to a solid tumor, its radiation should destroy the collection of cancer cells. That was the theory behind radioimmunotherapy in which a radioisotope is coupled with a monoclonal antibody that homes in on a specific biological target, like a guided missile. After 20 years of research, scientists have concluded that radioimmunotherapy is not effective on solid tumors. A large fraction of the antibody never reaches the tumor, and the fraction that does is not uniformly distributed among the cells.

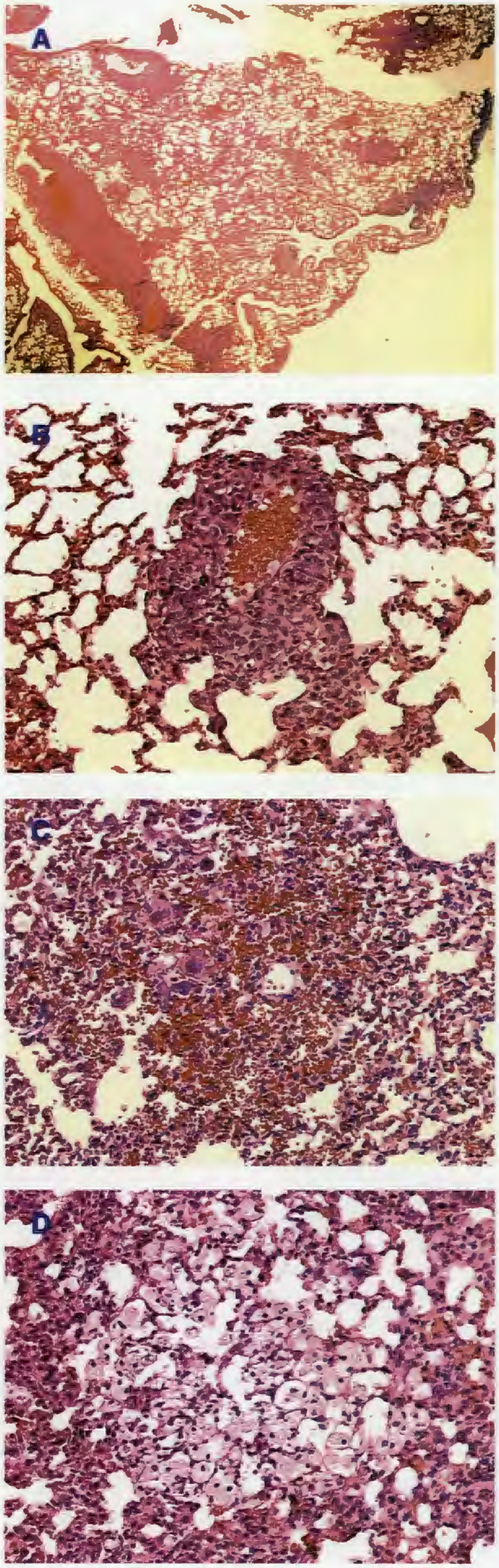
However, recent successes indicate that leukemia and other "liquid tumors" may be treatable by radioimmunotherapy. A number of clinical human trials are under way at Memorial Sloan-Kettering Cancer Center and other U.S. cancer treatment centers. ORNL will be supplying the radioisotope actinium-225 and radionuclide generators needed to produce bismuth-213 for early patient studies.

In the past two or three years, several research groups have shown that attacking tumor blood vessels with chemicals or antibodies retards tumor growth. But when therapy stops, resident tumor cell reproduction starts again. ORNL researchers have found that radioimmunotherapy that targets blood vessels, not solid tumor cells, can eradicate implanted lung tumors in mice. We are using an ORNL-developed monoclonal antibody that homes in on the inside of blood vessels in lung tumors. Bismuth-213, an alpha-particle emitter with a 45-minute half-life, is carried to the tumor vessels by the monoclonal antibody; our study is the only one that uses radiolabeled antibodies to attack tumor blood vessels. The bismuth-213 used is the final decay product of uranium-233, over a ton of which is stored in ORNL's Building 3019. Uranium-233 was originally produced at ORNL as part of the molten salt breeder reactor research program. Today ORNL is the western world's chief source of actinium-225 and bismuth-213.

A large fraction of the bismuth-213-labeled antibody parks in blood vessels in lung tumors and sprays out high-energy alpha particles. This radiation penetrates 6 to 10 tumor cell layers nearby, killing everything in their short path, including tumor cells and cells lining the blood vessels. The damage to blood vessels may reduce the supply of nutrients to the tumor.

In experiments in hundreds of mice with implanted lung tumors, our researchers showed that 100% of the mice treated with appropriate doses survived for 100 days (even though some normal lung cells were damaged by the treatment). The untreated mice died in 10 to 14 days.

To attach the bismuth-213 to the antibody, the molecule CHXb-DTPA is used. At one end of the molecule are "arms" that grab and envelop the bismuth-213 to protect it from being dislodged by competing metal ions; a functional group at the other end attaches the bismuth-213 to the antibody. The assembly of this therapeutic agent involves attaching the CHXb-DTPA molecule to the antibody. The altered antibody is then reacted with bismuth-213 from the actinium-225/bismuth-213 generator. At the top of the generator is actinium-225 (which has a half-life of 10 days)—a decay product of thorium-229, which in turn is a decay product of uranium-233. During the decay of actinium-225, bismuth-213 is formed. As often as every 3 hours, bismuth-213 can be "washed" from the



Photomicrographs of 5-μm-thick sections from mouse lungs. Panel A: low magnification of untreated lung—solid pink areas are untreated tumor cells. Panel B: higher (400×) magnification of a small tumor (clusters of pink cells) growing around a blood vessel (red area in center). Panel C: tumor after treatment with high dose of a monoclonal antibody to which bismuth-213 is attached. Tumor contains giant cells (dying) and lots of red blood cells from local hemorrhage. Panel D: 40 days after treatment—scarred area of lung where the tumor was growing before treatment. No live cells remain in the tumor area. Untreated animals had all died 20 days earlier.

We have shown that monoclonal antibodies labeled with radioactive bismuth-213 destroy implanted lung tumors in mice.

generator for reaction with the antibody. The therapeutic agent is then injected into mice.

ORNL researchers are still searching for the best doses and dose schedules as well as for an explanation of why bismuth-213 effectively destroys lung tumors in mice. A treatment like this might be available for humans in 5 years if an analogous antibody is found. In a decade or so, radioisotope-bearing molecular probes that can bind to tumor blood vessels throughout the body may kill cancer cells that have spread from nearly *every* kind of solid human tumor.

The research was supported by ORNL's Laboratory Directed Research and Development Program. The work is also funded by DOE's Office of Biological and Environmental Research, Health Effects and Life Sciences Research Division.

ORNL Closing In on Obesity Genes

For some people, being fat may be an unfortunate fate. Those with inherited obesity have a higher risk of suffering from diabetes, heart disease, and stroke. So, research is under way to target "fat" genes.

Most forms of human obesity are the result of a complex interaction of environmental factors and multiple, interacting genes scattered throughout the genome. These genes govern body weight by controlling appetite, metabolism, storage of body fat, and the balance of energy inputs and outputs. So far, five genes that act singly to cause obesity have been isolated in mice and humans and cloned by researchers at various laboratories. But it is estimated that less than 1% of obesity in the human population is controlled by single genes.

The complexities of the gene-environment interactions that cause most obesity make it difficult to investigate the role of genes that influence body weight in humans. Hence, ORNL is trying the promising approach of using mouse models to identify and characterize genetic factors influencing the quantity and distribution of body fat.

Although genes thought to influence polygenic obesity in mice and humans have been mapped, none of these genes has yet been isolated. Biologists at ORNL are striving hard to be the first group to isolate and clone one of these polygenic genes in mice.

From among the mouse stocks generated in radiation mutagenesis experiments carried out at ORNL since 1949, many mice were observed to have pink coats and pink eyes. The reason: the radiation knocked out DNA from a coat-color gene on mouse chromosome 7 called *p* (pink-eyed dilution). During such studies, we observed that when a certain defined region containing the coat-color gene and a region of its neighboring DNA on mouse chromosome 7 were deleted, the animals were about 35% fatter than age-matched animal controls. The actual physiological differences between the fat mice and mice of normal weight are being studied by a collaborator at Louisana State University.

By focusing on DNA from the *p* coat-color mutant mice that also get fat, ORNL researchers defined a small region on mouse chromosome 7 that might contain gene(s) affecting body weight in mice. Recombinant DNA techniques are being used to identify and characterize genes from this small region that might be logical candidates for polygenic fat genes. These findings should provide insights into the body fat regulatory mechanisms in mice and humans. Once polygenic fat genes are cloned and isolated, it may be possible to isolate the associated gene products that undermine control of body weight and use this information to develop an anti-obesity drug. With a little help from genetic studies and drug designers, being fat forever may not have to be some people's fate.

The research was supported by DOE's Office of Biological and Environmental Research. ornl

ORNL biologists are close to isolating and cloning a significant obesity gene in mice.

Dabney Johnson examines an obese mouse that carries a single-gene obesity mutation. *Photograph by Tom Cerniglio.*

Environmental Sciences and Technology

Digital image enhanced by Reneé Balogh

Keeping up with the demand for energy has a downside: energy development, production, and use release pollutants that foul the environment. At ORNL we take an interdisciplinary approach to understanding and solving major environmental problems. Our teams have experts in biogeochemistry, environmental biotechnology, global environmental chemistry, ecosystem studies, geosciences, hydrology, social sciences, and environmental assessment. We also develop instruments for the sensitive detection and monitoring of radiation and chemicals.

One of our goals is to improve understanding of environmental processes, such as the ecological effects of elevated levels of atmospheric carbon dioxide and climate-related increases in temperature, precipitation, and times of drought. Another goal is to develop a scientific basis for implementing environmental technologies (monitoring, mitigation, and remediation). For example, we have developed two approaches to removing radioactive cesium-137 from highly radioactive waste to reduce waste disposal costs.

Much of our research is possible only because of the existence of special natural areas at ORNL such as Walker Branch Watershed and the Oak Ridge National Environmental Research Park, a user facility. Other research makes use of the facilities of the Bioprocessing Research and Development Center as well as resources of the Center for Biotechnology and the Center for Global Environmental Studies. Through these resources, we are trying to keep up with the demand for new information and technologies to help preserve a clean environment.

Advanced Liquid-free Bioprocessing Technology

ORNL's revolutionary approach to bioprocessing eliminates the use of liquids, greatly reducing aqueous wastes from chemical production in bioreactors.

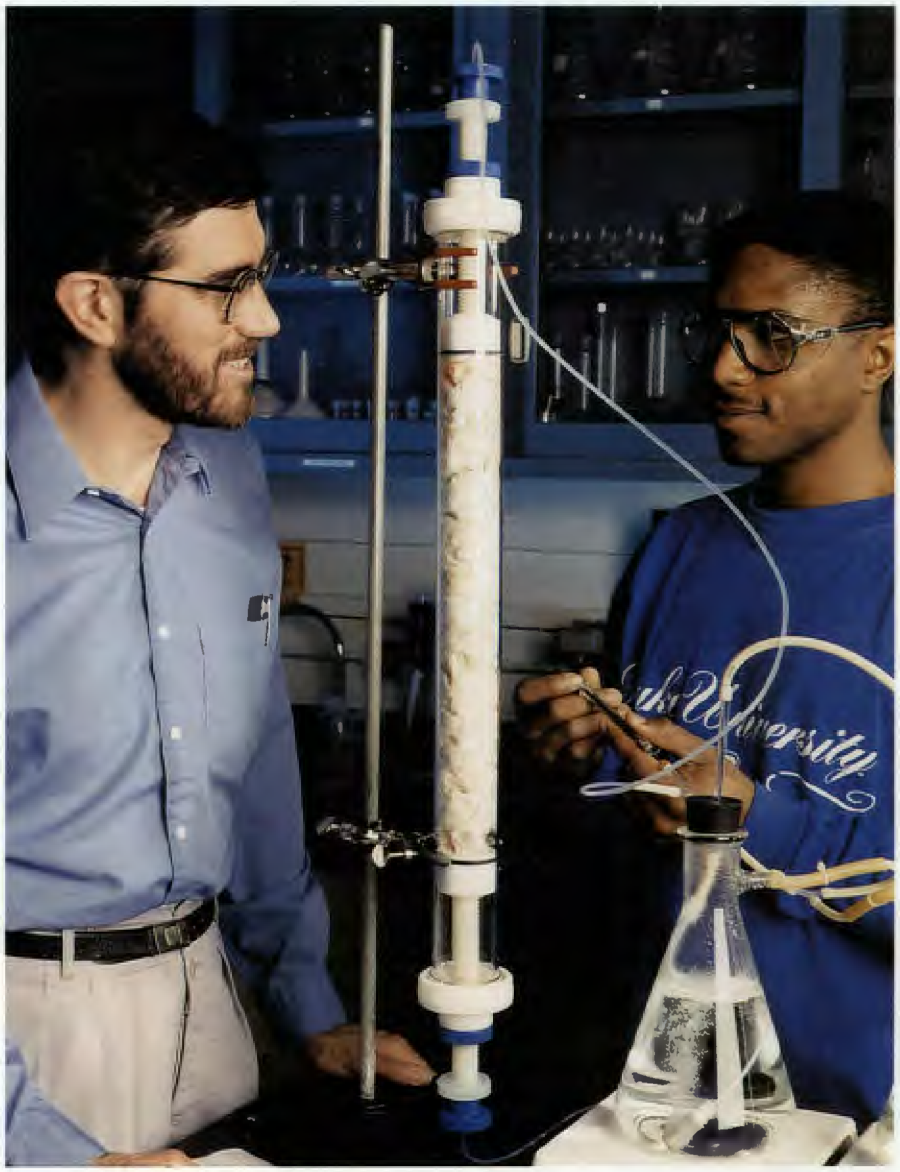
For every kilogram of chemical produced in the United States, some 10 to 100 kilograms of waste by-products are generated. These by-products consist mostly of water, but this waste liquid requires treatment using energy-consuming processes before it can be released to our waterways—at a high cost to industry and ultimately the consumer.

Synthesis of chemicals may require several steps; furthermore, each step may use a different solvent and reaction vessel. Significant waste is generated from one reaction step to the next as solvents are switched (e.g., from hexane to water), and more waste is produced when the product is separated from the final solution.

Over the years, ORNL researchers have developed bioprocessing methods for making products in liquids (water), using various types of bioreactors. Traditionally, chemicals in a liquid, phase are transformed to useful products by microorganisms that are attached to support material through which the liquid passes.

Now, ORNL researchers have devised a revolutionary approach to bioprocessing that eliminates the use of liquids (including solvents and diluents), greatly reducing aqueous wastes from chemical production in bioreactors. The technology could save money because it uses less energy for waste treatment and eases the separation and recovery of products. It also may allow new enzymatic products to be obtained.

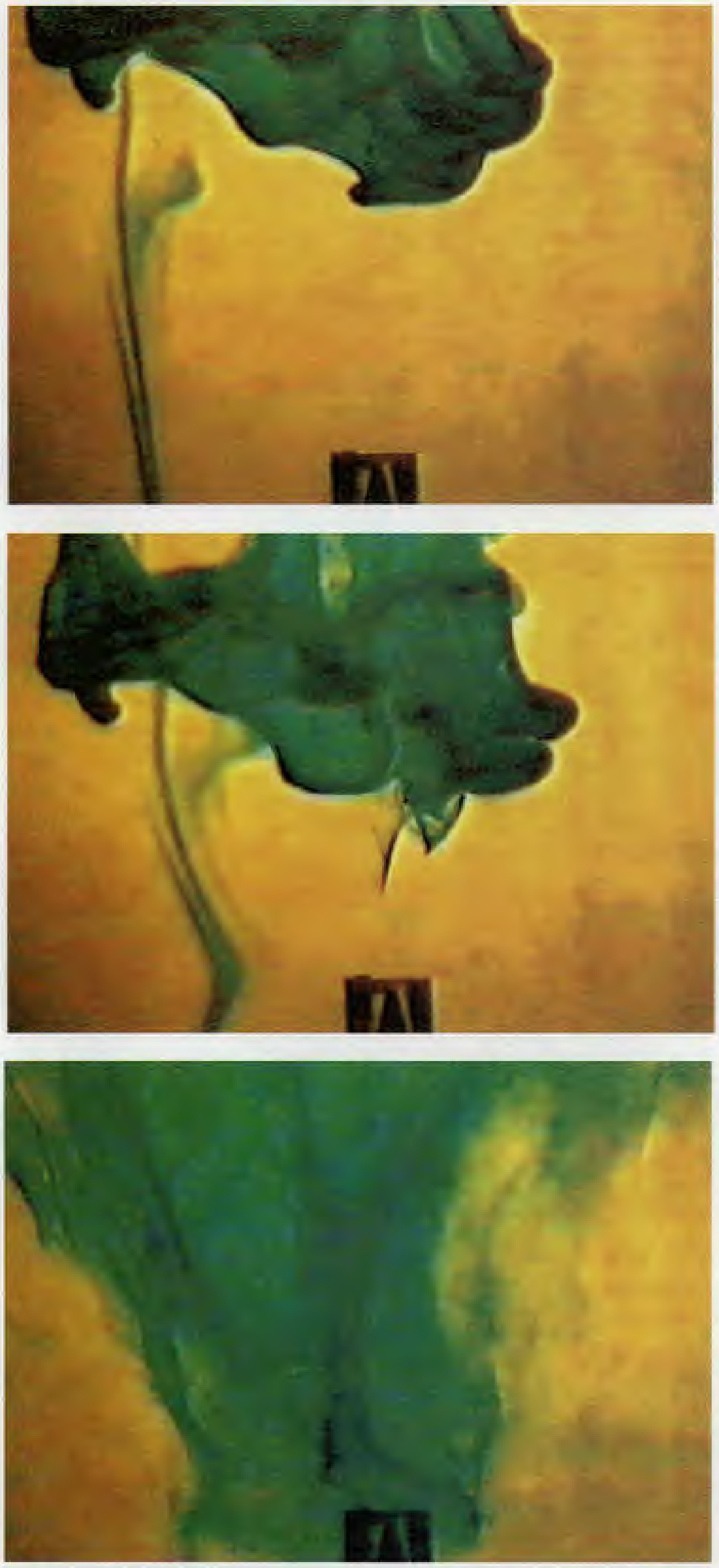
The approach both introduces reactants and recovers products in gaseous form. The process uses an immobilized enzyme (a protein extracted from living cells) to speed up the reaction that yields the product. Because all reactants are fast-moving gas molecules, they intermix with each other and the enzyme more readily than do liquid molecules. The recovery of products is also easier from the gas phase rather than from the dilute aqueous solution—typical of a traditional fermentation.



Brian Davison (left) and Chris C. Gable III (a student at the University of Tennessee at Knoxville) discuss ORNL's new bioprocess that introduces reactants and recovers products in gaseous form. The process uses an immobilized enzyme to speed up the product-yielding reaction. *Photograph by Tom Cerniglio.*

Just below or at its boiling point, a chemical compound can volatilize, producing a vapor in a gas stream. In the ORNL process, vapors of the starting material are pumped into a vertical column containing glass wool (like a tube filled with porous insulation) to which an enzyme is attached. The vapors diffuse through the column, where they come into contact with the enzyme. The enzyme catalyzes the reaction between the gaseous compounds, producing a gaseous product that flows out of the

It was once thought impossible to spray a nonconductive fluid into an electrically conductive one, but ORNL did it.



Inverse electrospraying mixes liquids well, as shown in the images of a tracer dye in water. Top image: time = 0 - ; voltage = 0 V. Middle image: time = 0 + ; voltage = 4 kV. Bottom image: time = 1 second; voltage = 4kV.

other end of the column, where it is collected. In one proof-of-principle experiment, ORNL chemical engineers used lipase, an enzyme extracted from a pig's pancreas, and vapors of ethyl acetate and isoamyl alcohol as the reactants. The products were two gaseous species that later condensed into liquids—ethanol (alcohol) and isoamyl acetate (an aromatic ester known as banana oil because of its banana fragrance).

ORNL researchers hope to show that this new bioprocessing technology can be used for many different esterifications, chemical reactions that produce esters. An ester is an organic compound formed from an organic acid and an alcohol.

They have also shown that the new process can be used for oxidation reactions, which may have applications in waste treatment. In preliminary experiments, an enzyme extracted from mushrooms, polyphenoloxidase, converted phenol vapors reacting with oxygen in the air into quinone, an aromatic compound used in making dyes, tanning hides, and producing photographs.

The ORNL process is limited currently to compounds that are volatile at 20 to 50°C. Higher temperatures and faster production rates may be possible as science harnesses enzymes that can tolerate higher temperatures and more extreme operating conditions (such as enzymes from thermophilic bacteria in hot vents under the sea). Then a wider range of starting materials could be used to make a wider range of products even more easily and more cheaply.

The research was supported by DOE's Office of Industrial Technologies, Division of Biological and Chemical Technology Research.

Inverse Electrospraying May Cleanse Polluted Water

Electrostatic spraying is used to paint cars and deposit herbicides on fruit trees. Such "electrospraying" is efficient because large drops are broken into a fine mist, providing a more uniform coating. In addition, the particles are attracted electrostatically to a grounded body, such as a car or tree.

Basically, electrospraying involves spraying an electrically conductive fluid into a nonconductive fluid, like water into air. It was once thought impossible to reverse this process and spray a nonconductive fluid into an electrically conductive fluid, like air into water. But ORNL researchers have proved that "inverse electrospraying" is possible; that

The liquid in this inverse electrospraying column appears red because of the pumping and spraying of dyed red kerosene microdroplets into water.

it can be explained; and that it makes possible a lighter, simpler, more energy-efficient device for speeding up chemical reactions and cleansing polluted water.

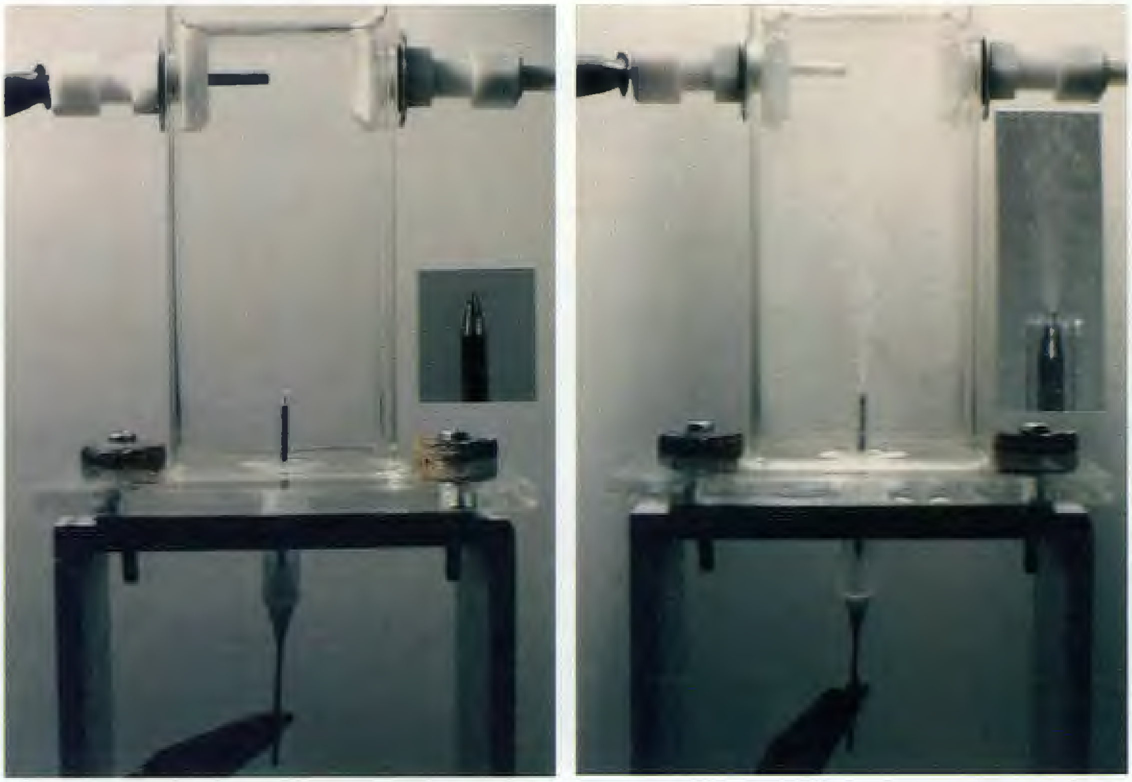
Two years ago, our researchers set up an apparatus consisting of a pump, a glass column, and two electrodes immersed in water in the column. In this configuration, one electrode is at the top and the other is a vertical capillary electrode at the bottom of the water column through which another fluid (such as air) is introduced. After pumping air into the water column, the researchers increased the voltage from 0 to 4000 volts, creating a nonuniform electric field. After several experiments, they observed that the electric field actually pumped the air deep into the water, obviating the need for a mechanical pump. The explanation? Charge carriers are attracted to the oppositely charged electric field, causing the fluid to flow. This phenomenon, called electrohydrodynamic convection, creates a low pressure near the capillary tip, thus causing pumping.

As air bubbles passed through the nonuniform electric field, they were shattered into micron-sized bubbles. Thus, the electric field induced simultaneous pumping and spraying of air, forming microbubbles.

Inverse electrospraying was also used to pump and spray organic liquids, such as kerosene, into water. Our researchers found that this technique is very effective at mixing liquids. In this case, they used color tracers and fluorescent particles that would glow when laser light was shone on them. By making the flow visible, they observed excellent mixing of kerosene and water.

Because inverse electrospraying mixes liquids well, the process could replace mechanical agitators, which are conventionally used for liquid mixing. Mechanical agitators convert electrical energy into mechanical energy, but inverse electrospraying uses electricity directly and thus is more energy efficient. In addition, a device based on inverse electrospraying would be simpler, lighter, and probably less expensive to build and operate than conventional mixing systems because it would require no mechanical devices such as pumps and agitators. Also, because it would have no moving parts, it would cause no vibrations.

Inverse electrospraying shows promise for removing organic chemicals and



Images show the apparatus, with an inset providing a closeup of the electrified capillary through which a nonconducting fluid enters a conducting fluid in a water column. Here, after a voltage of 4 kV is applied, a spray of bubbles is observed in the column. The bubbles come from the ambient air that is simultaneously pumped and sprayed into the water. *Photograph by Curtis Boles.*

toxic metals from water. The Electric Power Research Institute, the research arm of the U.S. electric utility industry, is sponsoring an ORNL project to use inverse electrospraying to introduce ozone into water contaminated with toxic organic compounds such as polychlorinated biphenyls (PCBs), pesticides, and chemicals containing benzene. Ozone breaks these compounds down into simpler compounds that can be removed by other chemical or biological treatments. In our approach, ozone would be rapidly dispersed through the water in the form of extremely small bubbles. Because the ozone would be carried more quickly into the water, it would make contact with and break down organic contaminants more rapidly than would conventional methods of ozonation.

Tiny bubbles are the key to removing trace amounts of heavy metals from water through a flotation method of separation. Inverse electrospraying can make microbubbles that collide with and attach to particles of heavy metals such as chromium, copper, nickel, and zinc. Because the microbubbles are buoyant, they carry the metal particles to an interface where they can be removed.

Inverse electrospraying may also have other applications. It could be used to make special materials that can be formed only from very small particles, such as ceramic precursors. It may be used to provide oxygen to aerobic bacteria that are introduced into oil by normal electrospraying to remove sulfur from the oil—a process being developed by ORNL in collaboration with several companies, including Texaco, Exxon, Chevron, and Energy Biosystems.

As information on inverse electrospraying becomes more widely dispersed, ideas on how to apply it should continue to flow.

The work was sponsored by DOE's Environmental Management Science Program and Office of Energy Research, Basic Energy Sciences, Division of Chemical Sciences. The ozonation research is supported by the Electric Power Research Institute.

ORNL a Leader in Global Change and Forest Studies

Hardwood forests on DOE's Oak Ridge Reservation don't get equal treatment. Thanks to ORNL's unique facilities for performing some of the world's largest ecological manipulations, white and chestnut oaks, red maples, and yellow poplar trees are exposed to more (or less) rain, higher levels of carbon dioxide (CO_2) or higher temperatures than other trees in the natural forest environment. Combined with our computer modeling capabilities for understanding biological processes such as foliar photosynthesis, tissue respiration, growth, nutrient cycling, and decomposition, our "user facilities" are attracting many outside scientists to help us study the impacts of global climate change on forest ecosystems. ORNL is unequaled as a national resource for gaining a better understanding of how future climates can affect southern forests in the United States.

In the throughfall displacement experiment conducted in the Walker Branch Watershed on the Oak Ridge Reservation, troughs intercept a fraction of the normal precipitation in one area and divert it passively through gravity flow to another plot. As a result, one-third of the trees in the experiment receive normal rainfall, another third get one-third less rain and snow, and the final third receive one-third greater precipitation.

After three-and a-half years, oak, maple, gum, sourwood, and yellow poplar trees were not noticeably affected by the manipulated soil moisture levels. However, during the 1995 drought, 20% of the dogwood trees in this forest died on the dry plot and only 3% died on the wet plot. This finding suggests that, in a consistently drier future climate, the presence of dogwoods in southern forests would be dramatically reduced.

Another key conclusion of the throughfall displacement experiment is that daily to weekly rainfall patterns during the growing season are far more important than fluctuations in total annual precipitation for understanding the ecological impacts of moisture variations. Computer modeling experts attempting to assess the impacts of climate change on forest ecosystems must recognize that no rain in June when trees are actively growing fast is more significant than no rain in late summer when trees hardly grow at all. We continue to study the implications of dormant season changes in rainfall to identify impacts on forest nutrient cycling that might produce long-term change in forest productivity and composition.

In our open-topped chamber studies of tree growth responses to elevated CO_2, we found little change in yellow poplar saplings but increased leaf area and more roots in white oak. A dozen similar experiments across the nation had widely different results. ORNL developed an analytical approach called the "growth per unit leaf area index" (the mass in grams of wood produced each year divided by leaf area in square meters) that shows the responses across different species and site conditions to be basically uniform. This approach enables extrapolation of individual tree species responses to predict the response of a whole mixed forest to elevated CO_2.

We found that the growth of maple trees was reduced in chambers where the temperature was kept 4°C higher than ambient temperatures and that sugar maples (found no farther south than Chattanooga) were more severely affected than red maples (found as far south as the Gulf coast). In both species, the negative growth effects of temperature were offset by the positive growth effects of elevated CO_2. This finding suggests that, for predicting tree growth in the future, the overall effect of both increased atmospheric CO_2 concentrations and global warming must be considered.

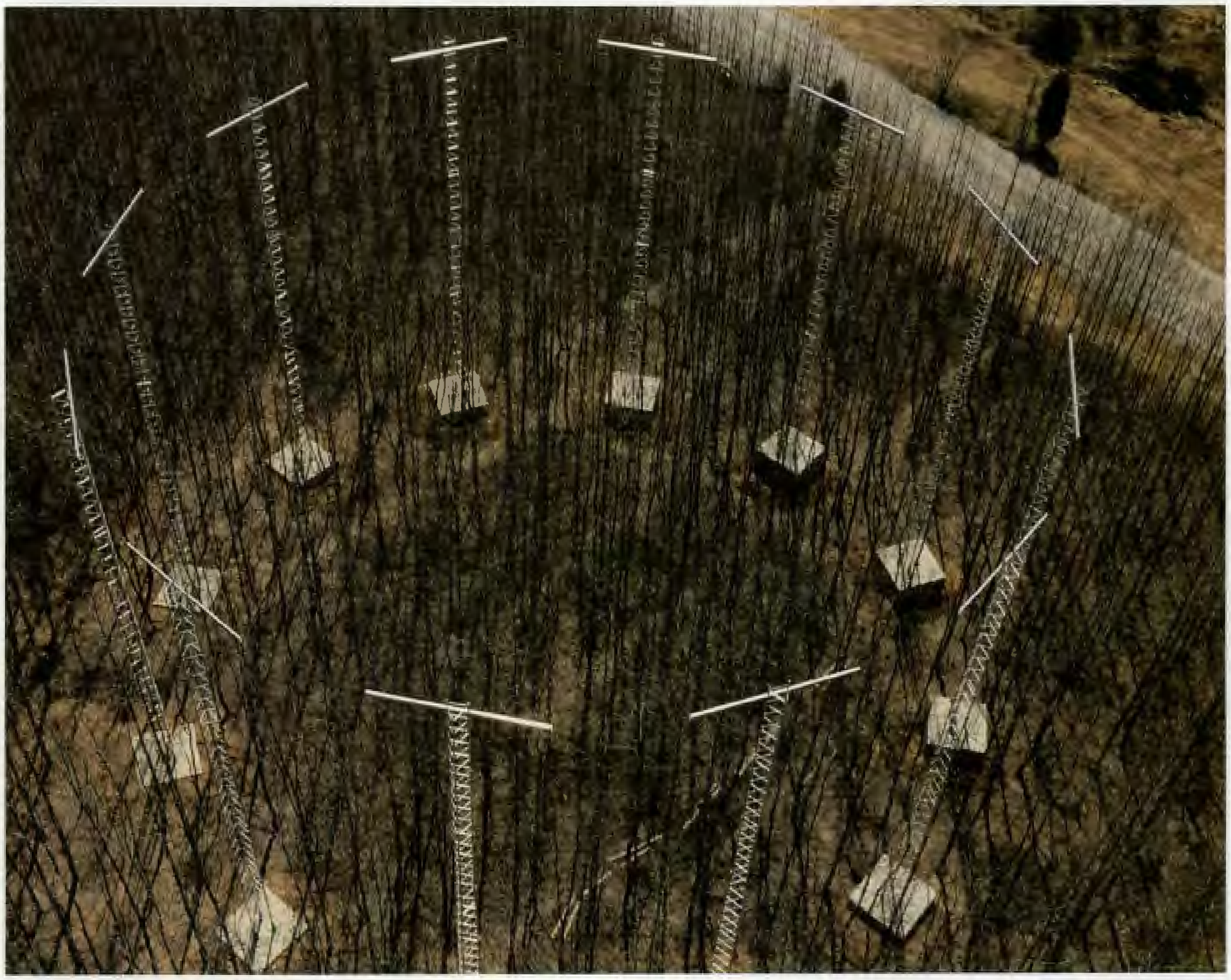
ORNL researchers seek to determine if forests could slow down the onset of global warming by soaking up additional CO_2 concentrations injected into the air by industrial activities. Some of this extra carbon from the air could end up in the soil following the decomposition of leaf litter and roots. Such a "soil carbon signal" may be seen in 10 years as a result of a new ORNL manipulation of a small sweetgum tree stand using the novel Free Air CO_2 Enrichment (FACE) technology. We have characterized this site and are now studying changes in biological processes and soil composition as FACE vent pipes suspended from a tower blow out extra CO_2 for the wind to carry to the trees. Eventually, we may be able to predict reliably whether the world's forests are equal to the task of removing some of the excess atmospheric CO_2 attributed to human activities.

The research was funded by DOE's Office of Health and Environmental Research, the National Science Foundation, and ORNL's Laboratory Directed Research and Development Program.

ORNL Process May Help Treat Hanford Tank Waste

Imagine a bottle of oil and vinegar in which the oil floats on a "vinegar" containing dissolved contaminants. Dissolved in the oil are special molecules that act like Pac-Man. When the oil and vinegar are mixed temporarily by vigorous shaking of the bottle, the Pac-Man molecules snatch the contaminant molecules from the drops of the vinegar and transfer them

ORNL studies the ecological effects on forest trees of increases in atmospheric carbon dioxide, precipitation, drought, and air temperature.



This aerial view shows the towers and vent pipes of ORNL's novel Free Air CO_2 Enrichment system for introducing additional amounts of carbon dioxide to a small sweetgum tree stand on the Oak Ridge Reservation. If the trees soak up the additional CO_2, the effects may include changes in the stand's biological processes and soil composition. *Photograph by Curtis Boles.*

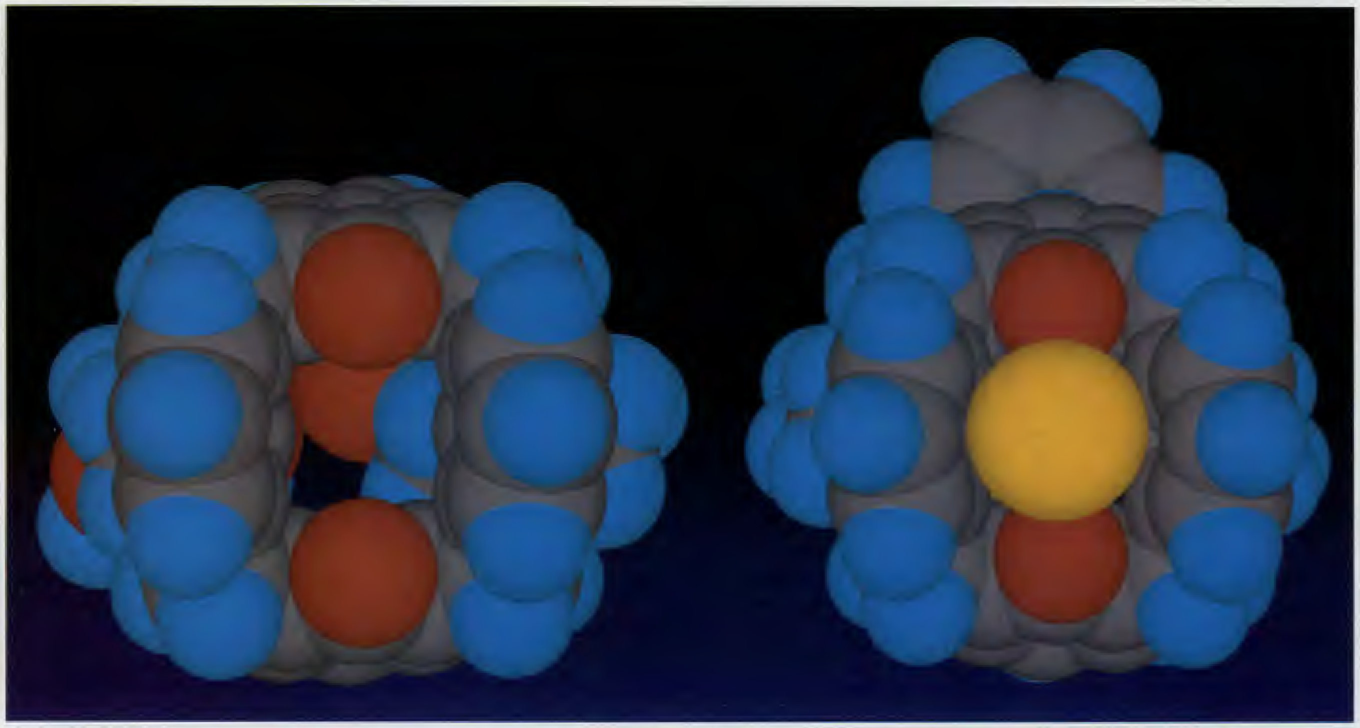
to the oil drops for final removal. A similar "solvent extraction" process is the basis of a practical system being designed by ORNL for the 55 million gallons of radioactive waste in the Department of Energy's 177 tanks (67 of which are leaking) in Hanford, Washington.

DOE is committed to cleaning up these tanks at the lowest possible cost. The waste will be vitrified as low-level glass logs that are safe enough to store on the Hanford site and as high-level glass logs that must be permanently isolated in a geologic repository.

The Hanford tank wastes contain fission products from reprocessing spent reactor fuel to recover plutonium for nuclear weapons production that started during World War II. The fission products are in an alkaline solution of sodium nitrate formed by adding sodium hydroxide to the nitric acid used for reprocessing. Although this treatment made the waste less corrosive to the storage tanks, it also created a need for new separations technologies for ultimate cleanup. The fission products targeted by ORNL's separation process are long-lived, mobile technetium-99 and highly radioactive strontium-90 and cesium-137, both of which have half-lives of about 30 years. Removal and concentration of these fission products would minimize the volume of high-level waste that must be vitrified, resulting in tremendous cost savings.

In the proposed process, the fission products would be extracted from the alkaline sodium nitrate waste solution into the "oil" phase—kerosene containing the extractants. The Pac-Man–like molecules in the oil are "crown ethers"—large, cyclic, designer molecules that each have a cavity sculpted to the right size and shape in which to trap a specific ion. A commercially available crown ether is used in the ORNL process to snatch strontium-90 ions or positively charged sodium ions that attract (and extract) technetium in the form of the negatively charged pertechnetate ion.

To seize cesium from the waste stream, ORNL researchers focused on a new, highly selective macrocycle whose basic framework was designed in France. Because the Hanford tanks contain a million sodium ions for every cesium ion, the French molecule was appealing because it can recognize and grab one cesium "needle" in every haystack of sodium ions. Although this molecule has the high selectivity needed, it still could not function adequately in a solvent extraction process adaptable for Hanford tank-waste separations. To overcome this problem, the ORNL researchers modified both the crown ether and the solvent system to develop an effective solvent extraction process for removing cesium from radioactive waste. They also took advantage of the



This Pac-Man–like crown ether molecule captures a radioactive cesium ion (yellow ball) from liquid waste because its cavity was sculpted to the right size and shape to trap this particular ion. *Images by Jeff C. Bryan.*

high concentrations of sodium and nitrate ions, which drive the solvent extraction reactions.

The process also uses water mixed with a little nitric acid to strip the fission products from the kerosene solvent. As a result, the solvent can be recycled many times and the fission products can ultimately be encapsulated in high-level glass canisters.

Technetium removal has been successfully tested on a batch scale on Hanford waste and waste from ORNL's own Melton Valley Storage Tanks. Tests on cesium removal from Hanford waste are being conducted in 1997. ORNL's goal is to develop a combined solvent extraction process using centrifugal contactors in which two crown ethers remove and concentrate the three fission products simultaneously. Such a process should prove attractive to Hanford and DOE because it leaves the waste otherwise unchanged, produces little secondary waste, provides a concentrated stream of fission products for vitrification, and is compact, cheap, safe, reliable, and fast.

The research is sponsored by DOE's Office of Environmental Management, Office of Science and Technology, Efficient Separations and Processing Crosscutting Program.

Cesium Removal Demonstrated at ORNL

ORNL developed, tested, and scaled up an ion-exchange continuous flow system for effectively removing cesium-137 from radioactive liquid waste.

Radioactive cesium-137 is a really bad actor in ORNL's mixed waste. Because the isotope emits the bulk of the waste's radioactivity as high-energy gamma rays, the waste must be shielded in lead or concrete. Currently, most of the cesium-containing liquid wastes are generated by ORNL's Radiochemical Engineering and Development Center and are concentrated in the Bethel Valley Evaporator, which also handles all liquid radioactive waste from other past and present operations. The liquid mixed waste is stored on site in eight stainless-steel Melton Valley Storage Tanks in an underground concrete vault.

Other bad actors in ORNL's waste are toxic metals that must be disposed of as hazardous waste according to the Resource Conservation and Recovery Act (RCRA). These metals include arsenic, barium, cadmium, chromium, mercury, lead, nickel, selenium, silver, and thallium. Because some of the ORNL radioactive liquid waste contains some of the RCRA metals at levels above legal limits, they are also classified as mixed waste—hazardous waste mixed with radioactive waste.

If cesium-137 could be removed from ORNL's mixed waste, the remaining

This aerial view shows six Melton Valley Storage Tanks (below crane, which points to ORNL's Hydrofracture Facility). *Photograph by Curtis Boles.*

compounds in a solution of sodium and potassium nitrate could be combined with grout, solidified as concrete monoliths, and disposed of on site as low-level waste. Such separations would reduce ORNL's waste disposal costs.

To help solve this problem, ORNL researchers have developed a method to remove both cesium-137 and some of the RCRA metals from the mixed waste, leaving low-level waste behind for disposal at a reduced cost. They have developed and tested a laboratory-scale ion-exchange continuous-flow system, scaled it up, and proved it works in the Cesium Removal Demonstration Project. The key to the system's success is a commercial preparation of crystalline silicotitanate (CST) manufactured by UOP's Molecular Sieves Division under a DOE program also involving Texas A&M University and Sandia National Laboratories. ORNL researchers, who had tested eight different cesium sorbents, were the first to show in a continuous hot-cell operation using real waste liquid that CST can effectively remove cesium-137 from radioactive liquid waste.

In the ion-exchange process, the liquid waste flows down a column through CST crystals, which contain sodium ions as a result of the manufacturing process. CST takes up and holds both cesium and some of the RCRA metals while releasing the sodium ions to the liquid waste passing through. CST prefers cesium and some of the other metals to sodium because they fit better in CST's crystal structure. The final waste-loaded CST product is a batch of dried granular material resembling white sand. A full-scale demonstration of the CST successfully processed 15% of the ORNL waste inventory. The first batch loaded with radioactive cesium from the Melton Valley Storage Tanks was sent to DOE's Savannah River Plant to be vitrified into glass logs. The remaining batches are being stored on site until they can be shipped to DOE's permanent disposal site (probably the Nevada Test Site).

Waste-loaded CSTs have passed several toxicity characteristic leaching procedure (TCLP) tests required by the Environmental Protection Agency. When the leach testing solution was contacted with the CST test batches, none of the RCRA metals were leached out at levels above the leach testing limits. As long as TCLP tests verify that the toxic metals are permanently trapped in each CST batch, DOE will accept it for long-term geologic isolation (unless it contains transuranic elements, in which case its destiny is likely to be DOE's Waste Isolation Pilot Plant in New Mexico).

The CST process is also being considered for cesium removal at DOE's Hanford, Idaho, and Savannah River sites. It has been estimated that the CST process would save Hanford $500 million in reduced waste disposal costs. CST also takes up strontium-90 (an emitter of beta radiation), but it's not the ideal sorbent for the task. Research is under way to find a better strontium sorbent to effectively remove another bad actor from DOE waste.

The research was sponsored by DOE's Office of Waste Management and Office of Science and Technology.

Novel Tracers Map ORNL's Underground

An environmental researcher uncaps an injection well on the Oak Ridge Reservation and pours in a container of what appears to be plain water. The clear solution actually contains trillions of microscopic silicon beads tentacled with DNA fragments. As stand-ins for different radioactive contaminants, their job is to show how contaminants in groundwater move through a subterranean maze of broken rock and soil.

As they drift down a groundwater current, some of the minuscule beads lodge against fracture walls or become trapped in dead-end fissures. The survivors seep calmly along until they near an intersecting fracture; the current accelerates, and soon they're navigating whitewater: a veritable tidal wave surges through the junction, shooting half the spheres upward into an ascending stream. There they careen into another fleet of beads flying their own DNA flags. This fracture soon empties into yet another, and spheres from both fleets finally sweep into a monitoring well to be taken into custody for analysis.

Those flag-flying silicon vessels represent a major advance in tracing the movement of radioactive contaminants through the reservation's tortuous underground environment. One of several novel types of tracers developed at ORNL, they hold great promise for aiding DOE's environmental restoration efforts, as well as for guarding against pollution of water supplies in other settings.

Tracers are "surrogate contaminants," harmless substances that mimic the behavior and physical and chemical makeup of specific toxic counterparts, such as radioactive waste or hazardous chemicals. They can indicate the origin and movement of contaminants by showing which sources do—and which sources don't—feed into a contaminated area.

The DNA tracers are silicon hydroxide beads, a fraction of a micron in diameter, tagged with fragments, each containing 20 pieces of the DNA constituents A, C, T, and G. The number of DNA tags available to label tracers is thus 4^{20}, more than a trillion. Therein lies a key strength of the technology: It allows production of virtually unlimited numbers of tracers that behave identically but that are easily distinguished because each DNA tag naturally pairs with complementary DNA fragments of a known sequence. Until the DNA tracers were developed, there were not enough different tracers to map all the intersecting groundwater pathways underlying the Reservation that various radioisotopes could take.

Groundwater under the reservation traverses fractured bedrock that transports it rapidly and porous shale that absorbs and then releases it slowly. Think of the subsurface as a huge sponge with a web of cracks. Water runs through the cracks quickly,

Beads tagged with DNA fragments are used to trace the routes of groundwater contaminants in the ORNL area.

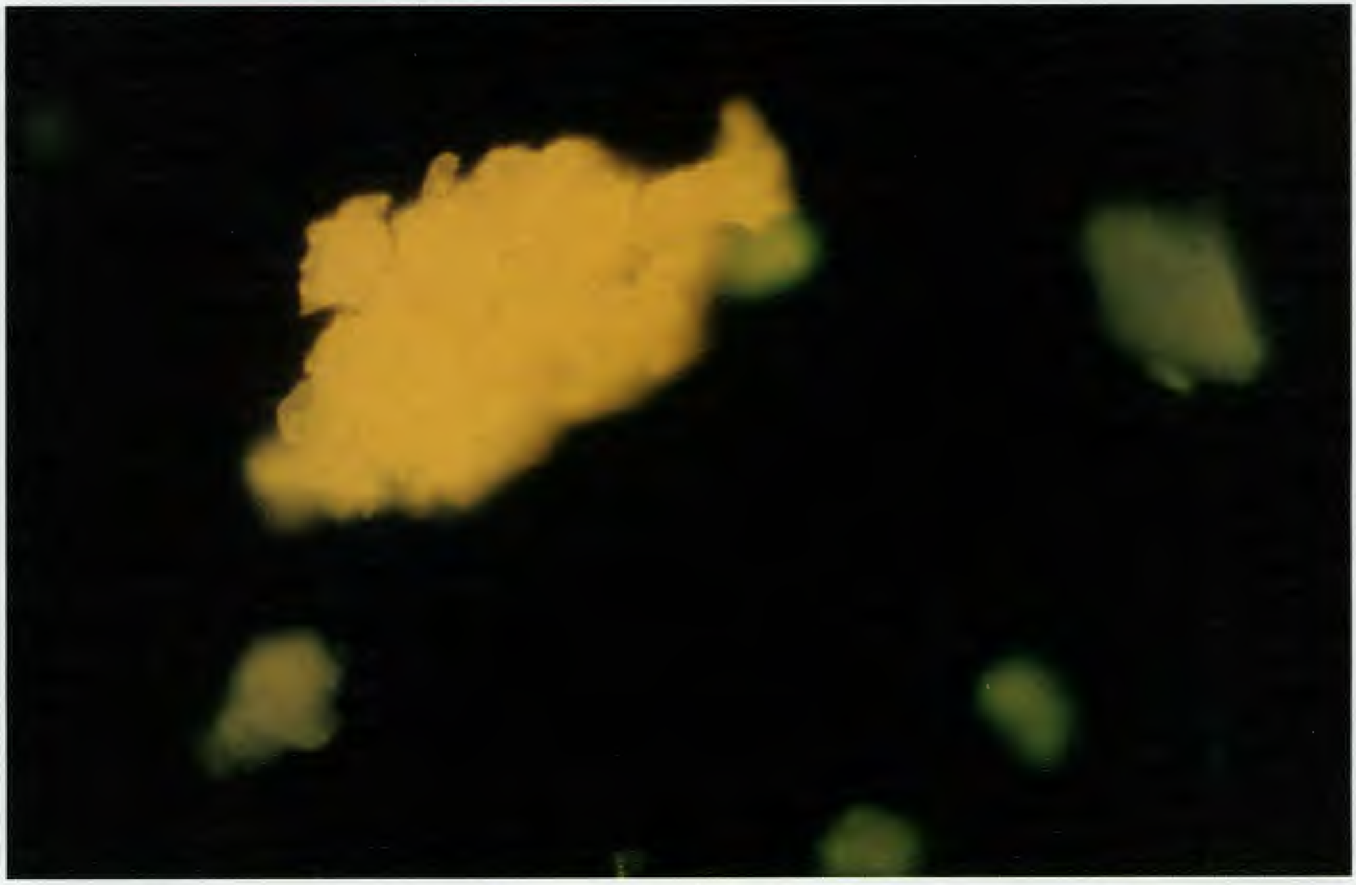
perhaps hundreds of meters per day, but seeps slowly through the sponge (matrix) itself, a couple meters per year at best. Travel time depends on the type of tracer and its interaction with the matrix. So several types of tracers are used to map the same area: reactive tracers mimic contaminants that attach onto matrix material; diffusive tracers mimic those that diffuse into the matrix; and colloidal tracers (the silicon beads) mimic those that travel the fractures rapidly because they are too big to diffuse.

In the case of our groundwater-surfing beads, the time it takes a tracer to migrate from the particular injection point to the monitoring well indicates how fast the contaminants it mimics would move through that area. When tracers introduced into different fractures in a zone turn up in the same monitoring well, researchers know that those fractures connect underground and that their contents, including contaminants, mingle. Other types of tracers indicate to what extent the radioactive counterparts of the tracers will attach to soil or diffuse into the shale and leach out slowly over years.

In addition to the DNA tags, ORNL uses other novel tracers, such as ice-nucleating bacteria, nonreactive gases, and rare-earth elements to map, model, and measure groundwater transport of radioactive contaminants. Their use has led to a new understanding of the direction and speed of radionuclide transport and the effectiveness of remediation methods such as pumping and treating groundwater.

The ORNL team is working on refinements to make the new tracers sufficiently economical for use in small-budget projects. The tracers promise to be valuable for detecting contaminant pathways in many settings. For example, tracers introduced at various points in a contaminated drainage system could pinpoint from whence a pollutant is coming. Environmental researchers now have an armada of informants to send down into the dark to shed light on subterranean waterways.

The research was sponsored by ORNL's Laboratory Directed Research and Development Program, ORNL's Groundwater Program Office, and DOE's Office of Technology Development and Office of Science and Technology. **ornl**



Silicon beads in groundwater collected from monitoring wells emit a green and yellow glow under ultraviolet light, indicating that they have been tagged with DNA fragments. The injection well from which each bead started through the groundwater system can be determined by identifying the specific DNA sequence with which each bead is tagged.

Energy Production and End-Use Technologies

Photograph by Tom Cerniglio, digital image enhanced by Reneé Balogh

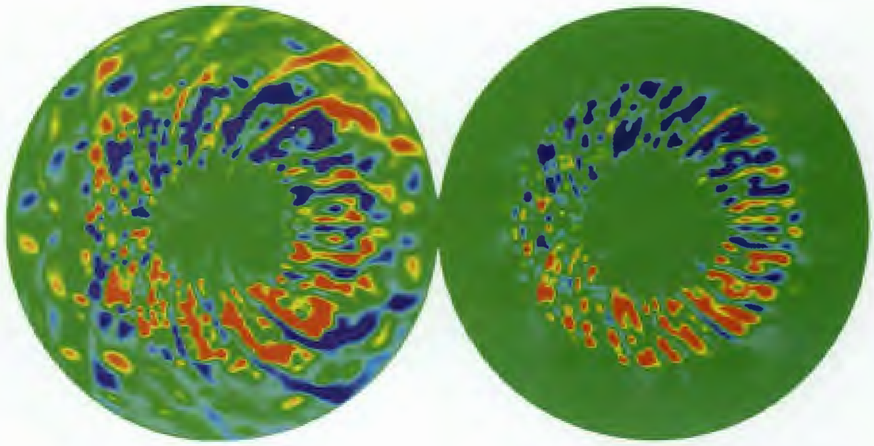
Fossil and fission energy now and fusion energy in the future. Efficient distribution of electricity by utilities and efficient use of energy in industrial processes. Leak-tight buildings and refrigerators on a strict energy diet. Transportation vehicles that go farther on less fuel to reduce our nation's need for imported oil. These are some of the targets of ORNL's energy-related research.

ORNL is one of the world's premier centers for research and development (R&D) work on energy production, distribution, and use and on the effects of energy technologies and decisions on society. As a primary performer of DOE-sponsored R&D in energy efficiency, ORNL brings to bear its remarkable capabilities in materials science, biotechnology, engineering, and technology development and evaluation. The objects of our expertise are transportation systems, buildings and building materials, industrial processes, and utility distribution systems. Our research on fission, fossil, and fusion technologies applies the Laboratory's strengths in physics and engineering to the improvement of existing systems and the development of new science and technology.

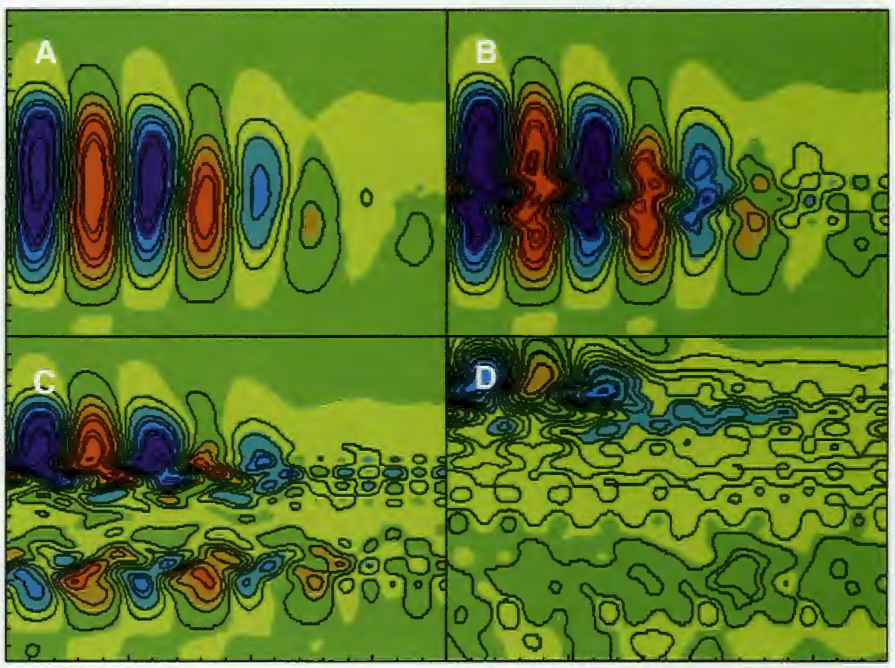
Unique facilities for energy-related R&D are used both for technology development and for fundamental investigations in the basic energy sciences that underpin the technology work. ORNL's scientific, engineering, environmental, economic, and social science expertise is integrated to supply the information needed in making decisions that ensure a sustainable energy future.

Fusion Plasma Turbulence Can Be Suppressed

ORNL-led experiments showed that plasma turbulence and associated heat losses can be reduced in a properly operated fusion device.



Turbulence at the DIII-D tokamak edge amplifies a global shear flow that, in turn, suppresses turbulence. These two snapshots of a time evolution of turbulence at the plasma edge show fully developed turbulence just before a transition (left) and suppression of turbulence at the edge (right).



Four successive stages in the evolution of plasma turbulence. The first snapshot shows the turbulent eddies. In the second, turbulence amplification of shear flow has started, with the eddies being distorted by the flow. The distortion increases and the eddies are sheared in the third frame. Finally, turbulence is totally suppressed.

In fusion energy, a key to getting heat out is to make sure that heat is initially locked in. That's why fusion energy researchers have tried to find ways to eliminate turbulence in experimental fusion devices.

Turbulence is a major cause of heat loss in fusion plasmas in doughnut-shaped tokamak devices. Heat losses must be avoided because the goal of a fusion energy device is to obtain an output of energy (heat to make steam to generate electrical power) that far exceeds the input of energy—electrical power. Electricity is needed to operate magnets that confine the charged particles (electrons and nuclei) making up the gaseous hydrogen plasma so that they are in close contact (high density). Also needed is electrical power to heat the plasma to high temperatures so the closely packed hydrogen nuclei overcome their natural repulsion and fuse, forming helium and releasing neutrons and large amounts of usable heat.

In the 1980s, it was found that as power to heat the plasma is increased, plasma turbulence is also increased. This irregular fluctuation in plasma velocity and pressure results in loss of heat (what fusion energy researchers call "energy transport"). It became a major concern that efficiency of plasma heating declined with increasing power. That was the bad news.

Now, here's the good news. Experiments led by ORNL in 1996 at the DIII-D tokamak in San Diego, together with experiments performed at the Tokamak Fusion Test Reactor in Princeton, New Jersey, showed that plasma turbulence can be suppressed by operating experimental fusion devices in the most advanced "plasma confinement mode." It was found that turbulence could be almost eliminated at certain power levels by properly controlling plasma temperature, density, and current. One change that was essential to turbulence suppression was ramping the current to make it peak towards the plasma edge rather than in the center. In future experiments, it is planned to use radio-frequency power for this purpose and to sustain the plasma discharges in a steady state.

In parallel, a theoretical effort involving scientists at ORNL, the University of California at San Diego, and the Princeton Plasma Physics Laboratory developed an explanation for the reduced turbulence seen on DIII-D. It was proposed that, under certain conditions, a plasma can "self-organize" and move from the state of chaotic turbulence to a state of order. A turbulent plasma consists of eddies, or small vortices, that increase the rate at which the energy leaks out. Flows in plasma, such as plasma rotation, are driven by the electric field generated by currents in the plasma in interaction with the tokamak's magnetic field. If plasma conditions are properly controlled, the same turbulence can amplify flows in different plasma locations to create a global "sheared flow" in which each eddy is pulled in two directions, breaking it up. In this way, turbulence and the resulting energy losses from the plasma can be nearly eliminated.

The ORNL-led turbulence suppression experiments enabled the DIII-D machine to achieve a record performance. Overall, the project was considered a sheer success.

The research was sponsored by DOE, the Office of Energy Research, Office of Fusion Energy Sciences.

ORNL Reviews Nuclear Plant Containments

In this example of a concrete containment being constructed for a nuclear power plant, some of the primary construction materials are evident.

In the United States, the biggest challenge to a concrete containment at a nuclear power plant was the 1979 Three Mile Island accident. In this case, a sequence of equipment malfunctions and operator errors caused a loss of reactor core cooling that led to partial melting of the fuel and a release of radiation into the concrete containment's environment. But the containment structure did its job. Despite the temperature and pressure buildup from the accident, the concrete containment limited the release of radioactivity into the atmosphere to a level low enough to cause the public no harm.

Today's nuclear power plants have a large containment structure made of either concrete or steel to limit radiation releases to the surrounding public. Of the 110 U.S. nuclear power plants licensed for commercial operation, over 60% have a concrete containment. The others use a steel containment but rely on concrete structures to provide additional radiation shielding and protection against environmental effects.

Although these plants' concrete structures have performed well and will continue to meet their

ORNL has developed a methodology for determining if concrete containments at aging nuclear power plants will continue to perform satisfactorily.

intended functions, some in all likelihood will undergo degradation from exposure to hostile environments, just as some U.S. concrete bridges and highways are deteriorating. Examples of potential threats to the integrity of nuclear-plant containment structures are listed in a document prepared in 1996 by ORNL and Johns Hopkins University for the U.S. Nuclear Regulatory Commission (NRC). The document is titled *Report on Aging of Nuclear Power Plant Reinforced Concrete Structures*.

One potential threat to these structures is corrosion of the reinforcing steel bars used to compensate for the low strength of concrete when it is loaded in tension. Another threat would be an attack by chemicals, which can either erode the concrete or cause harmful expansive reactions of its constituents. Also, concrete located in regions where moisture accumulates can crack from exposure to freezing and thawing conditions. Finally, if the concrete is exposed to elevated temperatures or irradiation, it can crack and lose its strength and rigidity.

The report's authors have documented examples of degradation already present in some nuclear power plant containment structures—corrosion of steel reinforcement in cooling-water-intake structures, greater than estimated losses of forces used to precompress the concrete in prestressed concrete containment designs, and cracking and spalling of containment dome concrete as a result of weather-induced freezing and thawing. As nuclear power plants continue to age, the authors state, the incidences of degradation can be expected to increase.

By the end of this decade, more than 60 U.S. commercial nuclear power plants will be more than 20 years old, with some nearing the end of their initial operating license period. Faced with the large costs of shutting down and cleaning up reactors and replacing lost generating capacity with other sources, many U.S. utilities are expected to seek extensions of their initial plant operating licenses (nominally a 40-year period). Although mechanical and electrical equipment in a plant can be replaced, it would be extremely difficult and economically unattractive to replace a concrete containment structure. To get approval from the NRC for a continuation of service, utilities must provide evidence that the concrete structures will continue to perform as designed.

Since 1988, ORNL researchers have been developing a methodology the NRC can use as part of the evaluation process for nuclear power plants seeking to continue operation. Under this program, ORNL's Structural Materials Information Center was set up to collect and disseminate, both on paper and electronically, data on how the properties of materials vary over time under the influence of environmental stressors. Currently, more than 140 materials are being evaluated in the center. We have developed an aging assessment methodology that uses ranking criteria to identify structural components and degradation factors of primary importance for managing aging structures. This methodology enables utilities to focus their inspection programs on structures or structural components most important to aging and identifies the type of degradation that might be expected.

We have established guidelines and criteria for assessing the condition of concrete containment structures. Also, a reliability-based approach has been developed that can be applied in evaluation of these structures to estimate their current and future performance. One application of this approach would be in the development of optimized in-service inspection and maintenance programs.

In addition, we have conducted in-depth evaluations of (1) several concrete-related technologies, such as knowledge-based systems for concrete and concrete-related materials; (2) in-service inspection and condition assessment techniques and methodologies for their application; (3) corrosion of metals embedded in concrete, including criteria for applying methods to halt or prevent corrosion (e.g., cathodic systems that protect the embedded steel reinforcement by forcing corrosion to occur at another location so the structure is not affected); and (4) ways to repair degraded concrete structures, such as filling cracks with epoxy or polyester materials, using chemical grouts to halt water seepage, and using inorganic and organic materials to replace spalled concrete materials.

Results of this program are summarized in the ORNL–Johns Hopkins University report mentioned earlier. Although this activity addressed concrete structures in nuclear power plants, our program results could be applied to buildings, bridges, roadways, and other infrastructure-related facilities. We know enough to provide sound advice on managing aging facilities, even though not all the answers are cast in concrete.

The project was sponsored by the NRC's Office of Nuclear Regulatory Research, Division of Engineering Technology.

ORNL Leads Study on Using Reactors To Burn Plutonium

Now that the arms race is over, the United States hopes that Russia will join a new race: ridding the world of excess weapons-grade plutonium as quickly as possible. This potentially hazardous material, along with highly enriched uranium in surplus nuclear weapons, is a legacy of the end of the Cold War between the United States and the former Soviet Union. To give the race a jump start, President Clinton announced his latest nuclear weapons nonproliferation strategy, whose formulation was influenced by an ORNL-led study.

On January 14, 1997, the Clinton Administration announced a two-pronged strategy to ensure that plutonium from dismantled U.S. and Russian nuclear weapons will never again be used in weapons production. A $2.3 billion, 20- to 30-year program was proposed for putting 50 metric tons of U.S. surplus plutonium out of harm's way. It was decided to permanently store some of the bomb-grade material by immobilizing it in glass or ceramic logs and mixing it with highly radioactive waste for storage in canisters in a U.S. repository. The remainder of the plutonium would be used as mixed-oxide (MOX) fuel in existing electricity-generating commercial reactors, which ordinarily are fueled with slightly enriched uranium.

In January 1994, President Clinton and Russian President Boris Yeltsin asked experts to jointly study options for the long-term disposition of fissile materials, particularly plutonium, taking into account the issues of nonproliferation, environmental protection, safety, and technical and economic factors. The Department of Energy's (DOE's) Fissile Materials Disposition Program was established soon after to implement the Presidents' directive. ORNL then became DOE's lead laboratory for characterization, assessment, and development of reactor-based plutonium disposition options.

In collaboration with utilities, other national laboratories, and the Canadian government, ORNL's Fissile Materials Disposition Program, managed by Sherrell Greene, led a 3-year study to identify and evaluate U.S. reactor options for plutonium disposition. The study, recently documented in a series of ORNL *Reactor Alternative Summary Reports*, examined the challenges and consequences of producing and burning MOX fuels. This study provided much of the scientific basis for President Clinton's recent decision to burn some of the plutonium as MOX fuel in American commercial light-water reactors.

The plan is to burn MOX fuel in 3 to 6 reactors for 10 to 15 years to dispose of surplus plutonium as quickly as possible. The plutonium would be used only once; the spent fuel from the reactor would not be reprocessed to extract residual plutonium and maximize the fuel's energy value, as is done in Europe. Instead, the spent fuel (which is unusable as weapons material) would go into long-term storage in a U.S. geological repository.

Partly because plutonium and uranium absorb neutrons differently, the ORNL-led study found that relatively minor reactor modifications would be required, along with some modifications in fuel-handling and spent-fuel systems, for selected reactors to burn MOX fuel. Also, safeguard and security measures must be upgraded at these reactors to ensure that plutonium-containing fuel is kept out of the hands of people bent on making an atomic weapon.

An ORNL-led study provided a scientific basis for President Clinton's decision to burn plutonium in U.S. power reactors.

The technologies needed to fabricate MOX fuel from dismantled nuclear weapons were described in the ORNL-led study. The heart of each nuclear warhead is a plutonium metal pit, a sphere smaller than a bowling ball. In one facility, each pit will be converted chemically to a mixed oxide, using a process being developed at DOE's Los Alamos National Laboratory: First, hydrogen will be added, producing plutonium hydride, and then hydrogen is driven off, leaving plutonium metal, which is then oxidized, producing a fine plutonium oxide powder. In a second facility, depleted uranium will be added to the powder to make mixed-oxide fuel elements.

The ORNL-led study concluded that new technology must be developed for the efficient conversion of plutonium pits to powder. Estimates indicate the facilities for fabricating MOX fuel could be ready in 10 years.

On the international front, the *Joint Russian-U.S. Plutonium Disposition Options Study* was recently issued, thanks partly to ORNL leadership. ORNL staff members Bruce Bevard and David Moses wrote major sections of this report. ORNL's Jim Stiegler sat on the 9-member U.S./Russian Steering Committee on Plutonium Disposition, which provided oversight for this report. Stiegler has since been replaced by Gordon Michaels, director of ORNL's Nuclear Technology Programs. Co-chairs of the committee are Nikolai Egorov, deputy minister of Minatom (equivalent to the nuclear part of DOE), and Bruce MacDonald of the White House Office of Science and Technology Policy.

In addition, ORNL has begun managing the implementation of two multiyear, multinational programs to demonstrate three different types of MOX technologies: American light-water reactors, Canadian deuterium-uranium heavy-water reactors, and the VVER pressurized water-cooled reactors in Russia. The Russian government, which is not enthusiastic about the immobilization option, plans to dispose of at least 50 metric tons of surplus plutonium by burning it as MOX fuel in electricity-generating reactors. Thanks to the moxie of ORNL and other U.S. participants, the race to disarm should forge ahead.

The ORNL research was sponsored by DOE, Office of Fissile Materials Disposition.

ORNL and Industry Seek Commercially Acceptable Wire

ORNL has developed industrially appealing processes for producing high-temperature superconducting tapes. Now, we are working with industry to determine how to produce wire of industrial strength—and an industrial length.

On April 10, 1996, at a scientific meeting in San Francisco, ORNL researchers rolled out a short superconducting tape that, when chilled to 77 K by liquid nitrogen, can carry large amounts of current without energy-wasting resistive losses. They announced the development of a process for making the backbone, or substrate, of superconducting wire using a pair of rollers, heat, and thin ceramic films. The rolling-assisted biaxial textured substrates (RABiTS™) process generated excitement among researchers in the electrical industry. It represented a leap forward in the race to develop fabricable superconducting wire. The substrate can be made with equipment like that used to produce labels on soft drink cans, videotapes, and liners inside snack food bags.

The ORNL process is faster and probably cheaper than competitive processes. It conditions the substrate, or template, upon which a high-temperature superconducting film of yttrium-barium-copper oxide is grown. The substrate is made of textured nickel covered with buffer layers of cerium oxide and yttria-stabilized zirconia that are 350 times thinner than a sheet of paper. These oxide layers are needed as a chemical barrier to prevent the substrate's nickel atoms from dislodging the superconductor's copper atoms. But the layers must be put down uniformly so that their crystalline structure closely mimics that of the nickel tape. The buffered substrate aligns crystalline grains in the superconducting film as it grows. Such a superconducting "sandwich" allows efficient flow of electricity in the presence of high magnetic fields if it is chilled by liquid nitrogen (which costs only 2% of the price of liquid helium, the coolant for low-temperature superconductors).

The goal is to develop industrially appealing processes, ranging from electron-beam evaporation to a chemical coating process, to produce these tapes, which on a laboratory scale are centimeters long, in kilometer lengths. Such wires could be used in transmission cables, transformers, steel and paper mill motors, generators, and magnet-containing devices such as medical diagnostic machines.

A nonexclusive license agreement has been signed

ORNL is working with industry to determine how best to fabricate longer, stronger high-temperature superconducting wire.

Mariappan Paranthaman recently used electron-beam evaporation to make a superconducting wire 7 centimeters long. He shows the nickel substrate on which buffer layers are deposited by e-beam evaporation. *Photograph by Tom Cerniglio.*

with Midwest Superconductivity to use the technology in research and development, with an option for wire and tape commercialization rights. Co-developer Westinghouse is producing the roll-textured nickel base metal. Recently, 3M Company and Southwire Company have announced plans to further develop RABiTS™-based wires for transmission cable. Our collaborations with industry should shorten the time it takes to make a durable superconducting wire that's acceptably long.

The RABiTS™ team received a NOVA Award for Teamwork from Lockheed Martin Corporation and captured top honors in the technical achievement category of the corporation's Oak Ridge awards competition. The project was conducted under joint sponsorship by DOE's Office of Energy Efficiency and Renewable Energy and DOE's Office of Energy Research.

Highly Efficient Refrigerator Design

The "fridge of the future" will use half as much energy as today's refrigerator-freezers, and it will change the way we chill our foods, easing fears about chewing holes in the protective ozone layer and warming the globe. At ORNL a popular refrigerator model has already been put on a strict energy diet, exceeding one turn-of-the century goal. The refrigerator-freezer was altered to reduce its energy use by 50%, from 2 kilowatt hours per day to 1 kWh/d. This reduction in energy use exceeds the limit called for in a new rule announced by the federal government on April 24, 1997. The rule requires refrigerators sold in 2001 to use 30% less electricity than those on the market today.

This laboratory prototype is the product of work by ORNL researchers and refrigerator manufacturer engineers in a cooperative research and development agreement (CRADA). The CRADA between ORNL and the Appliance Research Consortium (a subsidiary of the Association of Home Appliance Manufacturers) achieved a dramatic energy reduction in a standard 20-cubic-foot refrigerator with a freezer on top. More than 60% of the refrigerators sold in the United States are "top-mounted" refrigerators like the lab model.

Some 125 million refrigerators in the United States consume approximately 1.5% of the energy used in the country. If the energy used in units currently in homes was reduced to 1 kWh/d, refrigerators would consume only about one-half of one percent of the nation's energy, saving almost $6.5 billion annually. The accompanying decrease in demand for electricity from coal-fired power plants would also significantly reduce greenhouse gas emissions.

The CRADA's "technically feasible model," which exceeds the goal of government standards scheduled to go into effect in 2001, is more efficient because of four changes. Vacuum insulation panels were used around the freezer section to reduce heat gain. Polyurethane foam was added to the doors, doubling their thickness.

A popular refrigerator model has been altered at ORNL to cut its energy use in half.

Ed Vineyard checks the instrumentation in the highly efficient refrigerator model. *Photograph by Tom Cerniglio.*

Also, a high-efficiency compressor was installed. Three motors that used to operate on alternating current to drive two fans and the compressor were replaced with three direct-current, electrically commutated motors, which use less electricity and release less waste heat. Finally, the automatic defrost control, which daily removes ice from refrigerant coils to improve their heat transfer, was replaced with adaptive defrost, so that defrosting occurs only when needed—perhaps every other day in summer and once a week in winter, depending on the humidity and number of times the refrigerator door is opened.

ORNL and its CRADA partners—Amana, General Electric, Maytag, Sub-Zero, Sanyo, W. C. Wood, and Whirlpool—also developed a second model that is more cost-effective than the initial prototype. It has all the extra features except for vacuum insulation around the freezer and increased evaporator area. This second model would result in a savings of approximately $4.5 billion annually.

Vacuum insulation (such as the powder-evacuated panels being studied at ORNL) may be revisited in an ongoing CRADA between ORNL and Frigidaire. The CRADA's goal is a production model, leading to a highly efficient refrigerator on the market in three to four years; such an appliance should pay for itself in three years through reductions in electricity bills. The problem is that the hydrochlorofluorocarbon HCFC-141b that is now used as the blowing agent to insulate refrigerators will be banned in 2003. The replacement insulation will likely be less energy-efficient, making vacuum insulation look more cost effective.

Both the technically feasible and cost-effective models use the ozone-friendly refrigerant R-134a, which has been designated to replace CFC-containing refrigerants in new refrigerators because of its lack of chlorine.

Because it is a greenhouse gas and thus contributes to global warming, R-134a may also have to be replaced. One proposed replacement is a hydrocarbon, which raises the risk of house fires. Engineering problems must be solved to avoid house safety problems and adverse effects on global change. The idea is to keep our food cold without making the globe too warm.

The research was funded by DOE's Office of Building Technologies, State and Community Programs, and by the Appliance Research Consortium of the Association of Home Appliance Manufacturers.

ORNL's Soft-Switching Inverters Will Help Save Energy

Electrical power is often delivered or stored in a form different from what's needed for a particular use. So, to get power to the people, a device called an inverter is needed to convert incoming power from, say, direct current (dc) to alternating current (ac) at variable frequencies and voltages. Unfortunately, such conversions waste electrical energy and generate heat.

To address this problem, a new type of power inverter is being devised—one that may be a building block for technologies ranging from electric buses, to more efficient heat pumps, to safer brain surgery techniques. Called a soft-switching inverter (SSI), this device is more efficient, more compact, and more reliable than conventional inverters. Also, it produces little electromagnetic interference—those irritating magnetic fields that interfere with proper operation of other electronic devices.

The first SSI developed at ORNL was the resonant snubber inverter (RSI), which has been patented. Now, our researchers are developing the next generation of SSIs, which are expected to have a wide array of industrial and military uses.

A conventional hard-switching inverter uses six semiconductor transistors (switches) that open and close up to 20,000 times per second to create an alternating current. Every time a switch is turned on or off with full current or voltage running through it, high, instantaneous power losses are generated. These power spikes wear out switches and equipment and produce waste heat. The RSI adds small auxiliary components that temporarily divert the power from the main switches so that they are turned on and off without power loss.

Because the RSI operates more efficiently than a conventional inverter (98% vs 94% efficiency at high power), it produces less waste heat. It loses only 2% of the energy at high speeds and 20% at low speeds, compared with conventional inverter losses of 6% at high speeds and 30 to 40% at low speeds. Lower heat losses decrease the possibility of equipment degradation and failure and allow a more compact design. SSIs use lighter, cheaper "sinks" to absorb the operating heat, and device components can be safely placed closer together. Compared with the newest conventional inverter, the SSI weighs only about one-third as much and occupies one-tenth the volume.

Because the SSI is smaller and lighter, it may be used in electric cars or buses. Its greatest efficiency gains are at the mid-power range at which it would operate in an automobile.

An SSI-equipped heat pump would run continually at varying fan speeds instead of cycling on and off. It would use less power because heat pumps use five times as much power cycling on as is consumed during normal operation. Also, it would run more quietly while offering improved comfort.

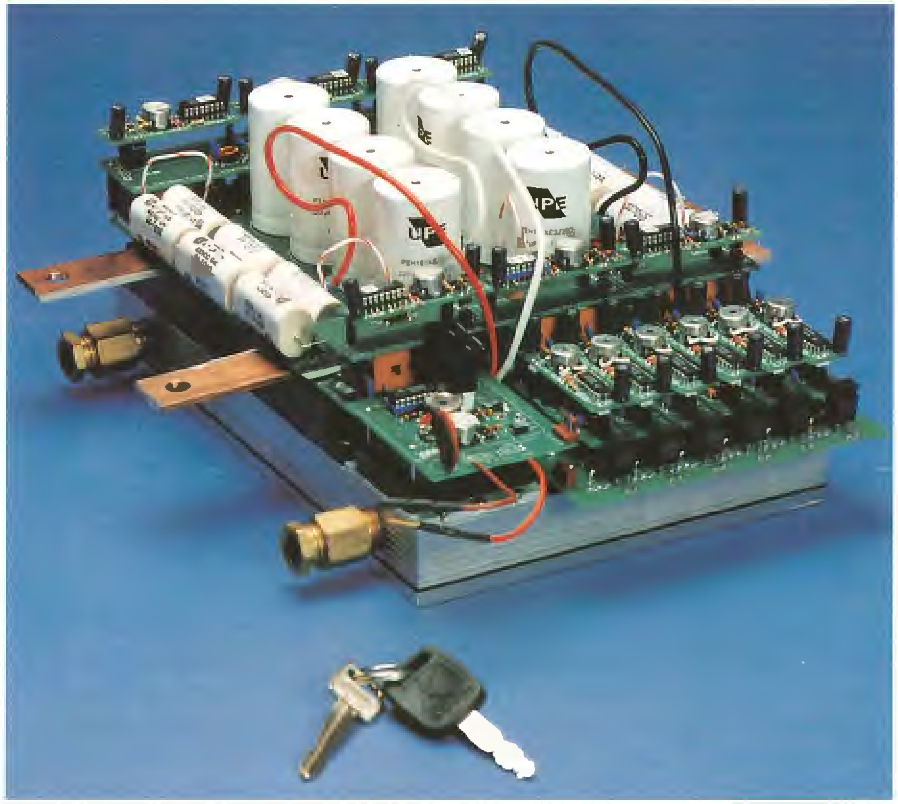
ORNL has a cooperative research and development agreement with Stereotaxis involving use of the RSI in a medical procedure that employs superconducting magnets to route tiny magnetic devices through the brain. The technology could be used to inject medicines, perform biopsies, thermally destroy targeted tissue, or deliver radioisotopes to a tumor, minimizing the amount of brain tissue involved in surgery or radiation treatment.

SSIs may also be used in industrial machinery such as pumps, compressors, and conveyor belts. Such inverters should improve the reliability of adjustable speed drives, increasing the efficiency of much industrial equipment.

ORNL researchers are developing SSIs in support of the DOE/U.S. Navy Power Electronics Building Blocks Program. The program's goal is to do for power electronics what integrated circuits did for computers: revolutionize the technology by making it possible to build compact, cool-running inverters. Such technology will empower people to use energy more efficiently.

The ORNL development of soft-switching inverters was initiated under ORNL's Laboratory Directed Research and Development Program. It is now being supported by DOE's Office of Energy Efficiency and Renewable Energy, Office of Transportation Technologies, as part of DOE's contribution to the DOE/U.S. Navy Power Electronics Building Blocks Program.

ORNL is developing highly efficient, compact, and reliable soft-switching inverters to convert dc to ac.



This compact, reliable, ORNL-developed soft-switching inverter is a key technology for efficient conversion of electrical power from one form to another (e.g., direct current to alternating current).

U.S. Vulnerable To Another Oil Price Shock

The oil price shocks of the 1970s and '80s sparked worldwide inflation and caused many nations to slip into recession. Could such a disruptive drop in oil supplies and rapid rise in prices happen again? Yes, according to an ORNL study. The United States is increasingly vulnerable to another oil price shock. Even the U.S. Strategic Petroleum Reserve wouldn't provide much of a buffer unless the disruption were very small and short.

The Organization of Petroleum Exporting Countries (OPEC), which represents many Persian Gulf nations, is poised to control more than half the world petroleum market again within 10 years. OPEC nations, which have most of the world's proven oil reserves, dominate world oil trade. Because they are drawing down their reserves half as fast as non-OPEC states, their share of oil resources is actually growing.

In the future, various situations could disrupt oil supplies from the Persian Gulf region: a revolution in a major oil-producing country, a Mideast war, terrorist activities, a political boycott, or the deliberate manipulation of supplies.

ORNL researchers examined changes in oil market fundamentals since the 1970s to see if a comparable price shock now would have a serious economic impact. They found that it would. Although some factors had improved (the rate of growth of oil demand is slower, for example), others were the same and still others worse (e.g., the United States now imports more oil than ever before). The ORNL team simulated the economic effects of a 2-year price shock in 2005 through 2006, assuming a 10% OPEC pumping slowdown in 2005 and an additional 7% cut the next year. Output then would increase at 0.5% per year through 2010. The reductions are roughly the same as those during 1979 through 1980 when OPEC repeatedly cut production to maintain high oil prices.

The simulation showed oil prices would jump from about $21 per barrel in 2004 to $54 per barrel in 2005, fall to $46 in 2006, and stabilize at $28 to $30 in the next few years. In contrast, if markets remain stable, the Energy Information Administration expects oil to hold steady at around $20 to $25 per barrel through 2015. In the ORNL simulation, the cost of the price shock to the United States economy, and the windfall to OPEC, would amount to about $500 billion through 2010.

The ORNL analysis also shows oil dependency has changed little since the 1970s. Almost half (46%) of the oil consumed annually in the United States is imported, equal to the record highs of the 1970s. Although many power plants have switched to other fuels, the transportation sector, which accounts for two-thirds of U.S. oil use, remains 95% dependent on petroleum for energy. Increased travel has outstripped fuel efficiency gains in automobiles.

What can be done to counter the threat of oil price shocks? The best defense appears to be increasing the price elasticity of oil (the ability of economies to respond effectively to changing oil prices). If demand is highly elastic, buyers can respond to a price hike by buying less until the price drops. If supplies are more elastic, OPEC production cuts can be compensated for by increasing supplies from the rest of the world.

A key to increasing price elasticity is developing new technologies. Needed are vehicles that use fuel more efficiently to make a barrel of oil go farther, and alternative fuels to substitute for oil when prices rise. Needed also are easier and cheaper methods of finding and producing oil, such as three-dimensional seismic imaging and advanced drilling technologies. These advances would both reduce the demand for oil and enable the rest of the world to supply more fuel faster and more cheaply if OPEC supplies decline. With highly elastic demand, non-OPEC nations should be able to respond effectively to future shocks and reduce the economic costs by half or more.

The research was sponsored by DOE's Office of Policy.

ORNL found that a price shock in the oil market now would have a serious economic impact on the United States.

David Greene, who led the ORNL oil study, surveys the gasoline storage tanks near Middlebrook Pike in Knoxville. The tanks are filled with fuel from the Colonial pipeline. Oil is refined into gasoline near the Gulf of Mexico and piped north by the pipeline. *Photograph by Tom Cerniglio.*

ORNL's Noisy Chaos Approach May Improve Engine Efficiency

Lay a drinking straw on the kitchen table, flick its middle gently with your finger, and watch it roll. Now flick it twice as hard and note that it rolls twice as far. This is what scientists and engineers call a linear system. Now, put the straw on its end so it balances on the table. Blow on it gently—a little change. Watch the straw topple to the table—a big change. The balanced straw is an example of a nonlinear system, something that's very sensitive to small perturbations.

Now, turn on the kitchen's gas stove. For a second, nothing happens and then, when the gas concentration reaches a critical level, poof!—up pops a flame. Like the balanced straw, the gas flame is nonlinear. Unlike the straw, however, the gas flame continues to fluctuate between unstable states, a process called flicker. In a sense, flicker is caused by the flame continually going out and relighting itself, over and over. A flickering flame is an example of chaos, the seemingly random fluctuation of nonlinear systems because of their sensitivity to small variations in the past.

One of the most important recent scientific discoveries has been that even very simple nonlinear processes can exhibit chaos. Chaos theory (or more properly, deterministic chaos theory) is concerned with how seemingly random processes can be explained using simple mathematical models that include nonlinear effects. Scientists have demonstrated that such models come surprisingly close to reproducing complex behavior seen every day, even when there is nothing explicitly random in the models. The apparent randomness comes from the

ORNL's noisy chaos theory considers external and internal "noises" that may affect the behavior of chaotic systems such as flames and engines.

nonlinear sensitivity feeding back into itself from moment to moment, causing a never-ending repetition of slightly different patterns. In the flame, flicker results when the fuel is depleted by burning, then the flame shrinks, then the fuel builds up again, then the flame suddenly flares up again, and so on.

ORNL researchers have added a new twist to chaos theory. We also take into account external and internal "noises" that perturb the nonlinear processes. Any real system is never completely isolated from its surroundings; likewise, other processes are always going on in the system at scales below our level of observation. Such noise, whether it comes from outside or inside, disturbs the ideal chaotic patterns that would otherwise exist, causing them to become "fuzzy" but not eliminating them completely. In the case of a flame, noise comes from the hiss of the gas jet and air currents in the room. To be more accurate, models of the flame should include how it responds both to its past history and to these noisy effects. We think this "noisy chaos" approach more accurately reflects how real systems behave.

We are applying our noisy chaos concept to better understand the behavior of internal combustion engines in today's cars and trucks. Like the gas flame, the combustion in your car engine fluctuates from moment to moment because of its nonlinearity. Such fluctuations are a problem because they increase pollution and reduce fuel efficiency. If combustion were the only process going on in the engine, it would probably be relatively easy to redesign the engine to reduce or eliminate the fluctuations. The problem is not so simple, however, because of the vehicle's other noisy processes, such as flexing belts, rattling gears, and pumping pistons. All these other processes perturb the combustion, making its chaotic patterns fuzzy and difficult to observe. If we can understand the resulting patterns in spite of their fuzziness, it is still theoretically possible to improve engine performance.

Improving the performance of internal combustion engines has both strategic importance for U.S. energy consumption and potential commercial applications. Thus, through a CRADA, ORNL and Ford Motor Company researchers measure the noisy chaotic patterns in internal combustion engines and develop improved computer models for explaining them. We believe the noisy chaos approach could be an important key to designing cars that use less fuel and emit less pollution. We also believe that the noisy chaos concept will have much broader applications than just automotive engines. For example, it may be applicable to utility boilers, precision machining, anti-skid brakes, and cardiac pacemakers.

Making nonlinear energy processes more efficient and less polluting is important but not easy. Results so far indicate that ORNL's noisy chaos theory could be a sound approach to this difficult challenge.

The research was supported by DOE's Office of Energy Research and Ford Motor Company. ornl

Stuart Daw conducts an experiment using an internal combustion engine to produce data to improve ORNL's "noisy chaos" computer models of engines. *Photograph by Tom Cerniglio.*

Instrumentation, Manufacturing, and Control Technologies

ORNL has unique capabilities in the development and implementation of technologies for measuring, monitoring, and controlling a variety of systems. We apply our expertise and instrumentation in electronics, photonics, imaging, and signal processing to biological, chemical, and nuclear concerns. Our goals are improved environmental quality and health protection as well as more accurate data to support science missions. The capabilities represented by this competency span the range from basic research in materials and processes through prototype development to production-scale facilities for precision manufacturing and inspection.

ORNL and Oak Ridge Y-12 Plant user facilities that promote the development of these technologies are the Metrology Research and Development Laboratories, the Metals Processing Laboratory User (MPLUS) Center, and the Oak Ridge Centers for Manufacturing Technology. With all these capabilities, we measure up to most people's expectations.

Photograph by Tom Cerniglio, digital image enhanced by Reneé Balogh

Helping U.S.Textile Firms Weave Quality Fabric

Faced with looming job losses because of stiff foreign competition, the U.S. textile industry is weaving new technology into its strategy to regain the competitive edge. Here's the problem. Since 1980 the U.S. textile industry has lost business—and 400,000 jobs—to foreign textile companies because of its higher labor costs; if the trend continues, another 600,000 jobs could be lost by 2002 in an industry that produces not only clothing but also carpeting, medical dressings, and automotive airbags. Here's a possible solution. The domestic textile industry can compete more effectively if it finds an economical way to produce visually flawless fabrics of a quality high enough that consumers will buy them in large quantities. To improve weaving technology to increase demand for its textiles, the U.S. industry has been collaborating with Department of Energy laboratories (including ORNL) in the Computer-Aided Fabric Evaluation (CAFE) Project.

Today's textile mills use high-speed looms to weave yarn into cloth. Inspectors in the mill manually feel and visually examine the cloth, looking for defects. Sometimes they miss the less obvious ones, and defective material passes through the entire textile system, eventually reaching the marketplace where retailers and consumers notice the flaws and the material is marked down or returned as a loss.

One strategy for stemming such financial losses is to develop a technology to inspect fabric while it is being woven. During the weaving process, horizontal filling, or "pick," yarn is laid down at a right angle to the "warp" yarns that run lengthwise through the fabric. Fabric quality and the amount of yarn used, both of which can affect product cost, strongly

Oak Ridge researchers have invented an optical device to detect defects in fabric while it's being woven.

ORNL's Jack LaForge is a member of a team that seeks to make the U.S. textile industry more competitive worldwide. ORNL and five other DOE laboratories contribute to the Computer-Aided Fabric Evaluation project, which incorporates on-line fabric inspection into weaving looms to dramatically increase the quality of U.S.-produced fabric. *Photograph by Bill Norris.*

depend on the regularity and density of the pick yarn (strands per inch). Thus, the CAFE project called for the development of a user-friendly inspection and defect detection system for industrial looms that measures pick density and locates flaws in fabric in real time. This system should help textile mills and apparel manufacturers minimize their production of reduced-price, second-grade merchandise and bad cloth that must be discarded, cutting their financial losses and saving jobs.

ORNL and Oak Ridge Y-12 Plant researchers have invented an optical device that meets the CAFE criteria. The new linear diode pick measurement device, which is cheaper than conventional camera systems and easily installed on existing looms, images and inspects textiles on the loom in real time. Using this simple and reliable combination of lasers, diodes, and lenses linked to a computer, loom operators can measure pick density and variability, map defects electronically, and identify fabric anomalies as the fabric is woven. From this real-time information, operators will instantly correct loom operation to halt production of defects and tag defective material for rejection—without stopping the loom. Tests of the on-line sensor system began at three U.S. textile mills in July 1996 and continue to run through 1997. Operation of the high-tech weaving systems was successful. Technology may save the day for U.S. textiles.

Funding for this development came from DOE's Defense Programs, Office of Technology Partnerships.

Heartbeat Detector Senses Persons Hiding in Vehicles

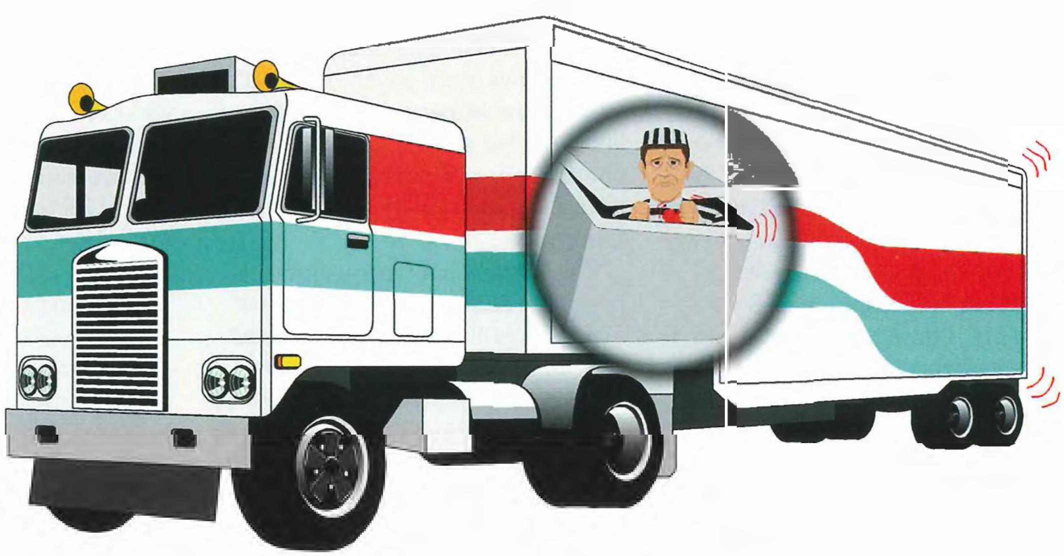
An 18-wheeler pulls into the portal of a nuclear defense plant to deliver heavy equipment. The guard says to the driver, "Please turn off your engine and everybody get out of the truck for a few minutes." A man and woman step out. The guard's next task is to search every nook and cranny, every box and package, in the truck. The object of the time-consuming search is a hidden armed terrorist bent on holding the plant's personnel hostage.

That was the old way. Now, the guard attaches six vibration sensors to the outside of the truck. These sensors are linked by cables to a signal-amplifying box attached to a sturdy laptop PC. The guard hits a function key on the laptop keyboard and watches signals ripple across the computer screen. In 20 seconds, a green rectangular "flag" appears at the top right of the screen. The message at the bottom of the screen says, "No intruder detected. PASS." But had the flag come up red, the message would have read, "INTRUDER DETECTED!! SEARCH."

In the early 1990s, the Department of Energy, concerned that terrorists concealed in vehicles could be sneaked into its defense installations (such as the Oak Ridge Y-12 Plant), called for the design and construction of "smart portals." Two Y-12 researchers began work to develop a heartbeat detector to find hidden intruders after learning that in 1991, researchers at Michigan State University had developed a microwave sensor to detect heartbeats at a distance. The Y-12 approach was to detect the "telltale" heartbeat using vibration sensors and a laptop computer to tease out the heartbeat signal from the truck's other vibrations induced by natural resonances, wind, and other influences.

Such an enclosed space detection system, popularly known as the heartbeat detector, has been built and installed at Y-12's "portal of the future," which will also incorporate undervehicle surveillance cameras, fiber-optic weigh-in-motion technology, and detectors of special nuclear materials and explosives. Portals of the future will economically reduce the time needed to inspect each vehicle while increasing the level of security. In fact, the heartbeat detector is 10 to 250 times faster than human

A device developed for detecting terrorists concealed in vehicles is being used to locate escaping prisoners.



The heartbeat detector can detect a prisoner or intruder hidden in a truck. *Drawing by Reneé Balogh.*

inspection, and its cost is only 3% that of conventional methods.

As the heart uses energy to pump blood, its regular, vigorous pulsations send shock waves through the body. The energy of the body's vibrations is transferred to any object the body touches, such as the inside of a truck. Amazingly, a hidden person's heart transmits pulsating energy that can be detected at the truck's exterior surface by vibration sensors linked to a computer.

To make it possible to detect the presence or absence of a heartbeat among the truck's other vibrations, ORNL researchers were asked to develop a mathematical procedure called an algorithm. The algorithm they developed uses a mathematical function called a wavelet—a small wave that rapidly dies out. The wavelets in the algorithm have a characteristic shape that closely matches typical human heartbeat signals. Using the wavelet function algorithm, the computer compares the wavelet functions to vibration signals from the truck. If there's a close match, the computer tells the guard to search the truck; if there's no match, the guard gets the green light and lets the truck pass through the portal without a search.

The heartbeat detector has other obvious applications. For example, it could detect any prisoner who tries to escape by hiding in a laundry truck. It could pinpoint illegal aliens from Mexico who sometimes sneak across the border to the United States in cars after taking the stuffing out of car seats and squeezing in under them. In 1996 the heartbeat detector was tested at two prisons: the Riverbend Maximum Security Institution in Nashville, Tennessee, and the Centinela State Prison in California. It was also tested for eight hours each at the San Ysidro and Otay Mesa portals at two border crossings between Mexico and the United States.

Because of its practical uses, the Oak Ridge heartbeat detector was licensed by Lockheed Martin Energy Systems to Geovox Security, Inc., which introduced a commercial version in the fall of 1996. The company has sold one heartbeat detector to the British Home Office (equivalent of the U.S. departments of Justice and the Interior), which operates all United Kingdom prisons. Many U.S. prison facilities are interested in purchasing heartbeat detectors, as well. They want to guard against letting the wrong people out just as DOE's nuclear defense plants want to guard against letting the wrong people in.

The project was funded by DOE's Office of Security Affairs.

ORNL Devises Way To Prevent Steam Explosions

In the metal casting industry worldwide, workers have been killed and large buildings and heavy equipment have been destroyed by steam explosions caused by contact of molten metal with water. According to data collected by the Aluminum Association, from 1980 through 1995 the aluminum industry experienced several hundred explosions during casting operations which resulted in hundreds of injuries, about 10 deaths, and extensive property damage. Three devastating explosions occurred in 1986 alone. The steel, magnesium, and pulp and paper industries also encounter steam explosion events. The most famous metal-water explosion of 1986, however, occurred not in these industries but at the Chernobyl nuclear power plant, causing an uncontrollable release of radioactivity over much of Europe.

The aluminum industry, which began conducting its own explosion experiments 40 years ago, concluded that, under certain conditions, a few organic coatings prevent explosions at surfaces submerged in water; however, there was no understanding of why or to what extent the coatings provided protection. The most widely used organic coating in aluminum casting pits is the coal-tar epoxy Tarset Standard. But when this industry mainstay and other similar paints were banned largely because of their toxicity, the industry turned to ORNL for help.

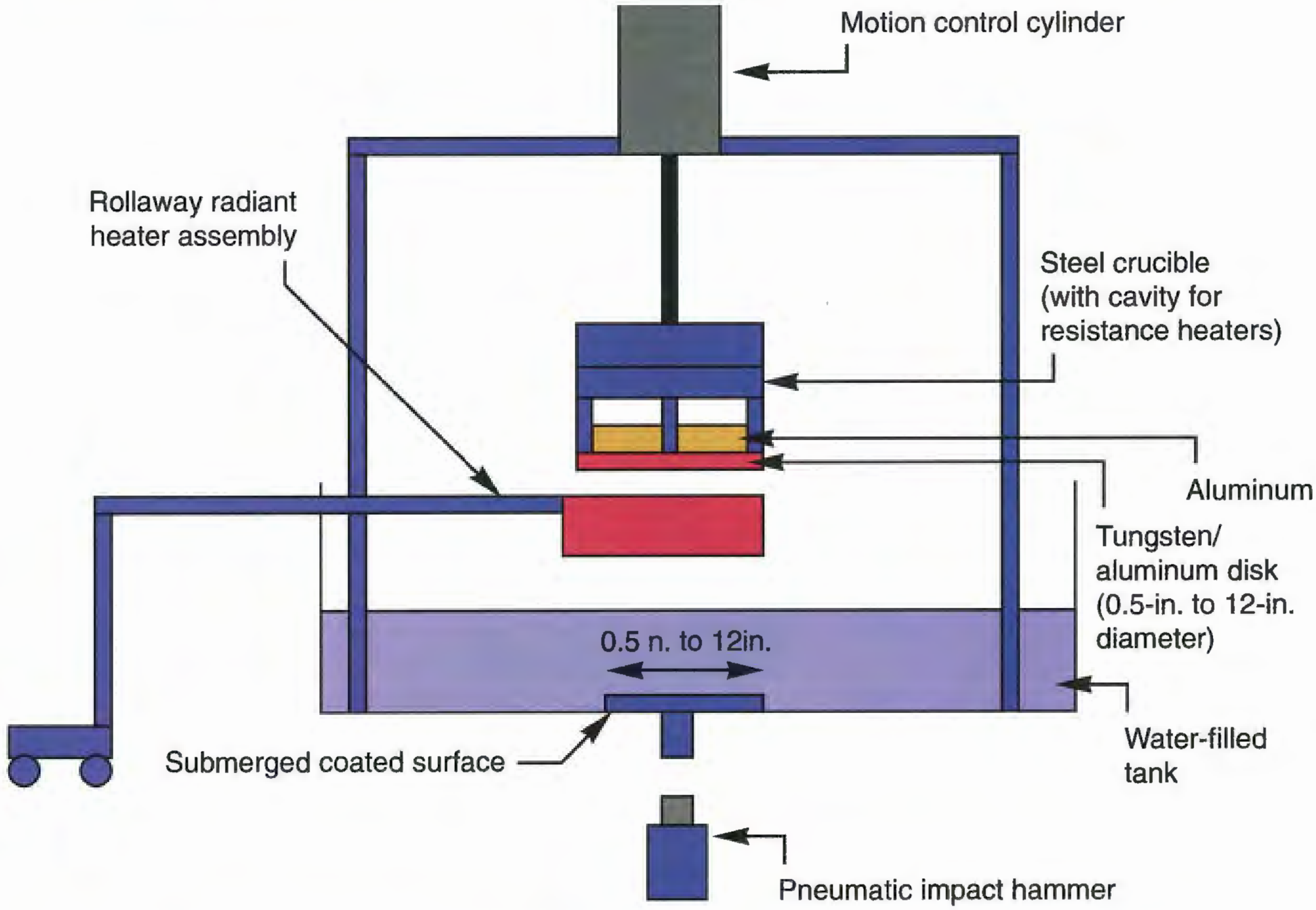
We were asked to conduct basic research to determine why, under what conditions, and to what extent these organic coatings prevent explosions. We were also asked to use this information to devise an alternative, environmentally friendly protective measure. ORNL was chosen because our researchers have been studying the potential problem of steam explosions in water-cooled research reactors in which fuel elements are made of uranium-aluminum mixtures sandwiched between aluminum plates.

In the aluminum industry, an aluminum ingot is formed by pouring molten aluminum into a steel mold that is lowered into a steel-lined (or concrete) pit of water. The water cools the mold, eventually solidifying the aluminum. Because of the chaotic nature of the process, significant quantities of molten aluminum can pour over submerged surfaces, sometimes leading to energetic explosions. To reduce the chance of a catastrophic event, the aluminum industry has coated the mold and pit linings with organic coatings such as Tarset Standard.

When molten aluminum first comes into contact with water, a protective steam film forms. It has been found that some sort of "trigger" causes the steam film to destabilize and collapse. As a result, the molten aluminum mass breaks into literally millions of hot particles, causing water they come in contact with to flash to high-pressure steam. ORNL researchers proposed that explosive boiling of entrapped water and external shocks (e.g., from jack hammers used in metal casting houses) could serve as triggers. ORNL researchers also suggested that noncondensible gases introduced into the steam film would cushion external triggers.

To test these ideas and find out why some coatings are more effective than others in preventing steam explosions, we developed a unique experimental apparatus called the Steam Explosion

ORNL has developed an environmentally friendly method for suppressing steam explosions in the aluminum industry.



Schematic of the SETS facility. Inside a steel crucible a pool of molten aluminum is supported by a tungsten plate that lets heat pass through it back and forth almost as fast as the molten aluminum would. However, tungsten melts at a much higher temperature. Therefore, accurate, instrumented, quick-turnaround, and safe lab-scale simulations of large and small amounts of aluminum pouring over submerged surfaces become possible. The plate is heated by a radiant heater. The energy of the molten aluminum is transferred through the plate to the entrapped water when the crucible is lowered toward the tank of water. A pneumatic impact hammer is used for some experiments to simulate an external shock. Coated samples (steel disks coated with epoxies, absorbent paper, lubricants, etc.) or uncoated samples (e.g., rusted steel or concrete disks) are mounted at the base of the tank for testing. Variations of back pressure and diameters of heater and base surfaces permit simulations of small- to large-scale events. The instruments detect early pressure pulses and heat transfer phenomena that would eventually trigger a steam explosion, but an actual explosion is avoided in this apparatus.

Triggering Studies (SETS) facility. In this facility, molten aluminum never comes in contact with water in a tank so there is no danger of a steam explosion. However, the facility can accurately simulate heat transfer from molten aluminum moving over submerged surfaces.

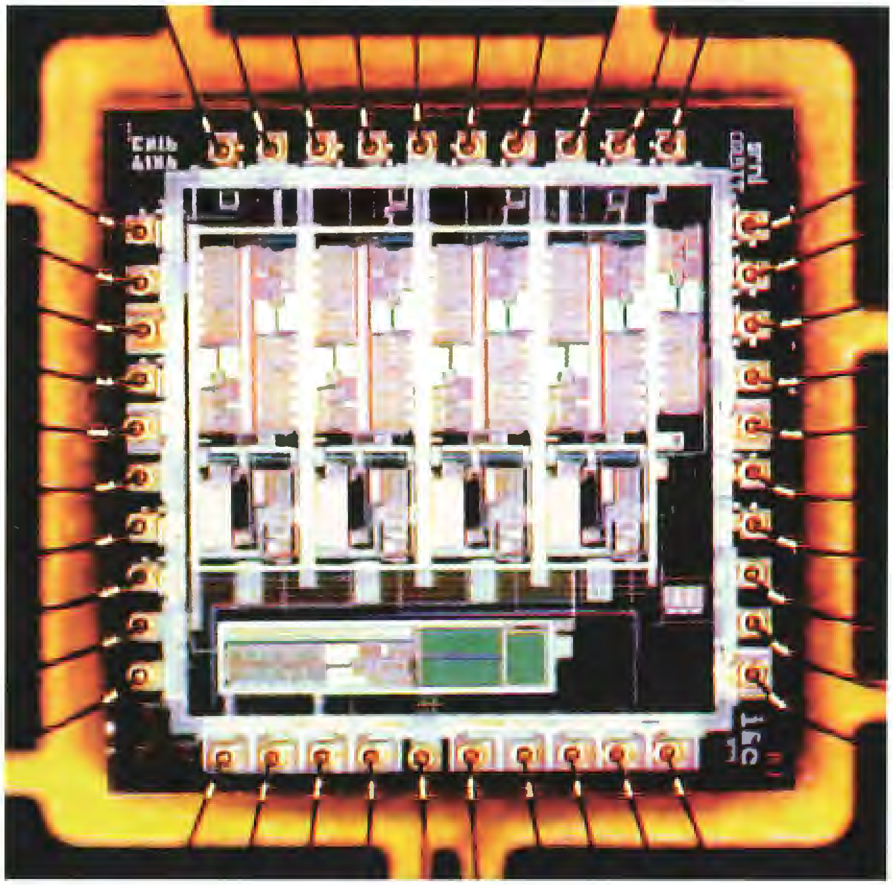
Tests on the SETS apparatus produced unique insights into the physics of steam explosion triggering. As the coated metal samples heat up, the coatings decompose and char, generating copious quantities of gases that tend to drive entrapped water away. Because there is no significant water to entrap, explosive forces for triggering are eliminated. Further, these gases migrate to the free aluminum surface and absorb external shocks like airbags. The charred areas and the gases generated by heating the coated surfaces repel water—beads of water easily roll off the samples when you blow them.

On the other hand, our studies of uncoated, rusted steel samples show they are quite wettable—water spreads and coats the steel. Thus, rusted steel traps a mixture of water and steam, making it available for explosive boiling heat transfer, which can send shock waves to trigger a steam explosion. SETS tests demonstrate that the buildup of potentially explosive energy was much greater over rusted steel than over samples with coatings thought to suppress steam explosions. Other tests showed that practically achievable external shocks in casthouses, such as jackhammers or large ingots accidentally dropped onto operating floors, were much less significant as potential triggers than explosive boiling of entrapped water from submerged surfaces.

Based on our studies of explosions and coatings, we postulated that steam explosions could be prevented by injecting air (or some other noncondensible gas) at critical locations and prescribed rates based on process conditions. Lab-scale experiments indicate that gas inclusion in the steam film around molten particles can significantly stabilize the protective steam film and cushion against destabilizing shock pressures. Field demonstrations of our new gas injection technique, which are planned to demonstrate its usefulness to the aluminum industry, will be carried out later this decade by ORNL and the Aluminum Association of America under a cooperative research and development agreement.

ORNL researchers have also suggested that gas injection and special coatings at the bottom of pressure vessels or reactor cavities may prevent steam explosions in DOE research reactors and commercial nuclear power plants. We hope our research results will help improve the safety of the metal casting and nuclear industries.

The research is sponsored by DOE's Office of Energy Research, Laboratory Technology Research Program, and by DOE's Office of Energy Efficiency, Office of Industrial Technologies.



ORNL researchers designed an integrated circuit that performs four channels of temperature measurement in oil well drill bits. *Electronic file enhanced by Mark Robbins.*

Monitor Warns of Need To Change Oil Drill Bit

One of the worst nightmares of oil and gas exploration companies is a broken drill bit. Suspended from an oil drilling rig by a "string" of pipes, this knee-high steel mechanism is the key to striking oil and gas. A succession of drill bits bores through up to 6000 meters (~20,000 feet) of rock with roughly 200,000 newtons (50,000 pounds) of weight on each bit while enduring downhole pressures that can reach 130 megapascals (~20,000 pounds per square inch). Operation of a drilling rig can cost as much as $10,000 an hour. If the bit breaks into pieces while drilling on the way down, the cost to a drilling company of the time required to fish the pieces out with a magnet before drilling is resumed could exceed $1 million for a single bit. Thus, to prevent failure, oil drilling companies replace drill bits well before they have reached the end of their useful lives.

Because of the potential to save money, oil drilling companies are interested in a drill bit that could be used much longer. The dream solution: incorporate a device in the bit that warns of telltale changes preceding failure, signaling the need to change out the drill bit just in time. Widespread use of such a device would lower the cost of petroleum exploration and production and help ensure that the U.S. market receives oil at a reasonable cost, which is a primary DOE mission.

To meet this need, ORNL, Hughes Christensen Company (a manufacturer of drill bits), and the Houston Advanced Research Center have developed an implantable incipient failure monitor for drill bits through a cooperative research and development agreement. About the size of a small battery, this monitor measures the rise in drill bit temperature, which is an indicator of a number of changes that lead to failure. When drill bits mechanically degrade (say, when the lubricant seals fail), increased friction results, generating heat. So a miniaturized, ruggedized temperature measurement and logging instrument was devised to measure temperatures in the drill bit. This temperature monitor is the first electronic device ever to be incorporated directly into an oil well drill bit.

The temperature monitor operates on very low power levels supplied by a battery. Its materials and components are tolerant of high temperatures (up to 150°C), vibrations, and mechanical shock. The heart of the device is a customized application-specific integrated circuit (ASIC) designed at ORNL. This ASIC consists of an analog circuit that performs the measurement and a mixed analog-and-digital circuit that controls the system and logs the measurements.

Several temperature sensors, whose resistance varies in a known manner with temperature, are implanted at critical points within the drill bit.

ORNL has developed an electronic temperature monitor that detects early signs of failure in an oil well drill bit.

David Holcomb (left) and Nance Ericson show where the electronic temperature monitor they developed will fit into an oil drill bit to warn of failure before it actually occurs. *Photograph by Tom Cerniglio.*

Measurements are currently being made in tests downhole to identify signatures of different incipient failures for a database. The recorded measurements are retained in the modules' "nonvolatile" memory, even if the power supply is interrupted. The information will aid the design of a more intelligent sensor module that will recognize specific types of expected impending failures.

Rather than measure electrical resistance directly with thermocouples or other conventional methods that require stable, accurate current and voltage sources, the researchers use a timing method that produces a digital result proportional to temperature even if the voltage supply is unstable. The device relies on an oscillator that generates a stable frequency (like a clock ticking, except there are many more ticks per second). The digital information on the incipient failure will be communicated from the sensor monitor by special signals that travel up the hole to oil rig drill operators .

There are other practical applications for this kind of temperature monitor. The device could be used to warn truck drivers that their brakes are on the brink of overheating. Food processors could use such a rugged temperature monitor to ensure that a large batch of stew is cooked throughout long enough and at the right temperature to sterilize it before canning. Other applications might be remote environmental sensing in the Arctic Ocean, monitoring heat-treatment furnace temperatures, and making temperature measurements on the thermal shields of vehicles re-entering the Earth's atmosphere from space.

As they seek to help industry find oil and gas more economically, ORNL researchers are finding ways to make smaller, tougher electronic devices that can help other people, too.

The development was funded by DOE's Office of Energy Research, Hughes Christensen Company, and the Houston Advanced Research Center.

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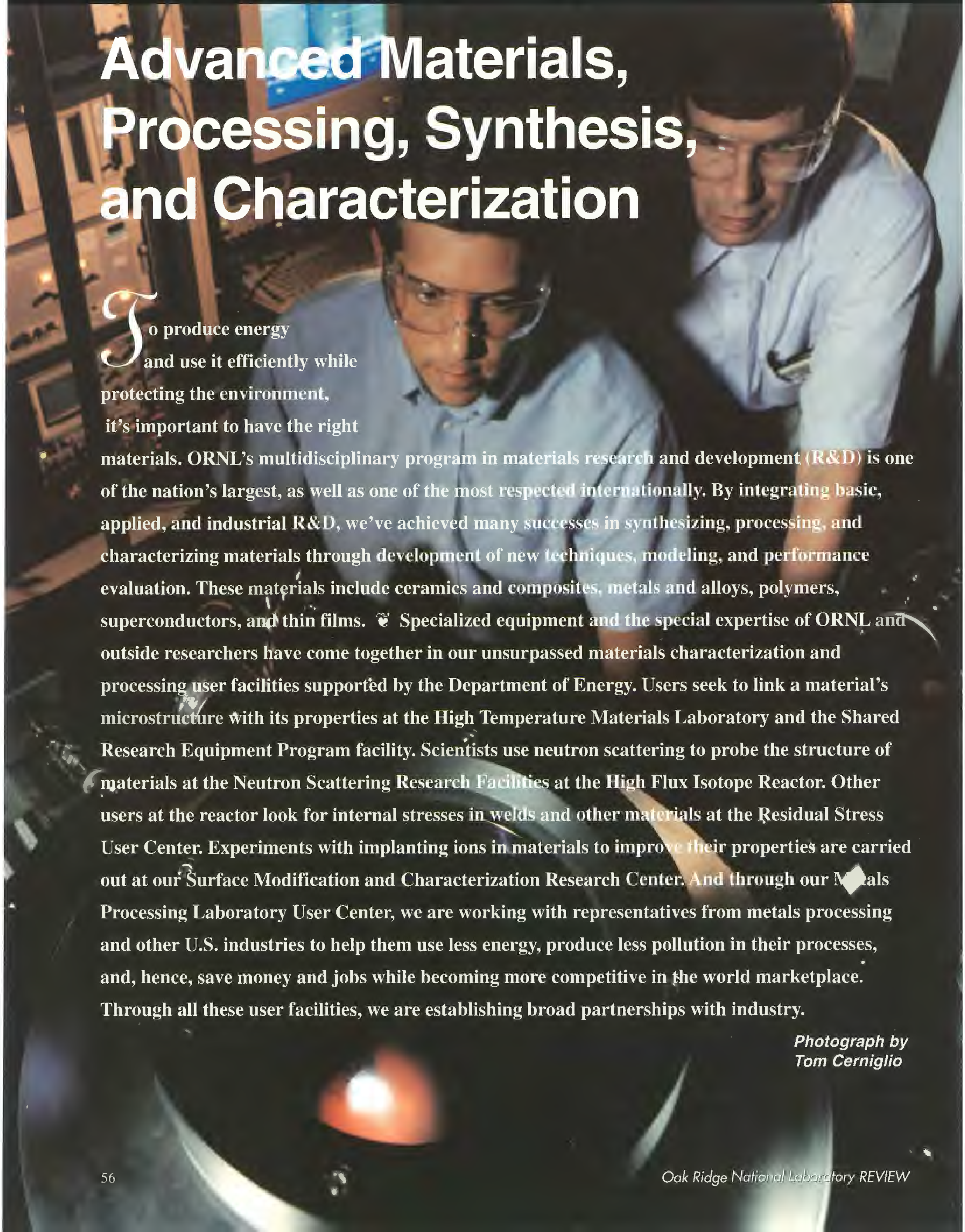
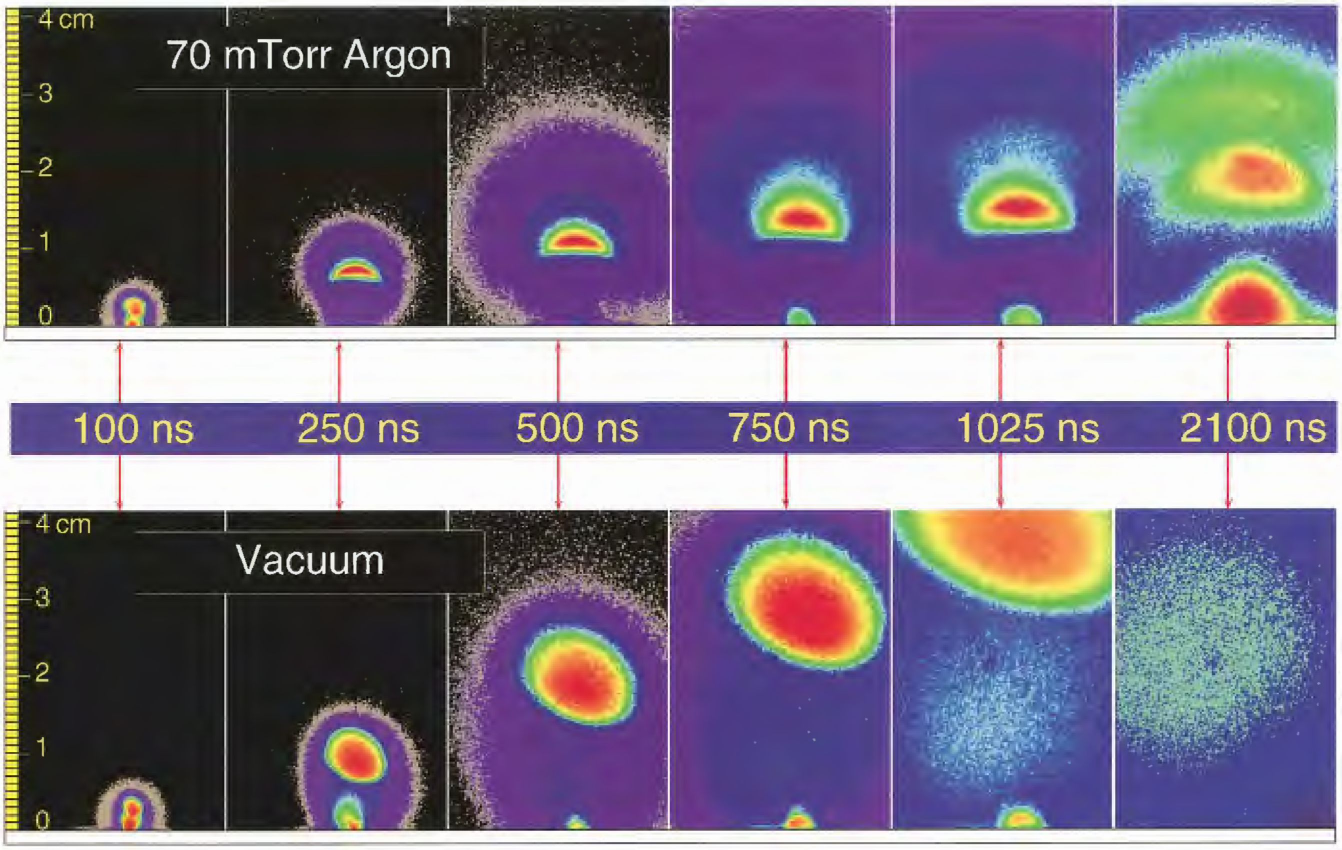


Advanced Materials, Processing, Synthesis, and Characterization

To produce energy and use it efficiently while protecting the environment, it's important to have the right materials. ORNL's multidisciplinary program in materials research and development (R&D) is one of the nation's largest, as well as one of the most respected internationally. By integrating basic, applied, and industrial R&D, we've achieved many successes in synthesizing, processing, and characterizing materials through development of new techniques, modeling, and performance evaluation. These materials include ceramics and composites, metals and alloys, polymers, superconductors, and thin films. ❦ Specialized equipment and the special expertise of ORNL and outside researchers have come together in our unsurpassed materials characterization and processing user facilities supported by the Department of Energy. Users seek to link a material's microstructure with its properties at the High Temperature Materials Laboratory and the Shared Research Equipment Program facility. Scientists use neutron scattering to probe the structure of materials at the Neutron Scattering Research Facilities at the High Flux Isotope Reactor. Other users at the reactor look for internal stresses in welds and other materials at the Residual Stress User Center. Experiments with implanting ions in materials to improve their properties are carried out at our Surface Modification and Characterization Research Center. And through our Metals Processing Laboratory User Center, we are working with representatives from metals processing and other U.S. industries to help them use less energy, produce less pollution in their processes, and, hence, save money and jobs while becoming more competitive in the world marketplace. Through all these user facilities, we are establishing broad partnerships with industry.

Photograph by Tom Cerniglio



Stop-action photographs reveal how a plasma plume composed of laser-vaporized carbon ions, atoms, and clusters moves away from a graphite surface into vacuum (bottom) and into a low-pressure background gas (70-mTorr argon, top). The digital images of the plasma light are taken at different times after the vaporizing laser pulse and are assigned false colors to reveal different regions of emission for spectroscopic identification. Expanding into vacuum (bottom sequence), the bright ball of fast carbon ions responsible for high-quality amorphous diamond films is the dominant plume component, while slower atoms and clusters are barely visible. However, the top image sequence shows how a low-pressure gas scatters and slows these ions, confining the plume so that carbon-carbon collisions can form clusters, such as buckyballs, near the target surface for fabrication of novel materials in the gas phase.

David Geohegan (left) and Alex Puretzky capture digitized snapshots of the vaporized plume of carbon species created during laser ablation of pyrolytic graphite to synthesize new materials. An intensified charge-coupled detector array camera is used in fundamental studies of the target vaporization, vapor transport, and deposition processes that occur during only a few microseconds. The studies are used to optimize vacuum growth of transparent films of amorphous carbon with the properties of diamond, or the growth of clusters in background gases to useful nanoparticles (e.g., buckyballs).

Laser-Deposited Films Improved with Aid of Plume Pictures

Just as solar rays turn comet ice into a blazing, cloudlike tail, pulsed beams of ultraviolet laser light can rapidly heat and vaporize a solid target in a vacuum chamber. But in pulsed laser deposition, the vaporized material travels in a luminescent plume toward a heated substrate where the material is deposited. The plume is a dense plasma of energetic electrons and neutral atoms, ions, and molecules in both excited and ground states. The plume's contents are laid down in the same composition as the starting polycrystalline target material, but in the form of a film whose crystalline structure is locked into place by the substrate's atomic template. Although the first pulsed laser deposition experiment was conducted in 1965, the technique has been employed widely only since 1987, when it was discovered that it can be used to grow high-temperature superconducting films.

ORNL researchers have taken high-tech snapshots of many a plume on its trip from target to substrate. They have used an assortment of sophisticated tools to get the picture. These include a fast-intensified charge-coupled detector camera to acquire images of the fluorescent plasma; optical emission and absorption spectroscopies that differentiate among the plume's atomic and molecular species and states; and an ion probe, which measures ion energy and plasma density. From these tools, scientists can learn how fast the plume is moving and how much material in different atomic forms is present in the plume's different parts.

By monitoring the plume, ORNL researchers can predict whether the film being produced will be uniformly thick. They can determine which conditions—laser beam energy and wavelength, gas pressure, substrate temperature—have changed and how much any change should be corrected to optimize film quality. From the diagnostics, they have found that most of the plume blasts from target to substrate in 20 microseconds and that the fast plume material moves from 1 to 5 centimeters per microsecond.

How fast the material moves, where it goes, how much rebounds from the substrate, and what type of product is formed depend partly on whether the plume is in a vacuum or background gas. For example, if the target is graphite in a background gas like argon, all-carbon buckyballs can be produced. If graphite is zapped in a vacuum with a laser beam, the product could be an amorphous diamond film that emits electrons when subjected to a strong electric field. Because this film is a superhard, transparent field emitter which can excite phosphor coatings, one company is using laser ablation to make amorphous diamond films for flat panel displays; these devices are needed to make much less bulky television sets and computer monitors, similar to the flat screens of notebook computers. ORNL researchers are looking at ways to deposit amorphous diamond films that could emit electron beams in lieu of light to pattern silicon chips. In this way, more circuits can be packed on each chip, making a chip both smaller and smarter.

ORNL's plume diagnostics have revealed just how different background gases and varying gas pressures slow down the plume, causing the material to cluster together. As a rule, the gas absorbs energy from collisions between the expanding plasma and gas molecules, slowing down many plasma species. As the gas pressure is increased, some of the rapidly expanding plasma escapes with few collisions, but most gets caught in a snowplowed pile of gas which acts like a shock wave. As a result, the plume splits into two or three components. ORNL researchers developed the first accurate model of plume splitting and were among the first groups to understand it.

By imaging the plume in pulsed laser deposition, researchers can influence the quality of the thin-film product.

Monitoring of many types of ablation plumes showed that clusters of bound atoms ejected from the target can sometimes ruin an amorphous diamond film, but that clusters created by collisions with a background gas—the "third component" of a split plume—can be useful in other ways. For example, in experiments involving doping zinc telluride films to learn how to make cheaper blue-light-emitting diodes, the nitrogen gas itself was incorporated in the film. When film growth was conducted using each of the three components of material observed with the plume pictures, researchers produced films that possess quite different electronic properties. The best films were obtained when the nitrogen pressure was high enough to kill the damaging superfast "first" component, but the nitrogen content was low enough to avoid formation of the clunky nanoparticles of the "third" plume component. ORNL researchers now are intentionally making larger clusters and nanoparticles at higher pressures, from supertough nanotubes to nanocrystallites (which emit light in electric fields), all of interest for flat panel displays.

In respect to laser deposition plumes, ORNL researchers don't use film to get good pictures, but instead use pictures to get good films.

The research is supported by DOE's Office of Energy Research, under the Division of Materials Sciences in the Office of Basic Energy Sciences.

New Approach To Thermoelectric Refrigeration

The most efficient refrigerators—the compressor-based kinds found in our kitchens—are noisy because they have moving parts. They are not, therefore, the best choice for chilling foods and beverages in nuclear submarines. Because subs must operate as quietly as possible, the needed cooling is provided by refrigerators using thermoelectric materials such as bismuth-telluride alloys. These thermoelectric materials are much less efficient than compressor-based refrigerators—they provide less cooling per watt of electricity consumed. But, although less economical, they are quiet, more reliable, and convenient. Some can reach temperatures as low as 160 K, or –113°C. Thus, they are also used for beer coolers, water coolers, and spot cooling of electronic circuits on chips.

Thermoelectric materials conduct electricity well, but they conduct heat poorly. If these materials could be designed to be much more efficient, they could be used to make car air conditioners and home refrigerators, avoiding the need for refrigerants that threaten the ozone layer or strengthen the greenhouse effect. It might even be possible to design a thermoelectric material that can chill high-temperature superconducting cables to 77 K, replacing liquid nitrogen, the cheapest coolant that enables such wires to conduct electricity without resistance.

ORNL researchers have demonstrated a novel approach to designing thermoelectric materials that could provide the required cooling at

ORNL researchers have demonstrated a novel approach to designing thermoelectric materials that could provide the required cooling at much improved efficiencies.

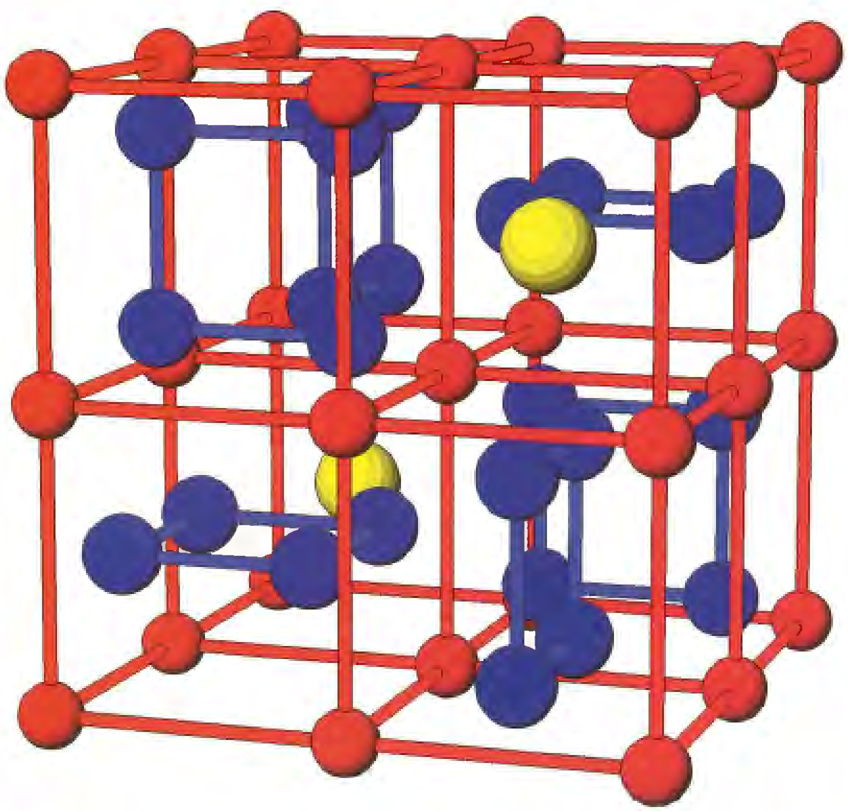
much improved efficiencies. This approach has been described in articles in *Science* (May 31, 1996) and *Physics Today* (March 1997).

Thermoelectric materials can provide electricity when heated, or they can provide cooling when conducting an electric current. In 1823 Thomas Seebeck observed that if two different metals are joined in a closed circuit and if the junction for the two materials is heated, an electric current will be produced—the basis for thermocouples and radioisotope thermoelectric generators in deep space probes. In 1838 Heinrich Lenz observed that, if electrical current is passed in one direction through the junction between dissimilar materials, cooling will result.

ORNL researchers have designed an intriguing thermoelectric material. Because it can be used in a temperature range of 800 to 900 K (500 to 600°C), this material shows promise for generating electricity from waste heat in power plants and chemical production facilities. The material is more efficient than currently used silicon-germanium alloys.

Because of the potential of the ORNL approach for developing novel materials for thermoelectric refrigeration, our researchers are working with Marlow Industries in a cooperative research and development agreement. Marlow manufactures thermoelectric cooling modules in which the two ends of the device are linked by two legs (made of semiconducting material) whose electrons (or positively charged electron holes—the vacant positions in a crystal left by the absence of electrons) carry heat. The negative terminal of a battery is connected to the end to be chilled, and the positive terminal is connected to the device's other end. Because like charges repel, the battery's electrons force the electrons in the legs away from the "cold" end, driving them and the heat they carry to the positively charged end. The cold end becomes colder, and refrigeration results.

Using an idea suggested by a researcher now at Rensselaer Polytechnic Institute, ORNL researchers developed a new crystalline solid with the "filled skutterudite" structure. The word skutterudite is derived from the name of a Norwegian location that has minerals with this same cubic structure. When iron, cobalt, and antimony are melted together, the iron and cobalt atoms form cubic "cages," many of which are filled with antimony atoms in groups of four. But the researchers changed the skutterudite structure by also filling the empty cages with rare-earth atoms (cerium or lanthanum), which are too small for the cages. As a result, while iron, cobalt, and antimony atoms conduct electricity, each rare-earth atom rattles around in its cage, scattering heat waves and making the material a very poor thermal conductor. This novel approach of trapping small atoms in large cages could make possible the design of more efficient thermoelectric materials for refrigeration, creating cooling modules whose only moving parts are the vibrating atoms inside.



In this filled skutterudite crystal structure, iron or cobalt atoms are represented by red spheres, antimony atoms by blue spheres, and rare-earth atoms (lanthanum or cerium) by yellow spheres. The "rattling," or thermal vibration of the rare-earth atoms, is thought to be responsible for the low thermal conductivity of these compounds.

The research is sponsored by DOE's Office of Energy Research, Basic Energy Sciences, Division of Materials Sciences.

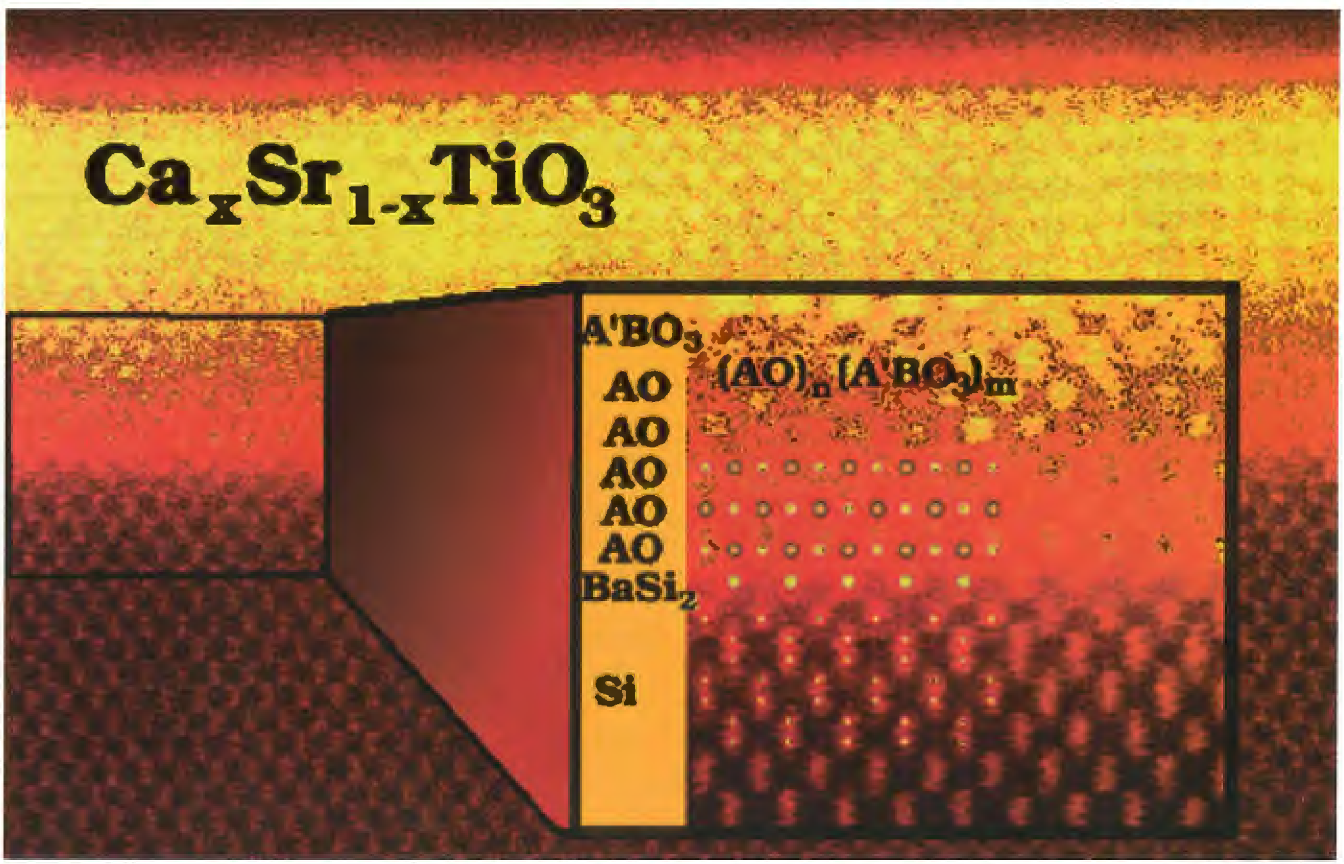
ORNL Technology Leading to Better Transistor for Computer Memory Chips

A faster transistor that doesn't forget has been shown to be feasible, thanks to an ORNL materials technology. This next-generation ferroelectric, or ferro-gated, transistor will enable the electronic industry to pack more information in smart cards and memory circuits in future processor chips for portable computers—and speed up retrieval of this information.

A smart card is a pocket-sized computer processor that could replace your bulky wallet. This invention for consumer convenience can be used as electronic cash, driver's license, credit card, information source, ticket for transportation services, and personal identifier. A smart card consists of a receiver (to accept signals from a card reader requesting information such as a credit card number), power supply, microprocessor, memory chip, and antenna (to send out requested information). Ferro-gated transistors are expected to be used in future smart cards' memory chips because, compared with today's smart card electronics, they cram in more information and require much less power to get information in and out.

The ferro-gated transistor is a kind of "smart transistor" because of its retentive memory. It will be especially useful for dynamic random access memory (DRAM) in computers because it is nonvolatile—the information stored as a bit on such a transistor during operation won't vanish when the computer's power is turned off. In today's computers, DRAM is volatile, so any application not saved to a hard disk drive or floppy disk is lost when the computer is shut down. A chip containing millions of the new transistors could act as the hard disk drive of a laptop computer

A new transistor being developed will allow computer memory chips to hold more information and enable users to read and write it faster, making the device ideal for smart cards and laptop computers.



$(AO)_n(A'BO_3)_m$: The above figure shows an enlarged panel of the initial interface between crystalline oxides and silicon. The enlarged panel (right) is an overlay depicting positions of silicon atoms, the repeated alkaline oxide (AO) planes, and the first layers of the perovskite, $A'BO_3$. The lattice image shows ORNL's series of oxides in which 4 atomic layers of BaSrO are at the interface between silicon and the perovskite, $Ca_xSr_{1-x}TiO_3$. This composite interface structure is commensurate to silicon and provides the basis for ferroelectric transistor development.

and extend the lifetimes of laptop batteries. Memory chips made of these new transistors will be able to retain up to a million times more information than chips of the same size today.

The ferro-gated transistor is a metal-on-oxide field-effect transistor, a very small semiconducting device that consists of three metal electrodes and a silicon base. When a conventional field-effect transistor is turned on, electrons injected by a source electrode flow as a current through the silicon base for collection at a drain electrode. To turn the transistor off, a gate electrode between the other electrodes applies an electrical voltage to a dielectric film which pinches off the current by raising resistance in the silicon base. In this way, a transistor can function as an on-and-off switch or as a repository of a bit of information coded as a combination of 1's and 0's (the "on" transistors are each storing a 1 and the "off" transistors are each storing a 0).

The new ferro-gated transistor is different from the conventional field-effect transistor in one way. The dielectric film between the gate electrode and the silicon base in the new transistor is formed from barium titanate, rather than silicon oxide. ORNL researchers perfected a technique for depositing barium titanate as a crystalline film on silicon, made metal oxide silicon capacitors, and proved that the properties of barium titanate meet requirements of a ferro-gated transistor.

The crystal structure of barium titanate gives it desirable ferroelectric properties—in certain regions, positive and negative ions separate, setting up an internal electric field. Alternatively, such an electric field is maintained in silicon oxide by using external power. The internal electric field of barium titanate remains unchanged and requires no external power unless it is flipped. Depending on whether it's up or down, the field either pulls up or pushes away electrical charges in the silicon substrate, facilitating or resisting the flow of electrical current.

The semipermanence of the barium titanate's internal field gives the new transistor two advantages. First, information held by millions of "on" and "off" ferro-gated transistors is retained when the power is shut off. Second, chips containing such transistors require less electricity because power is needed only when it is necessary to flip the internal electric field of any transistor's barium titanate film.

Because its dielectric constant is 250 times higher than that of silicon oxide, the barium titanate layer exerts a stronger influence on the transistor's conductivity; thus, less area is required for the gate electrode, making it possible to put the source and drain electrodes closer together. As a result, the transistor can be made smaller, and because electrons would travel a shorter distance between the source and drain electrodes, the device is faster.

In today's computers, two transistors and two power-hungry capacitors are required to store one bit. If ferro-gated transistors are used, only one transistor is needed per bit—a change in the "logic state" that greatly cuts power requirements. Memory chips made of these new transistors will be able to retain a thousand to a million times more information. For example, a one-centimeter-square chip today (about the size of a small shirt button) would hold 64,000 to 256,000 bytes, whereas a chip the same size containing ferro-gated transistors would hold one billion bytes (gigabyte) of information.

To make computers even faster in the future, memory circuits will be incorporated into the processor chip. The spinning hard drive will be a thing of the past. Today it takes hundreds of milliseconds to retrieve information from a gigabyte hard drive disk and to write information to it. If ferro-gated transistors are used for gigabyte memory circuits of processor chips, it will take only fractions of a nanosecond to read the information and a few hundred nanoseconds to write information for storage in future computers.

Rodney McKee received a NOVA Award for Technical Excellence from Lockheed Martin Corporation for this development. It was funded by ORNL's Laboratory Directed Research and Development Program and by DOE's Office of Energy Research, Basic Energy Sciences, Division of Materials Science.

Better Crystalline Substrates Open New Markets

They don't peer into a crystal ball to predict the successful materials of tomorrow. But ORNL researchers have helped transform crystals into new technologically important materials such as substrates for the growth of epitaxial electro-optic and superconducting thin films.

Electronic and optical devices can be made of thin crystalline films deposited on and supported by a durable substrate. A substrate is an underlying template that lines up the crystals of a thin film grown on it so that it conducts electrons or light. The substrate should not react with the film and, to avoid film breakage, it should expand at the same rate as the film when both are heated.

Few crystals can meet these criteria, but single-crystal magnesium oxide (MgO) is an excellent substrate for thin-film devices. However, for some devices, the typical MgO crystal has previously been too small. Through a cooperative research and development agreement, ORNL and Commercial Crystal Laboratories (Naples, Florida) developed new insights into the MgO crystal growth process, leading to the formulation of a new concept for the nucleation and growth of this material. Drawing on this concept, researchers can grow MgO crystals whose diameters are double or triple those previously produced—just the right size for customers needing larger substrates for developing new electronic and optical devices such as switches and modulators for light-based communication networks and all-optical computers. This new MgO crystal-growth technology will help U.S. high-technology firms avoid total reliance on foreign suppliers of MgO substrates.

Crystals of potassium tantalate/niobate grown at ORNL have also been shown to make excellent substrates because they are mechanically and chemically stable. By adding calcium and barium to potassium tantalate crystals, ORNL researcher Lynn Boatner found a way to make them either insulating or conducting. By adding niobium, he turned the crystal into a ferroelectric material whose separated positive and negative electrical charges can be switched when an electric field is applied. These new substrates are important because high-temperature superconducting films can be grown on them for applications such as magnetic sensors for medical, geological, and industrial applications; microwave components for radar and communication technologies; and ultrafast switches.

Potassium tantalate substrates can be produced as large wafers, reducing the fabrication cost of thin-film devices that are grown on the substrate material. Commercial Crystal Laboratories has developed improved ways to prepare epitaxial-quality surface finishes on these substrates and is currently marketing the material for commercial and research applications.

The development of these new substrates received an R&D 100 Award in 1996, and the technology for producing these crystals has been patented and licensed to Commercial Crystal Laboratories. The ORNL researchers, Boatner and Ron Feenstra, also received a 1997 Federal Laboratory Consortium Award for Excellence in Technology Transfer.

The commercial prospects for these ORNL-developed materials are not known, but it is clear that the collaborators have completed a gem of a project.

This research was funded by DOE's Office of Energy Research, Basic Energy Sciences, and the Laboratory Technology Research Program. ornl

ORNL and a Florida company learned how to grow larger crystals for use as substrates in advanced electronic devices.

An oriented substrate cut from a potassium tantalate crystal. Thin films can be grown on substrates like this, forming the heart of devices that depend on ferroelectric, waveguide, high-temperature superconducting, or superlattice materials.

Physical Sciences and Neutron Science and Technology

Image by Ross Toedte, enhanced by Renée Balogh

Physical scientists at ORNL are engaged in many studies, ranging from the structure of heavy nuclei to the explosions in stars that cast out heavy elements to the formation of rocks and energy resources in the earth. Our nuclear physicists, both experimental and theoretical, are concerned with the effects of excitation on the shape, structure, and other properties of various nuclei. They carry out research at ORNL's Holifield Radioactive Ion Beam Facility (HRIBF), which is the only U.S. facility that can produce and accelerate high-intensity, low-energy beams of radioactive nuclei, and the Oak Ridge Electron Linear Accelerator (ORELA), a unique, intense pulsed-neutron-source accelerator facility used for basic research in nuclear astrophysics and fundamental interactions.

Atomic physicists at ORNL conduct experimental and theoretical investigations of a broad class of phenomena occurring when multiply charged heavy ions interact with gases, solids, free and bound electrons, photons, and other ions; the EN Tandem Van de Graaff Accelerator and the Electron Cyclotron Resonance Ion Source Facility are operated in support of the atomic physics research community.

ORNL also conducts broad programs in chemical energy, separations and analysis, heavy-element chemistry, and advanced battery technology. Basic research improves the fundamental understanding of methods for separating mixtures as well as systems related to chemical conversions that underpin new or existing concepts of energy production and storage. Geoscience research at ORNL focuses on fundamental geochemical processes that control the transport of matter and energy in the earth's crust.

Stemming directly from the Laboratory's original mission, ORNL's competency in neutron-based science and technology includes the design and operation of neutron sources (reactors and accelerators) and the use of neutrons in science and technology (neutron scattering, isotope production, neutron activation analysis, materials irradiation, and molecular structure determination). This broad spectrum of research in the physical sciences at ORNL is supported by the Office of Basic Energy Sciences in DOE's Office of Energy Research, which supports most research in the physical sciences in the United States.

Radioactive Ion Beam Facility Dedicated

Scientists from all over the world are coming to Oak Ridge to study atomic nuclei that cannot be produced naturally from elements that exist on the earth. On December 12, 1996, ORNL's Holifield Radioactive Ion Beam Facility (HRIBF) was dedicated as an international user facility. The ceremony featured dignitaries from the White House's Office of Science and Technology Policy, DOE headquarters, the state of Tennessee, Oak Ridge Associated Universities, Vanderbilt University, and the University of Tennessee. The dedication was followed the next day by a symposium on radioactive ion beam physics.

Dave Hendrie, director of DOE's Division of Nuclear Physics, congratulated ORNL staff for designing and constructing the HRIBF. "You can count this effort as a success," he said, "and today is one of those glorious days for science in general."

Hendrie recounted the history of the project, which was conceived in 1991 as funding dwindled for ORNL's Holifield Heavy Ion Research Facility (HHIRF). "When HHIRF ran into funding troubles a few years ago," he said, "you had a good idea for a modest-sized, cost-effective facility. You sold the idea to DOE. You put it

The Holifield Radioactive Ion Beam Facility has produced its first beams for experiments to study nuclear structure and astrophysics.

This whimsical painting of the HRIBF by Edda Reviol (wife of a young research professor in the Physics Department at the University of Tennessee) indicates the production of radioactive ions when protons from the cyclotron smash a target (burst of color at bottom, left of center). After selection, a beam of these radioactive ions is accelerated to the top of the 100-foot, 25-megavolt tandem accelerator and then back down where the ions strike the target of the experimental apparatus, depicted in the lower right-hand portion of the figure. This sequence takes place in the HRIBF facility with ORNL's landmark tower (center).

together over the years. It turned out to be timely."

The HRIBF is the only facility in the world dedicated to the acceleration of radioactive ion beams with sufficient intensity and energy to be useful for nuclear physics and nuclear astrophysics. HRIBF's radioactive ion beams provide a tool for creating new superheavy elements, extremely large deformed nuclei, and nuclei beyond their limits of stability, helping to answer important questions about the nature of the nucleus. Two-thirds of the experiments at the facility will be devoted to studying the structure of exotic nuclei that exist for just a fraction of a second.

About a third of the experiments using HRIBF radioactive ion beams will be performed to solve mysteries in nuclear astrophysics. These studies will focus on the formation and fate of stars. One goal is to better understand spectacular nova and supernova explosions in which temperatures at the center of doomed stars reach billions of degrees, fueling exotic fusion reactions that produce iron and all the naturally occurring elements in the universe heavier than iron. As the star blows itself up, it scatters heavy elements such as the iron, calcium, silver, tin, iodine, gold, mercury, lead, and uranium isotopes that are the basis of life and of our civilization.

On August 30, 1996, the HRIBF (whose chief components include the Oak Ridge Isochronous Cyclotron and the tandem accelerator housed in ORNL's landmark tower) produced its first beams of radioactive ions and accelerated them using the tandem accelerator. Radioactive arsenic-70 ions were produced by bombarding a liquid germanium target with a proton beam from the Oak Ridge Isochronous Cyclotron. Although its intensity was only a few thousand ions per second, the beam was easily detected by stopping it on a moving tape system and observing its radioactive decay. A beam of arsenic-69 ions was produced in the same test. In March 1997, the HRIBF started its experimental program using beams of radioactive arsenic-69.

In 1997, scientists from universities and laboratories around the world will be conducting experiments they hope will answer questions about nuclear physics and nuclear astrophysics. The HRIBF facility will serve a national and international community of about 300 scientists from 33 states and 20 foreign countries, providing a unique new tool for understanding nuclear matter, the main constituent of the visible universe.

The HRIBF is the only facility in the world capable of supporting a wide range of nuclear astrophysics and nuclear structure physics studies—an exciting, fast-growing new field that has been identified by the U.S. nuclear science community as a top priority for future development.

Hendrie concluded the dedication by saying "I see the future of physics as quite bright."

HRIBF is supported by DOE's Office of Energy Research, Basic Energy Sciences, Division of Nuclear Physics.

ORNL Instrument Measures Fluid Densities under Extreme Conditions

Hot fluids form and circulate deep in the earth's crust. However, how they react with minerals and organic matter to form rock masses, magmas, ore deposits, oil, and natural gas is not well understood.

Using unique instrumentation, ORNL researchers are gathering data and developing "equations of state" that help geologists gain a more quantitative understanding of the origin and evolution of fluids in the earth's crust. It is now evident that frequently used equations published by leading scientists are seriously in error. The new data and equations will lead to improved geologic models that will either support or refute current theories about how rock masses and energy resources form.

Natural fluids in the earth's crust reach extreme, or "supercritical," temperatures and pressures at great depths. When water reaches the supercritical state—at temperatures above 374°C and pressures above 222 bars (approximately 222 times atmospheric pressure)—it acquires special properties. Compared with true liquids and gases, supercritical water-rich fluids are often more reactive with rocks, causing the formation of new minerals and hydrocarbons.

The new equations of state are based primarily on data obtained from a custom-designed, vibrating-tube densimeter constructed at ORNL. This unique instrument is used to determine the volumetric properties of fluids under extreme conditions. A commercial vibrating-tube densimeter that measures densities of fluids at ordinary temperatures and pressures was modified extensively to create an instrument that could be used at temperatures as high as 500°C and at pressures up to 2000 bars. Currently, measurements are being made on fluids in the carbon-oxygen-hydrogen-nitrogen (C-O-H-N) system. The fluid species of principal interest in this system are water (H_2O), carbon dioxide (CO_2), methane (CH_4), and nitrogen (N_2). Using the special ORNL densimeter, it is possible to mix these species in any proportion to create intermediate fluid compositions of interest. During experiments, fluids flow through a U-shaped tube, which vibrates in response to forces generated by magnets. By measuring the period of vibration of the U-tube (the denser the fluid, the slower it vibrates), the density of the fluid flowing through the tube can be calculated.

Additional research on C-O-H-N mixtures is being performed with another unique ORNL instrument: a hydrogen-service, internally heated pressure vessel. This apparatus is used to determine the effective concentrations (activities) of the species in supercritical aqueous fluids. By combining the data obtained from the vibrating-tube densimeter and the hydrogen-service, internally heated pressure vessel, ORNL researchers can determine how aqueous fluids of different compositions and densities behave at different temperatures and pressures.

The new equations of state derived from our research are useful not only to geologists but also to chemical engineers and waste management personnel. It has been shown in recent years that supercritical aqueous fluid plus oxygen converts hazardous wastes to harmless chemicals such as carbon dioxide and sodium chloride (ordinary table salt). The ORNL equations are also being applied to designing coal gasification facilities, fabricating specialty ceramics in which supercritical temperatures and pressures are needed to grow crystals of a particular size and shape, and predicting the availability of natural gas and geothermal energy. ORNL researchers are providing a "piece of the rock" of valuable information for understanding the earth and for improving human life on it.

The research is sponsored by DOE, Office of Basic Energy Sciences, Division of Engineering and Geosciences.

Analyzing Biopolymer Mixtures Using Mass Spectrometry

ORNL research using negative ions is having a positive effect on mass spectrometry applications. This work has led to sophisticated techniques for environmental analysis, explosives detection, engine exhaust analysis, and analysis of compounds of biomedical interest.

Using unique instruments, ORNL researchers are helping geologists better understand the origin and evolution of fluids in the earth's crust.

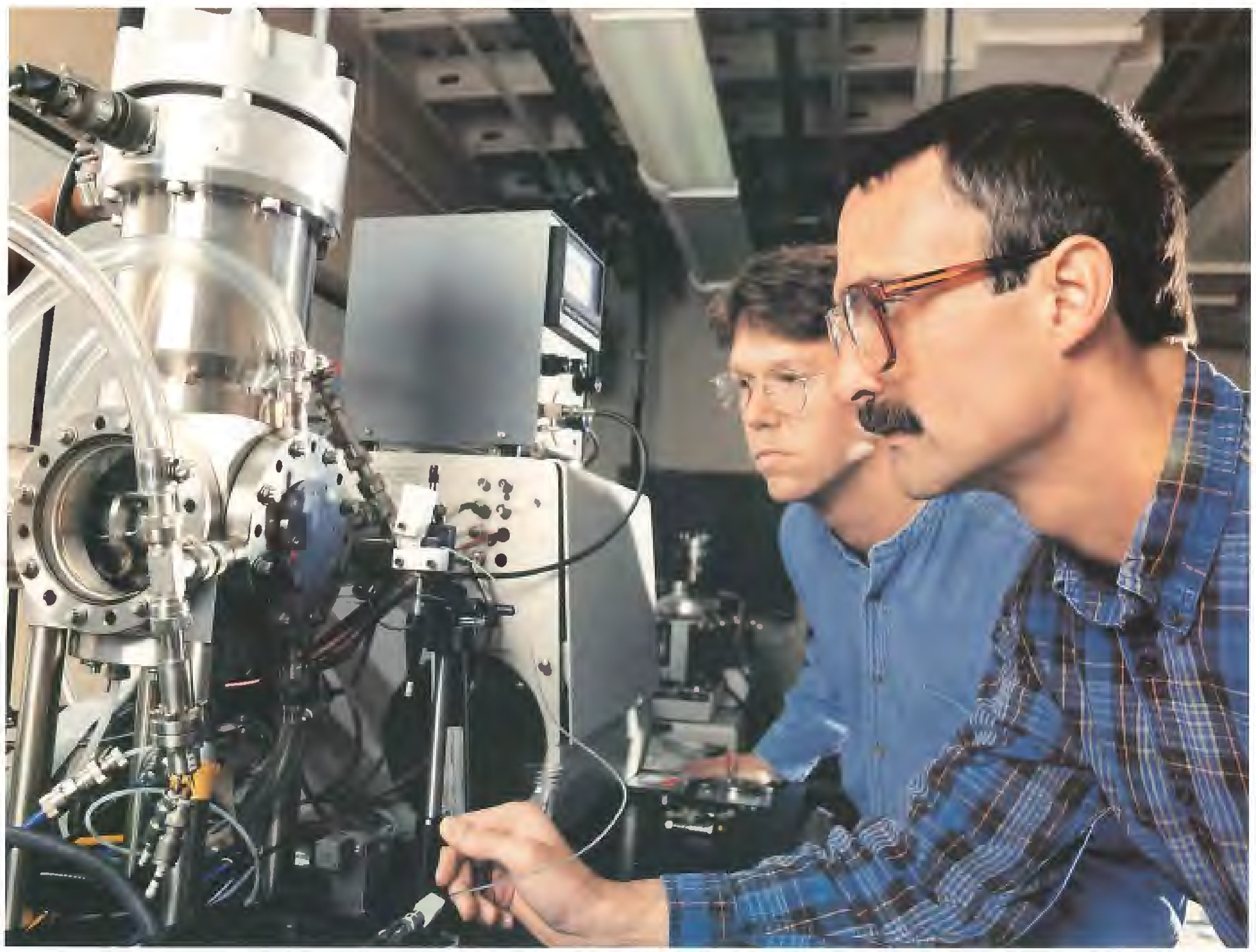
Jim Blencoe (left) and Jeffery Seitz check the pumps on ORNL's vibrating-tube densimeter, a facility that runs on the principle of a tuning fork. It enables geochemists to measure densities of fluid mixtures up to one part per million at temperatures up to 500°C and pressures up to 2000 bars. *Photograph by Curtis Boles.*

Several years ago, ORNL researchers connected different ion sources to a quadrupole ion trap mass spectrometer. One of these was the ORNL-developed and patented atmospheric sampling glow-discharge ionization source, which was originally developed to detect explosives. The technology was licensed to several ion trap mass spectrometer manufacturers. Although an explosives vapor detector has not been commercialized, the technology has been targeted for the environmental analysis market, which has been significantly larger and more reliable than the explosives detection market. These same ORNL researchers were also the first group to join the electrospray ion source (an effective method for generating ions of biopolymers such as proteins and DNA) with the quadrupole ion trap mass spectrometer. Two instrument manufacturers have recently started selling electrospray–ion trap instruments that were heavily influenced by the early ORNL work.

The glow-discharge source is particularly well suited to molecules present in air in trace concentrations, such as those that have vaporized from high explosives or organic pollutants. Many of these volatile and semi-volatile molecules form stable negative ions by readily capturing electrons in the glow discharge source. If a molecule in the source does not capture an electron efficiently, a proton usually can be added to it to form a positive ion. The positive or negative ions are injected into a quadrupole ion trap mass spectrometer where they can be analyzed according to their mass-to-charge ratio. By measuring the positions and sizes of the peaks in the mass spectrum, researchers can identify the constituents of a sample and their relative concentrations.

We are now studying the use of both negative and positive ions to improve methods for characterizing biological materials. Recently, the use of mass spectrometry to analyze biopolymers has been advanced by two techniques

ORNL researchers developed the ion-ion reaction technique for the electrospray ion trap mass spectrometer to more easily identify individual proteins in complex mixtures.



Scott McLuckey adjusts an electrospray ion trap mass spectrometer as researcher Jim Stephenson looks on. *Photograph by Tom Cerniglio.*

for forming gas-phase ions from involatile materials. One technique, called laser desorption, uses the laser. The other technique is electrospray, mentioned above, which is particularly well suited for liberating biopolymers in solution to yield gaseous ions. When the solution is passed through a hypodermic needle held at 3000 to 4000 volts, the liquid exiting the needle breaks up into a fine mist of droplets from which ions emerge. The ions are then drawn into the vacuum system of a mass spectrometer where they can be manipulated and measured.

Although widely employed in the biomedical community and, in particular, the drug industry, the electrospray technique had limited ability to help scientists directly analyze mixtures, because it tends to form multiply charged ions with a distribution of charge states. Hence, each mixture component tends to give many peaks that can result in a complex mass spectrum, even with just a few components.

This situation changed, however, when ORNL researchers developed the ion-ion reaction technique to enable identification of individual proteins in complex mixtures. In ORNL's demonstration of this technique, singly charged negative ions formed by glow discharge were introduced into the quadrupole ion trap and reacted with a positively charged protein mixture formed by electrospray. The negative ions plucked the excess protons, or positive charges, off the proteins in the mixture, reducing dramatically the number of peaks per mixture component so that each protein in the mixture could be readily identified in the simplified spectrum.

ORNL researchers have also introduced positive rare-gas ions to react with negatively charged DNA molecules, causing their fragmentation. In this way, ion-ion reactions can enhance the ability to sequence pieces of DNA. This capability could be useful someday for detecting an infectious organism or identifying a genetic disease. Because the motion of each ion in the ion trap mass spectrometer's oscillating electric field depends upon mass-to-charge ratio, ORNL researchers seek to develop methods for ion manipulation to enable ultrasensitive detection of targeted biopolymers in body fluids, such as proteins that signal the onset of disease. Because of its high speed, high sensitivity, and high specificity, ion trap mass spectrometry offers an attractive means for detecting disease in its early stages so it can be reversed in time to stop the negative effects.

Most of this research has been sponsored by DOE, Office of Basic Energy Sciences, Chemical Sciences Branch. Biomedical applications work has been sponsored by the National Institutes of Health, and bio-agent detection work has been initiated with DOE's Office of Nonproliferation and National Security.

New Insights into the Structure of Water

ORNL has long been a leading center for studying the molecular structure of substances using neutron scattering at research reactors. Using our powerful Intel Paragon supercomputers, we are now also a world leader in molecular simulation calculations. Here's a true story that illustrates these complementary capabilities, demonstrating ORNL's continuing leadership as a strong center for neutron science, computational science, chemical science, and materials science research.

In 1991 Peter Cummings (who at the time was on the faculty of the University of Virginia and since 1994 has been an ORNL–University of Tennessee Distinguished Scientist) and ORNL researchers Hank Cochran, Mike Simonson, and Bob Mesmer performed molecular simulations of supercritical water on the Oak Ridge Cray computer. The simulations showed hydrogen bonding in supercritical water—a non-liquid, non-gaseous state of water produced at high temperature and pressure.

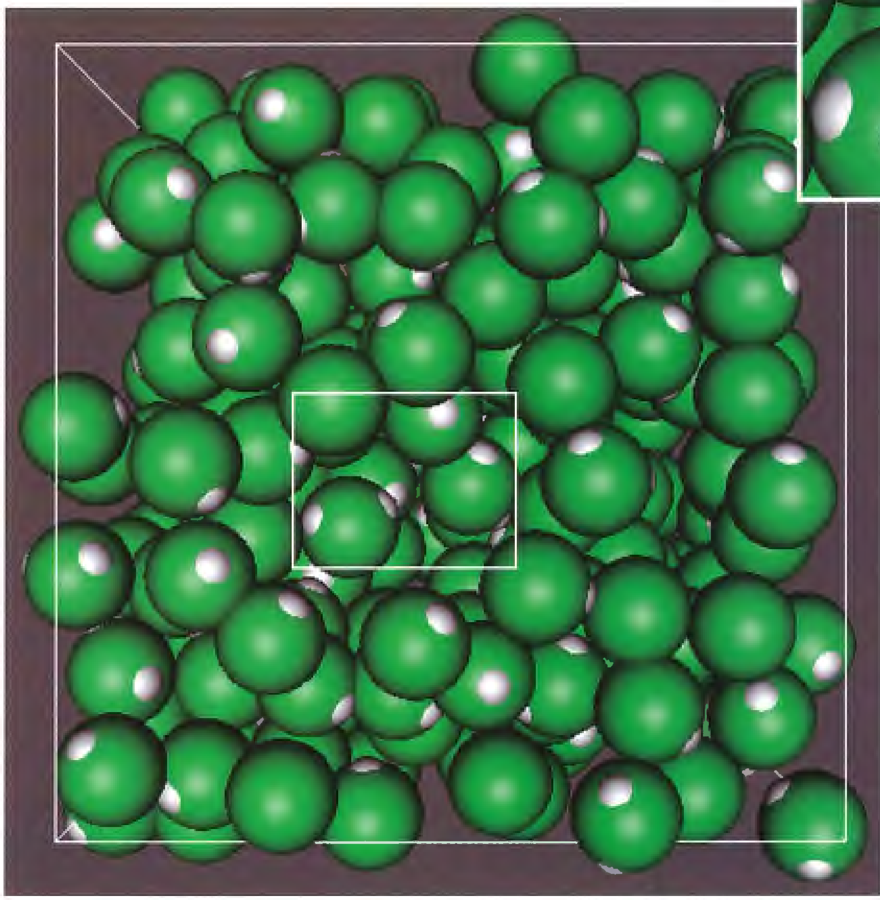
In December 1993 the prestigious scientific journal *Nature* published a paper that disputed the Oak Ridge results. It stated that neutron scattering experiments conducted at the Rutherford-Appleton Laboratory in the United Kingdom indicated that hydrogen bonding is essentially absent in supercritical water. The paper's authors asserted that the simple water model used in the Oak Ridge simulations needed modification. Subsequent publications based on molecular simulation calculations by the ORNL group and by other research groups challenged the results of the U.K. laboratory scientists and their collaborators from the University of Rome, showing that the scattering results were unphysical and suggesting possible error in the correction for inelastic scattering.

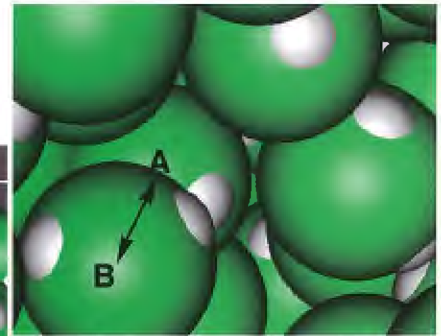
In response to the challenges, in 1996 the British-Italian group reexamined its neutron scattering data, using an improved correction for the results of inelastic scattering. From their reanalysis, group members found that hydrogen bonding is indeed present in supercritical water as predicted by the Oak Ridge simulation group. They also reanalyzed the data they had obtained a decade earlier for ambient water—data that had been the basis for understanding and modeling water structure by researchers worldwide.

As a result of the new analysis, the British-Italian group, led by Alan Soper, has revised the description of water at ambient conditions (i.e., at room temperature and atmospheric pressure). The structure of water at ambient conditions is extremely important because of water's role in many biological and chemical processes at ambient conditions.

Interestingly, the widely accepted data disagreed with an earlier understanding of water structure, as determined more than 20 years ago by ORNL chemist Al Narten through his neutron scattering studies at our High Flux Isotope Reactor (HFIR). Soper's revised results now agree much better with Narten's. The British-Italian group's paper correcting its previous neutron scattering results was published

As this true story illustrates, experimental science and computational science can make important contributions to each other.





This snapshot from a molecular dynamics computer simulation of supercritical water at a temperature of 573 K and a density of 0.72 g/cm^3 shows a number of water molecules. The green spheres represent the oxygen atoms, and the silver bumps on them represent the hydrogen atoms. In the blown-up portion is an arrow connecting water molecules A and B. Note that the hydrogen atoms on molecule B point away from molecule A, and one hydrogen atom on molecule A points toward B. This geometric arrangement between pairs of water molecules is called a hydrogen bond and has a very important influence on the properties of water.

in the January 1997 issue of the *Journal of Chemical Physics.*

Meanwhile, using the Intel Paragon supercomputers in the Center for Computational Sciences, the ORNL simulation group is refining models used in simulations of ambient water to get quantitative agreement with the results of the reanalyzed neutron scattering data. An improved model shows the ability to predict accurately the properties of water all the way from ambient conditions to supercritical conditions. And another ORNL group is currently studying supercritical water using neutron scattering at the HFIR.

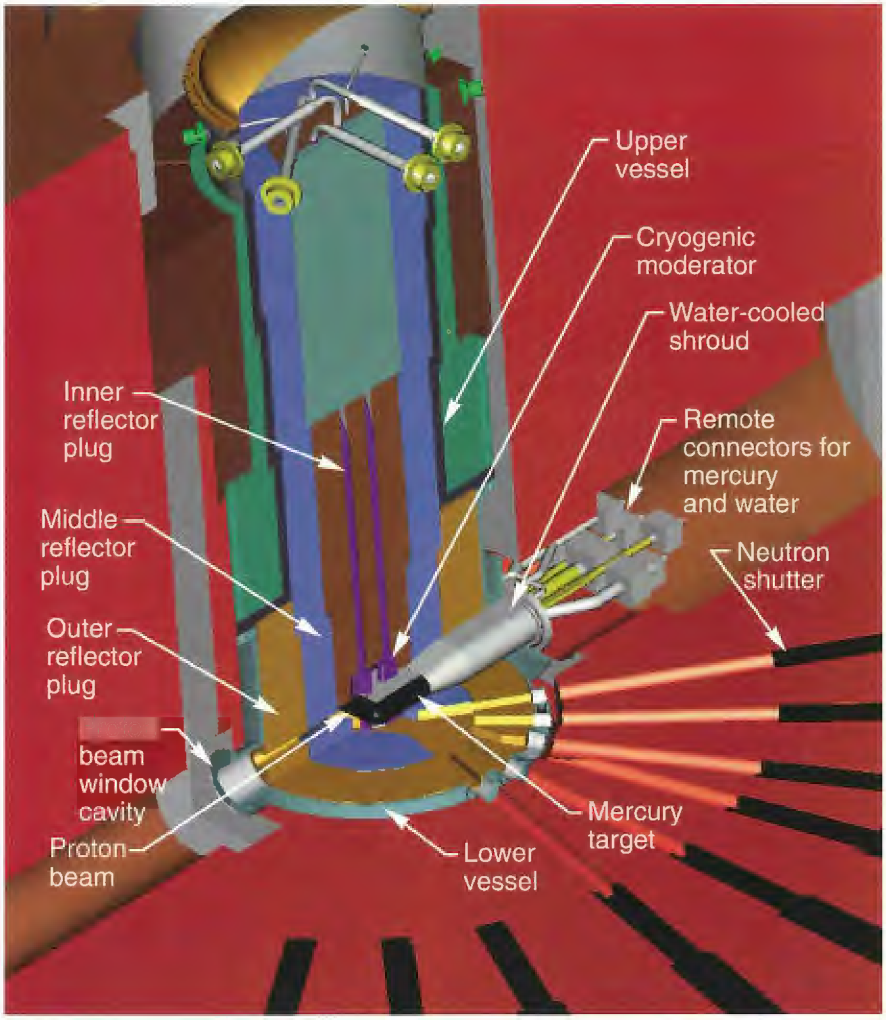
This story illustrates an unusual interplay between neutron scattering experiments and molecular simulation calculations in which both the interpretation of scattering results and the models used in molecular simulations have been improved. In the past, it has been believed that calculations alone must be revised to agree with the results of experiments. Now, it appears that experimental science and computational science can make important contributions to each other.

With its combination of world-class scattering and simulation capabilities, ORNL is well positioned to lead a new era of molecular-based engineering and science. Clearly, such research has improved our understanding of water, the most important but least understood substance on the earth.

The work has been funded by DOE's Office of Energy Research, Office of Basic Energy Sciences, Division of Chemical Sciences.

ORNL Designs Neutron Spallation Target System

Like the fist of the legendary Superman, neutrons can punch through centimeters of steel. X-rays and positrons can penetrate only fractions of a centimeter inside many materials, giving us only a glimpse of a material's surface layers. Neutrons, on the other hand, can reveal bulk structure and properties of materials. Although Superman achieves astonishing feats with the help of his X-ray vision, scientists rely on a more powerful tool—neutron vision—to "see" through matter. That's why researchers are excited about the proposed National Spallation Neutron Source (NSNS), which will offer



View of mercury target (black area, lower center) struck by a proton beam. Intense neutron beams will be produced from this target of the National Spallation Neutron Source.

pulsed neutrons of the highest intensity ever. No wonder the NSNS, which DOE seeks to locate in Oak Ridge, has been called "the microscope of the 21st century."

To get neutrons from the NSNS, you need protons. But first you have to start with negative hydrogen ions fed from an ion source into a high-energy linear accelerator. This "linac" accelerates the ion beam to energies of 1 billion electron volts (GeV) and injects it into an accumulator ring that produces short bursts of protons. Some 60 proton pulses per second (less than 1 microsecond per pulse, one pulse every 17 milliseconds) are directed onto a heavy metal target, where a nuclear reaction called spallation occurs, resulting in the production of neutrons for research into materials.

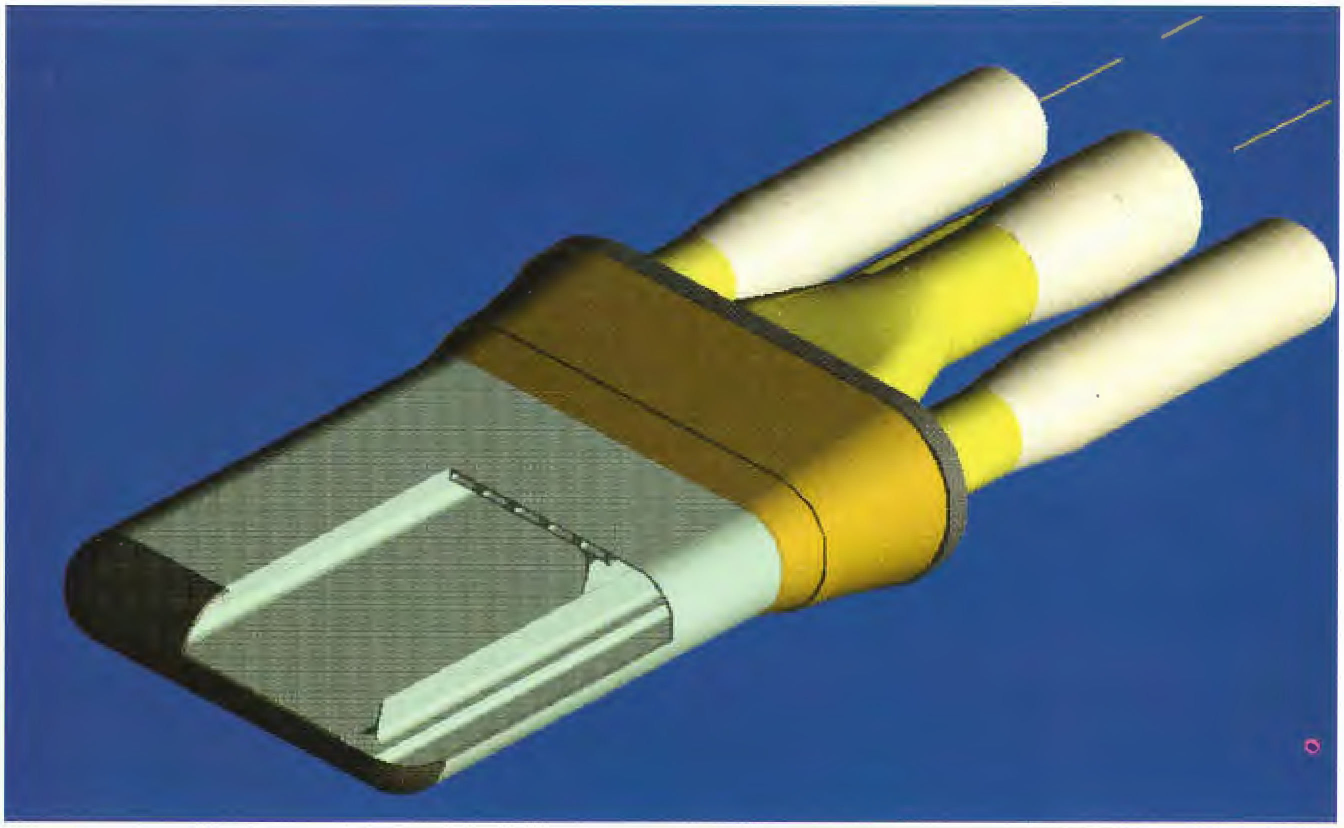
The NSNS is a collaborative project involving five DOE national laboratories. In addition to coordinating the NSNS project, ORNL's responsibilities include designing and constructing the liquid mercury target for neutron production. Because of the enormous amount of energy that the short, powerful pulses of the incoming 1-GeV proton beam will deposit in the spallation target, it was decided not to use a solid target such as tantalum or tungsten. The sledgehammer effect of the proton pulses will cause a large, rapid rise in temperature resulting in thermal shock, which could break the solid target material. In addition, the protons and neutrons will produce severe radiation damage in the solid target material.

Mercury was chosen for the target for three reasons: it is not damaged by radiation, as are solids; it has a high atomic number, making it a source of numerous neutrons (the average mercury nucleus has 120 neutrons and 80 protons); and, because it is liquid at room temperature, it is better able than a solid target to move heat away by flowing. It is calculated that only one cubic meter of mercury is needed as the target material and that it will last for the life of the NSNS facility. The NSNS will be the first scientific facility to use pure mercury as a target for a proton beam.

The production of neutrons through spallation reactions can be visualized by the following analogy. The nucleus is like a bucket of baseballs representing the neutrons and protons; throw another baseball into the bucket and watch a few balls spray out of the bucket. In a similar way, part of the neutrons are produced in what is called the fast, or high-energy, part of the nuclear reaction, or the "microscopic intranuclear cascade." After these fast particles are ejected, the remaining particles are still in a heated state, like the balls in the bucket bouncing around. Some of these lower-energy baseballs can still escape, and so can neutrons in the so-called evaporation phase. These evaporated neutrons make up the bulk of neutron production. In addition to the incoming proton beam, the higher-energy neutrons and protons that are produced can also collide with mercury nuclei in a "macroscopic cascade." The bottom line is that, for every incident 1-GeV proton, approximately 20 neutrons will be produced in the evaporation phase for potential use in neutron scattering experiments.

To maximize the safety of the facility, the NSNS will be designed with many levels of containment to keep potentially hazardous material from getting into the environment. Containment levels include primary and secondary vessels, concrete barriers, and the main building. For example, between the mercury target container and its shroud, helium gas will be circulated in a flow loop. If the

ORNL is designing a mercury target system for the National Spallation Neutron Source. When struck by an intense proton beam, the target will emit numerous neutrons for research.



Schematic of the mercury target system for the National Spallation Neutron Source.

container for the liquid mercury should rupture, the mercury would flow into the loop containing the helium, which would then be collected in a dump tank. The system will be monitored, and if escaping mercury is detected, the accelerator and mercury pump system will be shut down. The remaining mercury in the system would then be passed to the dump tank, and the container would be replaced.

The neutrons coming out of the mercury must be turned into low-energy neutrons suitable for research—that is, they must be at room temperature or colder. The emerging neutrons will be channeled by a beryllium or lead reflector into vessels to reduce their energy. Neutrons will be slowed down by passing them through cans of water (to produce room-temperature neutrons) or through cans of liquid hydrogen at a temperature of 20 K (to produce cold neutrons).

In 1997, containers of mercury will be irradiated with protons at DOE's Brookhaven and Los Alamos national laboratories. Results of these tests will help ORNL researchers refine their computer models and improve their capabilities for predicting neutron production, thermal shock, heating, and other phenomena in a mercury target system. Model results will be used to improve the design of the mercury target system, which is described in the NSNS *Conceptual Design Report* (published in mid-1997)—an important document about a super source of neutrons.

The NSNS is funded by DOE's Office of Energy Research, Office of Basic Energy Sciences, Division of Materials Sciences.

ORNL Helps Develop Cleaner Ways To Make Plastics

Plastics are popular, but pollution is not. There's the rub. Our lifestyles are being shaped by products increasingly made of plastics, such as polystyrene in coffee cups, Teflon® in pans, and fluoropolymers (e.g., Scotchgard®) that protect carpets against staining and soiling. These plastics are formed by joining many (poly) small molecules (mers) into giant, chainlike macromolecules called polymers. But the process of synthesizing polymers from monomers generates undesirable discharges that may include contaminated water, toxic wastes, or ozone-destroying chlorofluorocarbons. A cleaner way to make plastics is needed to improve our environment and meet environmental regulations.

At the University of North Carolina (UNC), Professor Joseph DeSimone is developing environmentally friendly methods for synthesizing polystyrene, fluoropolymers, and other plastics. The process produces no large volumes of toxic waste or contaminated water. The reason: it uses supercritical carbon dioxide (CO_2) instead of water or other solvents as the medium in which reactions or separations can be performed. Supercritical CO_2 is a solvent with almost no undesirable characteristics with regard to safety, environmental, health, or cost considerations. Supercritical CO_2 is made by pressurizing the gas from our atmosphere; when it's discharged by the process, it replaces the same amount of CO_2 that was extracted from the air, so there's no net addition to the greenhouse gas.

A supercritical CO_2 fluid is formed by raising the temperature and pressure of CO_2 so that all differences between CO_2's liquid and gaseous states disappear. By making small adjustments in the pressure or temperature of the CO_2, the solubility of monomers and other components needed for polymer formation can be very widely varied, ensuring that the CO_2 that is eventually released does not contain undesirable contaminants. But supercritical CO_2 is not a perfect solvent. Not all monomers are sufficiently soluble in CO_2 to mix well and form polymers. In such cases, a surfactant, or chemical "soap," must be added to enable the supercritical CO_2 to suspend enough of these small molecules that otherwise would sit at the vessel's bottom.

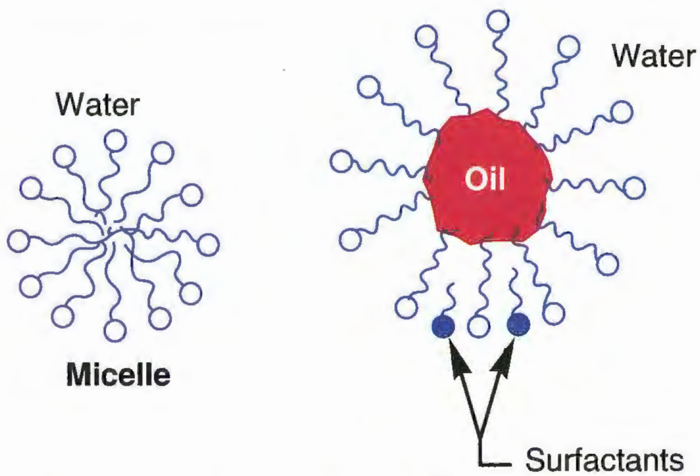
A surfactant is a surface-active agent such as a detergent. Water normally

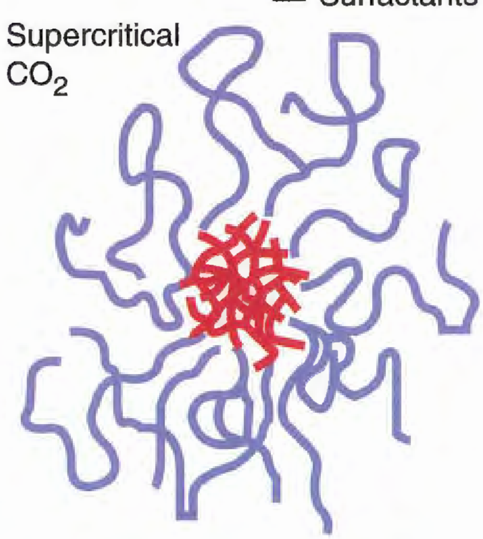
Polymers can be formed the pollution-free way by suspending small molecules in supercritical carbon dioxide with the help of detergent-like molecules called surfactants. When pressure is adjusted at constant temperature to increase the density of the supercritical fluid, surfactant molecules aggregate to form micelles with the CO_2-loving (green) segments, suspending the CO_2-phobic (red) segments in solution and shielding them from the carbon dioxide. *Drawing by Jamie Payne.*

Using small-angle neutron scattering, we helped determine the best ways to form polymers from chemicals in supercritical CO_2, an environmentally friendly solvent for making plastics.

cannot dissolve oil and grease to remove them from dirty clothes, but detergent molecules surround oil and grease molecules, holding them in the water so they can be washed away. A cluster of surfactant molecules, called a micelle, may look like twisted spaghetti lying around a meatball in the middle of a plate. The outside ends on the detergent molecule chains are attracted to water, and the inside ends prefer oil (and hold it there just as the spaghetti keeps the meatball from rolling on a slightly tilted plate); for polymer synthesis, the outside ends of the surfactant chains in a micelle are attracted to supercritical CO_2, and the inside ends have an affinity for monomers, which are strung together (synthesized) in the center of the micelle, where they are shielded from contact with CO_2.

Why do some monomers and polymers dissolve in CO_2 while others don't? Which surfactants are the most effective at suspending different monomers and polymers to keep them from dropping out of solution? Can we control the process and make the surfactants aggregate into micelles or break apart into individual molecules simply by "tuning" the CO_2 pressure? DeSimone, who devised more than a dozen surfactants that are effective with CO_2 and specific polymers, asked ORNL researchers if small-angle neutron scattering (SANS) could determine the answers. We said that it could, based on our experience in employing SANS to characterize micelles in water. Using SANS, in collaboration with visiting researchers from the University of Palermo in Italy, we characterized a number of different micelles and determined their relative effectiveness in suspending different monomers in supercritical CO_2 to enable the formation of polymers. We don't make plastic, but we take our best tools and talent to help others find better, cleaner ways to make it.

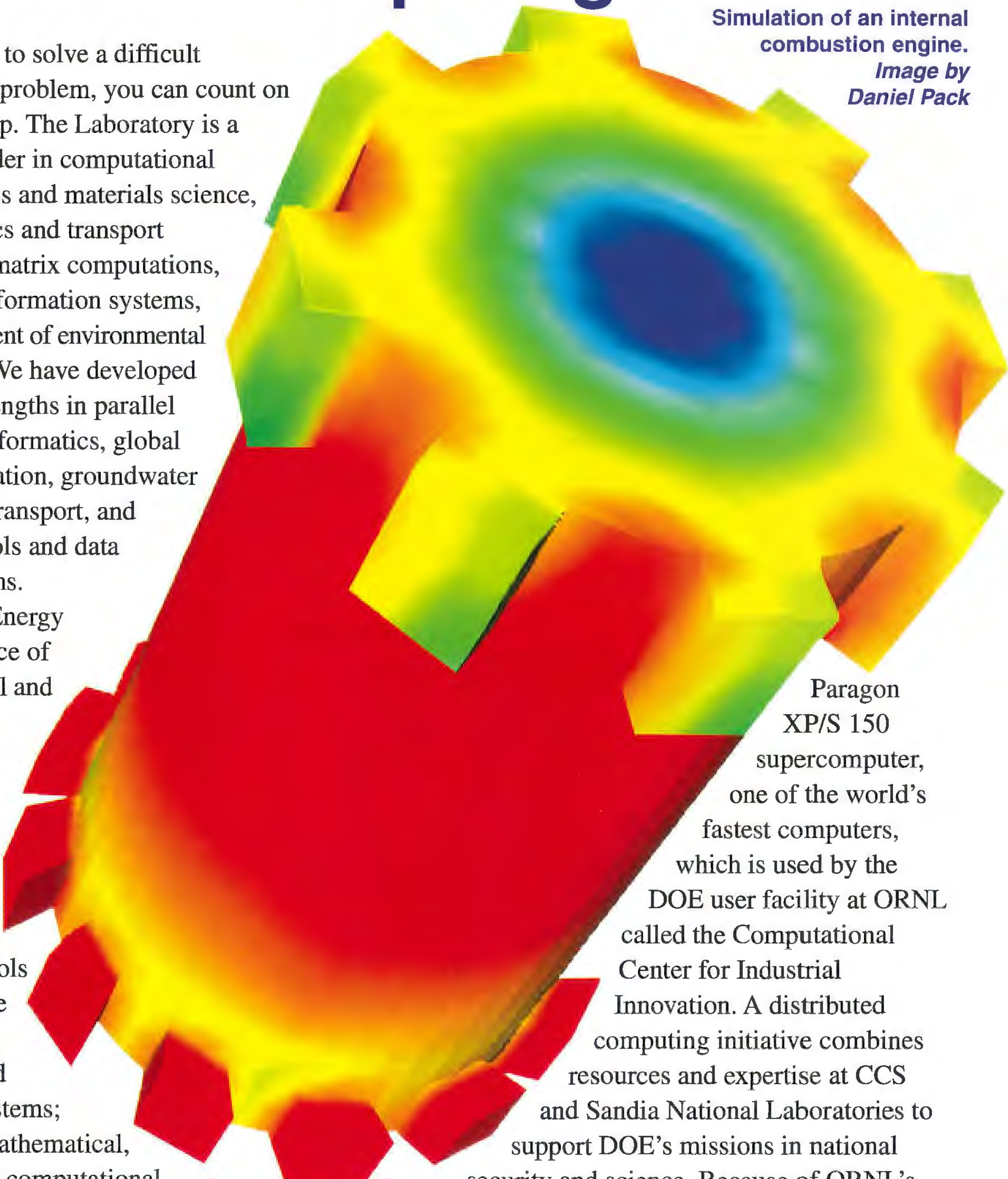




To remove grease from dirty clothes, a detergent must be added to water, which by itself cannot dissolve and remove oil and grease. Detergent molecules surround oil and grease molecules, holding them in the water so they can be washed away (see drawing above). A detergent is a surfactant (short for surface-active agent). Surfactant molecules form a cluster called a micelle (shown in all drawings), which consists of spaghetti-like chains whose tails prefer oil (on the inside) and whose heads are attracted to water (on the outside). For CO_2 surfactants, block copolymers (two different polymers covalently bonded together) are used. The different ends, which are either attracted to, or repelled, by CO_2, form micelles that suspend the growing polymer chains inside and shield them from contact with the supercritical solvent. *Drawing by Reneé Balogh.*

As a result of this work, ORNL's George Wignall, Hank Cochran, and David Londono were formally recognized for their contributions to research on the "Design and Application of Surfactants for Carbon Dioxide," which was selected to receive a Presidential Green Chemistry Challenge Award. The research team was led by Joseph DeSimone. The neutron studies at ORNL were initiated under the Laboratory Directed Research and Development Program. Additional funding was provided by DOE's Office of Energy Research (Division of Materials Sciences and Division of Chemical Sciences within the Office of Basic Energy Sciences) and Office of Computational and Technology Research. ornl

Computational Science and Advanced Computing



Simulation of an internal combustion engine. *Image by Daniel Pack*

If you need to solve a difficult mathematical problem, you can count on ORNL for help. The Laboratory is a long-time leader in computational plasma physics and materials science, nuclear physics and transport calculations, matrix computations, geographic information systems, and management of environmental information. We have developed additional strengths in parallel computing, informatics, global climate simulation, groundwater contaminant transport, and computing tools and data storage systems.

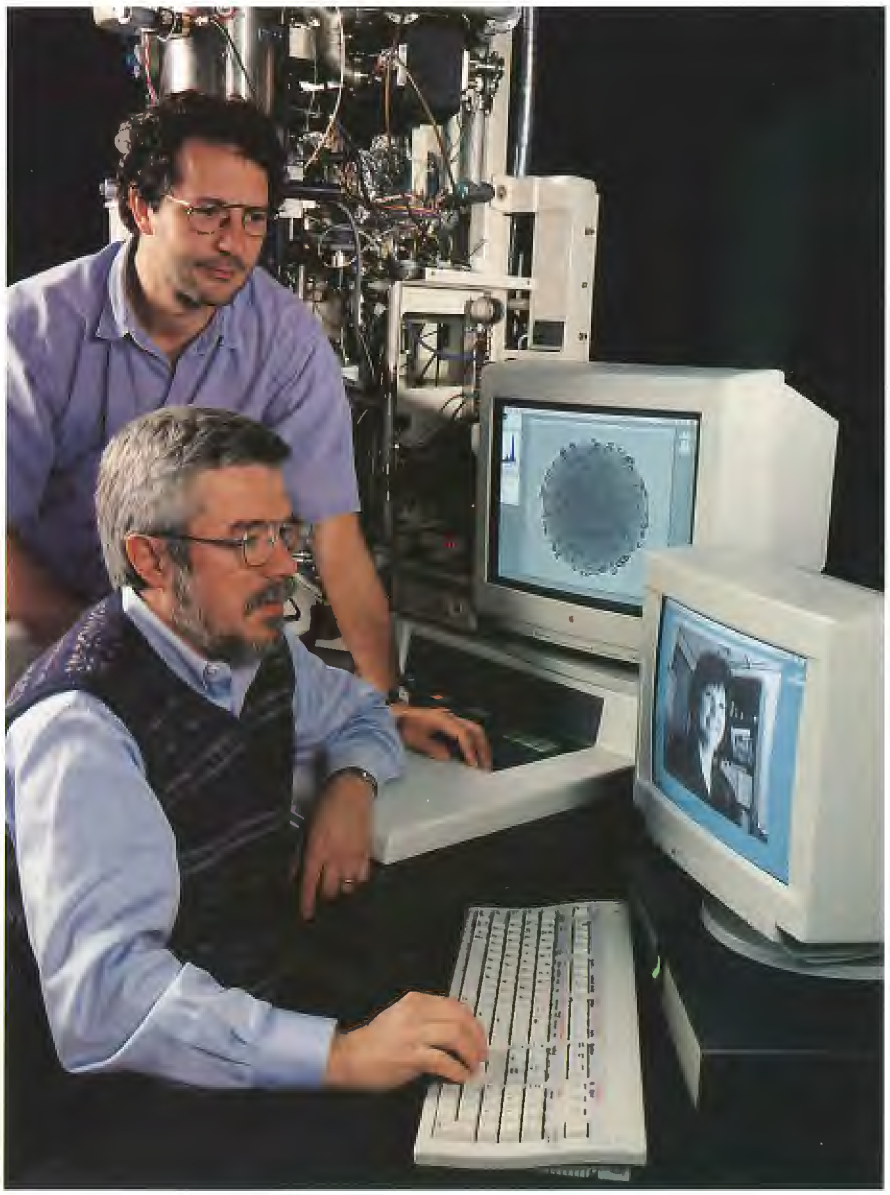
The DOE-Energy Research Office of Computational and Technology Research supports ORNL developments of parallel processing algorithms; tools to facilitate the use of parallel and distributed computing systems; and applied mathematical, statistical, and computational methods for analyses of physical processes. The DOE office also funds the operation of ORNL's Center for Computational Sciences (CCS); the heart of CCS is the massively parallel Intel Paragon XP/S 150 supercomputer, one of the world's fastest computers, which is used by the DOE user facility at ORNL called the Computational Center for Industrial Innovation. A distributed computing initiative combines resources and expertise at CCS and Sandia National Laboratories to support DOE's missions in national security and science. Because of ORNL's impressive expertise and equipment, we have become a computing power, a notable computational resource for a variety of DOE missions.

Remote Control of ORNL Microscopes

In November 1996, students in an electron microscopy class at Lehigh University focused on a virtual place in cyberspace. They took turns remotely operating an electron microscope by computer. Tapping a key or two on the computer keyboard, the curious students moved the specimen about, changed the image magnification, and adjusted the microscope's focus. On the computer screen they studied the sample as its different images appeared, transmitted across the Internet from the microscope located at ORNL. They also had live video and audio contact with their ORNL collaborator, using teleconferencing tools.

ORNL researchers and other scientists in the DOE laboratory system have been demonstrating the potential of using the Internet or other networking technology for remote operation of research equipment. At ORNL the Hitachi HF-2000 field emission transmission electron microscope has been used in demonstrations from Lehigh University, Detroit, San Diego, and Washington, D.C. Remote operation of the ORNL microscope was demonstrated to (now former) Secretary of Energy Hazel O'Leary at a DOE conference in March 1996 in Reston, Virginia.

ORNL researchers are helping to show the potential of using the Internet for remote operation of research equipment.



Larry Allard (sitting) and Edgar Voelkl demonstrate the remote operation of an electron microscope. *Photograph by Tom Cerniglio.*

The HF-2000 microscope and three other ORNL electron microscopes are now among nearly a dozen microscopes at DOE facilities that will be remotely operated as part of the new Materials MicroCharacterization Collaboratory pilot project supported by the DOE 2000 initiative. Other ORNL projects receiving DOE 2000 initiative funding are the development of electronic notebooks (see next story) and remote collaborations involving experiments at ORNL's High Flux Isotope Reactor and the Advanced Photon Source at DOE's Argonne National Laboratory.

According to DOE, a collaboratory is "an open laboratory spanning multiple geographical areas where collaborators interact via electronic means—'working together apart.' " It enables researchers to conduct experiments remotely and view and discuss the results immediately over the Internet.

In the materials collaboratory, ORNL researchers will be working on microscopy projects with researchers from Argonne, Lawrence Berkeley National Laboratory, and the DOE-funded microscopy center at the University of Illinois at Urbana-Champaign. Contributing partners in the research will be the National Institute of Standards and Technology and six manufacturers of microscopes and control systems: Philips; JEOL; Hitachi; R. J. Lee; Gaton, Inc.; and EMispec.

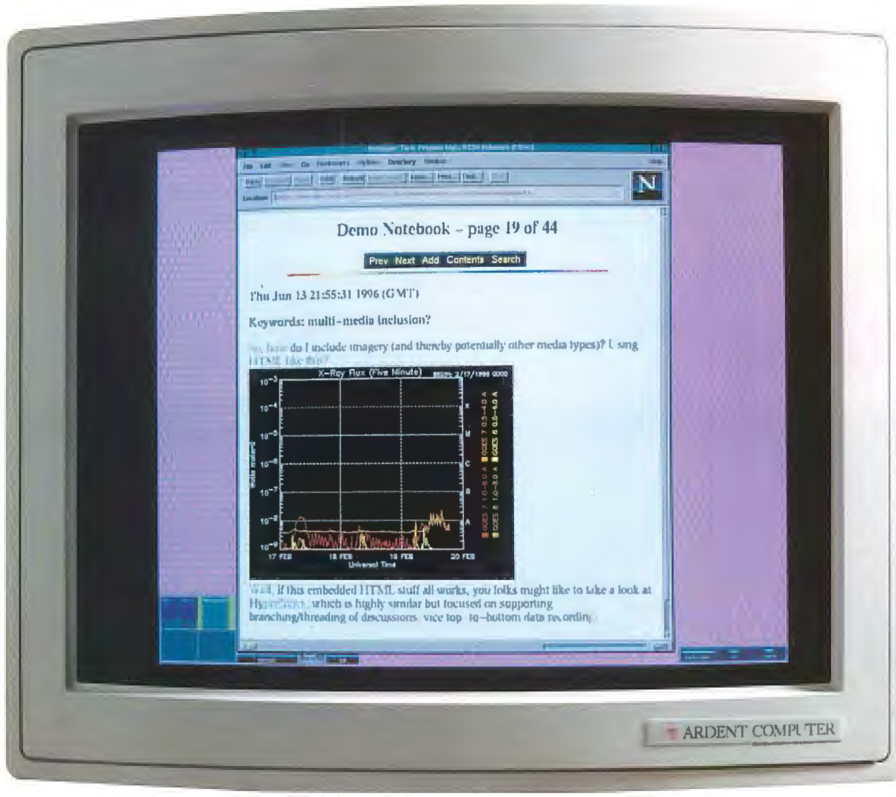
The collaborators will try not only to bring their "user facilities" to the user but also to make them more user friendly. They will automate routine functions as much as possible and provide an easy, effective, mouse-driven user interface. They will also add features to ensure data security and keep unauthorized users off the system.

Collaborative research projects among scientists at the participating laboratories will embrace critical problems involving surfaces and interfaces, which are important in controlling the behavior of advanced materials. Specific microscope research will focus on catalysts used to control emissions from automobiles and diesel trucks, as well as interfaces between substrates and coatings designed to protect them against corrosion. That ORNL will be a key player in the early development of virtual laboratories is a virtual certainty.

The research is supported by the Office of Mathematical, Information and Computational Sciences, the Office of Basic Energy Sciences, and the Office of Transportation Technology.

Electronic Notebooks for Scientists

We have developed an electronic notebook that's especially useful for scientific collaborations involving the remote operation of research equipment.



Closeup of a page of ORNL's electronic notebook on the computer screen. *Photograph by Tom Cerniglio.*

Scientists traditionally use paper notebooks to record their ideas for experiments and notes on experimental setups, observations, and research results. These notebooks are kept on bookshelves or in file cabinets.

Is there a more efficient alternative in the age of computers and the Internet? Why manually copy documentation into a paper notebook when you can cut and paste it electronically and later do searches to quickly find a special entry?

Some of our researchers recommend a new recordkeeping tool—the electronic notebook. An electronic notebook is a repository for objects that document scientific research. It can be used to enter, retrieve, or query objects such as text, sketches, images, tables, spreadsheets, and graphs. Electronic notebooks are not calculators, nor are they chat spaces. They hold a static record of ideas, experiments, and results.

A notebook accessed by computer offers scientists all the features of the traditional paper notebook, plus the capability to accept multimedia input (audio and video clips) and computer-generated images, tables, and graphs placed by drag and drop. Furthermore, electronic notebooks can be useful for scientific collaborations, especially those involving the remote operation of research equipment. They can be easily searched for information. They can contain hyperlinks to other information, such as a research paper or raw data stored elsewhere on the Internet.

We have developed a prototype for an electronic notebook that is being used by more than 30 different groups around the country. Commercial interest will quickly grow once the obstacle of legal acceptance of the electronic notebook concept is overcome. We anticipate that electronic notebooks will soar in popularity not only for collaborating groups but also for private users.

ORNL is collaborating with researchers from DOE's Lawrence Berkeley National Laboratory and Pacific Northwest National Laboratory (PNNL) to design a common notebook architecture that will allow interoperation of the different notebooks. That is, an ORNL researcher could use the Laboratory's notebook interface to view entries that were written by a colleague at PNNL using his own notebook. Also, the two researchers could share input tools they each developed.

In developing the Web-based electronic notebook architecture, ORNL researchers are focusing on ensuring the security of the notebook.

Our electronic notebook can be easily searched for information.

Electronic notebook entries can be digitally authenticated and signed, individually or collectively. They can be electronically time stamped and notarized. While entries cannot be modified once signed, the pages can be annotated and forward referenced. Entries can be secured by encryption, both in transit and in storage. All these security actions can be performed transparently to the users, thus adding no complexity to the user interface.

The ORNL prototype uses Common Gateway Interface scripts to access notebook pages. The researchers are developing Java applets (mini-programs written in the Java programming language developed by Sun Microsystems) to enter objects in the notebook, such as a pen-based sketch pad. Of course, as they make further developments in this project, they record their progress—in their electronic notebooks.

The research was initially supported by ORNL's internal Laboratory Directed Research and Development Program. Funding now comes from DOE's Mathematical, Information, and Computational Sciences Division. A demonstration version of ORNL's notebook is available on the World Wide Web (http://www.epm.ornl.gov/~geist/java/applets/enote). It can be accessed by any authorized user from any type of computer that has a Web browser.

Challenges of Linking Four Supercomputers

It would be nice to be able to solve any scientific problem using one computer. But one ordinary single-processor computer in an office isn't always enough: new problems continually demand more power and speed. Some scientific problems are so complex that the only approach is to divide and conquer. The problem is broken into small parts, and hundreds or thousands of computer processors are linked together to attack pieces of the problem at the same time for a rapid solution. The linked processors form one computer—but it's a parallel supercomputer that fits in a large room.

In the quest to solve increasingly complex problems, a project is under way to link geographically separated parallel supercomputers by a high-speed network to form one distributed supercomputer. An ORNL team is working with researchers from Sandia National Laboratories and the Pittsburgh Supercomputing Center to develop this system linking four massively parallel supercomputers: ORNL's XP/S 150 (2048 individual processors) and XP/S 35 (512 processors) Intel Paragons, one Intel Paragon at Sandia (1840 processors), and Pittsburgh's Cray T3E (512 processors).

Although the concept is simple, the task is not. For example, the supercomputers at the three centers use different operating systems and compilers. A program written for any one of the computers must be able to run on two to four machines simultaneously despite the system differences, a feat somewhat like flawless simultaneous translation into three languages at lightning speed. This translation is done using Parallel Virtual Machine (PVM) software developed at ORNL.

Another challenge is speeding up communication among supercomputers so that no processor is idle while waiting for data from another computer. The asynchronous transfer mode (ATM) interface card, developed by GigaNet, increased the intermachine communication rate from the 300 kilobytes per second possible with Ethernet to 72 megabytes per second (MB/s). But there are other bottlenecks.

Think of data exchange between computers as pumping water through a hose. One slowdown has been the pumping rate: the intermachine message routing systems currently move data through a service node—a "doorway" out of the machine—that carries only 17 MB/s. A PVM modification called "direct to ATM" routing will send data directly to the ATM network instead, enabling applications to use nearly all of the 72 MB/second bandwidth (the hose) between machines. The change will accelerate communication between the ORNL Paragons to about 72 MB/s.

The primary slowdown between ORNL and Sandia, on the other hand, has been the hose. The inter-site Energy Sciences Network (ESnet) moves only 1 to 2 MB/s between the two sites now; however, network capacity upgrades will increase the data flow to 12 MB/s soon and to 72 MB/s in a few months.

The two ORNL Paragons are already linked and running applications. Linking the geographically separated computers is more complicated: for some applications, individual processors must be added incrementally, the system tested, and the bugs worked out.

The first phase of a materials application for modeling the magnetic behavior of nickel-copper alloys is running on ORNL's Paragons. The materials code is set up to run one atom of the model per computer processor. A production run on 1372 processors across the ORNL Paragons completed more than 2.2 quadrillion mathematical floating point operations. Plans include a 2048-processor run that will involve the ORNL XP/S 150 and Sandia's Paragon, as well as a 2916-processor run that will involve the ORNL XP/S 150, possibly the XP/S 35, Sandia's Paragon, and Pittsburgh's Cray T3E.

A shock physics code developed to address nuclear weapons safety is running across the ORNL and Sandia Paragons at a gradually increasing scale. It involves predicting the response of a nuclear weapon to a hypothetical nearby chemical explosion to assess whether a sympathetic detonation would be likely. This code has run on 1024 processors at ORNL and Sandia, and will also be used for fundamental scientific studies such as the consequences for global climate of an asteroid striking an ocean.

A third application, a global climate model, will include two different codes (one for the atmosphere and one for the ocean) communicating with each other while running on multiple computers. Work on this application is focused on determining the best procedures for approaching such a complex calculation, which will predict climate over an extended time, in a distributed computing setup.

When the distributed supercomputer is complete, it will be big enough to tackle a host of complex problems that are virtually impossible to solve today. We will be counting on distributed computing using ever larger machines to solve the biggest problems in the future.

This project is funded by DOE's Mathematical, Information, and Computational Sciences Division.

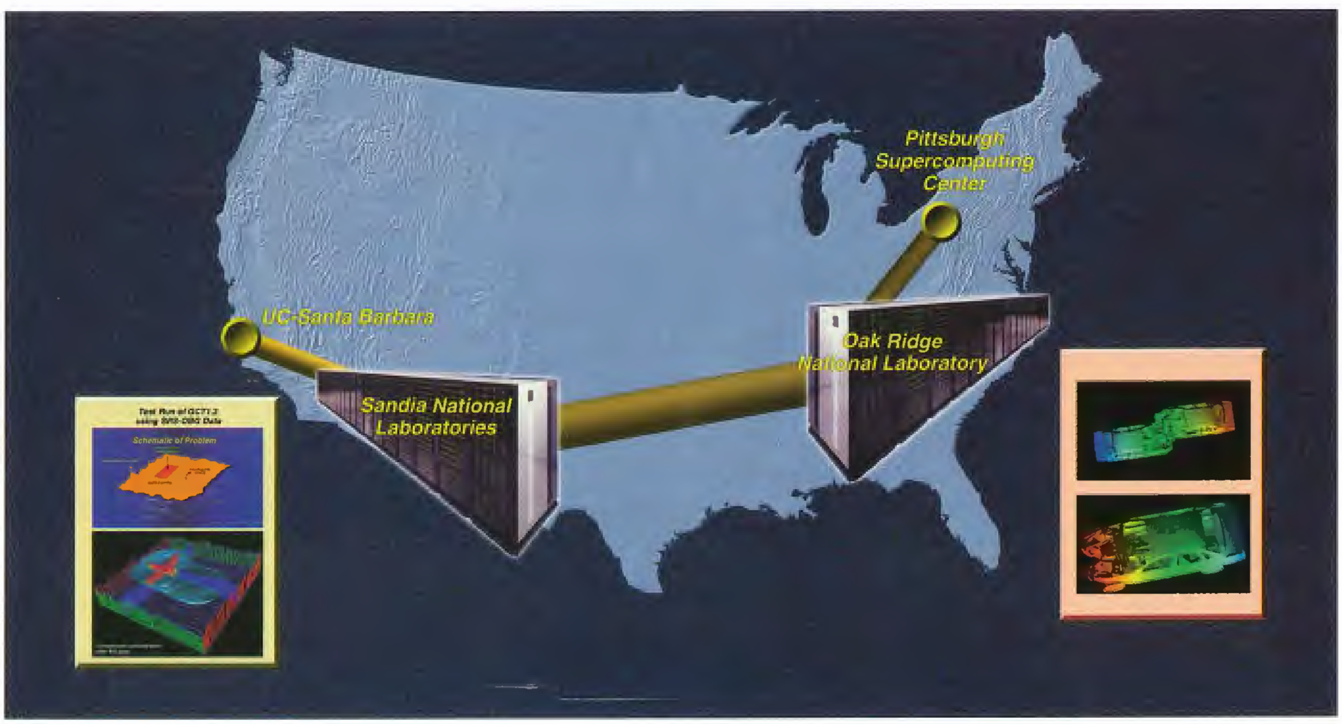
Operating Supercomputers Seamlessly

As research problems become larger and more complex, their solutions require more and more computing power. They inspire the development of advanced computing systems such as massively parallel supercomputers in which many processors are linked together. Some of these machines at different sites are becoming even more powerful because they are linked together by a high-speed network, forming a distributed supercomputer. One of the current challenges in computing research is making such a complicated environment seamless so that a user can run an application across these linked machines as if they were one computer.

ORNL is helping develop a seamless environment that spans the parallel supercomputers at ORNL, Sandia National Laboratories, and Pittsburgh Computing Center. The research team wants to make distributed supercomputing systems like this one so easy to use that they are accessible to any researcher whose project needs them, not just to computer scientists.

To achieve the goal of seamlessness, several complications are being worked out. For example, all three supercomputer centers use different operating systems, access policies, and communication networks. Connecting these heterogeneous computers is Parallel Virtual Machine (PVM) software developed at ORNL. PVM, which won an R&D 100 award in 1994, is specifically designed to make a heterogeneous cluster of computers appear as a single computational resource. As the seamless environment becomes more of a reality, a user will be able to specify the general requirements for an application (e.g.,

In the quest to solve increasingly complex problems, geographically separated parallel supercomputers are being linked by a high-speed network to form one "distributed supercomputer."



Parallel supercomputers in Oak Ridge, Pittsburgh, and Albuquerque are linked by a high-speed network to rapidly solve complex scientific and national security problems. *Images by Daniel Pack and Ross Toedte.*

ORNL is working to make the multi-site supercomputing environment "seamless" so that linked machines can be used as if they were one computer.

amount of memory, processing time, storage), and then PVM will decide the most efficient way to run it, do the necessary translations, and port it to the appropriate processors without further instruction from the user.

The formidable security systems and access restrictions around all three computer centers are another obstacle. Sandia, particularly, because it is a weapons laboratory, has a practically impenetrable firewall around its computing system designed to deflect anything from the outside. Methods had to be devised to get data through the security systems without compromising their effectiveness and to prevent interception of data traveling over the network. Sufficient progress has been made to allow shared computer runs between ORNL and Sandia.

One of the highest hurdles remaining is scheduling run time on the machines. Competition is stiff for time on even one of the supercomputers; negotiating simultaneous computing time and preparing each machine for shared runs is a logistical nightmare. At present, an expert must schedule each linked run manually. The goal is eventually to automate the entire scheduling process from input of code to output of results.

Most of the low-level infrastructure for the distributed system is in place. The seamless environment work is aimed at making access to the system progressively easier so that the user will see and use the entire collection of resources as a single computer. At present, only about five persons have the skills to set up an application to run at more than one site; the long-term goal is for any scientist with an appropriate application to be able to do so.

Several scientific problems are already being solved in our multiple-center distributed computing environment. The supercomputing team is working with researchers to meet their needs for more computing power and speed as it chips away at the obstacles to running these supercomputer clusters seamlessly in parallel.

This project is funded by DOE's Mathematical, Information, and Computational Sciences Division.

Speeding Up Storage and Retrieval of Supercomputer Data

The speed of parallel computer processors isn't the only thing that dictates how fast supercomputing applications can run. Just as essential is the speed with which processors can store and access data. In fact, given the development of lightning-fast parallel computers and the exponential growth in the sizes of data sets, some computing experts think the time required for data storage and retrieval will set the pace for computing for the foreseeable future.

The excellence of HPSS has just been recognized in a 1997 R&D 100 Award.

The pace has been quickened by the development of the High-Performance Storage System (HPSS) by IBM and a consortium of national laboratories, including ORNL. IBM began marketing the system in late 1996. The HPSS moves very large data files among high-performance computers, networked workstation clusters, and storage systems many times faster than was possible before.

Powerful parallel computers generate vast quantities of data (including results of calculations), and systems are needed to accept, store, catalog, and retrieve those data rapidly and with absolute reliability. The HPSS addresses those demands using standard but, for optimal effectiveness, top-of-the-line network and storage technologies and vendor products. It is largely a huge software application—about a million lines of code—that controls a user's storage hardware and network devices and generates and maintains the "metadata" (information that identifies the stored files in detail—labels, locales, sizes, access limitations, etc.) needed by a particular site.

An HPSS package consists of servers (central computers in local area networks) and "data movers," software modules that transfer data streams between processors and storage devices. The package is completely modular; any module can be upgraded or replaced without affecting the rest of the system. Like most storage systems, it is hierarchical: From the computer, it routes data into disk storage arrays (high speed but modest capacity) and later, for archiving, onto tape (high capacity but slower access). The HPSS manages these different classes of storage devices as a single system.

One secret to the HPSS's success is that all computer processors and storage devices are connected directly to the network so that data move directly between them at network speed. (Conventional storage systems route data through a server and a control interface, a big bottleneck.) Another HPSS plus is parallelism: Many data streams can move simultaneously among multiple computing processors and multiple storage devices, or a single huge file can be split into smaller subfiles that are transferred simultaneously. These advantages give HPSS the capability to transfer data at rates of gigabytes (billions of bytes) per second; the actual speeds for a given site are limited only by the amount of available hardware.

Advanced techniques are used to ensure security and protection of data. Client-server processes are structured as "transactions," related groups of functions that must occur together to maintain the integrity of the data set. If all parts of a transaction are not completed, the entire transaction is redone.

The HPSS is scalable and almost infinitely extensible. It can assimilate virtually any number, speed, and capacity of processors and storage devices.

ORNL's Center for Computational Sciences is converting its entire storage system from NSL-Unitree to HPSS. Sandia, Lawrence Livermore, and Los Alamos national laboratories already have adopted the system, as have a number of other high-performance computing centers. It will be used by these DOE defense labs to carry out their responsibility of ensuring the integrity of the U.S. nuclear stockpile in a world without nuclear testing.

The HPSS will be useful in any environment that involves high-speed transmission of substantial amounts of data, such as hospitals, corporations, universities, and some types of online services. (Cable services that provide movies on demand, for example, would be a natural for the HPSS.) ORNL is a member of HOST, a conglomerate of medical care institutions, medical groups, vendors, and research institutions interested in using the HPSS for storing and rapidly accessing medical records. The requirements for the task would be enormous: all medical records in the country must be retrievable quickly through one index, and security measures must eventually be in place to prevent unauthorized access to or tampering with records.

ORNL is developing additional features for HPSS and is working with Storage Tek, a maker of tape libraries, to ensure that HPSS works properly with that company's very fast Redwood drives. Work is under way on other compatibility issues to ensure that the HPSS is adaptable to platforms across the computer industry.

Given its unique combination of speed, parallelism, and scalability, the HPSS is expected to define the state of the art in advanced storage system software for some time. It will be setting the pace for high-speed computing into the 21st century.

The project was supported initially through a CRADA with IBM and now is funded through the Accelerated Computing Strategic Initiative, part of DOE's Defense Programs.

Advanced Lubricants and Supercomputers

The squeaky wheel gets the grease to reduce friction between moving parts and prevent them from burning up. But it's less widely known that motor oils used in our cars today will not be able to take the heat as lubricants in tomorrow's highly efficient vehicles. Because the lean, clean cars being developed for the U.S. Partnership for a New Generation of Vehicles will operate at higher temperatures and engine speeds, today's motor oils would break down too fast to be reliable. Thus, industry is searching for advanced lubricants that will stand up to the harsh conditions of advanced vehicles. The problem is that it would take many decades for researchers in the industry to synthesize and test billions of different hydrocarbon liquids to identify the most promising candidates for advanced lubricants. An attractive complement to experimentation is computation.

ORNL researchers have shown that molecular simulation calculations on our Intel Paragon supercomputers can accurately predict the performance of advanced lubricants. We have developed algorithms and parallel codes for use on the Intel Paragon so that we can simulate the behavior of lubricant molecules. This computational approach should provide industry with a much faster, cheaper way to identify suitable lubricants for advanced vehicles.

Many different lubricant candidates (i.e., hydrocarbon liquids) can be synthesized, and even more can be simulated. The properties of a hydrocarbon liquid depend in a complex way on two factors: the way in which molecules interact with each other and the conformations of the individual molecules themselves in the liquid—that is, the spatial arrangements of atoms in a molecule that stem from free rotation of the atoms about a single chemical bond. Complicating matters further is that these two factors are intimately interrelated (molecules interacting with each other affect their conformations, and vice versa). As a result, hydrocarbon liquid properties are found to depend on the number of carbon atoms in the molecule's backbone and the number, position, and length of branches along the backbone, as well as on temperature and pressure.

In our simulations, we have studied how the viscosity of various hydrocarbon liquids varies with all these factors. Viscosity is a measure of resistance to flow; it's high in corn syrup and low in alcohol. If the viscosity of oil changes during use, problems could ensue. If the oil viscosity is too high before you start your car on a cold morning, the engine might not start; if it's too low when you're driving on the interstate highway during a summer afternoon, your engine might fail.

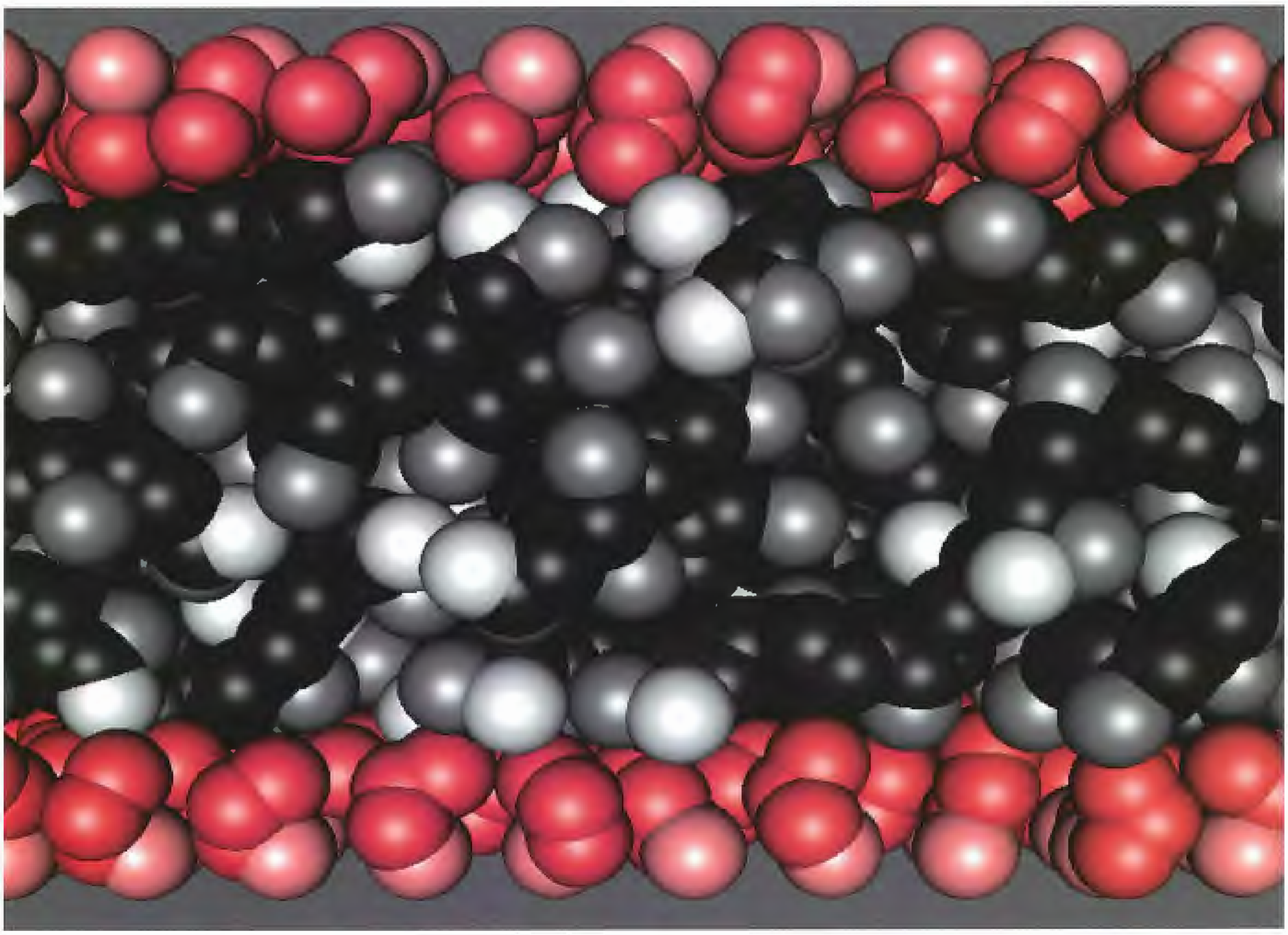
Viscosity of a lubricant can be changed by a number of factors. Because different fluids have different viscosities, the structure of the hydrocarbon molecules—backbone length, branching, etc.—is expected to affect viscosity. Temperature is a factor—liquids usually have a lower viscosity at a high temperature. A third important factor is the shear rate. The shear rate in a lubricant is determined by how rapidly the two solid surfaces being lubricated move past one another and how far apart the moving surfaces are. With a faster speed and narrower distance, the shear rate climbs.

At low shear rates most liquids, including lubricants, exhibit constant viscosity when the shear rate changes. This constant viscosity behavior is called Newtonian behavior because it is described by Newton's law of viscous flow. On the other hand, at the high shear rates that occur in automobile engine lubricants, most liquids (including lubricants) exhibit "shear-thinning" behavior—their viscosity decreases as the shear rate increases. The experimentally measured viscosity of a lubricant is usually its Newtonian viscosity because the shear rates at which the shear-thinning behavior occurs (shear rates that occur in your automobile engine today) are far too high for experimental viscosity measurement.

Finally, previous experiments and molecular simulations by other researchers have suggested that a lubricant's viscosity may change as the distance between the two lubricated surfaces decreases to molecular dimensions. Of course, this finding would be vitally important because engine wear occurs where surfaces are closest to one another.

We have simulated the performance of squalane, a hydrocarbon molecule typical of many lubricants. The squalane molecule has 24 carbon atoms in its molecular backbone and 6 short side branches (each 1 carbon atom long) symmetrically placed along the backbone. One measure of lubricant performance is the viscosity index, a measure used by industry to describe how viscosity changes with temperature. The viscosity index of squalane predicted by our simulations is in excellent agreement with experimental measurements. This was the first time that a substance's viscosity index had been predicted by molecular simulation. It was also the first time that accurate models had been extended to calculating the viscosity of molecules as large as those used in motor oils.

Such calculations were beyond the capabilities of earlier computers and computer codes. With this success, industry can now use molecular simulations with confidence to predict the viscosity index of new lubricants,



This visualization is created from a molecular simulation of squalane molecules in confined flow between moving surfaces. The red balls are the atoms of the moving surfaces; the top surface moves to the right, and the bottom surface moves to the left. The balls of other colors represent the carbon atoms of the squalane molecules (the hydrogen atoms are not shown). The black balls are the carbon atoms at each end of the 24 carbon backbone of the squalane molecules. The gray balls are the single-carbon branches along the backbone. The squalane molecules are shown in different colors so that it is easier to distinguish the carbon atoms of one molecule from those of another. Careful examination of the squalane molecules reveals that they are somewhat aligned in layers parallel to the moving surfaces rather than being randomly oriented as would be the case in the static bulk liquid.

ORNL has shown that computer simulations accurately predict lubricant performance.

even before they have been synthesized.

At the University of California at Santa Barbara and the University of Illinois at Urbana-Champaign, research groups have experimentally studied the viscosity of liquids between surfaces moving past one another separated by only a few atomic diameters. They found that the viscosity measured in this so-called "confined flow" appeared to be much higher than that of bulk oil, and they inferred that the flowing oil's molecules may be lined up in layers parallel to the moving surfaces. This behavior occurs at shear rates much lower than those in your engine.

Previous molecular simulations (using models of unknown accuracy) apparently supported these interpretations; however, our molecular simulations of squalane in confined flow (using models proven to be accurate) have challenged the earlier conclusions. We found that the viscosities of the confined and bulk oil are identical when correct attention is paid to all of the factors involved in either simulations or experiments. We concluded that at high shear rates, shear flow alone is sufficient to align the molecules, and the aligning of narrowly spaced surfaces affect the viscosity only at very low shear rates.

Our accurate computer simulations have challenged the consensus from results of previous experiments and simulations, but from this challenge has come a new level of molecular understanding. Just as the squeaky wheel gets the grease, we believe the exciting new results of molecular simulations will attract the attention of both experimental and theoretical scientists and of industry, as well.

The research was sponsored by the Laboratory Directed Research and Development Program at ORNL.

Modeling the Invar Alloy

Like people, some materials behave normally and others do not. Take a normal metal or alloy and heat it up. It will expand because the more the material is heated, the more its atoms vibrate and push apart. Take a normal magnet made of ferromagnetic metals such as iron, nickel, or cobalt. Its atoms are magnetic—like compass needles, they can be aligned up or down to north or south poles, producing a large magnetic field.

Now consider a disordered alloy of nickel and iron called Invar (short for "invariable"). Discovered 100 years ago by the Swiss-born French physicist Charles Guillaume (who received a Nobel Prize for physics in 1920 for his discovery), Invar is not normal. Heat it up to a certain temperature range and it won't expand or contract (it's invariable); however, its ability to maintain its dimensions over a wide range of temperature makes it useful for highly precise Swiss watches, pendulums in clocks, standards of measure, high-precision instruments, shadow masks for televisions and computer monitors (to reduce glare), and tubing surrounding fiber-optic cables.

Invar is also a magnetic material—but not a normal one. For one thing, based on neutron and X-ray scattering data obtained by ORNL researchers, Invar's resistance to contraction has been definitively linked to magnetic pressure: natural repulsion by iron atoms as they approach each other during cooling keeps the vibrating atoms from moving even closer together, nearly canceling the contraction effect. For another thing, the orientations of its atomic magnets are unusual for a magnetic material; they are not simply up or down—sometimes they point outwards at an angle, like a compass needle pointing north-northwest. Because it is so abnormal, Invar is one of the most studied and most complicated of materials.

ORNL scientists are using computer simulation to better understand the complex magnetic behavior of a disordered nickel-iron alloy in which the atoms are randomly arranged within a face-centered cubic structure. Using an ORNL-developed computer code on 256 nodes of the Intel Paragon massively parallel supercomputer, they calculated the orientations of 256 magnetic atoms of an Invar alloy that is 36% nickel and 64% iron. Such a material is highly magnetic but on the borderline—small changes in volume or composition (e.g., an increase in iron content) could result in loss of magnetism.

We started with atoms whose magnetic moments (orientations with respect to the direction of magnetization) point in random directions. Our computer code, which knows the position of each nickel and iron atom, performs the quantum mechanics calculations to determine which way the magnetic moment of each atom should point. The code calculates electronic charge density (how electrons arrange themselves about sets of nuclei), magnetization density (imbalance in up and down electron spins), and the average orientation of the magnetization associated with each atom.

When the volume of the Invar alloy is decreased or its iron content is increased, two changes might occur, according to earlier studies. The alloy can remain ferromagnetic with all its magnetic moments pointing in the same direction, parallel to the direction of magnetization (collinear), but getting smaller, accounting for the sudden drop in its magnetic strength. Or the magnetic moments of atoms on the cube corners of the face-centered cubic alloy could point up while the magnetic moments of atoms at the center of each face point down, making the alloy antiferromagnetic but still collinear.

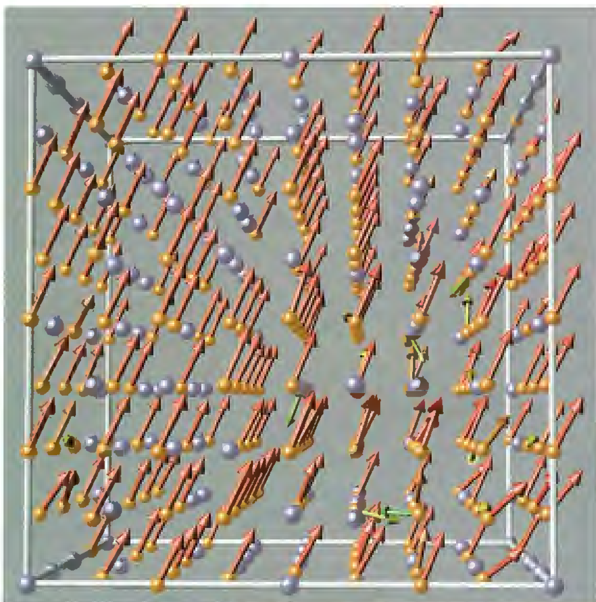
Our calculations suggest that some magnetic moments are antiferromagnetic and some are noncollinear (at an angle to the direction of magnetization) in the nickel-iron Invar alloy. All nickel magnetic moments point in the same direction as the magnetization, but some iron magnetic moments point at angles to it. In shells where 1 iron atom is surrounded by 12 iron atoms, the magnetic moment of the central atom wants to point down, not up like its neighbors. This neighbor shell is antiferromagnetic. If a central iron atom has fewer than 12 neighbors (8 to 11), the atoms in this neighbor shell act confused and unable to decide whether their magnetic moments should point up or down, so instead they become noncollinear as each points at an angle to the direction of magnetization. Some atoms' magnetic moments turn upside down or are noncollinear, and in both cases they are shorter than the ones that point up.

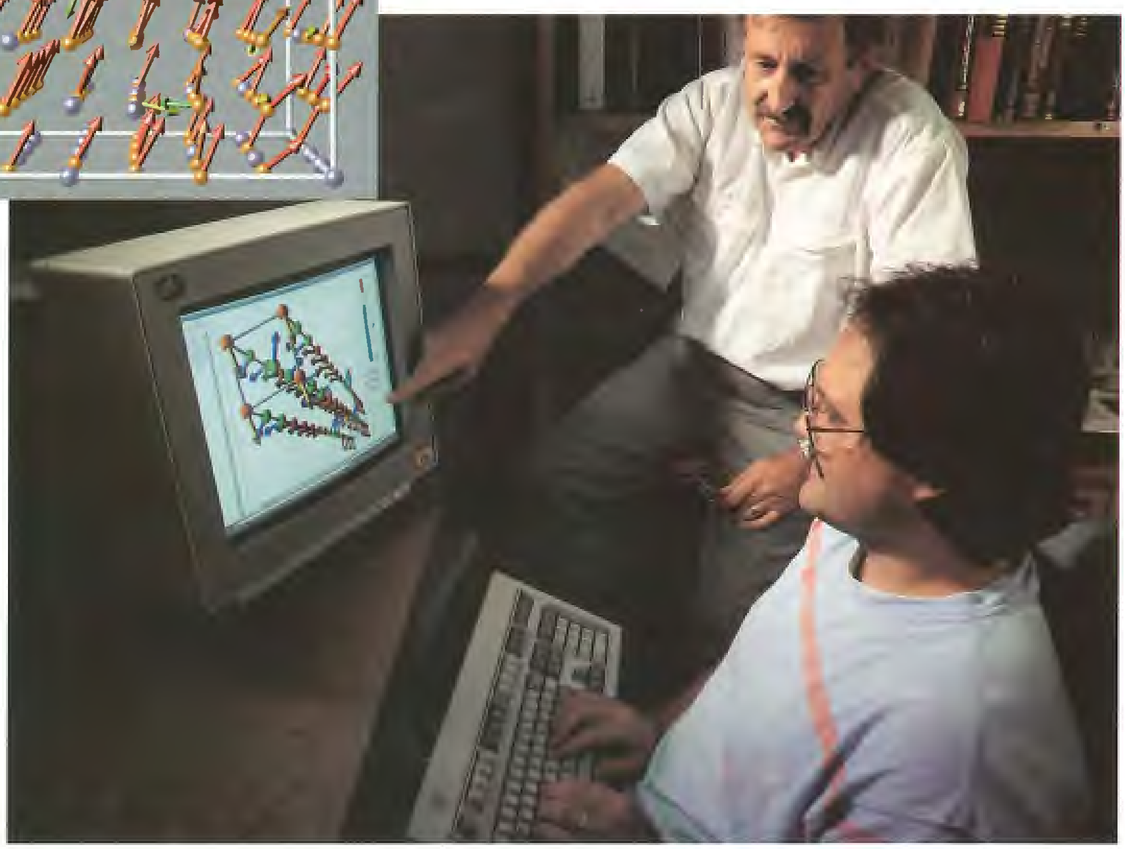
To improve our simulations, we will be collaborating with scientists at DOE's Ames Laboratory to understand the effects of temperature on the dynamics of magnetic moments, including the Curie temperature at which magnetism disappears. We have been working with other ORNL scientists performing neutron scattering experiments on Invar alloys at the High Flux Isotope Reactor to understand the complex magnetic structure of the alloys. And we have collaborated with ORNL scientists doing high-energy X-ray experiments using the National Synchronous Light Source at Brookhaven National Laboratory to study observed displacements of Invar atoms off their ideal lattice sites.

Scientists have long suspected that the Invar alloy contains a mix of magnetic orientations (ferromagnetic, antiferromagnetic, and noncollinear). Our simulations lend theoretical support to that idea. Thanks to the combination of experimentation and computation, we expect that advances in understanding this invariable alloy will be almost constant.

The research is sponsored by DOE, Office of Energy Research, Office of Basic Energy Sciences, Division of Materials Sciences and Office of Computational and Technology Research, Division of Mathematical Information, and Computational Sciences.

ORNL scientists are using computer simulation to better understand the complex magnetic behavior of a disordered nickel-iron alloy called Invar.





Malcolm Stocks and Bill Shelton view a computer image of the direction and magnitude of magnetic moments calculated for a disordered nickel-iron alloy called Invar. Inset: A simulation visualization of the Invar alloy. *Photograph by Tom Cerniglio.*

Robotics and Education

The TransRover wheelchair, based on a platform with spin-on-itself capability, offers a range of motion and maneuverability not possible in today's powered wheelchair.

A Revolutionary Wheelchair Concept

People who use powered wheelchairs enjoy freedom from strenuous physical effort and from constant dependence on caretakers. Soon, they will enjoy several degrees more of another kind of freedom. A revolutionary omnidirectional chair based on an ORNL invention will allow for a freedom of motion and maneuverability hitherto impossible in wheelchair mobility.

CyberTrax Innovative Technologies of Tampa, Florida, plans to begin manufacturing the TransRovr (transportable roving omnidirectional vehicle replacement). CyberTrax signed a licensing agreement in 1996 for the algorithms and engineering technologies patented by ORNL researchers that provide the vehicle's extraordinary maneuverability. The invention at the heart of the wheelchair, the omnidirectional holonomic platform (OHP), evolved from a DOE project to develop mobile robots for work in hazardous environments. The OHP was a 1993 R&D 100 award winner, and the TransRover was a 1997 *Discover Magazine* Award finalist.

The base of the battery-powered wheelchair is a platform propelled by three freely rotating spherical casters (instead of wheels) that steer around a vertical axis. Its wheels, power train, and infrastructure are all hidden within the platform.

The horizontal motion capabilities of the advanced wheelchair allow unrestricted, resistance-free, 360-degree movement. The chair freely

A wheelchair with revolutionary maneuvering characteristics is being developed by CyberTrax Innovative Technologies using an ORNL-designed platform. Steve Killough (left) and François Pin (not pictured) developed the algorithms and innovative engineering that make the platform work. Trying out the CyberTrax prototype, called the Transportable roving omnidirectional vehicle replacement (TransRovr), is Jenny Brewington. The invention was a *Discover Magazine* Award finalist. *Photograph by Tom Cerniglio.*

ORNL is using software to "train" robots to carry out tasks as a team, reducing the chances that a malfunctioning robot will cause an entire mission to fail.

spins in a circle, moves sideways, zigzags, moves at any angle without turning, and changes directions without having to be stopped and restarted. Because the casters rotate freely, steering does not depend upon forcing the front wheels of the chair into position, as with a conventional chair. The chair turns by simply rotating on its platform base, so the wide turning radius needed for conventional wheelchairs is eliminated.

The maneuverability of the advanced wheelchair will also eliminate the wasted motion and power consumption that results from fixed-wheel steering. It allows users to choose routes based on their own preferences, rather than on the maneuvering limitations of their wheelchairs. The agility of the chair allows access to places that are awkward for conventional wheelchairs. For example, it will be able to zip into and out of tight corners without turning.

CyberTrax plans several other improvements for its TransRover, including an improved seat design, superior ergonomics, and advanced battery technology. Improved circuitry will provide rapid internal recharging of the batteries, which will reduce downtime.

The light weight and three-piece modular construction of its design will make the wheelchair easy to pick up and transport in an automobile trunk or back seat. The cost of the advanced wheelchair is expected to be comparable to that of conventional electric wheelchairs. The TransRover has the potential to free users from the limitations of conventional powered wheelchairs, which may eventually become obsolete.

Funding for the research that led to this invention was provided by DOE's Office of Energy Research, Office of Basic Energy Sciences, Division of Engineering and Geosciences, Engineering Research Program.

Teaching Robots To Cooperate

You're helping some friends paint a room. After finishing a wall, you see that the guy painting the window trim needs help, so you grab a brush and pitch in. When the two of you are through, as the others finish painting the baseboards, you clean the brushes and wipe up the paint spots on the floor.

It seems easy enough, but that simple scenario represents a range of behaviors so complicated that science cannot explain them: perceptions, deductions, motivations, choices. No one really knows how humans make the constant adaptations necessary to work together. Imagine how difficult it is to program similar behaviors into robots so they'll work as a team.

In the past, robotics research tended to focus on developing a single robot that could do all the required jobs on a mission. One problem with that approach is that such a Renaissance robot would need to have an enormous range of capabilities. A bigger problem is that one malfunction in it could scratch the whole mission.

ORNL is focusing instead on developing multiple, less-complex robots that can work in teams to accomplish missions. A software system called ALLIANCE, developed by an ORNL researcher, is designed to "motivate" robots to carry out a mission together and enable them to make rudimentary adaptations to the work environment.

ORNL's robot team, four R2D2 lookalikes, has successfully demonstrated the ALLIANCE architecture in carrying out tasks such as cooperative manipulation, cooperative observation of multiple targets, and movement in formation.

ALLIANCE gives each robot the ability to select appropriate actions for itself in light of its teammates' actions and the status of the mission. Robots fail a lot, and researchers can't foresee and program a response for every possible failure. ALLIANCE enables the robots themselves to determine how to respond to mission-threatening failures.

"Motivational behaviors" are programmed into the individual robots to direct them in selecting actions. The primary motivations are called impatience and acquiescence: impatience drives a robot to take over a task that is not being completed by another robot; acquiescence allows a robot to give up a task it cannot complete successfully.

ALLIANCE distributes control equally to each robot team member, allowing each to select its tasks without any central command. Bandwidth limitations preclude extensive conversation or negotiation among robots to coordinate the work. Instead, each unit broadcasts information periodically to the others about what it is doing. The robots use sensory feedback to monitor their own and other robots' performance, to indicate whether adequate progress is being made on each task.

For example, Robot A may be periodically broadcasting, "I'm painting this wall." If Robot B's sensors indicate that, on the contrary, Robot A is just standing there waving a brush and the wall isn't being painted at all, Robot B will take over the task. Robot A will give it up gracefully. The task and the mission can be accomplished despite the failure of Robot A.

The potential applications for cooperative robot teams are legion: almost any task in which it is desirable to reduce human exposure in dangerous tasks or tedium in highly repetitive ones. The possibilities include hazardous waste cleanup, surveillance and monitoring in contaminated areas, industrial and building maintenance, earthmoving, mining, and military applications such as locating and detonating land mines.

During the 1960s, people thought robots would be doing housework and other disagreeable tasks by now. But it's harder than *The Jetsons* led us to believe. Developing algorithms (step-by-step problem-solving procedures) to program robots for cooperative behaviors and discretionary actions is enormously time-consuming. As a next step, ORNL is working on "automatic design" of behaviors, which involves generating algorithms automatically, to reduce the programming complexity.

ALLIANCE is an early step toward building functioning robot teams that can handle real tasks. Developing a robot to play chess, with its strict rules and set scenarios, is nothing compared with developing one that can choose its next move in the real world.

The development was supported by DOE's Office of Energy Research, Basic Energy Sciences, Engineering Research Program.

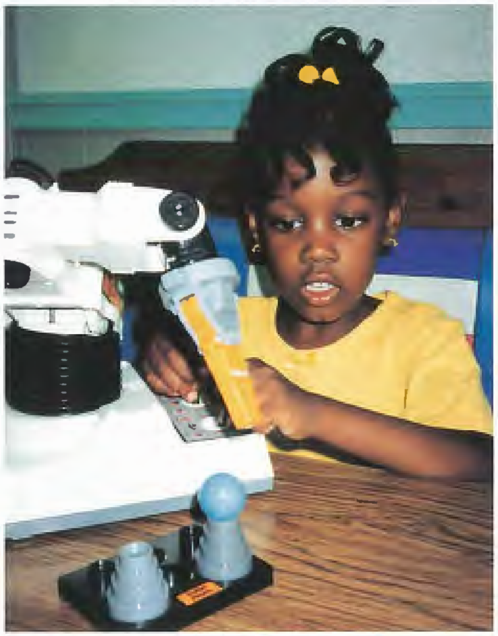
ORNL's Partners in Learning Science

In addition to kicking soccer balls on grassy fields, some of today's students are doing hands-on science, mathematics, and technology in the lab or field at ORNL. In the summer, they attend science camps. In the winter, they participate in classroom activities such as using computers to perform difficult calculations or to search out scientific information on the Internet.

Teachers participate in similar learning activities, all arranged through ORNL's Office of University and Science Education. Through educational partnerships with schools and school systems in the southeastern United States, ORNL provides science, mathematics, and technology training for precollege students and teachers. Teacher and student development programs have been offered not only at the Oak Ridge complex but also at other sites, including those in states served by two of our partners—the

A goal is to develop a robot that chooses its next move in the real world.

Parents watching over their children at play? No, Rich Sincovec, then director of ORNL's Computer Science and Mathematics Division, and Lynne Parker, robotics researcher who developed ALLIANCE, test ORNL-developed software that can direct teams of robots like these in carrying out missions cooperatively. *Photograph by Curtis Boles.*



Whitney Brown operates a robot used for educational purposes in one of ORNL's Ecological and Physical Sciences Study Center programs.

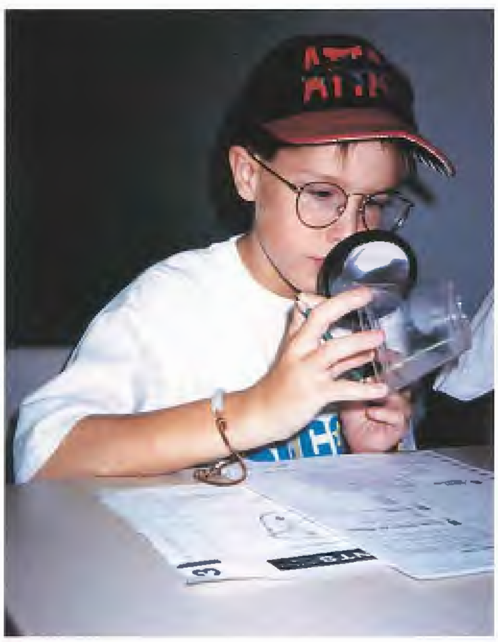
Through partnerships with schools, ORNL provides science, mathematics, and technology training for precollege students and teachers and research opportunities for college students and professors.

Appalachian Regional Commission and the Appalachian Rural System Initiative.

In support of the Oak Ridge Centers for Manufacturing Technology, headquartered at the Oak Ridge Y-12 Plant, student programs have been presented for the Governor's School for Manufacturing, which engages students in the study of engineering, technological, and business strategies that govern advanced manufacturing. It is a real challenging program of study and practical application for the high school students interested in manufacturing. Working with the Office of National Security Programs at the Y-12 Plant, we developed and provided a program for teachers on nuclear weapons nonproliferation issues.

Thirty-one teachers from school systems across the state participated in our Adventures in Supercomputing program. They learned to be system administrators of special workstations. They were trained to "empower" fellow teachers and students by giving them local control in establishing and maintaining electronic mail accounts and in using advanced scientific visualization capabilities.

Many of the students in these programs will return to ORNL in later years to join the diverse groups of university science, math, engineering, and technology students who perform research annually at ORNL as undergraduates, graduates, and postgraduates. These higher-education students serve as members of teams that explore and solve cutting-edge problems or help develop state-of-the-art techniques and instrumentation that provide approaches to answering important scientific questions.



Lee Irons examines a fingerprint on a glass in the SciCops program administered by ORNL's Office of University and Science Education, in partnership with ORNL's Center for Applied Science and Technology for Law Enforcement, and the Knox County Sheriff's Department.

Consider these two success stories involving university students working at ORNL. The designs of a former DOE high school honors student, who participated later as a University of Tennessee senior in mechanical engineering, are being built and used at ORNL and in a national textile research project. A student from Purdue University analyzed emissions of carbon dioxide from the cement industry and published a report that has become the international standard; it is now cited in United Nations documents as part of the recommended methodology by which all nations will report emissions of greenhouse gases.

Our young students may be joined, or even brought, by university faculty who collaborate with ORNL scientists and engineers and take advantage of facilities at the Laboratory that aid them in their campus-based research. These collaborations help achieve a higher potential in research, both for the Laboratory and for the universities. University visitors often say that the ORNL experience has steered their career paths into specific technical areas.

Whatever the level, wherever the interest, ORNL, through its technical staff of scientists and engineers working with the Office of University and Science Education, stands ready to nurture the future scientists, engineers, and leaders of U.S. industry, universities, and laboratories, including ORNL. As in kids' soccer, everybody wins. ornl

Operations, Environment, Safety, and Health

The day-to-day operation of ORNL is generally the responsibility of ORNL's Operations, Environment, Safety, and Health Directorate. We perform the necessary maintenance of infrastructure; provide health services, including physical examinations; assist line organizations in compliance with federal and state regulations in such areas as radiological protection, environmental protection, and industrial safety; and provide emergency planning and response. In addition, we provide financial and budget services for all operational and research areas at ORNL.

ORNL Director Alvin Trivelpiece and Jim Hall, manager of DOE's Oak Ridge Operations, sign documents showing approval of the Necessary and Sufficient Standards for ORNL. Looking on is Martha Krebs, director of DOE's Office of Energy Research. *Photograph by Curtis Boles.*

In 1996, ORNL cut its payroll in response to tighter budgets and program changes. Some services were transferred from Energy Systems to ORNL.

In 1996 as in other years, we found several opportunities for saving money, making our operations more efficient, and doing business in more innovative ways.

Restructuring the Work Force

During 1996 ORNL continued to reduce employment levels in response to declining budgets and changing program emphasis. Two reduction-in-force (RIF) programs were requested of DOE and approved. The first in March, to accommodate mid-year funding adjustments, included a voluntary reduction-in-force (VRIF) program. Twenty employees were terminated, including five voluntary reductions. The second program was approved for September in anticipation of a fiscal year (FY) 1997 budget decrease. This reduction included an enhanced VRIF program with 150% normal severance pay; 66 employees were terminated, including 49 volunteers. In November, DOE's Oak Ridge Operations (ORO) announced FY 1997 work force restructuring for about 1680 positions in the Oak Ridge area, including 230 at ORNL.

In January 1996, Lockheed Martin Energy Research Corporation was formed to manage and operate ORNL. Many services have been and continue to be purchased from Lockheed Martin Energy Systems, Inc. Some services, however, were transferred from Energy Systems to ORNL. Initial transfers included 88 employees to the Office of Public Affairs, the Human Resources Division, the Office of Technology Transfer, and the Legal Department. The transition continued, and on January 1, 1997, 326 positions were transferred to provide needed support and service in waste management, information management and technology, human resources, property and materials, and engineering.

ES&H Oversight Reduction and Multiple Standards

During the years following the technical safety appraisals and the Tiger Team reviews in the late 1980s and early 1990s, it became obvious that DOE national laboratories faced reduced productivity and rising costs that stemmed from excessive DOE oversight and the labs' compliance with multiple government standards. In 1995, for example, some ORNL facilities were audited more than five times, resulting in excessive costs and lost productivity. These same facilities were subject to DOE orders and requirements that added significant costs—but no value—to their operations.

ORNL has been a leader in addressing the issue of too much DOE oversight, which has resulted in excessive costs and lost productivity.

Questions were raised. Was so much oversight of the labs by DOE really needed to ensure their safe and efficient operation? Which standards were really necessary? Which actions were sufficient to meet the intent of environmental, safety, and health (ES&H) regulations?

These issues were identified by a number of review committees, and resolving the problems became critical to the Lab's survival. By boldly embarking on two programs simultaneously, ORNL took the lead throughout the DOE complex.

In a January 1995 meeting, the national laboratory directors pressed then Energy Secretary Hazel O'Leary for relief from excessive oversight. In April 1995, ORNL, working in partnership with DOE-ORO and DOE's Office of Energy Research, proposed a pilot program to reduce ES&H oversight. The pilot program, which ran throughout FY 1996, was based on enhanced self-assessment by ORNL, meaningful performance measures that were mutually agreed upon with DOE, and a focused appraisal of short duration. What was the outcome? ORNL maintained quality ES&H programs, while DOE significantly reduced ES&H oversight. Thus, the pilot program was the model for the current way of doing business at ORNL. In fact, the pilot was so successful that DOE's ES&H oversight policy is being rewritten to incorporate the principles of operation tested at ORNL.

As the ES&H pilot was progressing, ORNL also addressed the issue of multiple standards. DOE has a "requirements process," a system of orders and directives that begins in DOE Headquarters and flows to DOE-ORO and other operations offices. ORNL operations are directed by DOE through written information in the form of orders, manuals, and guidance documents. The problem was that the regulations in these documents duplicated provisions of "external requirements"—laws, regulations, and enforceable requirements from non-DOE regulators with authority at ORNL (e.g., the state of Tennessee and the U.S. Environmental Protection Agency). Sometimes the DOE requirements were even in conflict with external regulations and subject to varying interpretations throughout the DOE complex.

ORNL, in concert with DOE, launched the "necessary and sufficient" process to determine the standards appropriate for the research and support activities at ORNL. ORNL research and operations staff, supported by ES&H staff, developed a set of standards that are in keeping with the standards that industry and academia would be expected to meet in

ORNL is taking part in a DOE pilot program to conduct business operations economically using best management practices to achieve continuous improvement.

conducting similar work. Incorporating external standards wherever possible, this new set of standards, approved and in our contract with DOE, allows us to work to accepted and understood requirements. By modifying our ES&H procedures and practices to reflect the requirements of the approved standards, ORNL will be a safer place to work, and, because of reductions in ES&H costs, we will be able to compete more effectively for government research funds.

Business Management Oversight Pilot

On March 30, 1995, Under Secretary of Energy Charles Curtis issued a memorandum describing DOE's Business Management Oversight Pilot (BMOP) program. This pilot was successfully implemented at ORNL and Lockheed Martin Energy Systems. The overall pilot process received Vice President Al Gore's Hammer Award for Quality in 1996.

The BMOP reflected a growing partnership between DOE and its management and operations contractors, encouraging and rewarding performance and continuous improvement. BMOP facilitated a paradigm shift from compliance-based to performance-based, or outcome-oriented, oversight. The pilot also contributed to improved communications between ORNL managers and their DOE counterparts through cooperative efforts such as the development of mutually agreed-on performance objectives and measures.

To implement the BMOP, we defined the requirements and shared information. A comprehensive BMOP self-assessment was also developed and submitted to DOE-ORO. The BMOP performance objectives and measures and the annual self-assessment reports were combined with operational awareness to provide DOE-ORO reasonable assurance that business operations at ORNL were being conducted in a cost-effective manner using best management practices and were conducive to achieving continuous improvement.

We found that the BMOP had many benefits. It received an overall positive acceptance by DOE-ORO and ORNL management. It strengthened communications and fostered a more effective working partnership between DOE and ORNL management teams. It established a clearer focus on required outcomes and results, enabling management to change its focus from compliance-based to performance-based improvements. BMOP reduced performance appraisal and review efforts, leading to significant cost savings in the past year. It recognized value added when the self-assessment process is based on prenegotiated performance objectives and measures. It established databases that will allow baselining and trend analysis to support productivity improvements and benchmarking (the baselines being established will help to identify conditions, based on facts and data, with the potential for subsequent cost and productivity improvements). BMOP identified the need for continued efforts to train personnel in performance-based management processes and to communicate information about performance-based management systems. It focused greater management attention on performance results and cost effectiveness, helping to foster a change from rigid rules to guiding principles and from audit compliance to the evaluation of management controls.

On May 15, 1996, based on the success of the BMOP and upon recommendation of the BMOP Steering Committee, the Deputy Secretary of Energy signed a memorandum institutionalizing the performance-based oversight process. The BMOP is now referred to as the Business Management Review (BMR) process. The 1997 BMR assessment covers budget and cost management, financial management, human resources, industrial partnerships, information resource management, maintenance and operations, procurement, project management, property and materials management, real estate, and transportation management.

The BMR process is recognized as an evolving process that should complement ongoing communication efforts and aid in establishing a participative relationship with our main customer, DOE. Performance-based oversight offers tremendous potential for improved cost-effectiveness and efficiencies. The success of the pilot encourages ORNL to continue striving for improvements and refinements of the BMR process.

Improving ORNL's Cost Efficiencies

ORNL is committed to devoting more resources to research and development and to making operations more efficient. During 1996, 41 specific new actions were taken to reduce and avoid costs, resulting in a savings of nearly $14 million. Projects from previous years that had cost impacts for 1996 totaled nearly $7 million, bringing the total savings to $20.8 million.

How have we reduced our costs? Organizational streamlining and restructuring reduced overhead. ORNL's Engineering Technology Division effectively consolidated several functions over the past two years to realize significant annual cost savings. The division experienced a net reduction of 28 full-time employees. Several overhead organizations reduced costs by consolidating their operations. The organizations include the Office of Safety and Health Protection, the Office of Radiation Protection, and the Office of Environmental Compliance and Documentation.

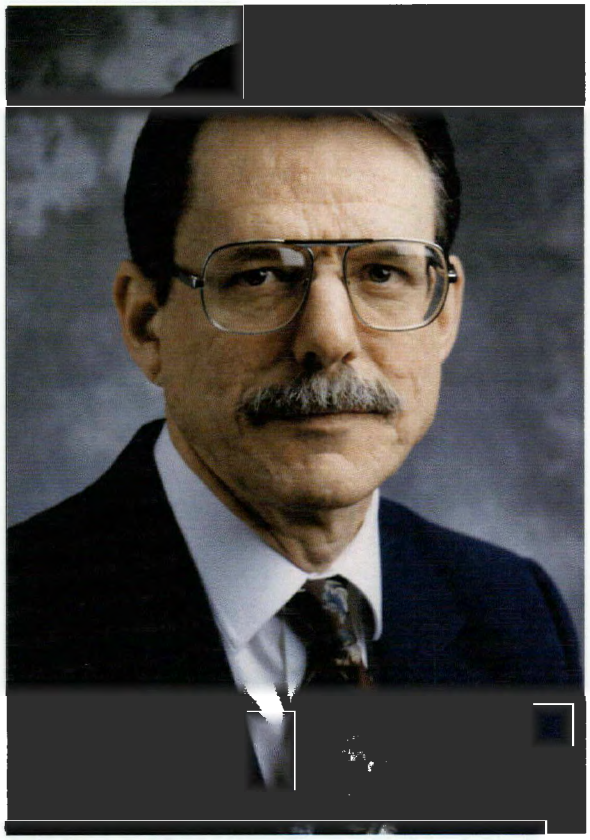
Significant costs were avoided in other ways. For example, we recycle lead from our legacy lead supplies. Instead of purchasing an expensive recoil separator for accelerator physics experiments at our Holifield Radioactive Ion Beam Facility, we acquired the Daresbury Recoil Separator at no cost from a United Kingdom laboratory; all we had to pay was the cost of shipping and installing the device.

We continue to seek ways to reduce and avoid costs.

ORNL Creates New Division

Where at ORNL can you get library services; access to our local data networks from your office and home or while on travel; help creating a Web page; integrated publishing, illustrating, and digital imaging support for technical papers, marketing materials, or proposal generation; or technical support for a UNIX workstation? The answer is ORNL's new Computing, Information, and Networking Division (CIND).

This new division supports the ORNL research mission in the areas of scientific and business computing, information management, and data networking. In these areas, division staff offer cost-effective services and consulting, provide leadership and strategic planning, and assist in attracting funds to the Laboratory.



Richard Hicks is the director of the new Computing, Information, and Networking Division.

CIND, whose director is Richard Hicks, was created October 1, 1996, by incorporating functions previously performed by the former ORNL Office of Computing and Network Management and two central organizations of Lockheed Martin Energy Systems—Information Management Services and Information Technology Services.

CIND also has the unique role of providing user advocacy and Laboratory-wide coordination for computing issues. In this role, the staff seeks customer feedback through the leadership of several ORNL-wide user committees: Scientific Computing User Advisory Committee (John Cobb); Administrative Computing Steering Committee (Russ Overbey); and Network Forum (Bill Wing). This advocacy role has been expanded to the information management arena with the appointment of Bob Conrad as advocate for the library and information area.

The division has the following groups, which provide these services.

The *Business Applications* group provides overall coordination of business computing at ORNL and helps obtain computer programming solutions.

The *Information Integration* group helps ensure that information systems being developed communicate well with one another, provides WebWorks to assist with Web-related projects, and offers desktop software solutions.

Networking groups manage, maintain, and improve the underlying data networks and software necessary for efficient network operations, maintain public local area networks and ORNL connections to the Internet. The *Network Computing* group manages system software on the primary ORNL internal and external Web servers, provides Web application software development services, and provides technical support for electronic mail applications. The *Workstation Support* group provides system administration and technical support for workstations and maintains workstation-related software and documentation.

In the *Information Management Section, Graphic Services* enhances scientific and technical communication through the design and production of illustrations, presentations, posters and displays, brochures, multimedia, and Internet graphics. *Publishing Services* provides personalized technical publishing services, including writing and editing, publishing project management, proposal development, word processing and desktop publishing, Internet publishing, and CD-ROM publishing. *ORNL Libraries* provide information support to ORNL staff through library collections, a large electronic network of databases, and Web interfaces allowing researchers to access information from their desktops. *Records Management* manages all Laboratory records and ensures ORNL compliance with document control regulations. The *Technical Information Office* serves as the control point for releasing scientific and technical information and maintains the Comprehensive Publications Registry.

A more complete and current list of CIND services can be found on their internal Web page: <http://www-internal.ornl.gov/cind>.

Reengineering at ORNL: Where Are We Going?

Reengineering will enable ORNL employees to perform their jobs better at a lower cost.

It's 1999 at ORNL. You sit at your desktop computer and quickly access all the financial and human resource data you need to manage your project. You look out the window and watch the new construction under way. You're pleased that your brother, also an employee at the Lab, no longer complains about not having the transportation, tools, or supplies he needs to do his job in research support services. Reengineering of the ORNL organization, you decide, has been a good thing.

On January 1, 1996, Oak Ridge National Laboratory began operating under a new corporation, Lockheed Martin Energy Research Corporation (LMER). This was a watershed event for the Laboratory because it provided the opportunity for us to choose on our own how best to operate our organization. As part of this new corporate arrangement, LMER established several stand-alone activities, such as the Legal Department and the Human Resources (HR) Division, which had previously been provided by our sister company, Lockheed Martin Energy Systems (LMES).

Early in February 1996, ORNL senior management decided to engage an outside consulting company to examine the Laboratory and make suggestions for improving the numerous processes we use to perform our mission. We wanted to be better able to compete for scarce federal research funds, so our goal was to improve our research productivity while cutting costs through reengineering—fundamental rethinking and radical redesign of business processes to bring about dramatic improvements in performance. Ernst & Young LLP was ultimately selected based upon several evaluation factors, but most importantly on their deliberate approach to reengineering.

In late spring, senior management formed the Reengineering Steering Committee under the leadership of Jim Roberto to consider the results of the work of Ernst & Young and the contract transition teams that had functioned prior to January 1, 1996. This committee's major accomplishments were:

- Formation of reengineering teams to examine our processes of finance and business management, HR, and research support services.
- Establishment of overhead reduction goals for both research and development (R&D) and support divisions. Goals include a 40% improvement in the cost-effectiveness of support and services, reduction of Lab overhead below 40% (excluding reengineering costs) by 1998, and an overall increase of 15% in direct scientific and technical effort per dollar by the end of fiscal year 1998.
- Initiation of organizational reengineering activities in all ORNL offices and divisions.
- Integration of the Ernst and Young recommendation into the results of the LMER transition teams.
- Integration of the overhead review process with reengineering.
- Identification of cost savings and efficiency improvements totalling $17 million in FY 1996.

Examining our Processes

During the fall and winter of 1996, Jim Stiegler assumed leadership of the reengineering effort, and new teams were formed to examine various processes. The Environment, Safety, and Health team is rewriting our environmental, safety, health, and quality (ESH&Q) procedures to ensure that they are "necessary and sufficient"—that is, that their intended functions meet various governmental agencies' ESH&Q expectations in an affordable, timely way. The Science and Technology Partnerships team is examining ways to (1) improve ORNL's relationships with outside organizations, (2) make it easier for guest researchers to start work here, and (3) expedite the formation of partnerships with industry, academia, and other federal laboratories to help ORNL compete more effectively for research funds. To help cut the overhead of research divisions, the Waste Management team is looking at ways to manage newly generated wastes as efficiently as possible and to reduce waste management costs by 50% over a five-year period.

The Engineering Design and Construction team is examining ways to simplify design and construction to attract federal funds so we can construct needed new facilities or maintain existing ones. The HR team is developing a new competency-based performance management and job evaluation system that will simplify the processes and transfer responsibility and accountability to line managers. HR has hired Towers Perrin, one of the top international HR consulting firms, to help lead development of these new systems.

The Finance and Business Management team, in concert with LMES, recommended the implementation of a commercial, off-the-shelf, enterprise information system to replace a number of our existing finance, project management, acquisition, and HR systems. This new system is a product of Systems, Applications and Products (SAP), an international company based in Germany. SAP R/3 is a highly integrated information system that will eliminate the need to maintain and update multiple databases. Installation of SAP R/3 also meets one of our goals in reengineering our fundamental business processes: introducing recognized "best business practices." Over the long term, it will reduce the costs of maintaining multiple nonintegrated business systems. SAP, whose products are installed in more than 7000 companies, leads the global market in enterprise information systems. We have established with LMES a joint project team to implement the SAP system. Jim Ball is directing the project, Becky Verastegui serves as technical director, Mike McNeely is the business management director, and Richard Green is the change management director. The system will be available for service in fiscal year 1999. Ernst & Young is serving as our implementation partner and will play a major role in this endeavor.

Revision of Human Resources Practices

We have embarked upon a major revision of most of our HR practices. Employees will see significant changes in compensation and performance management, training and employee development, the workplace, and information systems.

In October 1996, ORNL's Compensation Office, which is part of the HR organization, introduced an enhanced pay for performance program, an accelerated growth-to-midpoint program, a focal date salary increase program, and a new variable pay program. Also, a revised and simplified performance appraisal form will be introduced this year to simplify the appraisal process. A new competency-based performance management system will be developed and piloted for introduction in 1998. In addition, ground work for the development of a new job evaluation system is just beginning under the leadership of Fred Shull, ORNL's compensation director. We expect to pilot that new system in 1998, with full implementation in the fall of 1999, if all goes well.

We will overhaul employee development activities, especially in leadership.

The HR organization will use the SAP HR module as our HR information system. As a result, ORNL will have a single system that integrates all of our business and HR information requirements.

Many employees recently have spent most of their "classroom" time satisfying training requirements to ensure that the Laboratory is in compliance with environmental, health, and other regulations. We have separated employee development from compliance training. HR personnel will renew their focus on overhauling employee development activities to improve career skills, especially in the area of leadership. Compliance training will be implemented through the Operations, Environment, Safety and Health Directorate.

Improving Research Support Services

The reengineering team that has been studying research support services rendered by ORNL's Plant and Equipment (P&E) Division focused on removing barriers to productivity and creating long-term cultural change. Six subteams were established and are co-chaired by P&E management and union representatives. The six subteams are Strategic Investment (Carpenter Shop); Strategic Investment (Field Sheet Metal Shop); Transportation; Materials Acquisition, Control, and Delivery; Customer Relations; and Heating, Ventilation, and Air Conditioning (HVAC) Work Group.

The team found that the high costs of the services are linked only partially to the hourly rate. We have room to bring these service costs down and intend to do so. The major source of the costs, however, comes from inefficiencies in our work practices because of insufficient planning and coordination. Our workers, who are dispersed over several sites, cannot always get to a work site because they lack transportation. Others can't do the job requested because either needed supplies are unavailable or workers' tools are antiquated (the average age of our tools is 38 years, and our oldest piece of equipment is a 1906 rolling mill). Our goals include procuring newer tools and improving job coordination to ensure that workers have needed transportation and that parts are always available so that workers can make needed repairs or installations.

The carpenter shop team has completed on schedule and under budget all work necessary to reopen the 7009 Carpenter Shop. This shop had been shut down since the early 1980s because of asbestos contamination.

The field sheet metal shop team has located and procured a used power shear that will be installed in Building 3044. The availability of the shear will substantially reduce travel time for personnel at the west end of the Lab who need sheet metal work. The team is now studying how best to organize field sheet metal work to optimize service to our customers.

The transportation team has focused on identifying ways to better meet the transportation needs of the P&E Division without adding costs. Improved, staggered shifts for the taxi service have been implemented to increase the availability of transportation to craft workers at the beginning of the work shift and during lunch when usage peaks. Division vehicles have been redistributed for more effective support, and a small rental pool of vehicles has been made available to meet short-term needs. The team has implemented a west-end transport service team consisting of four truck drivers who will have access to an assortment of vehicles.

To ensure a reliable source of needed supplies, the materials team opened a pilot bench stock area and acquired Building 3023 from the Instrumentation and Controls Division to house the operation. To stock the area, the team acquired most of the equipment and material from the Oak Ridge K-25 Site at no cost. Computing and telecommunications equipment was later installed, and material clerks were hired to run the operation.

The customer service team is continuing to identify better ways to achieve and measure customer satisfaction. Plans are being made to provide customer service training to division staff.

The HVAC team has recommended a reorganization of the HVAC work group that should provide more focused and cost-effective support for customers.

Cultural change activities are beginning to gain momentum. Our consultants from the University of Alabama at Huntsville and the Saturn car company continue to provide us state-of-the-art advice on tapping the strength of an effective union-management partnership to achieve customer enthusiasm. As joint teams experience this strength through successful completion of projects, support for cultural change grows.

Work Smart Standards

The Necessary and Sufficient process has been used to develop "Work Smart standards" for ORNL. Using these standards as ESH&Q requirements for all work at ORNL, we expect to improve ORNL's ESH&Q performance while reducing costs and other impacts on research. All ESH&Q functions and tasks have been evaluated against the approved Work Smart standards by a team led by Doug Craig, director of ORNL's Metals and Ceramics Division, and Frank Kornegay of the Central Management Offices. From this effort, four key areas were identified in which significant improvements could be made. As a result, our goals are to maintain our set of Work Smart standards; communicate expectations and requirements to staff, guests, and subcontractors; provide meaningful, cost-effective compliance training; and provide assurance that operations are in compliance with work smart standards. We continue to make improvements in these areas.

ORNL will continue to be a world-class research institution because we recognize the need to ensure high quality in our research and the ease and effectiveness of our partnerships.

All required ESH&Q training has been evaluated against our approved Work Smart standards. We anticipate significant savings in training costs as we incorporate better methods to deliver the material (on the World Wide Web, for example); grant requests for exemptions, allowing some training to be given by subject matter experts rather than training staff; and hire the most cost-effective contractor to provide the required training.

All Laboratory-level ESH&Q procedures are currently being reviewed. Each requirement is being evaluated against our work smart standards. Our goal is to significantly reduce the number and complexity of the procedures, while enhancing the usefulness and flexibility of the documents.

Roles and responsibilities of organizations and individuals that best ensure compliance with requirements are being determined. Enhanced self-assessment programs will help research and support organizations find and fix problems in the most cost-effective manner, using experience from successful organizations. Some organizational changes may be recommended to ORNL senior management.

Science and Technology Partnerships

ORNL will continue to be a world-class research institution because we recognize the need to ensure high quality in our research and the ease and effectiveness of our partnerships. ORNL researchers collaborate with researchers from industry, academia, and other federal laboratories through user agreements, cooperative R&D agreements, work-for-others agreements, licenses, and a variety of other agreements. Through these mechanisms, guest researchers work at the Laboratory or our researchers do research at other laboratories.

Having an agreement in place before performing collaborative research is necessary in order to establish intellectual property rights and to address liability issues. It is important, however, that establishing the agreement does not consume so much time and effort that it hampers collaborative research. The current process for establishing partnership agreements and for getting guests and users into ORNL does just that. Depending on the nature of the agreement, as many as five or six offices are involved in the current process. When guest researchers arrive at ORNL, it can take hours or even days before they can get beyond the red tape and begin research.

A Science and Technology Partnerships reengineering team is

Reengineering involves starting over, challenging assumptions about how we should do business, and restructuring the organization around processes rather than structures.

Jim Roberto (left) and Jim Stiegler (right) have led ORNL's reengineering efforts.

evaluating the entire process. The team is led by Ron Bradley of the Metals and Ceramics Division and made up of representatives of the Office of Technology Transfer, the Office of Science and Technology Partnerships, R&D divisions at ORNL and the Y-12 Plant, the Oak Ridge Centers for Manufacturing Technology, and DOE's Oak Ridge Operations. The goal is to design a new process that will be significantly more efficient, cost-effective, and user-friendly than the current process. Successful reengineering of this process will have many positive benefits as partnerships with industry, academia, and other federal laboratories become increasingly important in the competition for research funds.

Waste Management

The responsibility for managing our active waste processes was returned to the Laboratory in January 1997. The new management and integration contractor will manage our legacy wastes. We recently established a Waste Management reengineering team under the leadership of Tim Myrick (manager of Environmental Management Programs at ORNL) to examine how best to deal with our current processes of waste generation. The core team has subteams concerned with pollution prevention (including material recycle), waste characterization, waste certification and verification, hazardous and mixed waste streams, communications, reporting and records, disposal end points, and waste treatment and storage processes. Process mapping and benchmarking activities are under way.

Engineering Design and Construction

An Engineering Design and Construction (ED&C) team led by L. E. McNeese has been working on reengineering ED&C processes at ORNL. The team has examined selected past, present, and expected ED&C projects at ORNL to identify potential barriers to implementation of efficient ED&C processes. Information is being gathered to verify that the identified potential barriers are real and important. Approaches for eliminating the important verified barriers that do not result from laws or regulations will be developed and recommended. Final recommendations will be made by mid-1997.

Reengineering is not downsizing, automation, reorganization, or total quality management (remember "quality circles" and "empowerment," concepts that are more narrowly focused than reengineering?). Reengineering involves starting over, challenging assumptions about how we should do business, and restructuring the organization around processes rather than structures. It is designed to take work out of the system. If we do our reengineering right, by 1999 we will be more productive at a lower cost, making us better able to compete for hard-to-get research funds. As a new company, Lockheed Martin Energy Research will be doing more with less.

Technology Transfer: CRADAs, Licenses, and Patents

Technology transfer activities at Oak Ridge played a major role in influencing six private companies to either relocate or open operations close to DOE facilities here.

Oak Ridge Technology Makes Its Mark

Recently released statistics show that technology developed at ORNL and other Oak Ridge facilities is making a difference among U.S. industries. A total of $18.3 million in commercial sales from Oak Ridge licensed technologies was reported for the 1996 fiscal year—an increase of 18% over the 1995 figure. Also, during the past fiscal year, the Office of Technology Transfer for Lockheed Martin Corporation in Oak Ridge executed 59 new cooperative research and development agreements (CRADAS) worth $48.6 million. It also executed 39 new licenses and 2 options for a total of 41 deals.

Technology transfer activities at Oak Ridge played a major role in influencing six private companies to either relocate or open operations close to DOE facilities operated by Lockheed Martin here.

Licenses can be either exclusive or nonexclusive, depending on the technology involved and the agreement reached by the licensing executive and the licensee. A license allows a company to use a technology, to manufacture a product, or both.

One license issued recently is for an optical biopsy system that uses a laser to determine if a tumor is malignant. The system, licensed to Optical Biopsy LLC, a subsidiary of Venture Alliance of Knoxville and Pioneer Surgical of Loxahatchee, Florida, may soon replace conventional tumor biopsies. It is already in use at the Thompson Cancer Survival Center in Knoxville.

Another license was issued last fiscal year to Turtle Mountain Communications of Maryville for a button-sized lens system that may enable the manufacture of video cameras and transmitters no bigger than a microcassette. (See p. 102 for a story on a partnership and license.)

Other noteworthy accomplishments for the 1996 fiscal year include $1 million in royalty income from licenses and execution of the first municipal CRADA with Los Angeles County. This CRADA focuses on solving water pollution problems caused by urban storm water.

Through CRADAS, government and industrial partners collaborate on ideas, share costs, and pool the results of a particular research and development program to bring technologies to the marketplace. Private partners provide resources for the research effort, while ORNL or other DOE laboratories provide personnel, facilities, and equipment.

Customer surveys show that industrial firms are pleased with the services provided by government partners in CRADAs. In 1996, the amount of cash brought to Oak Ridge ($1.5 million) by private companies in support of CRADAs exceeded the typical "in-kind support" of any previous year. So it's been a win-win situation for all.

CRADAs Executed in 1996 in Oak Ridge

Partner(s)	Technology	Principal Investigator
NCMS	Rapid response manufacturing	W. D. Cain
Golden Technologies, Inc.	Design, development, and fabrication of an inorganic membrane to separate hydrogen from petroleum refinery purge gases	G. E. Roettger
Golden Technologies, Inc.	Design, development, and fabrication of enhanced inorganic membranes in systems to remediate the problem of volatile organic compounds in water	D. E. Fain
Golden Technologies, Inc.	Inorganic membrane for hydrogen separation in olefin	D. E. Fain
USCAR/INEL	Intelligent welding of thin metal sections	M. W. Richey
Surface Optics Corp.	Surface inspection machine (infrared)	G. L. Powell
ConnectWare, Inc.	Asynchronous transfer mode (ATM) adapter device driver for digital UNIX	L. MacIntyre
Osram Sylvania, Inc.	Gelcasting polycrystalline alumina	M. A. Janney
E. I. du Pont de Nemours and Company	Evaluation of air conditioner air refrigerant cross-flow heat exchangers with R22 and zeotropic refrigerant mixture	V. C. Mei, F. C. Chen
American Society of Mechanical Engineers	Non-heat-treatable aluminum alloy sheet products	H. W. Hayden
Doble Engineering, Kahn Instruments	Moisture sensor for sulfur hexafluoride–filled circuit breakers	D. R. James, I. Sauers
Thermshield International, LTD.	Test bed demonstration project—radiation control coatings	T. W. Petrie
GelTech, Inc.	Novel cost-effective process for the replication of hybrid diffractive/refractive optical elements	B. E. Bernacki, L. C. Maxey
Serotech, Inc.	Surface-enhanced Raman optical data storage (SERODS) system	T. Vo-Dinh
Cincinnati Milacron Marketing Co.	Expert system for machine tool coolant selection	H. A. Fell

CRADAs Executed in 1996 in Oak Ridge (continued)

Partner(s)	Technology	Principal Investigator
Applied CarboChemicals, Inc.	Production of chemical derivatives from renewables	B. H. Davison
SPRI/Roof Consultants Institute	Whole building roof re-cover and drying demonstration project	A. Desjarlais
Hyper Velocity, Inc.	Position and velocity control of pneumatic cylinders for flexible assembly systems	J. G. Parrott, T. L. Williams
Advanced Lithography Group	HIP densification project	E. A. Franco-Ferreira
Medtronic, Inc.	Development of thin-film batteries for implantable medical devices	J. B. Bates
Commercial Crystal Laboratories, Inc.	New crystal-growth methods for producing lattice-matched substrates for high-temperature semiconductors	L. A. Boatner
Midwest Superconductivity, Inc., Westinghouse Electric Corp.	Advanced temperature superconductor film-based process using RABiTs™ substrates	A. Goyal, R. Hawsey
PDMA Corp.	In-service motor performance diagnostic	S. L. Bunch
Advanced Optical Equipment and Systems Corp.	Development of advanced photolytic iodine laser cutting and joining technologies for manufacturing	M. W. Richey
GelTech, Diffraction International, University of Rochester	Advanced micro-optics characterization using computer-generated holograms	L. C. Maxey, J. E. Rogers
Apeiron, Inc.	Advanced hardware and software methods for thread and gear-dimensional metrology	A. C. Miller
GaSonics International	Energetic neutral beam cleaning	D. E. Schechter, C. C. Tsai
Materials and Electrochemical Research Corp.	Hydrogen storage in organometallic fullerenes	F. C. Chen
Clinical Neuro Systems, Inc., Ben Franklin Techology Center, Delaware Valley Industrial Resource	Vascular occlusive device prototyping	W. Morrison, P. A. Evans
Innovative Computing Technologies, Inc.	Sensor-driven intelligent control system for plasma processing	V. B. Campbell
ERC, Inc.	Intelligent machine learning analysis for fuel cell operations	F. C. Chen
Charles Evans & Assoc.	Feasibility of correlating V-Cr-Ti alloy weld strength with weld chemistry	M. L. Grossbeck

CRADAs Executed in 1996 in Oak Ridge (continued)

Partner(s)	Technology	Principal Investigator
Utron, Inc.	A 7-km/s electrothermal light gas gun pellet injector	S. L. Milora
Lambda Technologies, Inc.	Advanced ECR ion source with large resonant plasma volume	G. D. Alton, F. W. Meyer
Visual Computing Systems Corp.	Flywheel motor alternator for hybrid electric vehicles	J. W. McKeever
Stereotaxis, Inc.	Superconducting coil amplifier for magnetic stereotaxis neurosurgery	J. Lai
Geltech, Inc.	Cost-effective, high-precision fabrication technologies for radiation-resistant advanced optical components	B. E. Bernacki
Frigidaire Company	Accelerated development of efficient refrigerator technologies	E. A. Vineyard
Micro-Grain, Inc.	Microwave treatment as a pesticide alternative for stored products	T. S. Bigelow
Dow Corning Corp.	High-temperature particle filtration technology	T. M. Besmann
Roofing Industry Committee	Investigating the durability of roofing systems in the aftermath of a major wind storm	A. Desjarlais
Tinsley Labs	Deterministic fabrication of optical components using ion-beam milling	D. O. Hobson
Union Camp Corp.	Overcoming constraints to high-yield plantation-grown hardwoods in the southeastern United States	G. A. Tuskan
DynEco International, Inc.	Orbital vane compressor-expander development for vehicle fuel cells	F. C. Chen, V. C. Mei
Detroit Diesel Corp.	Motor-generator augmentation of diesel turbocharge	R. Graves, D. Adams
Pall-Pass	Reverse osmosis membrane (pharmaceutical) and cleanable HEPA filter panel project	D. Fain
Angstrom Tools, LLC	Computational toolbox for molecular nanotechnology	B. G. Sumpter
Los Angeles County Department of Public Works	Conceptual development of an environmental data management system for National Pollutant Discharge Elimination System compliance	M. J. Sales

CRADAs Executed in 1996 in Oak Ridge (continued)

Partner(s)	Technology	Principal Investigator
Red Zone Robotics	Generalized operator interface for remote system control	G. Armstrong
Solar Turbines, Inc.	Evaluation of stainless steels for primary surface recuperator applications	R. W. Swindeman
DCH Technologies, Inc.	Development of low-cost hydrogen sensors and detectors	B. S. Hoffheins
American Magnetics, Inc.	Development, design, and fabrication of hybrid high-temperature superconducting leads	D. M. Kroeger
Maytag Appliances	Demonstration and evaluation of high-efficiency, horizontal-axis clothes washer	J. J. Tomlinson
Perkin-Elmer	Ion source and inlet system fundamentals and applications	G. J. VanBerkel
SciBus Analytical, Inc.	Commercialization of technologies developed in the Contaminant Analysis Automation (CAA) Program	L. Klatt

Licenses Executed in 1996

Licensee	Technology
Advanced Systems Technology	Active and passive neutron examination and assay
Angeion Corporation	Thin-film batteries
Applied CarboChemicals, Inc.	Fermentation process to produce succinic acid from corn (see p. 102)
CyberTrax Innovative Technologies, Inc.	Omnidirectional and holonomic rolling platform for wheelchair
DCH Technology, Inc.	Thick-film hydrogen sensor
DeRoyal Industries, Inc.	Concentration of pertechnetate and perrhenate solutions
Environmental Systems Corp.	Lumscope/Lumscan/ScopeCTL software
GeoVox Security Corp.	Enclosed Space Detection System (heartbeat detector)
Insight Inspection Technology	Robotic vehicle
Lambda Technologies, Inc.	Variable-frequency microwave technologies
LoTEC, Inc.	Ceramic powders
Midwest Superconductivity, Inc.	Structures having enhanced biaxial texture and method of fabricating same
Optical Biopsy, LLC	DNF method for cancer diagnosis
Pioneer Surgical, Inc.	DNF method for cancer diagnosis
Powell River Laboratories	Environmentally safe projectile (lead-free bullets)
SciBus Analytical, Inc.	PCR algorithm software
SenSiv, Inc.	Monolithic spectrometer
Serotec	Biological material transfer of monoclonal antibodies
Spire Corporation	Polymer surface-hardening process
Supelco, Inc.	Sol-gel sorbent trap for environmental sampling
Turtle Mountain Communications	Miniature hybrid optical imaging lens
Turtle Mountain Communications	RF beacon integrated circuit (mask works)

Licensee	Technology
UCB Chemicals Corp.	Ionization radiation curing of epoxy resin systems using cationic photoinit
United Defense, L.P.	Nickel-aluminum (Ni_3Al) alloys
Venture Alliance II, LLC	Synchronous luminescence system

Turning Corn into Chemicals the Biological Way

In England, it's the term for wheat; in Scotland and Ireland, it's oats. But in America, corn is the grass called maize that was domesticated and cultivated by Native Americans long before Europeans reached the New World. Although Americans consume considerable amounts of fresh corn on the cob, canned and frozen corn, cornbread muffins, and popcorn, corn in the United States is used primarily as animal fodder and also for making ethanol fuel and high-fructose syrup for soda beverages.

Now, scientists from four DOE laboratories, including ORNL, and a private company propose another use for corn. They have developed a revolutionary process for turning corn into chemicals needed to make consumer products. In this process, a new microorganism efficiently ferments glucose sugar in corn to succinic acid, which is an essential ingredient in the manufacture of plastics, clothing, paints, inks, food additives, and automobile bumpers.

In 1996 ORNL and three other DOE labs signed a $7 million agreement with Applied CarboChemicals, a Pennsylvania specialty chemicals company, to manufacture chemical feedstocks from renewable farm crops like corn. The agreement involves use of the new process, which has been licensed to Applied CarboChemicals and which received an R&D 100 Award in 1997.

This bioprocessing method is significantly less expensive than conventional petroleum-based methods for producing succinic acid. In addition, it eliminates gypsum, an undesirable by-product that must be hauled to landfills. Also, the new process promises economic benefits by reducing reliance on imported oil or at least by freeing up petroleum as a source of chemicals so it can be used as fuel. For example, if chemical feedstocks normally produced from petroleum were instead generated using a single combined biological and chemical plant, the oil saved could be used to heat 80,000 single-family homes for a year. Finally, the new process could expand markets for corn and other renewable feedstocks and provide greater job security and perhaps job growth within agriculture and related industries.

The new process, developed by ORNL, Argonne National Laboratory (ANL), National Renewable Energy Laboratory (NREL), and Pacific Northwest National Laboratory (PNNL), generates, separates, and purifies succinic acid and uses it as an intermediate to produce 1,4-butanediol, tetrahydrofuran, N-methyl pyrrolidone and other chemical feedstocks used to make a wide assortment of products. Existing domestic markets for such chemicals total more than $1.3 billion.

ORNL was the technical project leader, and ORNL researchers Nhuan Nghiem and Brian Davison developed the fermentation process. This process uses a novel microorganism, developed by ANL, that converts corn-derived glucose to succinic acid at very high yields. ANL also determined a way to purify the succinic acid product. NREL analyzed the economics of the new process, and PNNL found ways to catalyze succinic acid to produce commodity chemicals, the final step in the conversion process.

This research is part of DOE's Alternative Feedstocks program, which is intended to forge new links between the agricultural community and the chemicals industry through support of research and development that uses crops to produce chemical feedstocks. The research is funded by DOE's Office of Industrial Technology, Alternative Feedstocks Program. Funding is also provided through the cooperative research and development agreement with Applied CarboChemicals.

Using bioreactor columns to ferment corn, ORNL researchers recently produced 50 liters of a succinic acid product in each fermentation and shipped the broth to ANL for purification. Later this year 500-liter fermentations will be performed. If this DOE technology is commercialized and used widely to process corn, the United States may harvest rich rewards.

1996 Patents Issued to ORNL Inventors

Inventor(s)	Technology
T. Scott	Biparticle fluidized-bed reactor
R. Tyndall	Amoeba/bacteria consortia for degrading wastes and contaminants
R. McKee, F. Walker	Improved process for depositing epitaxial alkaline earth oxide onto a substrate and structures prepared with the process
R. Lauf, C. Holcombe, N. Dykes	Process for manufacturing multilayer capacitors and like articles
T. Scott, R. Petersen, B. Davison	Continuous fluidized-bed contactor with recycle of sorbent
T. Vo-Dinh	Articles of protective clothing adapted for detecting chemical permeation
J. Bates, N. Dudney	Method of making an electrolyte for an electrochemical cell
T. Vo-Dinh	Photoactivated luminescence sensor and method of detecting trichloroethylene and related volatile organochloride compounds
R. Devault, B. McConnell, B. Phillips	Hermetically sealed superconducting magnet motor
R. Lauf	Method for producing textured substrates for thin-film photovoltaic cells
M. Harris, O. Basaran, T. Kollie, K. Weaver	Silica powders for powder-evacuated thermal insulating panel and method
G. Eres, J. Sharp	Externally controlled closed-loop feedback apparatus for digital epitaxy
H. Haynes, J. Moyers, B. Stewart, D. Casada	Method and system for measuring gate valve clearances and seating force
M. Santella, V. Sikka	Intermetallic alloy welding wires and method for fabricating the same
T. Stovall, J. Tomlinson	System for energy-load management for heating and cooling of buildings
T. Vo-Dinh, A. Viallet	Chemical sensor probe for calcium and other metal ions
R. Tyndall, A. Vass	Methods of degrading napalm and trinitrotoluene
J. Moyers, H. Haynes	Method and apparatus for monitoring armature position in dc solenoids
L. Hively	Smart, passive sun-facing surfaces
D. Lowndes, J. McCamey	Method for continuous control of composition and doping of pulsed-laser deposited films
C. Scott, T. Scott, B. Faison, B. Davison, J. Woodward	Enhanced attrition bioreactor for enzyme hydrolysis of cellulosic materials

1996 Patents Issued to ORNL Inventors

Inventor(s)	Technology
O. Basaran, M. Harris, W. Sisson, T. Scott	Improved nozzle for electric dispersion reactor
J. Bates, N. Dudney, K. Weatherspoon	Packaging material for thin-film lithium batteries
S. Smith, K. Castleberry	Motor current method for monitoring machine tool performance
D. Casada	Motor monitoring method and apparatus using high-frequency current components
H. Haynes	Monitoring method and apparatus using high-frequency carrier and method of forming electrical pathways in indium-tin-oxide coatings
G. Alton	Microwave electron cyclotron resonance (ECR) ion source with a large, uniformly distributed, axially symmetric, ECR plasma volume
A. Akerman, C. Ayers, H. Haynes	Ultrasonic speech translator and communication system
S. Rajic, J. Muhs	Smart material fiber-optic connecting method
J. Bates	Rechargeable lithium battery for uses requiring a low-to-high power output
L. Dickens, H. Haynes, C. Ayers	Method and apparatus for monitoring rotating aircraft components
P. Box	A robotic vehicle
E. Wachter, W. Fisher (ORAU)	Method and apparatus for evaluating structural weakness in polymer matrix composites
K. Alexander, T. Tiegs, P. Becher, S. Waters	Alumina-based ceramic composite
R. Lauf, D. Bible, et al.	Apparatus and method for processing of materials
P. Maziasz, G. Goodwin, C. Liu	High-temperature corrosion-resistant iron-aluminide alloys exhibiting improved weldability
T. Vo-Dinh et al.	Laser-induced differential normalized fluorescence method for cancer diagnosis
D. Casada	Method and apparatus for monitoring motor-operated valve motor output torque and power at valve seating
C. Britton	A method of pedestal and common-mode noise correction for switched-capacitor storage arrays
H. Haynes, C. Ayers, D. Casada	Instrument for analysis of electric motors based on slip-poles component
R. Taleyarkhan	Method to prevent or mitigate steam explosions in casting pits

Awards and Appointments for 1996

Two current ORNL researchers were named corporate fellows in 1996: **Robert O'Neill** and **Stephen J. Pennycook.**

Stan David was named recipient of the William Irrgang Memorial Award by the American Welding Society. He also was selected as a U.S. delegate to the International Institute of Welding Annual Assembly held in September 1996 in Budapest, Hungary.

Roger S. Carlsmith, retired director of ORNL's Energy Efficiency and Renewable Energy Program, received the Sadi Carnot Award in Energy Conservation—one of three prestigious DOE Energy Science and Technology Awards.

Kathleen Alexander was selected one of 1996's 10 "Outstanding Young Americans" by the U.S. Junior Chamber of Commerce and was honored in Washington, D.C. She also was elected a fellow of ASM International.

J. Michael Ramsey received a Technology Award from *Discover* magazine for his innovative development of a lab on a chip, called "The Incredible Shrinking Lab" by the magazine. He also received a 1996 NOVA Award from Lockheed Martin Corporation.

Phil Jardine, Michael Smith, and **Thomas Thundat** each received a DOE Young Independent Scientist Award for 1996, as did three scientists from three other national laboratories. Four of these six scientists, including **Jardine** and **Smith**, received Presidential Early Career Awards for Scientists and Engineers. **Jardine** also was appointed an adjunct professor in the Department of Geological Sciences at the University of Tennessee and was elected chair of the Soils and Environmental Quality Division of the Soil Science Society of America.

In 1996 ORNL received six R&D 100 awards from *R&D* magazine, bringing ORNL's total for these coveted techology awards to 85. ORNL winners were **H. Craig Dees** (Gencell 101, bacterial cellulase for textile finishing and other uses); **J. Michael Ramsey** and **Stephen Jacobson** (lab on a chip for minute chemical separations); **John Bates, Nancy Dudney,** and **Chris Luck** (thin-film rechargeable lithium batteries); **Tuan Vo-Dinh, Kelly Houck,** and **David L. Stokes** (surface-enhanced Raman gene probe for gene mapping, DNA sequencing, and other uses); **Lynn Boatner** and **Ron Feenstra** (potassium tantalate or niobate crystals as substrates for the growth of oxides for electronic devices); and **Thomas Thundat, R. J. Warmack, Eric Wachter, Patrick Oden,** and **Panos Datskos** (noncontact micromechanical thermometer and microcantilever mercury vapor sensor).

Tuan Vo-Dinh was named the 1996 Tennessee Inventor of the Year by the Tennessee Inventors Association and the 1996 Inventor of the Year by the Inventors Clubs of America, Inc., which sponsors the International Hall of Fame Awards. Receiving Hall of Fame Awards were nine ORNL researchers in 1996: **Vo-Dinh, Michelle Buchanan, H. Craig Dees, Curtis C. Travis, Tim C. Scott, Jih-Shing (Jason) Lai, R. J. Warmack, Eric Wachter,** and **Thomas Thundat.**

Barbara Hoffheins, **Robert Lauf**, **Roddie Judkins, David Stinton**, **Ogbemi Omatete,** and **Claudia Walls** received the Award for Excellence in Technology Transfer from the Federal Laboratory Consortium.

The Radiation Research Award presented by the Radiation Research Society was renamed the Michael Fry Research Award after **Michael Fry**, a cancer researcher in ORNL's Life Sciences Division. The new name recognizes Fry's achievements as editor-in-chief of the journal *Radiation Research* and his many other contributions to the Society.

ORNL winners of three 1996 DOE Materials Sciences Awards were **Stephen J. Pennycook,** for studies of atomic structure and properties of grain boundaries in ceramics; **John Budai, Dave Christen, Amit Goyal, Charles Klabunde, Don Kroeger, David Norton, Mariappan Paranthaman,** and **Eliot Specht** for development of biaxially aligned, high critical current density, high-temperature superconducting deposits on textured metallic tapes; and **George Wignall, Brian Annis, Tony Habenschuss,** and **David Londono,** for theoretical studies and neutron/X-ray scattering investigations of structures of polymer blends.

Dorothy M. Skinner was selected to the first group of fellows of the Association for Women in Science (AWIS).

Don Batchelor and **Martin Peng** were elected fellows of the American Physical Society.

Fang C. Chen was elected a fellow of the American Society of Mechanical Engineers.

Ed Frome was named a fellow of the American Statistical Association.

John G. Merkle was elected a fellow of the American Society for Testing and Materials.

Terry Tiegs was named a fellow of the American Ceramic Society.

ORNL was honored with a Corporate Technical Achievement Award from the American Ceramic Society.

Vinod Sikka received an award in industrial technology at the 1996 National Energy Efficiency and Renewable Energy Awards ceremony in Washington, D.C., for the Exo-Melt

Robert O'Neill

Stephen Pennycook

Kathleen Alexander

method of efficiently melting nickel and iron aluminides.

Ada L. Olins received the Humboldt Research Award for Senior U.S. Scientists from the Alexander Von Humboldt Society.

Balasubramaniam Radhakrishnan received the Warren F. Savage Memorial Award from the American Welding Society.

Myint Thein received the Founder's Award at the 41st Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry.

Margaret (Peggy) Emmett received the Distinguished Service Award from the Radiation Protection and Shielding Division of the American Nuclear Society.

Buddy Bland, **Tim Sheehan**, **Al Geist**, **Malcolm Stocks**, **Phil Papadopoulos**, **Ken Kliewer**, **Bill Shelton**, and **Ross Toedte**, who combined expertise in parallel computing and materials science, received the Gold Medal at the Supercomputing '96 Conference "for their metacomputing approach that will connect ORNL's Paragon supercomputers with Sandia National Laboratories' Paragon supercomputer and the Cray T3D supercomputer at the Pittsburgh Supercomputing Center." ORNL winners of the Silver Medal in the innovation category were **Geist**, **Papadopoulos**, **Jim Kohl**, and **David Semaro**.

Shafik Iskander, Mikhail Sokolov, and **Randy Nanstad** received a Significant Contribution Award from the American Nuclear Society's Materials Science and Technology Division.

Philip Maziasz won the grand prize for the 1996 American Powder Metals Industries (APMI) Powder Metallurgy Metallography Competition.

David E. Reichle, ORNL associate director for life sciences and environmental technologies, was presented a 1996 Muskingum (Ohio) College Alumni Distinguished Service Award.

Lockheed Martin Energy Research and **Energy Systems** received the Department of Energy Headquarters Management and Operation Contractor of the Year Award for stellar performance in the Socioeconomic Programs arena.

John Sheffield was named a member and later chairman of the Fusion Energy Sciences Advisory Committee of the Department of Energy's Office of Energy Research.

Nermin A. Uckan was named a member of DOE's Fusion Energy Sciences Advisory Committee.

Lisa Stubbs was appointed a member of the Department of Energy Human Genome Coordination Committee.

John C. Miller was appointed a member of the National Research Council's Committee on Atomic, Molecular, and Optical Sciences.

Gregg Marland was appointed a member of three committees concerned with global change: National Technical Advisory Committee for the National Institute for Global Environmental Change; Global Emission Inventory Activity Committee (which he chairs) of the International Geosphere/Biosphere Programme; and an International Panel on Climate Change committee charged with estimating rates of greenhouse gas emissions to the atmosphere.

Barbara Walton was elected to a three-year term on the board of directors for the Society of Environmental Toxicology and Chemistry.

Steven E. Lindberg received a sabbatical award from the International Institute of Hydrophysics at the GKSS Research Centre to conduct research projects in Germany. He also was named associate editor of *Environmental Reviews*.

Gerilynn R. Moline was appointed press officer for the American Geophysical Union hydrology section.

Jim Roberto was appointed vice chair of the Committee on Condensed

Phil Jardine

Michael Smith

Thomas Thundat

Matter and Materials Physics of the National Research Council.

Rufus H. Ritchie was named to the Iberdrola Chair in Spain. Iberdrola, a major power company in Spain, recently established this chair at the Basque Country University in San Sebastian, Spain, to promote university research.

Marilyn Brown was appointed to a four-year term on the Board of Scientific Counselors for the U.S. Environmental Protection Agency.

Patrick J. Mulholland was appointed to the Everglades Nutrient Threshold Research Review Panel of the Florida Department of Environmental Protection. He also coauthored a chapter on hydrology and freshwater ecology for the United Nations Environmental Programme's document *Impacts, Adaptations and Mitigation of Climate Change: Scientific-Technical Analysis.*

Oakley H. Crawford and **Debra L. Joslin** were elected scientific members of the Böhmische Physical Society.

Osman Yasar was elected chairman of the worldwide Intel Supercomputer Users' Group.

George Wrenn was named Outstanding Engineer of the Year by the Tennessee Society of Professional Engineers.

Jerome Dobson was elected president of the University Consortium for Geographic Information.

Robert D. Hatcher was elected president of the American Geological Institute.

William E. Doll was elected secretary of the Near Surface Geophysics Section of the Society of Exploration Geophysicists.

Bruce Bevard and **David Moses** were elected members of the U.S. delegation to the international P-8 Meeting on Plutonium Disposition.

The American Society for Microbiology named **Robert S. Burlage** a member of the Committee on Environmental Microbiology and of the editorial board for the *Journal of Microbiological Methods.*

Linda L. Horton was appointed a member of the Council of Fellows of ASM International.

Cam H. Hubbard was named a member-at-large of the board of directors of the International Centre for Diffraction.

Po-Yung Lu, Kowetha Davidson, James Norris, Sylvia Talmadge, and **Robert Young** were appointed members of the National Advisory Committee of the U.S. Environmental Protection Agency.

George N. Miller was elected vice president-elect of the Automation and Technology Department of ISA, the International Society for Measurement and Control.

Eric Mulkey was named a diplomate of the American Academy of Environmental Engineers.

Frank Southworth was appointed a member of the board of directors of the Association of American Geographers.

Janet Strong-Gunderson was appointed a member of an ad hoc work group for the State of California Environmental Protection Agency.

Gerald A. Tuskan was appointed a member of the Forum for the Board on Biology and the Board on Agriculture of the National Research Council.

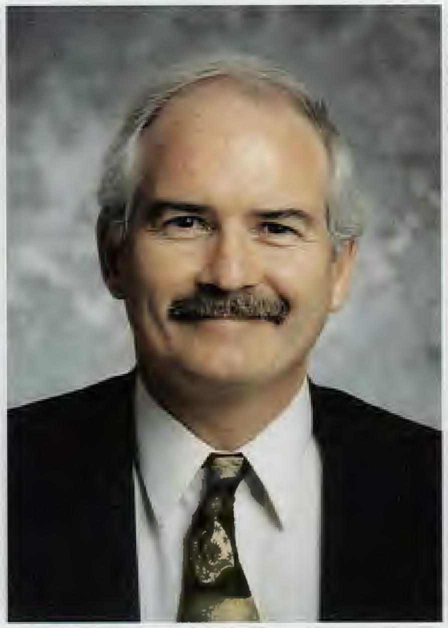
S. Y. Lee served as general chairman for the 1996 annual meeting of the Clay Minerals Society.

Patricia Hu was appointed a member of the editorial advisory board of *Accident Analysis and Prevention,* of the National Research Council's Transportation Research Board, and of the Expert Panel on Aging Scenarios for the U.S. Department of Transportation.

David J. Bjornstad was named a member of the editorial council of *The Journal of Environmental Economics and Management.*

Eric Hirst was named a member of the editorial advisory board of *The Electricity Journal.*

Michael Fry



Jerome Dobson

R.D. Hatcher, Jr.

Jonathan Nyquist was named co-chair of the Publications Committee for the Environmental and Engineering Geophysical Society. He also was named a member of the editorial board of *Geotimes*, a publication that covers geosciences news and information.

Lynne E. Parker was appointed to the editorial board of the *International Journal of Emerging Mechanical Engineering Technology.*

Ajay Rathi was appointed a member of the editorial advisory board of the *Journal of Transportation Engineering*.

Dave Schoenwald was appointed a member of the editorial board of the Institute of Electrical and Electronic Engineers' *IEEE Magazine*.

Lee Shugart was appointed a member of the editorial board of the journal *Biomarkers*.

Marina B. Ruggles was named associate technical editor of the *Journal of Pressure Vessel Technology*, the premier international journal for pressure vessel and piping technology.

Laura E. Toran was appointed associate editor for two journals, *Water Resources Research* and *Ground Water*. She was also appointed a member of the Committee to Select Outstanding Student Papers for the Hydrology Section of the American Geophysical Union.

Marc Wise was appointed a member of the editorial advisory board of *Field Analytical Chemistry and Technology*.

Edward C. Uberbacher, Ying Xu, and **Victor Olman** received a best paper award from the Institute of Electrical and Electronics Engineers, Inc. (IEEE) International Symposium on Intelligence and Systems. The winning paper, "A Segmentation Algorithm for Noisy Images," discusses their development of a computer algorithm to make it easier to extract objects from an image that contains many different objects.

Fang Peng received the First Prize Best Paper Award of the Industrial Power Converter Committee at the annual meeting of the IEEE/Industry Applications Society.

Jeff Christian and **Andre Desjarlais** received a Best Paper Award at the Conference on the Thermal Performance of Polyurethane Insulations.

C. T. Liu was a co-winner of a Best Paper Award from the Japan Institute of Metals and was appointed advisory professor at the Shanghai Jiao-Tong University in China.

Michael Muhlheim won the 1996 Mark Mills Award from the American Nuclear Society for best technical paper.

Steve Lindberg was appointed adjunct professor of environmental and public health at the University of Michigan.

ORNL's **Isotope Enrichment Facility** earned an international quality registration from the International Organization for Standardization. This is the first time that a DOE facility has been presented with an ISO 9000 registration.

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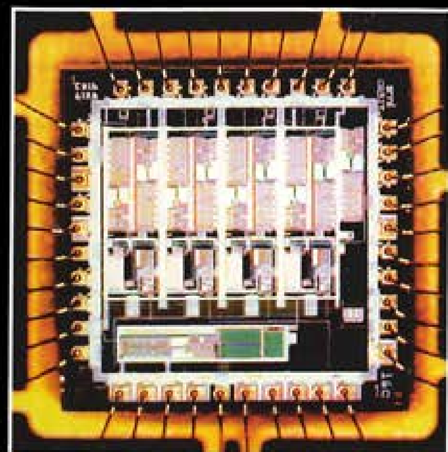

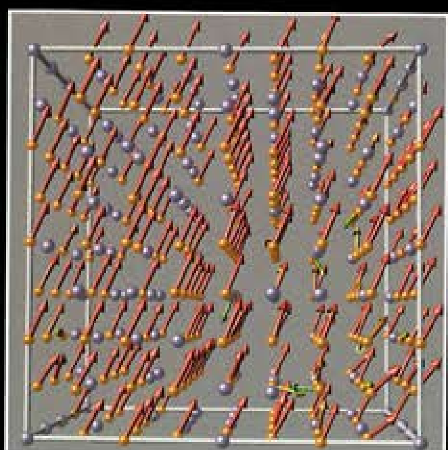
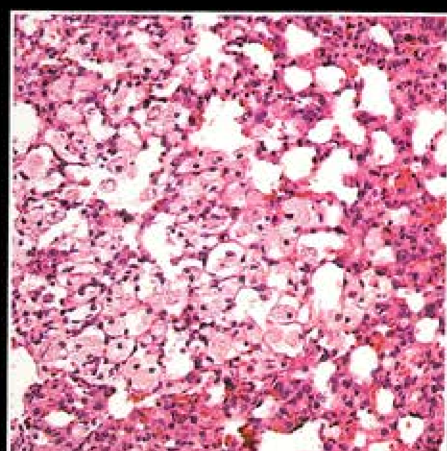
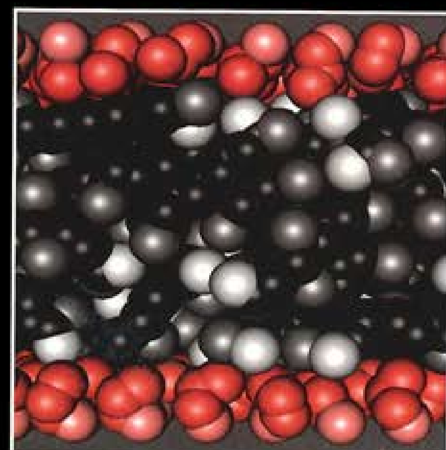


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