Summer 1979

Oak Ridge National Laboratory review

Physicists, both at the Laboratory and elsewhere, have been awaiting the completion and initial functioning of the Holifield Heavy Ion Research Facility now for over five years. When in operation, it will be unique in its capabilities throughout the world. Some of the questions it is expected to answer are discussed by Joe McGrory in the lead article.

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Oak Ridge National Laboratory

review

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DEPARTMENTS

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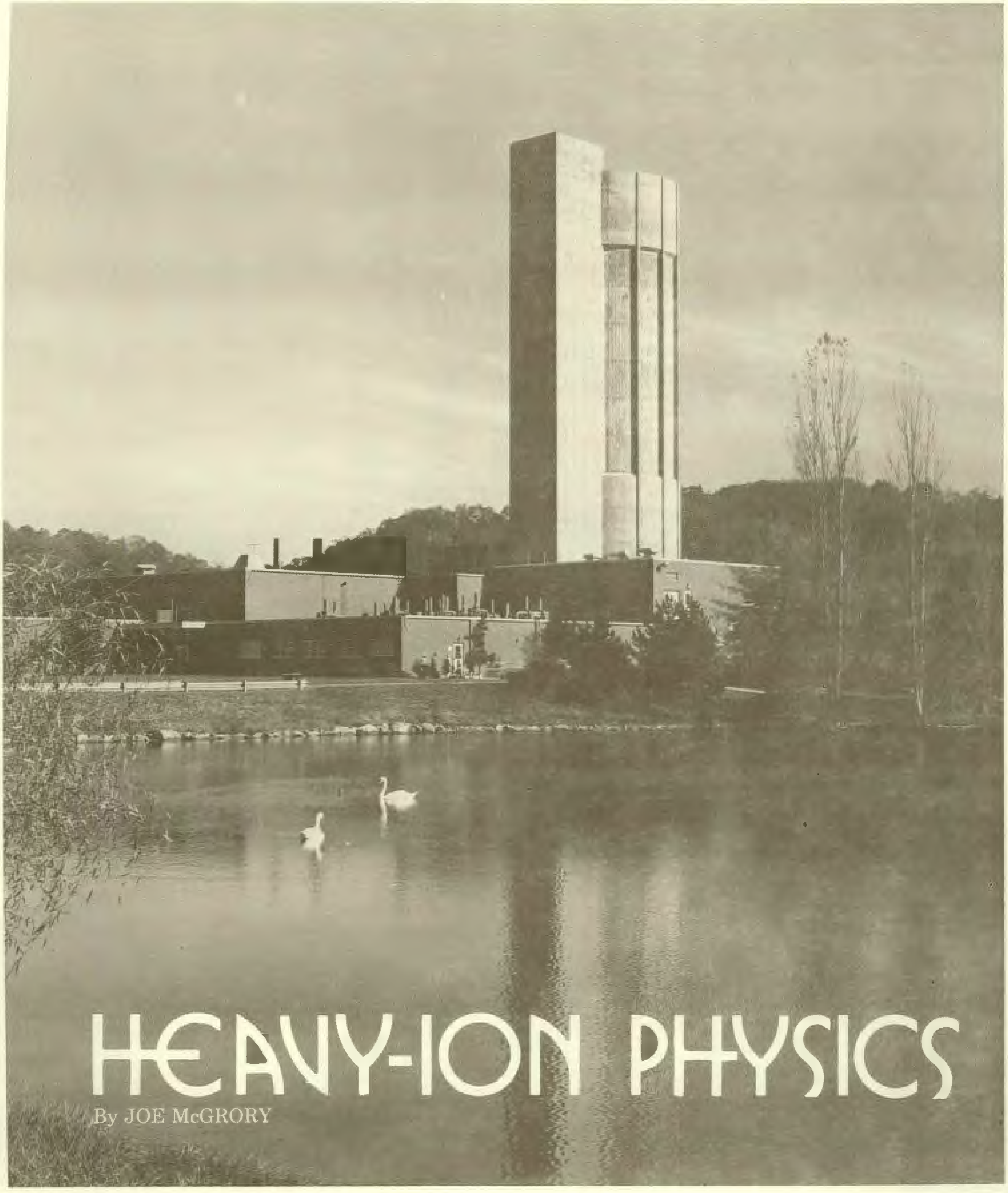


HEAVY-ION PHYSICS

By JOE McGRORY

A dream of heavy-ion research at ORNL that began with the publication in 1969 of a proposal for *An Accelerator for Physics and Chemistry of Heavy Elements (APACHE)* will be realized late this year when the Holifield Heavy-Ion Research Facility (HHIRF) is dedicated and opened to local researchers and users groups. Watching the tower "accelerate upwards," as the sign charged us during the more than two years of its construction, Joe McGrory has been anticipating the research results that will come out of the new facility. A veteran physicist at the Laboratory, Joe holds a Ph.D. in physics from Vanderbilt University and has been head of the nuclear theory group in the Physics Division since 1976. He is shown here (right) discussing his work with Tom Davies, another member of the group. When asked recently by a nonphysicist, "Why heavy-ion research?" he delivered himself of the following painstaking explanation.

The dominant structure of the skyline at Oak Ridge National Laboratory is the new tower to the east of Swan Pond, soon to house the 25-MV electrostatic tandem accelerator which will be the principal component of the Holifield Heavy-Ion Research Facility (HHIRF) in the near future. When completed, the accelerator facility will produce a variety of beams of heavy nuclei with very high energies in reasonably large quantities.

Until the last few years, most low-energy nuclear physics research has involved accelerating the lightest nuclear systems—protons, neutrons, deuterons (one neutron, one proton), and alpha particles (two neutrons, two protons)—at energies up to 50 million volts (MeV) per particle and scattering these beams from targets of nuclei of naturally existing atoms such as carbon, calcium, and uranium. In contrast, HHIRF will produce useful beams of much heavier nuclei, such as bromine, which has 35 protons and 44 or 46 neutrons. These beams will have energies up to 15 MeV per particle (total energy 1200 MeV).

Why do we want to attack the nuclear fortress with such heavy atomic artillery? Haven't we already learned all that is important about nuclei? Since we anticipate starting experiments on HHIRF in early 1980, this seems to be an appropriate time to explain some of the reasons for the development of this facility and to discuss recent progress in heavy-ion theory made by the nuclear theory group in the Physics Division at ORNL.

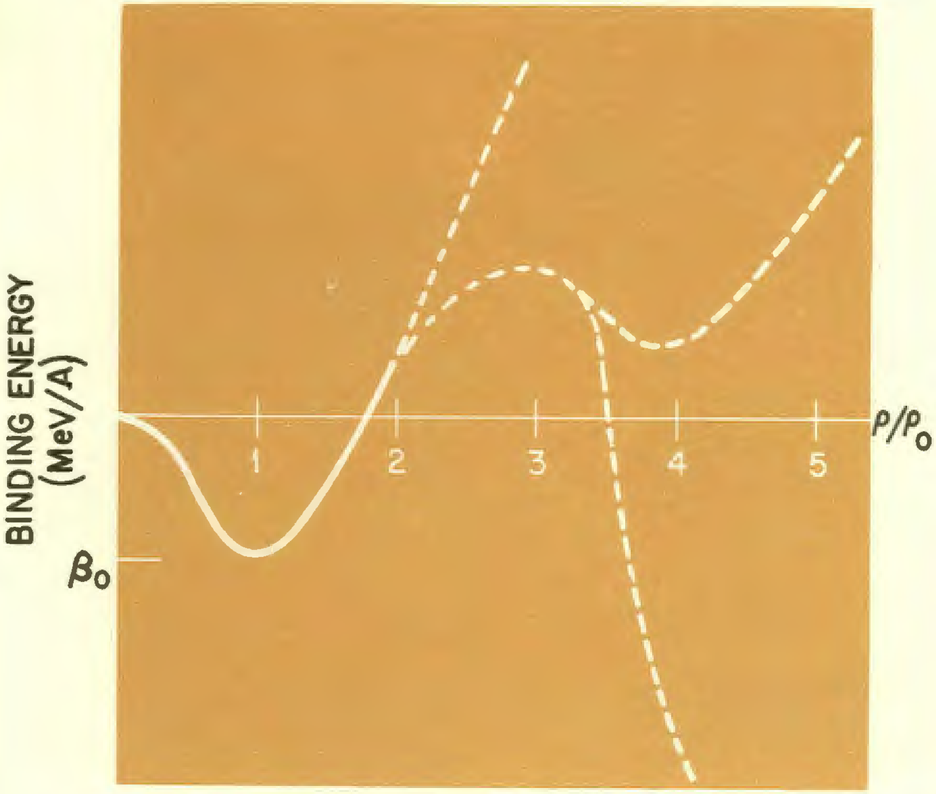
Just as HHIRF has become a dominant feature of the ORNL skyline, nuclear physics has been a dominant part of the intellectual and technological development of twentieth century science. But the scope of nuclear physics has been limited in the following ways:

1. Only those nuclei that are very close in mass and charge to nuclei that naturally occur have been studied.
2. We have been able to study nuclei only when they are "cold" (i.e., in states very close to the lowest possible energy).
3. We know about nuclei only at small angular momenta (i.e., only when they are rotating slowly).
4. We know about nuclei only at one density of nuclear matter.

A very loose analogy would be that we have studied matter only in its solid state, and we know essentially nothing about the liquid or gaseous state. These limitations deserve a little more detail.

Nuclei Far From Stability

How have we been limited in the nuclear species we could study? As a



Plot of the energy-per-particle of condensed nuclear matter as a function of its density, ρ. The density of normal nuclear matter is designated by ρ_0. The value of B at the point $\rho/\rho_0 = 1$ and the shape of the curve where the line is solid are the only parts of this curve known from experiment. The dashed lines represent various theoretical speculations as to the remainder of the curve.

Figure 1

first approximation, one can characterize a given nuclear system by the number of protons and neutrons and by the total energy of the system. Two forces basically determine the configuration of these neutrons and protons. One force is the well-known Coulomb force, the repulsive force between any two electrically charged protons. The other force is the nuclear force. The force between two nuclei varies in character as a function of their separation. At very short distances ($<10^{-13}$ cm), the force is strongly repulsive. At greater ranges, it is attractive. In terms of these several attractive and repulsive forces, we understand why only a certain finite number of nuclei exist in nature. If one tries to add a neutron or a proton to a naturally occurring nucleus which has the largest possible number of neutrons or protons for that species, the resulting system will be "unstable," and will disintegrate by emitting one or more nucleons or electrons. Unstable nuclear species can be produced by bombarding stable, or naturally occurring, nuclei with light particle beams such as proton or deuteron beams. In this way, we have extended the study of nuclei a few small steps away from the region of stability. With heavy-ion beams, the possibility to form new nuclei far from stability is dramatically increased. For instance, one can bombard $^{238}_{92}U$ with $^{81}_{35}Br$ and, in principle, form nuclei with a proton number (Z) as high as 127 and with a neutron number (N) as high as 192. This possibility of forming superheavy nuclei was a major reason for the initial decision to build up heavy-ion physics. Nuclear theory predicts that nuclei with $Z \approx 114$ might "live" long enough to be observed. To date, the search for such superheavies produced in heavy-ion reactions has been unsuccessful. There remains, however, the fascinating question of whether such new nuclei can be formed; and if so, which ones will be formed.

Hot Nuclei

Nuclear physics is just beginning to heat up with the availability of heavy-ion beams. When a nucleus is bombarded, some of the kinetic energy of the incident projectile can be transformed to internal excitation energy (heat) in the target nucleus. Most of our knowledge of nuclei to date concerns their behavior at relatively cold temperatures. The use of the word "temperature" in nuclear physics can be understood by analogy with classical temperature. In nuclear physics, temperature is a measure of the more-or-less random kinetic energy of the nucleons moving in the nucleus. In the single scattering of light ions at high energies, such as the scattering of protons and alpha particles, it is not possible to transfer much of the incident kinetic energy into excitation energy into the nucleus. In a heavy-ion-induced reaction, a large amount of kinetic energy can be brought into the system by a large number of nucleons, each of which is at a relatively low energy per particle. In this case, it is much more probable that much of the incident energy goes into the target nucleus to produce a high temperature. Thus, the availability of energetic heavy-ion beams offers us the possibility of studying the nucleus at much higher excitation energies (temperatures) than previously possible.

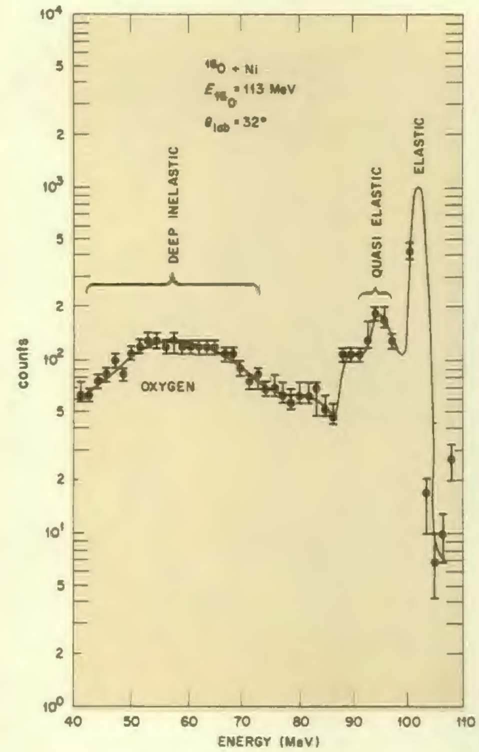
Properties of Nuclei with Large Rotational Frequencies

What happens to nuclei as they rotate faster and faster? The fact that one can describe a nucleus as "rotating" is somewhat surprising in itself. Nuclei have from 1 to about 250 particles. Thus, the typical nucleus is neither a few-body system nor a many-body system (as is a gas). In addition, since the nuclear dimensions are so small ($\sim 10^{-12}$ cm), one must use quantum mechanics to calculate nuclear properties. When a typical constituent nucleon in a nucleus travels a distance about equal to the nuclear diameter, it makes one or two collisions with other nucleons. In contrast to this behavior, for a classical fluid one deals with dimensions such as liters or cubic centimeters and Avogadro's number ($\sim 10^{23}$ molecules per liter). In a classical fluid, the constituent molecules make so many collisions with nearby molecules that for many properties, such as viscosity, one can ignore boundaries (i.e., there are no surface effects). By definition, quantum mechanical effects are negligible for classical fluids. Thus, fluid systems and nuclear systems are qualitatively different.

Yet one of the most successful models of nuclear physics is the liquid-drop model, proposed in the 1930s by the Danish physicist Niels Bohr. The model assumes that nuclei are made of particles tightly packed at a uniform density, with a sharp surface. The model assumes the nuclear force gives rise to a surface tension. As a result o. the competition between this surface tension and the repulsive Coulomb forces, the nucleus can rotate and vibrate as a liquid drop might. In such a model, it is possible to transfer energy to internal energy, analogous to heat, and to collective motion such as rotations or vibrations of the system as a whole. The frequency with which the nucleus rotates can be related to a quantity called the angular momentum of the nucleus. The angular momentum is a measurable quantity.

Figure 2

A plot of the observed final kinetic energy of ^{16}O fragments produced in the inelastic scattering of ^{16}O ions with 113 MeV of energy from a niobium target. The x axis shows the measured final kinetic energy of the ^{16}O ion, and the y axis shows a measure of the relative number of ^{16}O ions scattered with this final kinetic energy.



Just as a collision with a light particle is unlikely to raise the temperature of a nucleus, it is not possible with a light ion to introduce much angular momentum to a nucleus (i.e., to increase the spinning rate) with a light ion. With a heavy ion, it is possible to form states with very large angular momenta. Before heavy-ion beams were developed, high angular momenta meant values of 6 to 8 in some units. With heavy ions, nuclei with 40 to 60 units of angular momenta can be made. At these large values of angular momenta, the nucleus rotates so fast that the centrifugal forces should become significant. What happens to the shapes of nuclei when this happens? How is nuclear matter spewed out by this high frequency rotational motion?

Properties of Dense Nuclei

The concept of a phase change is a familiar one. One of the most familiar is the change from ice to water to steam as the temperature of the fluid is increased at a constant pressure. If one increases the pressure on a piece of ice at 0°C, it will melt, since the pressure lowers the melting point. We've all taken advantage of this to make snowballs or to ice skate. But what would happen if we could squeeze a nucleus? In other words, what are the properties of nuclear matter as a function of the density? One particular question we must address is how the energy-density of nuclear matter depends on the matter density? Figure 1 shows a plot of the total energy density of the nuclear system as a function of the matter density. The nucleus is stable, or lives a relatively long time, at those points on the curve where the energy density is a minimum. Our only knowledge of nuclei concerns their behavior at normal nuclear density close to the first minimum (Fig. 1). Recently (in part from experiments by Fred Bertrand of the Physics Division), we have learned a little about the shape of this curve very near this point. That is all the knowledge we have of this curve. There is wide speculation as to what happens at higher densities, a question of particular interest in astrophysics. The densities of so-called neutron stars are much higher than nuclear densities. Are there other minima where nuclear matter would be stable or long-lived? As the density increases, the constituent nucleons are forced close together. We have stated that when nuclei are very close together, there is a very strong repulsion between nucleons. One possible result of this strong repulsion is that other elementary particles such as pi-mesons (pions) may be produced. Pions are subnuclear particles with mass of about one-fourth that of the nucleon mass. Furthermore, as the nucleons are pushed even closer

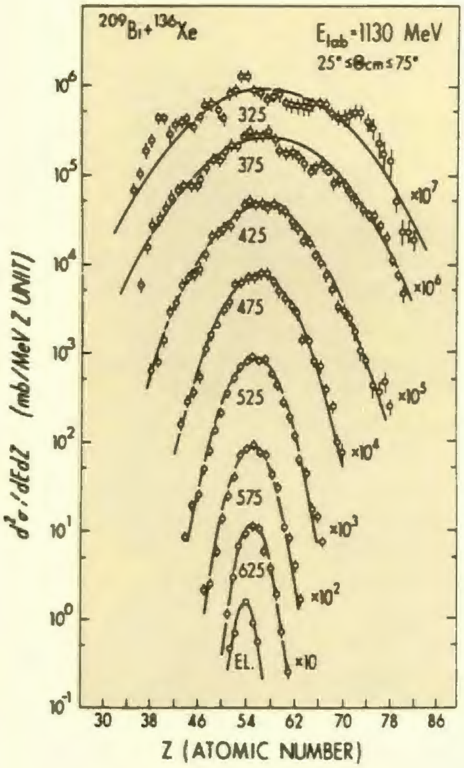


Figure 3

A plot of the final fragment charge distribution in the inelastic scattering of ^{136}Xe with a kinetic energy of 1130 MeV from a ^{209}Bi target. The x axis shows the charge of the final observed fragment, and the y axis shows a measure of the relative probability that an ion with a given charge Z is produced as a result of the scattering. The number on each curve indicates the kinetic energy of the observed final fragments. "EL" stands for elastic scattering, where the final kinetic energy roughly equals the initial kinetic energy.

together, even quarks may be produced. Quarks are the conjectured building blocks of the nucleons and other elementary particles which carry a fractional (1/3) electric charge. How the presence of these other elementary particles will be manifested in heavy-ion reactions is a completely open question.

How can high nuclear densities be formed? If two identical nuclei were to be overlapped, with the same volume for each nucleus maintained, the density would be doubled. It is not so easy to achieve such an overlap. For an ordinary classical spherical particle, the volume is proportional to r^3, where r is the radius of the sphere. If the spheres are incompressible solids, it is not possible for the volumes of the spheres to overlap in space. In the case of nucleons (protons and/or neutrons) which obey the equations of quantum mechanics, there is a six-dimensional volume proportional to $(\Delta r)^3$ $(\Delta p)^3$, where Δr and Δp are related to the spatial position and the linear momentum of the particles. The nucleons must satisfy the Pauli Principle, which says essentially that these elementary particle "spheres" cannot overlap in the total six-dimensional position-momentum space, called phase space. Thus, the larger the available volume in momentum space, the more closely packed the particles can be in position space. As the relative energy of the heavy ions is increased, the total amount of linear momentum is increased, or phase space is increased. It is then possible to pack more particles into a given volume in ordinary space—in other words, to achieve higher densities. It may be that densities even higher than twice the normal nuclear density can be attained if there is some sort of "pile-up effect" as the ions overlap. When two heavy ions collide, the "front" between the normal and the high-density regions might move faster than the velocity of sound in nuclear matter, and shock waves might form. (The same thing happens when sonic booms are created by jets moving through air at supersonic speeds.) Since we do not yet have appropriate heavy-ion beams to study these phenomena, the area is ripe for speculation.

Atomic Physics Applications

To this point, we have discussed purely nuclear physics. There are a number of very interesting questions to be answered in the field of atomic physics (the behavior of electrons in the electric fields produced by the nucleus). These questions will be studied with the new heavy-ion facilities. One such question concerns the behavior of electrons in very strong electric fields. An outstanding success in modern physics has been P.A.M. Dirac's relativistic quantum-mechanical theory for the motion of an electron in an electric field. An electron moving in the closest allowed orbit around a positive point charge Z is referred to as a 1s electron. The energy of this 1s electron in the Dirac theory is defined only for those cases where the charge, Z, is less than 137. For $Z > 137$, the energy becomes imaginary. How does the electron behave when $Z > 137$? All observed nuclei have $Z \leqslant 106$, so there has been no chance to investigate this question. There has been a great effort, particularly by Walter Greiner and collaborators at the University of Frankfurt, Germany, to predict theoretically what will happen. One of their predictions is that above a certain critical $Z_c \approx 170$, there will be the spontaneous production of positrons. (Positrons are particles with the same mass as the electron, but with positive charge. Dirac predicted the existence of positrons in 1930, and they were observed subsequently in experiments conducted by Carl Anderson at Cal Tech. Positrons are produced when a proton transforms to a neutron by shedding its electric charge as a positively charged electron. Another common source of positrons is in so-called pair production, where an uncharged gamma ray is converted into two particles, a positron and an electron.)

With the availability of beams of heavy ions, it is now possible to study the behavior of electrons in the field of charges with $Z > 137$. When two uranium atoms (each with $Z = 92$) collide at relative energies of 10 to 20 MeV/A (A = atomic number), for some time the electrons behave as if they were in a field of a nucleus consisting of the two uranium nuclei. This "nucleus" has a Z of 184, well beyond the critical $Z = 137$. There have already been experiments carried out at the new heavy-ion accelerator at Darmstadt, Germany, to look for the production of positrons in U + U collisions. Many positrons are observed to be produced in the reaction. Unfortunately, there are also several competing, more conventional, mechanisms for positron production in U + U collisions (similar in nature to the pair production). It is not yet clear whether the spontaneously produced positrons of the large-Z field have been observed.

With the availability of good, high-quality beams of heavy ions such as those that will be produced at HHIRF, there are many avenues of research open. In the last five years, greatly increased emphasis has already been placed on experimental and theoretical research in heavy-ion physics at a number of installations around the world (e.g., in the United States, at Lawrence Berkeley Laboratory, Argonne National Laboratory, Texas A&M, Brookhaven National Laboratory, Michigan State University, and ORNL). The theoretical heavy-ion-physics research effort is also international in scope. In the past three or four years, most of the effort of the nuclear theory group in the Physics Division at ORNL has focused on heavy-ion physics. Low-energy, heavy-ion physics has already revealed a surprising phenomenon, the deep-inelastic scattering process, and considerable theoretical progress has been made here and elsewhere to understand this process.

Deep-Inelastic Scattering

The new nuclear process which has emerged from experiments on heavy-ion physics is most often referred to as deep-inelastic scattering, discovered at Orsay, France, in the early 1970s. A brief digression here concerning conventional nuclear-physics scattering experiments will provide a framework in which to describe this new process.

Much of conventional experimental nuclear physics has concerned simple scattering experiments. If a proton is shot at a nucleus, up to a certain incident energy the proton is usually deflected, but no energy is transferred from the proton to the nucleus. This process is referred to as elastic scattering. As the incident proton energy is increased, at least one other process is possible: Energy can be transferred from the projectile to the target. Both the final energy and the final momentum of the proton are changed, and the target nucleus is left in an excited state. This deposition of energy in the nucleus by the projectile is the so-called inelastic scattering. A knockout process can also occur, by which a proton or neutron or a more complicated set of nucleons can be knocked out of the target nucleus. In most light-ion-induced inelastic scattering reactions, a relatively small part of the total energy of the incident proton is transferred to the target.

When the incident projectile and the target are heavy ions, many more mechanisms are possible. The two ions can scatter elastically with no energy transfer. As the energy increases, many particles can be transferred to and from the target. Even if there is no particle transfer, *both* the target and projectile can absorb energy from the energy of the incident relative motion of the projectile with respect to the target. Thus, there are many more "inelastic" channels open in heavy-ion reactions. Many experiments have already been done to study inelastic scattering of heavy ions at relatively low energies.

Figure 2 shows some results of typical heavy-ion inelastic scattering experiments. Conducted by Bob Stokstad and collaborators in the Physics Division, an investigation of the scattering of ^{16}O ions with an energy of 113 MeV from a ^{58}Ni target produced the results shown in this figure. The ordinate shows the relative probability that after the scattering, an ion very close in mass to ^{16}O is observed with a given final kinetic energy. The abscissa shows the final kinetic energy. The largest probability is for a final kinetic energy of about 100 MeV. This is essentially elastic scattering, but there is a large second peak at around 55 MeV, or at a kinetic energy loss of about 50 MeV. In this latter bump, a large fraction of the incident kinetic energy has been transformed into excitation energy of the target and scattered fragment.

What is the underlying physics of such reactions? There are primarily two important forces in such heavy-ion collisions. One is the electrostatic Coulomb force between protons in the ions of the beam and the target. The net effective Coulomb force between the ions can be characterized as a relatively weak, but very long-range repulsive force. It is the only force which is felt when there is a significant separation between the ions. If the incident ion energy is not very large, it cannot overcome this Coulomb repulsion. Thus, there is mostly elastic scattering, and the nuclear force is irrelevant. The second force is the nuclear force that exists because of the nuclear forces between constituent nucleons. The total nuclear force between ions is a short-ranged force, but it is a very strong one, and it is essentially attractive. As the incident ion energy is increased, the two ions can get close enough to feel this attraction, and they stick together for a short time before they separate in the final channel. What many experiments have shown is that in an unexpectedly large fraction of the time, any energy of relative motion that is not used up in overcoming the repulsion of the Coulomb force is absorbed by the "target" and the "projectile." In the final state, these two ions are highly excited (hot), and they are emitted with velocities one might expect for two classical spherical systems with the charges and the masses of the detected fragments.

Cheuk-Yin Wong and Edith Halbert are members of the nuclear physics group that are working on heavy-ion theory at ORNL.

A strong correlation observed in deep-inelastic reactions is seen in Figure 3, which shows some results obtained by John Huizenga and collaborators at the University of Rochester for the reaction ^{136}Xe on ^{209}Bi at an incident energy of ~8 MeV per particle. During the scattering, some particles are exchanged between the ions of xenon and bismuth, so there are a number of different ions produced in the scattering. In the experiment, it is possible to identify the charge and mass of the ions produced and to determine a relative probability that an ion of a given charge and mass is produced. The figure is a plot of the relative probability that an ion with a specific charge (indicated on the abscissa) will be produced. Curves are shown for a series of relative kinetic energies between the final fragments. The Z of xenon is 54. For all final kinetic energies, the most probable final fragment is xenon, so the most probable event is no net change of charge during the reaction. The figure shows that as the final relative kinetic energy decreases (as we go from the lower to the upper curves), there is an increasing probability that ions with more widely differing charges will be produced—which means that as more kinetic energy is transformed into internal heat, more charge is transferred between ions. A similar correlation is found for total mass transfer. The angular distribution of the final fragments with respect to the incident beam direction is measured. There is a consistent feature that the fragments whose charge and/or mass is most different from the incident beam or target nuclei are scattered through larger angles.

All these features are consistent with a very simple picture of the deep-inelastic process. The projectile and target nuclei come together and stick for a short time in a sort of dumbbell configuration which starts to rotate. While they stick together, a window is formed at the junction of the two nuclei, through which neutrons and protons pass back and forth freely. Mass and energy are transferred between the two nuclei. After they make part of a rotation, they come unstuck. The longer they stick together, the more energy is transferred between them, the more mass is exchanged, and the further they can rotate together. Thus, the mass transfer and the angular distributions observed in the deep-inelastic collisions can be interpreted as a measure of the sticking time.

Until now, much theoretical effort in low-energy, heavy-ion physics has been devoted to the study of the deep-inelastic process. The models that have been applied have been mostly collective models into which such classical concepts as friction, mass diffusion, or thermodynamic equilibrium have been introduced. There is no a priori justification for these concepts for a nuclear system because there are many reasons why nuclei might not act as classical fluids. The nuclear theory group in the Physics Division has devoted a significant fraction of its efforts in the last few years to the question of whether the observed features of low-energy, heavy-ion scattering experiments can be described by a nuclear model which is microscopic (i.e., in terms of discrete neutrons and protons as opposed to a continuous fluid) and which is fully quantum mechanical. The principal efforts in this area at ORNL have been by K. T. R. Davies and C. Y. Wong in the Physics Division, by R. Y. Cusson, a consultant to the Physics Division from Duke University, and by J. A. Maruhn and Vida Maruhn-Rezwani, who were with the nuclear theory group until the fall of 1977.

Hartree-Fock Theory

Most of the calculations done so far have been within the framework of the so-called Time-Dependent Hartree-Fock (TDHF) theory. A basic assumption of the theory is that at any moment, the motion of any one particle is affected by all the other particles in the system, and that the effects of all the other particles can be approximated by one central field, so that the motion of a nucleon in a nucleus has similarities to the motion of an electron in the electric field. Reducing the theory to usable computer programs has involved several man-years of effort. In the summer of 1978, the most complete calculations to date of the scattering of two heavy, unlike, ions (krypton as a projectile and lead as a target—^{84}Kr + ^{208}Pb) were performed by Tom Davies and Vida Maruhn-Rezwani of the Physics Division, in collaboration with Steve Koonin of Cal Tech and John Negele at M.I.T.

The results of their first calculations of the scattering of ^{84}Kr on ^{208}Pb at 494 MeV/A can be summarized as follows:

1. The calculations indicated a large damping of the incident kinetic energy into internal excitation. The amount of energy damping was in good agreement with experimental results.
2. The angular distributions of the krypton ions in the strongly damped collisions are roughly reproduced by the calculations.
3. There is a very small probability that during the deep-inelastic reaction ions are produced which differ significantly in mass and/or charge from the initial projectile and target ions, in agreement with experiment.

An analysis of the calculated results suggests that during the time the krypton and lead ions stick together, about 50% of the nucleons in the krypton ion are exchanged with the nucleons in the lead fragment. These particle exchanges are an important mechanism for the transfer of energy from kinetic energy of relative motion to internal excitation.

That these calculations do so well in accounting for this new feature of low-energy, heavy-ion scattering is very gratifying. It clearly indicates the TDHF approximation is a good first-order theory for the description of low-energy, heavy-ion physics.

High-Energy Collisions

In addition to the data on heavy-ion collisions at reasonably low energies (~10 MeV/A), a considerable amount of experimental information is available on heavy-ion collisions at extremely high energies (i.e., 200 to 300 MeV per particle; for example, ^{20}Ne accelerated to 4000 MeV). At these energies, the effects of the Pauli exclusion principle are much less important, and the concept of the nucleons' feeling an average mean force due to all the other nucleons is not so useful. One might expect more classical, thermodynamic models to be valid. One such model has been developed by Edith Halbert of ORNL's Physics Division. In simplest terms, the model assumes that the colliding ions can be treated in many ways like two groups of billiard balls colliding. The "nucleons" are allowed to bounce off each other according to classical Newtonian mechanics laws (Force = mass × acceleration). This is a very simplistic description of the calculations. However, Halbert's calculations, and a number of other similar calculations, yield a reasonable qualitative description of the experimental observations on the emission of light particles (protons, neutrons, alpha particles) in these high-energy, heavy-ion collisions. The results suggest that heavy-ion collision processes in the energy region above 200 MeV per particle can be described as simple collisions between individual constituent nucleons. The high-energy data are also described in a qualitatively successful way, by classical fluid dynamic calculations (in which each ion is assumed to behave like a water drop). These results are consistent with a picture in which there is a change in the physics of heavy-ion collisions as a function of projectile energies. At low energy, the concept of an average nuclear field is relevant; each particle motion is affected by all the other particles in the ions, and quantum-mechanical effects such as Pauli exclusion effects are important. In higher-energy, heavy-ion collisions, the ions behave more like classical systems of independent particles.

Cheuk-Yin Wong, of the Physics Division, and Henry Tang, a graduate student at Yale University, are already working on a microscopic model that might be capable of describing the physics in this transition region. In their theory, the TDHF solution for the heavy-ion scattering problem is considered to be the first approximation to the exact solution of the problem. A very significant contribution of their work is that it allows one to define certain functions of the microscopic nucleon coordinates, whose functions behave very much like classical temperature, entropy, viscosity, and thermal conductivity. In a parallel effort, Wong and Tang are completing the development of a computer program which will allow one to calculate the properties of collisions of two liquid drops which have arbitrary shapes, viscosities, compressibilities, and conductivities.

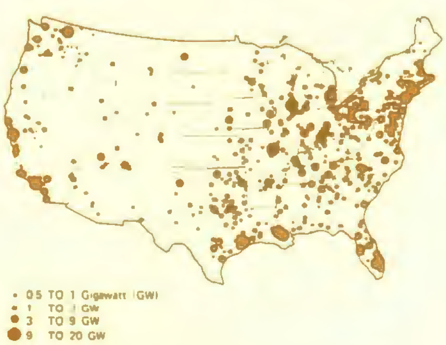
At ORNL, we are developing a capability that has the potential to describe the evolution of heavy-ion physics from low energies to higher energies as the physics evolves from quantum mean-field physics to classical fluid physics. There are many fascinating new classes of nuclear properties which will be amenable to study with the availability of high-quality, high-energy, heavy-ion beams. The field has already provided some surprises, and more are certainly in store. In the absence of unambiguous experimental information, the field is ripe for theoretical speculation. The nuclear theory group is already heavily involved in research which is tied closely to the type of physics that will be done with new accelerators, such as Phase 1 of HHIRF. With the onset of HHIRF operation, there is promise of a long period of intellectual stimulation and challenge. ornl

BOOKS

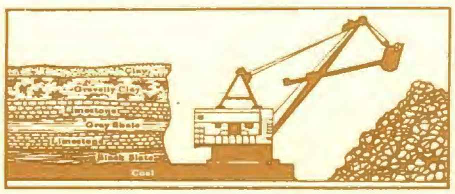
Energy Handbook

by Robert L. Loftness, D.Sc., Van Nostrand Reinhold, New York (1978). 737 pp + index, $47.50. Reviewed by Bill Fulkerson, director of the Energy Division.

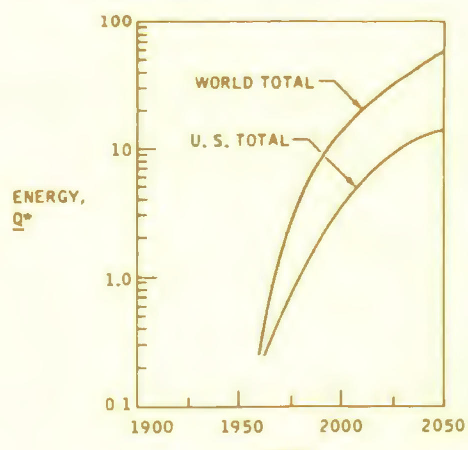
This book, written by the director of the Washington office of the Electric Power Research Institute (EPRI), is a very interesting compilation of tables, maps,



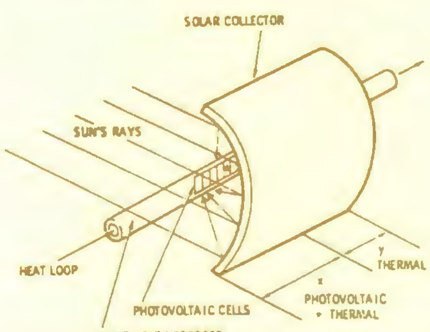
and graphs covering virtually every aspect of energy in the United States. It contains very little text. Instead, this data book simply organizes information from the current literature into a compendium which is bound to become a valuable document. For each energy technology, the book describes the major processes that are either being used or being developed. The book goes into energy use, energy resources, and—of particular interest to



me—energy conservation. Relative to the last topic, I must say I found the coverage only adequate, as it did not contain many of the references I would have picked out. Interestingly, it had several figures that have been taken from Eric Hirst's work. If a specialist looked at the particular section of the book that was in her or his field, it would probably be found wanting. However, for a brief pictorial view of any aspect of the subject from a selection of graphs, tables, and other illustrations, the book is really marvel-



ously full of good stuff. For instance, it would be invaluable as a help in preparing talks, or, if there's a subject area that you don't know about, and want a quick education in, it's a good reference work. The balance in subject matter is pretty good, ranging all the way from resources to supply, demand, and, finally, to environmental aspects and costs. The coverage, in short, is conscientious, comparing favorably with the data books that ORNL is preparing, such as the



transportation energy conservation data book or the buildings data book. One of the handbook's big pluses is that all of the tables and pictures and graphs are well documented, making it very easy to delve deeper into any area in which you have more than a superficial interest. All in all, the *Energy Handbook* appears to be a highly useful document, especially if there is going to be an attempt to update it every two or three years. It is an important resource book, and probably ought to be in every library, just as a dictionary is. ornl

Air Pollution and Vegetation

By SANDY McLAUGHLIN

The susceptibility of vegetation to damage from high levels of air pollution has been recognized for more than 100 years. However, intensive research on the toxicity of atmospheric pollutants to plants has occurred only in the past two decades. This emphasis reflects a growing concern over adverse aesthetic and economic impacts to vegetation from pollutants produced by increased industrialization in the United States. In addition, air pollutants adversely affect human and animal health, reduce visibility, accelerate corrosion of metal and erosion of stone surfaces, and have potential, long-term impacts on climate and the biogeochemical cycles influencing both terrestrial and aquatic ecosystems. Thus our concern over the extent of air pollution effects on terrestrial vegetation is one of several indices by which environmental costs of our technological choices are measured.

First, let's examine the historical basis of our concern. Probably the most dramatic evidence of pollutant impacts on vegetation has come from investigations conducted around smelting operations in the first half of this century. One of the more spectacular incidents, and one which had international implications, involved the smelting operations at Trail, British Columbia. Several years of intensive research were required in this case to verify that fumes (primarily sulfur dioxide) were being transported down the Columbia River Valley into Washington where thousands of acres of trees were being injured or killed. Very much closer to home, the many acres of still barren hills at Copper Hill, Tennessee, bear testimony to the excesses of uncontrolled emissions of sulfur dioxide (SO_2) from copper smelting operations 50 years ago and to unregulated logging which combined to alter drastically the structure and composition of the terrestrial vegetation and the stability of its soils.

Fortunately for us, public awareness and the establishment

For many green plants, some power plants may not make good neighbors. An increasing body of evidence indicates that some of our farms and forests may be suffering ill effects from continued exposure to air pollution from nearby industrial and power plants fired with coal. One of the contributors to this evidence is Sandy McLaughlin of ORNL's Environmental Sciences Division. Holder of a Ph.D. degree in forest tree physiology from Duke University, McLaughlin worked for the Tennessee Valley Authority for four years performing field and laboratory studies concerning the effects on vegetation produced by atmospheric emissions from coal-fired power plants. Since joining ORNL's staff in 1974, McLaughlin has conducted ecological studies on basic physiological processes of forest trees and on developing methods for detecting plant responses to air pollutants, particularly those from coal combustion. Many of the results of his studies are presented in the following article. Here, McLaughlin surveys growth chambers used to compare the effects of clean and polluted air on plant productivity. Some of the results of the study conducted by him and colleague Dave Shriner are told in the accompanying account.

of regulatory agencies have eliminated or reduced large-scale, uncontrolled, point-source emissions from industrial operations. These differences, together with the shift to electric power produced by large fossil-fuel electric generating plants with tall stacks and the continued increases in industrialization and urbanization, have changed the whole nature of our present day air pollution problems. Our primary concerns are no longer with individual point sources involving intermittent exposures to high concentrations of single pollutants but rather with mixtures of pollutants occurring at lower concentrations over longer duration and over broad regions. In short, the type of stress has changed from acute (high concentrations and rapid concentration changes) to chronic (long term, generally with lower levels). Chronic effects are a major concern because of the large areas potentially affected, and they are also the most difficult to study because they involve multiple interactions.

What are the pollutants of primary concern and what is their origin? At present, the three major phytotoxic pollutants recognized are sulfur dioxide (SO_2), ozone (O_3), and nitrogen dioxide (NO_2). Sulfur dioxide and nitrogen dioxide are derived primarily from combustion of fossil fuels while ozone is produced naturally by sunlight as well as by myriad reactions involving hydrocarbon residues of combustion and residues produced naturally by vegetation. Peroxyacetyl nitrate, produced by photochemical reactions in urban smog, and fluoride, produced primarily by phosphate fertilizer, aluminum manufacture, and uranium conversion technologies, are problematic on a smaller scale.

In the United States we are currently releasing approximately 31 million tons of sulfur oxides (primarily SO_2) and 24 million tons of nitrogen oxides (primarily NO_2) into the atmosphere on an annual basis. Approximately 70% of the SO_2 and 42% of the NO_2 are derived from stationary combustion, approxi-

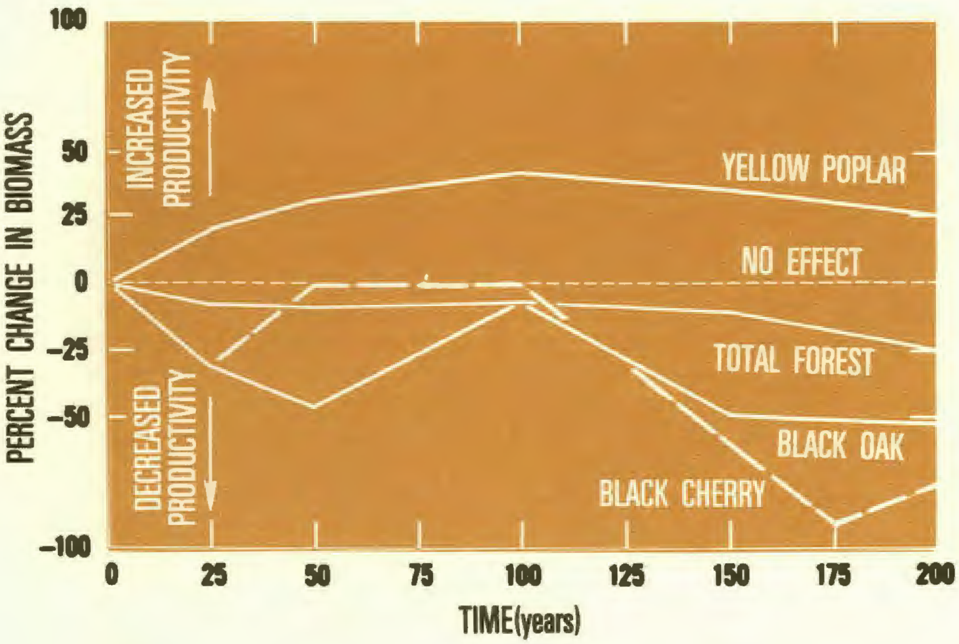
Absorption of gaseous pollutants by plant leaves may lead to physiological changes, ultimately causing reduced plant productivity. Rapid uptake of high concentrations leads to collapse of leaf cells and tissue death as shown following an SO_2 exposure of giant ragweed, a sensitive weedy species.

Dave Shriner examines a red kidney bean plant at the rainfall simulator. This device simulates the physical and chemical properties of rainfall to help ecologists assess effects of rainfall acidity and compositional changes on plants and soil.

mately two-thirds of which is associated with electricity generation. In addition to the amounts of these pollutants released, an important consideration is the distribution of the sources because this factor will determine ultimate ground-level concentrations to which vegetation is exposed. At present, over 80% of the nation's fossil-fueled power plants are located in the eastern half of the country, and approximately 50% are located in the Northeast. The high density of power plants in the East is combined with a high density of urban and industrial centers. In addition, the high frequency of air-stagnation systems in the eastern United States (second only to southern California) contributes to high levels of pollutants and poses a threat to valuable agricultural and forest crops.

Acid Rain

In addition to gaseous pollutants, a recently recognized phenomenon, acid rain, has added to both the complexity of the problem and the level of concern. Normal rainfall is slightly acid (pH 5.6) due to the uptake of CO_2 from the atmosphere and the formation of a weak carbonic acid solution. With increased input of sulfur and nitrogen oxides in recent decades, rainfall has become increasingly acid, primarily due to sulfuric and nitric acid formation in the atmosphere. Rainfall in the Oak Ridge area, for example, now has an average annual pH of about 4.1, a 40-fold increase over natural levels. Acidity of individual rainfall events in this area has exceeded normal levels by more than a hundredfold. The areal extent of these changes is impressive. Rainfall over most of the eastern United States is currently 10 to 40 times more acid than normal. Streams and lakes in the Adirondack region of the Northeast, where soil and water buffering capacity is low, are already experiencing significant impacts on growth and survival of fish populations. Current rainfall acidity exceeds by an order of magnitude that required to affect fish growth adversely. The effects of increased acidity on growth and survival of aquatic



ORNL ecologists have used simulation models as tools to examine the effects of air pollution stress on forest systems. This approach permits the study of chronic stress over time frames beyond the limits of ordinary laboratory and field studies. Results have indicated that competition between trees will strongly influence ultimate stress effects. Resistant species, such as white oak, and fast-growing, slightly sensitive species, such as yellow poplar, may show growth improvement. Other sensitive and less competitive species showed a much greater than expected loss of growth in the simulation.

organisms can be attributed both to direct effects of the acidity on the organisms and to the indirect effects of aluminum toxicity. Aluminum becomes a problem as increased acidity results in the accelerated leaching of the ionic species from soils and its enhanced availability in aquatic systems. Impacts on terrestrial vegetation due to direct contact with plant parts or indirectly as a result of changes in soil fertility have not yet been documented under field conditions, however. There is, in fact, evidence to indicate that in some areas of the southern and western United States where soil is deficient in sulfur, an essential plant nutrient, low levels of sulfur input from either acid rain or SO_2 may improve plant growth.

Our present concern about the threat from current levels of air pollutants to terrestrial ecosystems comes from laboratory studies, in which a variety of plant physiological processes have been shown to be affected, and from field studies, in which growth and yield of test plants have been measured. The p imary action site of gaseous air pollutants is upon plant leaves where pollutants enter by diffusion through stomata, the small pores in leaf surfaces. Pollutants ultimately enter the photosynthesizing cells after dissolving in the moist layer on internal cell walls (much in the same manner that gases enter the human blood stream following exchange through walls of the alveoli of the lungs). Once pollutants are inside leaf cells, they may produce biochemical and physiological effects as a result of a wide variety of reactions including biochemical oxidations or reductions, inhibition of specific enzymes, or breakdown of membrane systems leading to loss of cellular integrity. Where pollutant concentrations are high, leaf cells may be killed, producing foliar damage patterns that sometimes help in identifying the primary pollutant responsible. If foliar injury is either very extensive or repeated frequently, severe impacts on growth and even death of vegetation may occur. Large variations in sensitivity to air pollutants exist both within and among plant species. Symptoms of visible damage by ozone, a pollutant frequently occurring in high levels in the Oak Ridge area, include tan to silver flecks on upper leaf surfaces. Garden species on which these symptoms are most likely to appear include beans, cucumber, grape, petunia, potato, radish, spinach, and tomato.

More typical of the effects of present stress on plants are reduced plant growth (in the 0 to 20% range), altered reproduction (reduced seed size or numbers), or increased susceptibility of plants to other stresses such as insects or disease. A classic example of the latter response has been documented in the San Bernadino National Forest in southern California where ponderosa pine trees, weakened by ozone and other oxidants transported down valley from Los Angeles, have been heavily damaged by bark beetles.

Invisible Injury

An important concept in air-pollution research which has emerged (and which has been challenged) over the past four decades is the idea that plant growth and development may be adversely affected *in the absence of visible injury to foliage.* Opponents of the concept point to the fact that some plant species may experience yield reductions that are equal to or even considerably less than the fraction of total foliage area which is destroyed by high concentrations of pollutants. A considerable body of evidence has emerged in recent years, however, to support the validity of the concept of invisible damage. This concept is a cornerstone of our concern about the reality of present and potential levels of stress on plants from air pollution.

The challenges are many to plant researchers who are evaluating the impacts of air pollutants on terrestrial ecosystems. How do we measure the integrated effect of multiple pollutants on plant systems? Where an impact on plant growth, yield, or reproduction is measured, what pollutant or pollutant combination is responsible? How do the stresses that are a natural part of the plant environment (e.g., moisture, nutrition, insects, disease) influence plant response to pollutant stress?

The chronic nature of present-day air-pollutant stress dictates that realistic studies be made that consider the effects on plant response of both individual pollutants and pollutant mixtures. The duration and frequency of the stress episodes throughout the life cycle of test plants are also important because plant growth stages may greatly influence the effects of a given pollutant dose. Temperature, humidity, and light, which influence plant sensitivity to air pollutants, are also important variables to consider. The ultimate objective of research in defining these relationships is to assess accurately the extent to which present-day stress regimes may be influencing plant growth and development and to develop the capability to project the biological effects of potential changes in air quality associated with future technological development.

Current Research at ORNL

The Environmental Sciences Division (ESD) has been involved in research on the effects of air pollution on vegetation since 1975. Dave Shriner, Ron McConathy, Bill Johnston, Bill Selvidge, and I constitute the ESD staff directly involved in this research. The project evolved as a natural consequence of the formation of ERDA and the broadening of Laboratory-wide research programs that encompass both nonnuclear and nuclear technologies. The impetus for the present research has been the concern about the projected large-scale increases in our nation's dependence on coal for our future energy demands. Our attention has focused on the effects of effluents derived from coal combustion as well as from the developing coal conversion industry in which a variety of still rather poorly defined organic and inorganic gases may be released to the atmosphere. To date, our program has emphasized defining concentration thresholds for plant response to pollutants and identifying physiological stress indices from SO_2, O_3, and acid rain (primarily coal combustion problems), as well as benzene, carbonyl sulfide, and hydrogen sulfide, which are expected to be released from coal conversion facilities.

Since there are obvious limits in the extent to which controlled laboratory studies can approximate the complexities of real stress of biological and nonbiological origin, a variety of approaches have been used. These have included controlled laboratory experiments with gaseous pollutants, greenhouse experiments with acid rain, field studies evaluating the effects of our present-day air-quality regimes, and the application of simulation models designed to extend present-day knowledge into the relatively unexplored area of stress interactions over long time frames.

Laboratory Studies

The primary objective of our laboratory studies has been to determine concentration thresholds for plant response and to identify the biologically relevant indices of stress from pollutant doses. We are seeking the answers to many questions concerning the way in which plants react to various pollutants. For instance, do plants respond more to an average concentration of pollutants over a specified time interval or to short-term fluctuations during that interval? What is the maximum averaging interval that reflects the potential damage from an exposure? How much is plant response influenced by previous exposure history? Do our present air-quality standards adequately protect vegetation, or should they be revised? Answers to these questions are essential if we are ever to develop the capability of using air-quality monitoring data to predict vegetation response to pollutants. At ORNL, research has been aided by the fabrication of a programmable SO_2 exposure system which permits reproduction of a variety of concentration regimes in test chambers. This system provides a much more realistic representation of exposure kinetics (rate of change, peak-to-mean concentra-

ORNL ecologists are studying the effects of a variety of air pollutants currently causing chronic regional scale stress in the eastern United States. Their research is aimed at assessing potential effects of increased coal utilization on agricultural and forest productivity.

tion ratios, etc.) than do conventional steady-state systems. It also permits introduction of one or more additional pollutants for conducting interaction studies.

In the studies we have made thus far, we have used kidney beans in the test system because this species has the advantage of a relatively short growing cycle and is a member of the economically important legume (nitrogen-fixing) plant group. In the future, we will expand our work to include other species of both crops and forest trees. Physiological responses of test plants, such as CO_2 uptake (photosynthesis) and water loss (transpiration), are measured as indices of stress potential of various concentration regimes. Measurements of these processes are performed using infrared gas analyzers which can detect slight changes in CO_2 and H_2O in the air within experimental chambers where plants are placed for pollutant exposure. Results from studies with SO_2 indicate that the peak concentration during an exposure episode is much more important in determining plant response than the average concentration over the 3-hr averaging interval currently specified for protection of vegetation from sulfur dioxide by the Environmental Protection Agency. Photosynthesis, the process by which plants use the energy of sunlight to manufacture carbohydrates for growth and development, is quite sensitive to SO_2 and may be inhibited by approximately 30% when SO_2 concentrations reach approximately two-thirds of the present air-quality standard. This inhibition appears transitory, however, and recovery to normal rates is generally attained within 24 hr. So far, our studies have not detected a sensitization of this response by previous SO_2 exposure. A study of the influence of relative humidity on response of plants to SO_2 has also shown that high humidities typical of the eastern United States ($\geq$70%) significantly enhance the inhibition of photosynthesis and, apparently, the uptake of SO_2.

Greenhouse Studies

Our greenhouse studies with acid rain have been directed toward characterizing both the range of plant responses and the acidity threshold for producing these responses. Essential to this effort has been the development by Dave Shriner of a rain simulator with which the chemistry and physical characteristics of rainfall can be closely approximated. Initial experiments with daily exposure to a pH of 3.2 (the approximate highest acidity level that has been recorded in the Oak Ridge area during the past three years) show a broad range of effects on the kidney bean test system. These included reduced leaf chlorophyll, reduced photosynthesis, and reduced plant growth. Detailed examinations with a scanning electron microscope by Dave Shriner and Frances Ball (of the Analytical Chemistry Division) indicate that weathering of the protective waxy layer on leaf surfaces may be accelerated by acid rainfall. Changes of this type have important implications for energy exchange by leaf surfaces and for possible alterations in leaf resistance to pathogen invasion. Of the responses measured thus far, we have found that plant growth appears to be the best indicator of stress produced by acid rainfall. An additional preliminary finding from experiments at these rather high acidity levels is that interactive effects of SO_2 and acid rain on photosynthesis may be greater than the combined effect produced by either pollutant acting singly.

Recently, we have tried to characterize effects of treatments in which both the acidity level and the rainfall frequency approximate that in East Tennessee. Results indicate that present acidity levels are at or just barely above the threshold for growth inhibition. When additional pollutants such as ozone are present, growth—particularly of root systems—may be retarded. Such studies of interactions among pollutants represent a particularly relevant area for further research involving acid rain.

Field Studies

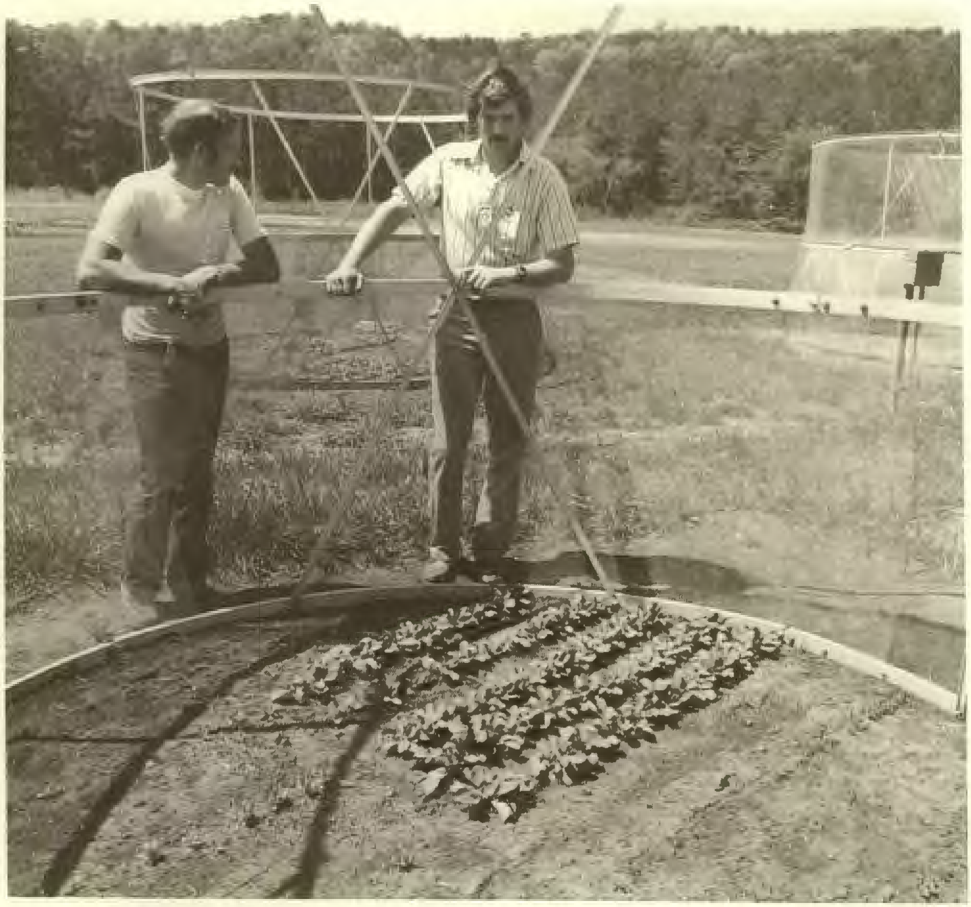
Although there are many advantages to controlled laboratory and greenhouse experiments, there is no substitute for field research to evaluate the response of biological organisms to environmental stress. However, field conditions with their many uncontrolled variables can provide a frustrating array of problems. For example, Tennessee Valley Authority biologists in the past have had to investigate claims of yield losses to agricultural crops, primarily soybeans, growing in the vicinity of some of their coal-fired power plants. Multivariate statistical techniques can account for only part of the changes in crop yield that would be expected with differing cultural practices, soil fertility, crop varieties, and disease incidence. Of course, the ultimate question is whether crops under these same conditions would have responded similarly if SO_2 injury to foliage had not occurred.

An important advance in our ability to address this question has come from the U.S. Department of Agriculture, where researchers have developed charcoal-filtered field chambers. Using an air-purification system, these chambers permit side-by-side comparisons of field plots grown in clean air with those grown in either ambient air or air to which additional pollutants have been added. These chambers have been used in a variety of locations across the United States. Yield losses of beans in Maryland have been as high as 27%, and losses of tobacco in North Carolina of 30% have been detected under chronic stress regimes. Productivity losses of up to 50% of citrus fruit have been measured in California.

We are currently setting up a system of field chambers at ORNL to measure the effects of chronic stress on productivity of both agricultural crops and forest tree seedlings. Preliminary results from studies conducted last summer showed 40% reductions in growth and yield of a variety of bush beans that is sensitive to air pollution. These data were obtained from comparisons of plants grown in unfiltered air with those grown in charcoal-filtered air in adjacent plots. Studies are continuing at this site to examine responses of other species and to determine the physiological basis for observed responses. An important objective of our work is to define the relationship of physiological and growth effects to the distribution of exposure episodes in time and to their respective concentration levels.

Simulation Modeling

Although field-chamber studies appear well suited for evaluating responses of agricultural crops and tree seedlings, measuring impacts of stress on forest systems presents a much more complex problem. Because of their perennial life form, much longer time frames are needed to evaluate the effects of stress on forest trees. Because diverse species are normally present, the effect of competition among forest species must be considered. This process plays an extremely im-



An important ultimate objective of air-pollution-effects assessment is measurement of responses of vegetation grown in the field. Here McLaughlin, r., and Bill Selvidge examine study plots which are used in comparing growth of plants in polluted air and air purified by charcoal filtration.

portant role in species composition during succession (the developmental process by which forest stands grow and mature).

To address these problems, researchers are using a simulation model developed by Hank Shugart and Darrell West of the Environmental Sciences Division. The computer model, FORET, was developed to study the successional dynamics of our eastern forests and provides a useful tool for testing the effects of stress on forest growth and development. An important feature of FORET is that it permits evaluation through time of changes in biomass both of individual species and of the forest stand. By varying the levels of imposed stress (in the form of growth limitation) for species of differing sensitivity to air pollutants and by changing the forest maturation stage at which that stress is imposed, the interactions of competition, stress, and time can be studied. Results thus far have indicated that competition will have a very important influence on the way our forests respond to long-term stress. Depending on the species, the effects of air pollutants may be either greatly enhanced or reduced from levels predicted from studies conducted in a noncompetitive environment. This modeling approach helps us to examine some important questions that cannot be addressed with conventional experiments. In this capacity, modeling provides a framework within which to ask new questions and to design new experiments.

Considering our present air-pollution problems and our research findings thus far, what might we anticipate in the future? Much can be expected to depend on the rate and direction of our future energy consumption. It seems certain that at least in the near term increased utilization of coal will occur. The location of these new coal-burning or coal-converting facilites and the emission-control strategies employed will greatly reduce the impact on the environment.

Measured in terms of regional-scale impacts on vegetation, the most significant pollutant appears to be ozone, which is produced as a secondary pollutant from many sources. Ozone levels and associated photochemical haze build up very rapidly during summer months whenever stable air conditions exist for more than a day. The rapidity of this buildup has produced visible injury to sensitive white pine trees in the Oak Ridge area on several occasions during the past few summers. Such a buildup attests to the extent to which wastes dumped into the atmosphere from many industrial and urban sources are influencing both local and regional air quality. The rate at which our air quality will continue to deteriorate depends on three important considerations: (1) changes in the national need for energy and industrialization, (2) technological advances in emission controls, and (3) realistic quantitative estimates of the nature and extent of environmental damage. It is our hope that these factors are considered with both balance and foresight.

take a number

BY V. R. R. UPPULURI

Paired Comparisons Yielding a Ranking

Suppose we have four stones with unknown weights, and we wish to rank them according to their weight. Let us assume that we are good at comparing objects two at a time. In other words, we can determine for a pair of stones (S_3, S_4) whether stone S_3 is heavier than stone S_4 and vice versa. Let us also assume that if stone S_3 is heavier than stone S_4, we can be more precise and determine how much heavier stone S_3 is than stone S_4. For instance, stone S_3 may be 1.5 times as heavy as stone S_4, which is equivalent to saying stone S_4 is 1/1.5 times as heavy as stone S_3. We also assume that when we are comparing two stones, we do not think of the others. Since humans tend to be inconsistent, it is likely that the resulting pairwise comparisons will not necessarily be consistent. This is not surprising in the light of Arrow's paradox, and we should be able to use the data of pairwise comparisons to draw valid conclusions. Given the information concerning the relative comparisons of pairs, the problem is to determine a ranking of the weights of the stones S_1, S_2, S_3, and S_4.

In 1976, Thomas L. Saaty at the Wharton School of the University of Pennsylvania proposed a method of ranking objects according to their weight, given the information on pairwise comparisons. For instance, let the pairwise comparisons of four stones S_1, S_2, S_3, and S_4 result in the matrix given below.

	S_1	S_2	S_3	S_4
S_1	1	2.5	3.0	3.5
S_2	1/2.5	1	1/4	2
S_3	1/3.0	4	1	1/1.5
S_4	1/3.5	1/2	1.5	1

This matrix summarizes the data obtained by pairwise comparisons. The first row of the matrix shows that stone S_1 is as heavy as itself; S_1 is 2.5 times as heavy as stone S_2; S_1 is 3 times as heavy as stone S_3; and S_1 is 3.5 times as heavy as stone S_4; and so on. Just as the first row determines the comparisons of the first column, the second row determines the comparisons of the second column, and so on.

The application of Saaty's method* to this problem yields the following ranks to the weights of the stones $S_1 > S_3 > S_4 > S_2$. In other words, S_1 is the heaviest stone; S_2 is the lightest stone; and S_3 and S_4 are in between as shown. Actually, if the total weights of the four stones are normalized to unity, the weights of the four stones S_1, S_2, S_3, and S_4 expressed in percentages are 45.3, 15.2, 23.9, and 15.6 respectively.

*Saaty's method involves finding the eigenvector associated with the largest eigenvalue of the observed matrix and normalizing the components of the eigenvector so that they add up to 100%. At Oak Ridge, the Mathematics and Statistics Department has developed an alternate method to that of Saaty based on logarithmic least squares. Although the answers are not identical, both the methods give comparable rankings. For instance, in the above problem, the logarithmic least-squares approach gives identical rankings for the weights of the four stones.

Fred Hartman and Lucile Norton examine spinach in a growth chamber at the Biology Division. The carboxylase used in their studies is extracted from spinach and from photosynthetic bacteria. Carboxylase is the enzyme that initiates the series of reactions that enable plants to convert atmospheric carbon dioxide to a useful food.

Enzymes, Plants, and Drugs

By CAROLYN KRAUSE

A half century ago, British bacteriologist Alexander Fleming was inspecting some petrie dishes with cultures of staphylococci that he had made several days before in his laboratory at a London hospital. One particular dish caught his eye because its normal colonies of the pus-forming bacteria were interspersed with areas on the nutrient agar where bacteria had failed to grow. After noticing that these areas were contaminated with common bread mold from an unknown source, Fleming made subcultures of the mold and observed its antibacterial action. Because the mold has the scientific name *Penicillium notatum,* he affixed the name "penicillin" to the substance in the mold that is lethal to bacteria. Although he reported his results in 1929, penicillin was not produced in substantial quantities until World War II

Fred Hartman was born, reared, and educated in Memphis. He received his B.S. degree in chemistry from Memphis State University in 1960 and his Ph.D. in biochemistry from the University of Tennessee medical units in Memphis in 1964. After completing two years of post-doctoral studies at the University of Illinois, he joined the ORNL staff in 1966. Since 1975 he has been section head of the Molecular and Cellular Sciences Section, which envelops much of the Biology Division's basic research. In 1976 Hartman served as acting director of the Biology Division while J. B. Storer was on leave of absence. His primary research interests are enzyme mechanisms and the design and use of affinity labels for defining structure-function relationships in biologically active macromolecules. This year he was chosen the recipient of the coveted Pfizer Award in Enzyme Chemistry, established in 1945 to stimulate fundamental research in enzyme chemistry in the United States. It is presented annually to a researcher not more than 40 years of age who is engaged in noncommercial work and has performed outstanding work in enzyme chemistry. Hartman, 39, will receive the award in September at the Washington, D.C. meeting of the American Chemical Society.

when it was used to save many lives. It has proven an effective weapon against a variety of infections, including meningitis, pneumonia, and syphilis.

In the same decade that Fleming made his serendipitous discovery, a German biochemist was performing important experiments on the uptake of oxygen in tissues. Working in Berlin in the 1920s, Otto Heinrich Warburg devised an instrument for measuring the rate of uptake of oxygen and conducted a number of studies with his "Warburg manometer" on normal and cancerous tissues. In one of his experiments he exposed plants to above-normal levels of oxygen and observed that plant growth was stunted. Subsequent corollary experiments by other scientists have shown that subjecting many species of plants to artificial atmospheres enriched in carbon dioxide (CO_2) and/or low in oxygen content resulted in an increase in plant growth by as much as 50 to 100%. Except for corn and sugar cane, most food crops have been found to respond favorably to elevated CO_2 levels and diminished oxygen concentrations.

These two discoveries by Fleming and Warburg may appear to have nothing in common except that the discoverers were Nobel Prize winners in medicine and physiology who did their best work in the 1920s. But a closer look reveals that the phenomena observed are dependent on the action of enzymes—proteins which speed up chemical reactions in living things without being consumed or altered in the process. These organic catalysts are essential to life; if certain enzymes in an organism are rendered inactive by poisons or drugs, the organism will die.

In 1966, it was discovered that penicillin's antibacterial action can be attributed to its ability to inactivate certain enzymes unique to many bacteria that catalyze the synthesis of cell walls in young and actively multiplying microorganisms. Thus, penicillin acts not by killing older bacteria, but by preventing the survival of new microbes.

The unfavorable response of plants to elevated oxygen levels and the ability of plants to grow better in an artificial atmosphere rich in CO_2 or depleted in oxygen are explained by a property of an enzyme unique to plants which initiates a series of reactions that convert atmospheric CO_2 into a useful sugar. A carboxylase, this enzyme hastens the reaction of CO_2 with a basic plant sugar named ribulosebisphosphate to form another product which is transformed after a series of reactions into glucose, the main plant foodstuff. But this same enzyme also speeds the reaction of ribulosebisphosphate with atmospheric oxygen, leading to the eventual formation of a product of no benefit to the plant. Thus, the enzyme catalyzes a reaction which wastes energy and consumes part of the ribulosebisphosphate, diverting it from use for making carbohydrates and thereby inhibiting plant growth. This Jekyll-and-Hyde ability of a carboxylase to catalyze both useful and unproductive reactions using CO_2 and oxygen, respectively, was discovered in 1973 by N. E. Tolbert, a Michigan State University biochemist who worked at ORNL in the 1950s.

If this carboxylase's ability to catalyze reactions with oxygen could be eliminated, plant yield

"If this carboxylase's ability to catalyze reactions with oxygen could be eliminated, plant yield for most food crops would be greatly increased..."

for most crops would be greatly increased, making available more food. Finding out whether this agronomical Holy Grail is attainable is one goal of Fred Hartman, head of the molecular and cellular sciences section in ORNL's Biology Division. In his 12 years at the Laboratory, Hartman has made great strides in enzyme chemistry. His applications of the "affinity-labeling" technique have been received enthusiastically by the community of pharmacologists because many naturally occurring antibiotics, such as penicillin, and synthetic drugs work by reacting with active sites in enzymes. An understanding of the mechanism by which some drugs work has been gained from studies in affinity labeling; likewise, the technique shows promise for systematically designing new therapeutic agents. The affinity-labeling technique was first introduced into enzymology by Elliott N. Shaw, director of the Biology Department at Brookhaven National Laboratory.

As a result of the ORNL biochemist's work, the American Chemical Society (ACS) has selected Hartman as the recipient of the Pfizer Award in Enzyme Chemistry for 1979. Sponsored by the Pfizer Pharmaceutical Company, the award is a prestigious one, shared by many members of the National Academy of Sciences including Howard Temin, a recent Nobel laureate. Hartman will receive it at an ACS meeting in Washington, D.C., this September. At that time, a half-day symposium will be devoted to his prize-winning work on affinity labeling and to techniques developed elsewhere for understanding what makes enzymes tick.

Life-Giving Enzyme

In human cells, there are at least 5000 different enzymes, each of which is selective for speeding up a single chemical reaction. The simplest enzymes are composed of about 100 amino acid units, while the most complex have several thousand units. Amino acids, of which there are 20 different types, are molecules made primarily of carbon, hydrogen, nitrogen, and oxygen with an amine group (NH_2) at one end and a carboxyl group (COOH) at the other.

The carboxylase is not one of the 5000 enzymes in human cells, because it is unique to plants. Even so, it is a complex enzyme, with 5000 amino acid units, and it is absolutely essential to all life on earth. It is the key to the carbon cycle of photosynthesis, the process by which plants use carbon dioxide, water, and the energy of sunlight to make carbohydrates. This enzyme is necessary not only for satisfying the nutritional needs of people and animals indirectly, as well as those of plants, but also for maintaining the earth's oxygen supply. Without plants, the atmosphere would become overloaded with CO_2, asphyxiating animal life. Says Hartman: "Only some species of life contain the carboxylase enzyme, but all species, except for a few primitive microorganisms, are dependent on it for food and oxygen."

Technically called ribulose-bisphosphate carboxylase, this life-giving enzyme was discovered in the 1950s by Melvin Calvin, who received the Nobel Prize in chemistry in 1961 for describing the process of photosynthesis. Calvin found that the five-carbon sugar ribulosebisphosphate accepts CO_2 in leaf chloroplasts in a reaction catalyzed by carboxylase to yield two molecules of phosphoglycerate, a three-carbon sugar. Following a series of reactions selectively catalyzed by five different enzymes, the two phosphoglycerates are put together to make the six-carbon glucose phosphate, the ultimate food product of photosynthesis. Meanwhile, ribulosebisphosphate is regenerated after the six cycles required for incorporating enough carbon to generate glucose phosphate.

Plants discharge oxygen to the air during photolysis when chlorophyll (the nonprotein that makes plants green) uses the energy of sunlight to catalyze the splitting of water into oxygen and hydrogen, which provides chemical energy to drive the ribulosebisphosphate cycle. Thus, light energy from the sun, which causes loss of oxygen or gain of electrons (reduction), is converted

"If we can characterize the active site of an enzyme, we can learn much about the mechanism of catalysis."

to chemical energy in plants with the help of catalysts.

The Food Problem

Atmospheric oxygen is used by plants in an unproductive process called photorespiration. As Tolbert discovered, carboxylase accounts for photorespiration by catalyzing the reaction of some of each plant's ribulosebisphosphate with oxygen, a pathway which reduces the net synthesis of carbohydrate. If a way could be found to reduce or eliminate this unproductive oxygenase activity of carboxylase without interfering with its ability to fix atmospheric carbon dioxide, then it might be possible to grow crops with increased mass.

Boosting crop yield per unit of land is a desirable way to increase food production because the alternative—expanding crop area—seems unlikely since almost all fertile land is already under cultivation and there will be greater competition for this land to raise plant biomass for an energy source. Thus, much research is focused on increasing crop yield to meet the rising food demands of the world's growing population. To avert mass starvation in the next century, it is estimated in a National Academy of Sciences study that crop yields must increase about 2.5% a year for the next 25 years.

Researchers supported by the U.S. Department of Agriculture and agricultural chemical companies are currently trying two approaches to improving crop yields through alteration of the carboxylase:

Genetic manipulation. Scientists use chemical mutagens to produce plant mutants and then screen these mutants for plants that exhibit efficient growth. The desired mutation would be loss of oxygenase activity, but so far no plant mutant with this trait has been found.

Chemical manipulation. The larger agricultural chemical companies are testing a variety of chemicals in the hope of finding one that favorably alters the properties of carboxylase. Is this massive trial-and-error effort of screening for effective chemical agents worth the time and money? Fred Hartman hopes to shed light on this question.

Active Sites

Of the 5000 amino acid units in this carboxylase, only a few units play a critical catalytic role. But the other units apparently have a function, like the razor to hold the blade. They give the enzyme size and shape. An enzyme must be large enough to be confined in plant cells; if it were too small, it would diffuse through cellular membranes and be excreted. If an enzyme were a straight chain, its catalytically active acids would be widely separated. The presence of hundreds of amino acid units allows the molecular chain to be coiled into a three-dimensional conformation characterized by folds and loops, as in a tangled Slinky. This geometric arrangement brings the catalytically functional amino acids together in a close-knit unit called the active site.

Hartman has devoted most of his career to the arduous task of characterizing active sites of enzymes. Now he is focusing much of his effort on identifying the amino acid units in the carboxylase that are essential to catalysis.

"If we can characterize the active site of an enzyme, we can learn much about the mechanism of catalysis," Hartman says. "What amino acids are involved in catalyzing the carboxylation and oxygenation? What happens if these amino acid residues are chemically altered? Can alteration provide a means of changing the ratio of oxygenase to carboxylase activity? Are the same amino acids operative for both pathways or are there several amino acids used for oxygenase activity but not for carboxylase activity? If so, could these acids be chemically modified or altered so that the plant's ribulosebisphosphate is used solely for CO_2 fixation?"

If Hartman should find that specific amino acids are critical to oxygenase activity only and could be selectively modified by a chemical agent, a potential benefit to world agriculture could be realized by chemical treatment of food crops.

Claude Stringer adjusts the amino acid sequencer used to determine the order of amino acid units in enzymes such as carboxylase. About 50 amino acid units can be clipped off in succession and their sequence thus determined.

Putting it cautiously, Hartman says, "With this information, we would be in the position to consider the feasibility of altering the enzyme's activity for the benefit of mankind. That doesn't mean we could actually make these changes, but we could determine if beneficial changes might be possible."

If Hartman learns that chemical modification of crops to increase yield is not practicable, then this information will provide guidance to government policymakers and executives of agricultural chemical companies who make decisions on spending money aimed at genetic and chemical manipulation of plants. And whatever the results of the research, basic biology should benefit. Says Hartman: "Any detailed characterization of an enzyme's active site will have valuable fallout in understanding the complexities of catalysis."

National Interest

The implications of Hartman's research for food and energy production as well as for basic understanding of catalysis have stimulated considerable interest in his work, as reflected in the support he is receiving from two federal government Cabinet departments—Energy and Agriculture. The U.S. Department of Agriculture is seeking information on the structure of carboxylase and the possibility of chemically altering it to elevate crop yield. DOE's Health and Environmental Research Division supports Hartman's work primarily because of its potential contribution to basic enzymology but also recognizes the relationship of this work to energy generation from biomass, such as fast-growing woody plants.

Hartman and his associates have embarked on a five-year project to determine the structure of carboxylase and to pinpoint the mechanism by which the enzyme catalyzes the initial reactions for photosynthesis and photorespiration. His present associates are I. Lucile Norton and Claude D. Stringer. An ex-associate, John V. Schloss, was a doctoral student at the University of Tennessee-Oak Ridge Graduate School of Biomedical Science and is now doing postdoctoral work under the University of Wisconsin's W. W. Cleland, generally regarded as the world's foremost enzyme kineticist.

The amino acid composition of carboxylase is known, but Hartman and his associates will be undertaking the laborious task of determining the linear sequence of the amino acid units in the protein chain. The project involves using chemical procedures to clip off amino acids one at a time, then to analyze the residues. To acquire additional insights into the enzyme's structure, Hartman is collaborating with an investigator from the Massachusetts Institute of Technology who specializes in x-ray crystallography.

Affinity Labeling

In late 1974, Hartman published his first paper on his new methodology for identifying active site residues in carboxylase. It is this methodology, called affinity labeling, that earned him the Pfizer Award of 1979.

Until recently, the characterization of active sites in enzymes entailed primarily the conventional method of treating the enzyme of interest with a chemical and observing whether the enzyme's activity was reduced or abolished. If the enzyme is inactivated, then it is possible to determine which amino acids in the enzyme are "turned off" by the chemical. The problem is that many amino acids are repeated many times throughout the coiled protein chain, so it is difficult to determine which of the amino acids modified by the chemical reagent are actually located in the active site. To overcome the nonspecificity of chemical reagents in general, Hartman uses the technique of affinity labeling.

The enzyme carboxylase reacts with ribulosebisphosphate, which is the substrate—that is, the substance whose reaction is catalyzed. Every enzyme binds its substrate in a highly selective fashion, the way a key fits into a lock. By binding the substrate with noncovalent (loose) bonds, the enzyme speeds up the substrate's reaction with another compound, such as CO_2 in the case of ribulosebisphosphate.

Affinity labeling is the technique of creating a compound that is similar to the substrate in that it has a built-in affinity for the enzyme's active site. The difference is that this chemically similar compound, or synthetic analog, can become bound to the enzyme by covalent bonds—linkages that are not easily broken in which electrons are shared. In addition, this chemical agent, tailor-made to fit into the enzyme, has the ability by virtue of its covalent bonds to inactivate the active centers of the enzyme. By use of conventional chemical procedures, Hartman and his colleagues can pinpoint where the substrate analog is attached to the enzyme.

One active-site amino acid that Hartman identified in carboxylase is lysine. To do this, he had to design an analog agent never before synthesized. He searched for an agent which, like ribulosebisphosphate, contains a phosphate group at both ends of its carbon chain but, in contrast to ribulosebisphosphate, is chemically reactive toward certain amino acids. To meet these criteria, Hartman and his associates synthesized bromobutanone bisphosphate, which, due to the presence of the halogen bromine, is a reactive compound. When this synthetic analog was reacted with carboxylase, the halogen group in this new compound was displaced by the amino group of lysine. The nitrogen in the lysine was covalently fixed to the carbon in the new compound. Thus, the lysine could no longer carry out its function and the enzyme's catalytic activity vanished.

"In treating and observing this enzyme," Hartman says, "we saw the covalent incorporation of the labeling agent and the concomitant lowered activity of the enzyme. To see where the labeling agent was attached to the enzyme, we clipped out the appropriate segment of the protein chain and analyzed it chemically." The only problem with this new compound, Hartman adds, is that it is not absolutely specific for the active site, but it certainly is superior to nonspecific chemical reagents.

Hartman has worked with other enzymes besides carboxylase, which he obtains from spinach and the photosynthetic bacterium, *Rhodo-*

spirillum rubrum. In the 12 years that Hartman has been at ORNL, he has experimented with half a dozen enzymes and synthesized many labeling agents. In selecting Hartman for the Pfizer Award, the ACS cited him "for important contributions to enzyme chemistry through the synthesis and utilization of active-site-directed covalent inhibitors of several important enzymes. These studies have included inhibitors of triosephosphate isomerase, aldolase, ribulosebisphosphate carboxylase and oxygenase, alcohol dehydrogenase, and several others."

Designing New Drugs

Most drugs are chemicals with the ability to inactivate specific enzymes. The therapeutic value of the drug penicillin lies in its ability to react covalently with enzymes essential to the biosynthesis of cell walls of bacterial pathogens. Such enzymes are not present in the human body. Mold bacteria make penicillin to protect themselves against infection from foreign bacteria. Another common therapeutic drug, aspirin, thins the blood and depresses blood clotting by inactivating an enzyme responsible for making blood platelets.

One anticancer agent, deoxyfluorouracil, works through enzyme inactivation to treat leukemia. This drug inactivates an enzyme essential to the biosynthesis of DNA, the genetic material of cells. Deoxyfluorouracil is a toxic agent which preferentially kills cancer cells because they divide more rapidly than normal cells. Thus, cancer cells have a greater dependence on the enzyme that catalyzes the synthesis of the genetic material passed onto new generations of cells. Because the whole body is dependent on the enzyme essential to DNA biosynthesis, this type of cancer chemotherapy has deplorable side effects, especially if improperly administered. Physicians strive to control the dosage of anticancer drugs to minimize side effects.

If one knows of specific enzymes essential to the existence of a disorder or of unwanted cells or pathogens, one can use the technique of affinity labeling to synthesize a compound that has an affinity for the enzyme and inhibits it by covalent bonding. There are compounds now being tested clinically for certain kinds of tumors and certain nervous disorders which were synthesized as affinity labels for specific enzymes.

One such drug designed systematically through the application of affinity labeling might benefit the chronically depressed. Explains Hartman: "People with some types of nervous disorders have either an excess or a deficiency of neurotransmitters, chemicals that stimulate nerve endings for the transmission of nerve impulses. Some people who are depressed all the time have an abnormally high level of antagonists, chemicals which block transmission of nerve impulses. Certain enzymes regulate the levels of neurotransmitters and antagonists. To treat depression, a drug has been synthesized—using the principles of affinity labeling—which inactivates an enzyme involved in the synthesis of antagonists. The drug is of potential benefit in those cases where depression is a consequence of an enzyme whose excess is responsible for the elevated level of antagonists."

Affinity labeling presents an effective means to characterize and alter active sites of enzymes and to control their effects. If the technique exploited at Oak Ridge is used to its full potential, it might help solve problems of curing illness, increasing energy supplies, and producing more food for a growing population. ornl

Staff quote:

"One of the more impressive features of our tour of Feldt's facilities was the sophisticated system for waste treatment of radioactive liquid effluents which are produced by the Laboratory. Commercial radioactive-waste-disposal equipment, which functions to concentrate, solidify, and encase the Laboratory's radioactive waste in concrete, has been installed in the lower basement of the Institute. The final disposal site will be either in salt mines or in the deep sea. The treatment process is fully automated and can be monitored electronically."—F. Owen Hoffman, discussing his visit last year to the Isotope Laboratory, Federal Research Center for Fisheries, Hamburg, F.R.G.

information meeting highlights

CHEMISTRY DIVISION, March 20

Halides and Corrosion

In the search for a mechanism that would explain two well-known aspects of localized corrosion (i.e., crevice corrosion, pitting, stress corrosion cracking, etc.), Gene Kelly has conducted a comparative study of the electrochemical behavior of titanium in acidic sulfate and acidic chloride media. The two previously inexplicable phenomena are (1) the "random" occurrence of spontaneous cessation (self-healing) of localized corrosion, and (2) the notorious association of halide ions with localized corrosion.

In the microscopic lesions present in the protective oxide film, both active (oxide-free) and passive (covered with a thin film of TiO_2) titanium surfaces are present, the former obtaining in the innermost tip region of a crack or crevice. As corrosion occurs on the active surface, the dissolution product, Ti(III), is oxidized along the passive walls to join Ti(IV), which diffuses back to the active surface. When the concentration of Ti(IV) at the active surface attains a certain critical value, repassivation (self-healing) of the active surface occurs, meaning that localized corrosion stops.

The kinetic parameters in the sulfate and chloride systems are such that the critical concentration of Ti(IV) required to passivate the active surface is approximately ten times as great in the chloride system as in the sulfate system, and the time required for its attainment is one or two orders of magnitude greater in the chloride system. Consequently, the halide ion functions as a promoter of localized corrosion. It seems likely that the mechanism is applicable to other metals and alloys. In steel, for example, a minor alloying element such as chromium may provide a couple analogous to the Ti(III) or Ti(IV) couple.

Structure of Molecular Liquids

Fluids consisting of nonpolar molecules—such as gasoline, lubricating oils, and other hydrocarbons—are amenable to theoretical analysis. But water and ionic solutions, such as salt dissolved in water, are examples of molecular fluids whose structure is not well understood by theorists. These fluids consist of atoms or molecules with strong attractive forces.

Now, Elijah Johnson, former Eugene P. Wigner Fellow and currently a theoretical chemist on the ORNL staff, is formulating a theoretical method that he hopes will describe the structure of fluids which have strong attractive intermolecular interactions. The theory makes use of statistical mechanical methods to compute the average relative location of molecules.

Tests of a number of molecular liquids have been conducted by Al Narten of the Chemistry Division. These liquids include carbon disulfide, carbon tetrachloride, and hydrocarbons like benzene and neopentane. To measure fluid structure—that is, the relative average location of molecules—Narten scatters radiation, x rays and neutrons, with a wavelength comparable to the spacing between molecules and then analyzes the diffraction pattern.

Narten's x-ray scattering experiments are now performed with a conventional x-ray source, but he plans to do collaborative measurements using synchrotron x-radiation at the National Synchrotron Light Source at Brookhaven National Laboratory. Narten conducts neutron scattering experiments at the High Flux Isotope Reactor, which offers the world's highest thermal neutron flux. Both types of scattering radiation are used to complement each other, since x rays are scattered by electrons and neutrons are scattered by nuclei.

Understanding structure is not the ultimate goal of these studies, however. Johnson sees the determination of structure as a prerequisite for understanding thermodynamic properties of these fluids, such as freezing and boiling points.

Understanding structure, Narten says, will help chemists make correlations between structure, such as molecular chain length, and bulk properties. For example, he notes that oil mixtures with an average chain length of 15 carbon atoms tend to have the best lubricating properties. Good correlations between structure and properties are important because they make possible accurate predictions.

In the future, Johnson plans to treat theoretically the molten salts, whose molecules or atoms exhibit strong attractive interactions. More work will be done to shed light on the structure of liquid hydrocarbons, such as the alkanes—methane, ethane, propane, butane, and others. Results of such studies could prove extremely relevant in a research laboratory striving to find economic and technically feasible methods of converting coal to liquid and gaseous fuels. ornl

Frank Modine, a Solid State Division physicist, is on assignment for a year to the Program Planning and Analysis Office. There he has become coordinator of the Seed Money Program and a member of the Proposal Review Committee, shown here in conference behind him. Members at the time this picture was taken were Carlos Bamberger, Bob Clausing, John Moyers, Ed Bondietti, Loucas Christophorou (chairman), Bob Hightower, and David Crandall. Not pictured are Charlie Nowlin, James Selkirk, and James Roberto. Since this picture was taken, retiring members Bamberger, Clausing, Moyers, and Selkirk have been replaced by Pat Callahan, Virgil Haynes, Marvin Poutsma, and Ray Tennant. Modine, who has been at the Laboratory since 1971, and who has his Ph.D. in physics from the University of Oregon, shares with us in the following article what he has learned about the Seed Money Program.

The Seed Money Program

By FRANK MODINE

Have you noticed more new R&D lately? When you read the ORNL *Review* or when you hear a State of the Laboratory address, have you noticed new R&D on coal, solar cells, and environmental hazards? Have you heard about the new methods for detecting single atoms, measuring burn severity, and raising exotic fish? If you are aware of these and other recent developments, you know that the Laboratory's R&D is changing, and you also may know about the Seed Money Program.

R&D at ORNL has changed in the past. The policy has always been to direct our R&D to meet national goals, a policy which means changing with the times. After starting with research in support of the war effort during World War II, the Laboratory moved toward research on peaceful uses of nuclear technology. In recent years, however, broader roles in energy technology and new environmental missions have brought more and more change. The rate of change was increased by the transition from AEC to ERDA to DOE, and the change has continued to accelerate because of the energy crisis and new national policies.

How does the Laboratory meet new and rapidly changing demands? Mainly, by trying harder, but there is one special way that stands out—the Seed Money Program. The program was started in 1974, principally to facilitate R&D change and growth at ORNL, which it does by attracting, encouraging, and developing new ideas. The success of the Seed Money Program has led to its

"... more than two-thirds of the ideas considered are funded for development."

current annual budget of nearly $1 million, a sum completely devoted to sponsoring new R&D.

The Seed Money Program succeeds for a reason. Analogous to a suggestion box for the Laboratory's technical staff, the program does more than collect ideas; it transforms good ideas into new R&D projects. This program is especially well suited to ORNL because it matches research needs with capabilities in a large, highly technical institution. Ideas for new R&D are often technically complex and, consequently, difficult to evaluate; the program overcomes this problem by relying heavily on the diverse talents of the technical staff. Ideas for R&D often need preliminary development before they can be fully appreciated; the program funds this development.

Encourages Creativity

The Seed Money Program is notable not only because it fulfills an important need by promoting new R&D but also because it encourages the staff to be more creative and because it is run largely by the R&D staff. The Laboratory benefits because the program identifies new R&D possibilities, thus defining the options for change and expansion. However, much of the Seed Money Program's success probably stems from the fact that it benefits the staff by supplying opportunities, which often would not otherwise exist, to pursue interesting ideas and thereby to obtain much personal satisfaction.

How does the Seed Money Program function? Under the program, technical staff members take ideas for new R&D to a committee of their peers rather than to Laboratory management. The committee helps evaluate the merits of the ideas and their possibilities for further development. It enlists additional staff members to serve as expert reviewers for help in making decisions. Many staff members participate: More than two hundred have taken ideas to the committee, over three dozen have served terms on the committee, and several hundred more have willingly served as technical advisors for specific proposals. Throughout the review process, the emphasis is on idea development. Instead of keeping the reviewers anonymous, the committee urges them to discuss the ideas openly with the proposers and to make helpful suggestions whenever possible. Rather than reject an idea, the seed money committee will try to suggest ways to improve or reformulate it. The result is the maximum implementation of some very good ideas. In fact, it is a credit to the creativity of the staff and to the efforts of the committee that more than two-thirds of the ideas considered are funded for development; and most of these are successfully developed. Ideas receiving committee approval are sent to management with a recommendation that their development be funded at an appropriate level. Management has responded with more than $3 million for developing ideas to a stage at which regular R&D funding can be sought. The development of a good idea has seldom been curtailed by lack of funds.

What kind of ideas are sponsored? Not all ideas are appropriate for seed money. A research laboratory is by nature full of ideas, but most pertain to ongoing work and can be implemented without seed money. A few ideas for research outside existing programs are the ones for which seed money is primarily intended because they can lead to new R&D. The objective of this program is to establish a new project which will become self-sufficient by attracting funding from an agency. The funding is usually, but not necessarily, direct. An exception and good example is the project undertaken by Nancy Larsen and Connie Begovich of the Computer Sciences Division to develop pattern recognition as a tool for data analysis. Because their division is service oriented, a proposal for outside funding was not a consideration. Nevertheless, the project clearly succeeded; its results have found application to problems in several of the Laboratory's R&D divisions. The major requirement for consideration of a proposal is that seed money funding may be reasonably expected to initiate a significant contribution to a Laboratory mission.

The Seed Money Program can support an idea at any stage of its development. Most often, an idea is funded as a one-year project. However, if an idea is already well developed, it may be adequate to fund only the preparation of a proposal to a funding agency. On the other hand, seed money can sponsor the development of an idea from the ground up. It is possible to obtain funding for a short feasibility investigation

"... the programmatic impacts ... are of even more significance than the individual successes"

and literature search. Then, if the idea still appears promising, funds can be obtained for preliminary development, proposal preparation, and, if necessary, travel to a funding agency.

How successful has seed money been? The program's accomplishments clearly exceed all reasonable expectations. Although the ORNL staff has become increasingly familiar with the Seed Money Program, the prominence and impact of the program are probably not generally recognized. Even avid readers of the ORNL *Review* may not realize that many of the *Review's* feature articles have described seed money projects. For example, Ron Canon's "Metals from Fly Ash" (Winter 1979), Sam Suffern's "Waste Heat Aquaculture at ORNL" (Summer 1978), Ron Goans's "How Deep Is the Burn" (Spring 1978), and Sam Hurst's "One-Atom Detection" (Winter 1978) discuss projects initially sponsored by seed money. Incidentally, both the burn project and the one-atom-detection project earned IR-100 Awards. Very little mention of these projects is needed, because you probably know of them, even if you missed the *Review* articles.

There are many other prominent developments that have been given a major impetus by seed money— or just some essential help over a rough spot. The very first seed money project was in this latter category. Early in 1974, Dave Novelli was well up on the latest transfer-factor developments. He knew that in some cases an immunity factor from the blood of one individual could be transferred to another individual to provide a treatment for some diseases and certain types of cancer. He also recognized that ORNL's expertise in high-pressure chromatography might be used to separate this factor, but he lacked the necessary financial support. Then, in Novelli's words, "a great thing happened: the Laboratory decided to start the Seed Money Program." He was first in line. If you have been at the Laboratory for a few years, you may remember some of the exciting results that were obtained when he began fractionating transfer factor. In fact, these results were written up in the *Review:* "Transfer Factors of Cell-Mediated Immunity" (Spring 1975). Clearly, the Seed Money Program succeeded in its first effort, and the success has continued. Of course, there also have been some glorious and not so glorious failures, but that is to be expected of a program that takes chances on innovative ideas, when regular funding agencies would be reluctant.

Programmatic Impacts

What are the programmatic impacts of seed money? These are of even more significance than the individual successes. Seed money has contributed to many of the recent changes in Laboratory programs, but one of the most pervasive contributions has been to the biomedical and environmental sciences, where the combination of broader energy missions and new environmental awareness has had great impact. For example, the program has given a total of over $800,000 to 25 projects in the Biology Division, and the funding has helped bring about a pronounced change in research emphasis. The shift from studies in radiology and mutagenesis to those of chemical hazards is most notable. Much new biology research concerns the carcinogenic, mutagenic, teratogenic, and toxic effects of environmental chemicals. In comparison with radiation, the biological and environmental effects of chemicals are more numerous, more complex, less understood, and more urgent.

The examples of seed money projects that illustrate the changes in biology research are too numerous to allow more than mention of a few. In an early project, George Singer and Willie Lijinsky developed new procedures for detecting and separating nitrosamine compounds. Such compounds derive from the sodium nitrite commonly used as a food preservative, and they are believed to be a major contributor to the carcinogenic load of modern man. Research in this area is beginning to have an impact on the food industry.

Biology studies of improved methods for prescreening and identifying carcinogens, cancer initiators, and promoters have also been sponsored. Tom Slaga has studied the prescreening potential of skin esterase changes; and in work that is associated with the mutagenic activity of fractions of synthetic oils, Kameswar Rao and Jim Epler have utilized a bacterial assay to predict biohazard. Carol Heckman recently combined her expertise in electron microscopy and cytohistochemistry with computerized pattern recognition to detect shape changes in respiratory tract cells that had been transformed by carcinogens derived from coal tar. Bruce Jacobsen, a *Drosophila* geneticist, is now studying the toxic effects of cadmium in enzymes responsible for eye pigmentation. In other current projects, Frank Kenny, John Papaconstantinou, and Sankar Mitra are each doing molecular biology research that also relates to biochemical effects of carcinogens. These projects are examples of research being modified to enter the area of energy byproducts and environmental hazards. Clearly, seed money has had a large programmatic impact.

New Energy Projects

The Seed Money Program has helped initiate several research programs in energy technology in areas that are completely new to the Laboratory. One of the best examples is the Laboratory's research on the direct conversion of solar energy to electricity by the photovoltaic effect. As early as 1973, Dick Wood and John Cleland recognized that Cleland's work in the early 1950s on transmutation doping of semiconductors might have significant applications to solar cell technology. A seed money grant in 1975 for nuclear doping of silicon for solar cells was the official beginning of what has become a highly successful program. The effort can be credited with initiating the use of transmutation-doped silicon in several industrial applications.

A seed money grant again contributed to the photovoltaic program when Bill Appleton was given support for a study that included using ion implantation as a technique for making junctions in solar cells. Although ion implantation was already established as a method for solar cell fabrication, it was costly and time consuming due to the elaborate procedures needed to anneal lattice damage created by the implantation process. Initially, the solar cells made by ion implantation at ORNL were of very low quality. In searching for better annealing methods, Rosa Young, who came to ORNL under the seed money grant on transmutation doping, learned of references in the Soviet literature to the use of high-powered pulsed lasers for removing lattice damage in ion-implanted silicon. Young immediately sought out every laser at ORNL which might be used for "laser annealing." After several failures, she found what was needed in a Q-switched ruby laser in the Fusion Energy Division. The rest is now ORNL history. For reasons that are still not clear, Soviet scientists were slow to develop the new technique, and the results of the first reported application of laser annealing to solar cell fabrication were given by R. T. Young and collaborators of ORNL at the photovoltaic Solar Energy Conference held in Luxembourg during September 1977.

Laser annealing and related phenomena, in which the ultra-rapid heating and cooling achievable only by intense pulsed-laser radiation are used for modifying the properties of materials, now constitute one of the very hottest areas of materials research. Although it would be an oversimplification to attribute ORNL's leading role in this exciting development entirely to seed money, there is absolutely no doubt that seed money grants to members of the Solid State Division were very significant factors.

Seed money also started Solid State Division research in another area of energy technology. John Bates began basic studies of fast-ion conduction in solid electrolytes with a seed money grant. This project also has developed into a significant effort that someday could have a large impact. Because solid-electrolyte batteries have a lower cost and a higher energy density than standard lead-acid batteries, they just might make electric vehicles a commonplace reality.

Seed money also initiated the now sizable program, currently under the direction of Loucas Christophorou in the Health and Safety Research Division, which promises a general conservation of electrical power by reducing transmission losses. A substantial energy savings will result if the electrical power that is lost in transport can be reduced by using higher transmission voltages. Out of long-range basic research on the behavior and interactions of low-energy electrons, ions, and molecules, Christophorou and his co-workers are developing new and better gaseous and liquid dielectrics for various high-voltage applications in the power industry. Although the program has its roots in basic research, it embraces practical development and testing. Among the results achieved thus far are a determination of basic criteria for optimum dielectrics, establishment of the concept of multicomponent gaseous insulators, the discovery of new ways to tailor dielectrics, and the development of new multicomponent gaseous dielectrics that are more than twice as good as those commonly used. Clearly, this seed money project has flourished and is now making a significant contribution to an essential part of the energy industry.

These last three seed money projects not only started successful programs in new areas for the

Laboratory but have also had an interesting spin-off in common. The photovoltaics effort led in 1977 to a conference at ORNL for the purpose of informing American industry of the advantages of transmutation doping of silicon for many applications. Originally planned as a relatively small gathering, the meeting grew and became international in scope. Now it is referred to as the First International Conference on Neutron Transmutation Doping; the third conference in the series is scheduled to be held in Denmark in 1980.

In 1978, at the request of DOE and in cooperation with EPRI, ORNL hosted the First International Symposium on Gaseous Dielectrics. Plans are now being made to hold the second such symposium at ORNL in 1980. The program on solid electrolytes was started more recently than the others; ORNL will host its first International Conference on Ionic Transport in Solid Electrolytes in 1981. These programs have not only prospered but they have also attracted national and international recognition.

Coal Research

One of the Laboratory's new thrusts is in the area of fossil energy, and the Seed Money Program has already committed more than $500,000 to promote this effort, sponsoring such projects as basic studies of the chemical and physical properties of coal, new technology for coal combustion, better methods for monitoring pollutants from coal smoke, and new ways for managing and even using coal slag and fly ash. The atmospheric, fluidized-bed-combustor model, which was constructed under the direction of Bob Holcomb and John Jones in a joint effort of the Engineering Technology, Engineering, and Metals and Ceramics divisions, is the largest single project ever sponsored by seed money. The funding has helped to provide a new facility which will support broadly based R&D for a clean, more efficient method of burning coal. The facility is only now nearing completion, but a TVA commitment for additional funding has already been obtained.

The R&D on new ways to use coal slag and ash is as impressive as the R&D on new ways to burn coal. The Chemical Technology Division's resource recovery program started as a feasibility study modestly funded by seed money. Under Vic DeCarlo, Ron Canon, Jack McDowell, and Jack Watson, the effort was so successful that the program is now funded by DOE's Basic Energy Sciences and Fossil Energy divisions, as well as by the Electric Power Research Institute. Promising processes for recovering metals such as aluminum, iron, and titanium have been identified, and the problem of disposing of coal residues may be ameliorated by extracting these and other valuable resources. In a current project in the Metals and Ceramics Division, Vic Tennery and Larry Harris are also working on coal by-products. They are studying methods for making stable solids, including a mineral-wool insulating material, from coal waste.

It would be possible to go on and mention other seed money projects, but the message is clear. In a few years, seed money has permeated the Laboratory, has initiated many successful programs, and has significantly influenced the kind of R&D performed. Moreover, seed money has created opportunities which have brought considerable recognition to the Laboratory and its staff.

Can the program's success be quantified? There have been attempts to quantify the accomplishments of the Seed Money Program. More than 50% of the projects obtain further funding. The funding brought in by these projects has been examined, and it appears that the program as a whole is achieving a return on investment of at least 2:1 and possibly as much as 5:1. The results are still preliminary because the program is only five years old, and return lags several years behind the investment. The return will never be calculated precisely because, to some extent, the Laboratory's budget is constrained by funding-agency controls; thus, the subsequent funding of seed money projects often represents program redirection rather than growth. In such cases, seed money contributes by changing the Laboratory's R&D so as to increase quality and relevance rather than quantity. A quantitative assessment is also difficult because R&D programs are merged, assimilated, and redirected as the Laboratory continues the evolution promoted by seed money. Of course, a return on any investment is impressive, but it's not the bottom line for a national laboratory. The program has promoted new national goals, technology transfer, innovative R&D, and professional fulfillment. These are more significant. By whatever standard, the Seed Money Program is a success! ornl

lab anecdote

Master Spies

Not everyone in Oak Ridge during the first several years knew Hazel White. As a civilian, I was not privileged to know her. And not all the soldiers knew of her. The select group that knew Hazel and who sent information to her were the enlisted men who were assigned to wartime work at the several plants in Oak Ridge and who also had master's degrees.

That last requirement was learned by induction. Some of the members of the SED (Special Engineers Detachment) had been asked by their superiors to keep their eyes and ears open and to report any conversations they heard or overheard that might breach information security. In other words, they were asked to be spies. However, they couldn't go once a week to an office with an "Intelligence Services" sign on the door and make a report. No, they had to write a weekly report and mail it to "Miss Hazel White" at a post office box. The Army paid for the 3¢ stamps. The spies soon learned who the other members of the spy corps were through encounters with them at the post office stamp window, and later, over beer at the PX. On comparing notes, they came to realize that all of them had master's degrees.

Cy Feldman told me that there was one hardship for him. His wife wondered why she found, one day, an envelope that bore a stamp and was addressed to Miss Hazel White when the soldiers were permitted to send their mail free. She learned the answer after the War when a visiting friend asked Cy whatever happened to Hazel?

Did Hazel's work shorten the War? The only test Feldman ever made of the system to see whether it worked was a conversation he held in German with a chemist friend as they rode to work on a bus. Apparently, they were not reported to Miss White.—*Herbert Pomerance*

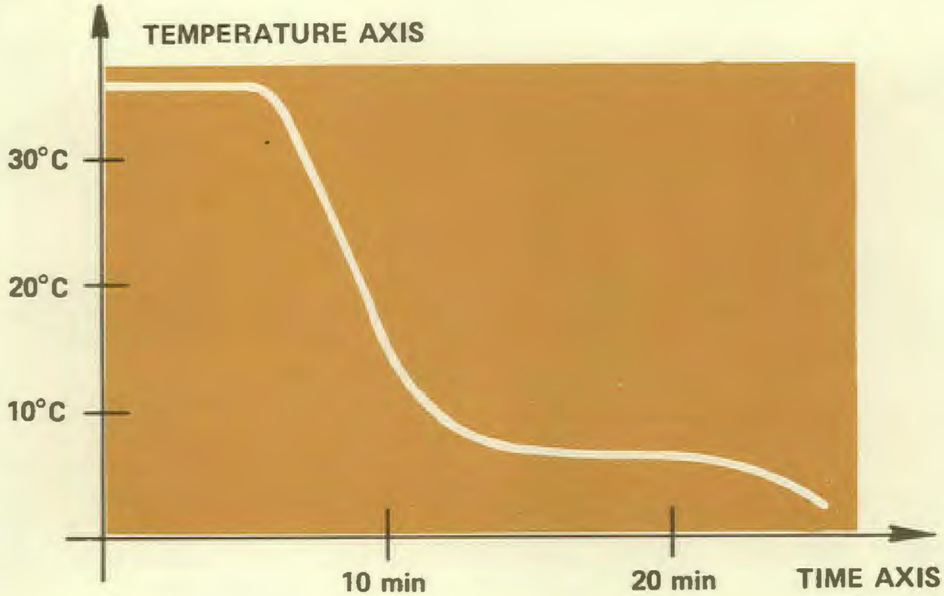
Coming up with a mathematical model for the way in which a frozen substance melts into a liquid is a complex achievement; yet it is being done by Alan Solomon in the Mathematics and Statistics Research Department. It is of use in the design of energy-saving buildings that employ walls containing phase-change materials (i.e., materials that change from liquid to solid and back as they release and store latent heat). Alan is shown here discussing the data gathered by the microprocesser, which has been programmed to conduct his experiment, with Ralph Deal, who is at ORNL on a year's assignment from Kalamazoo College, in Michigan. A graduate of City College of New York, Solomon holds the Ph.D. in mathematics from New York University. After teaching there for four years, he joined the staff of Tel Aviv University in Israel. In 1970, he moved to the newly created department of mathematics of Ben Gurion University, becoming chairman in 1974. He has been at ORNL since 1976.

The Mathematics of Moving Boundaries

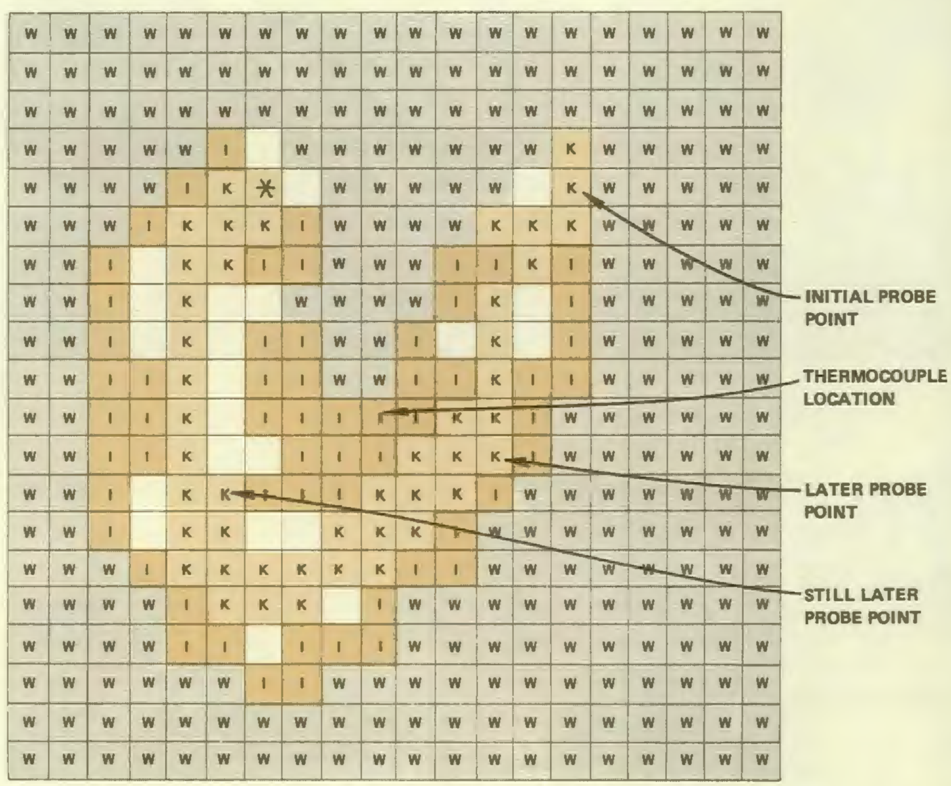
By A. D. SOLOMON

A "boundary" is a border or edge around a region. A stationary or unmoving boundary is, for example, the location of a fence around a house. In a broad sense, a moving boundary is one that moves with the passage of time. When mathematicians (such as I) speak of a boundary, they usually refer to the boundary of some geometrical region. Sometimes we imagine that the region contains material of interest in a physical context. When we use the words "moving boundary," we indicate that the boundary may be changing with passing time. Let us be more specific.

Upon waking on a cold winter day, you observe a large, beautiful



Computed thermocouple measurements for the simulated cryosurgical procedure. This is the kind of curve that the surgeon will obtain from thermocouples placed in the tissue.



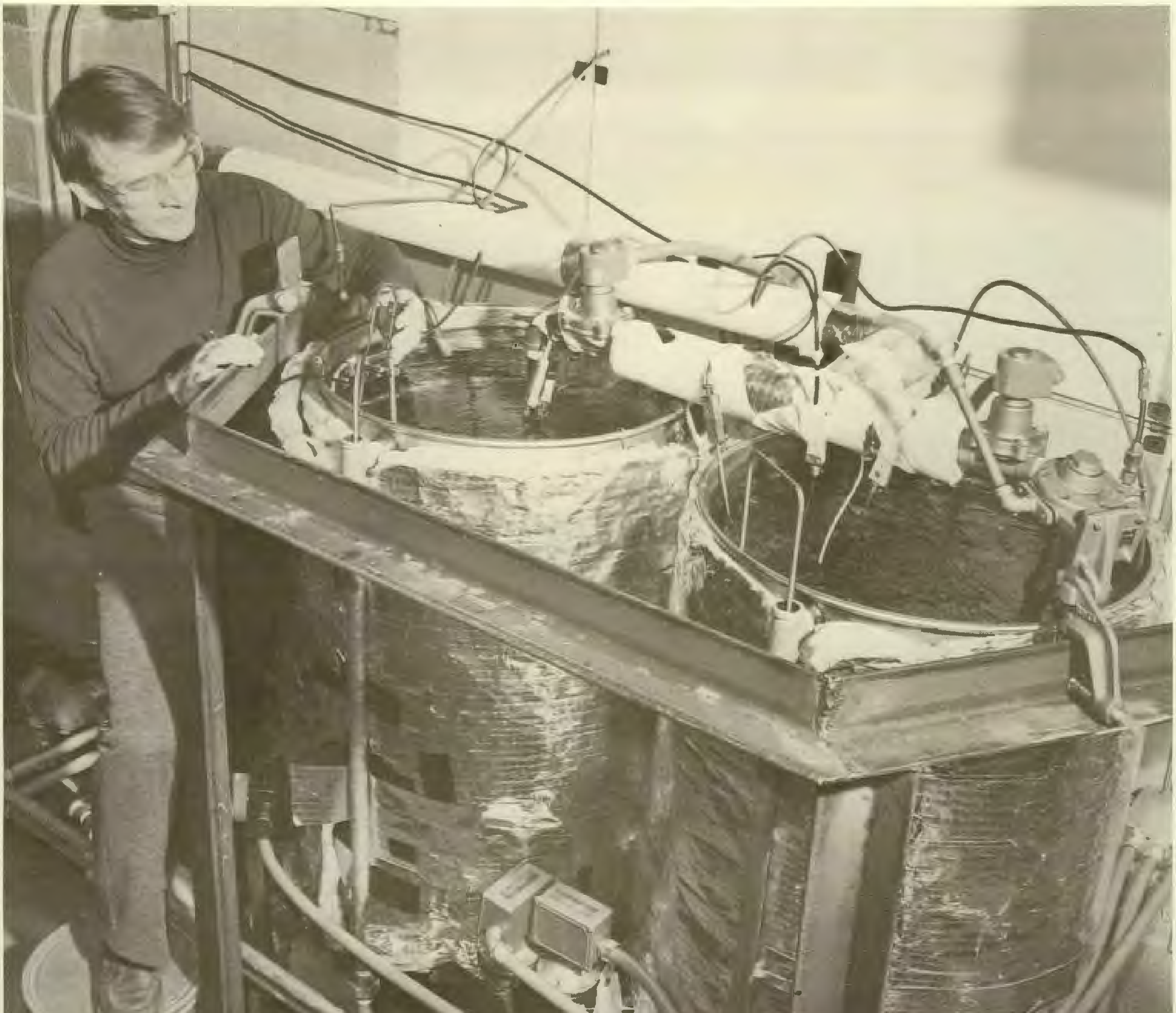
A simulated cryosurgical procedure in two space dimensions. Here a cold probe has moved through an arc-like path. After 25 min it has left a swath of killed tissue (denoted by the letter K), injured tissue (represented by a blank space), frozen but as yet uninjured tissue (denoted by I) and unfrozen tissue (denoted by W). The final probe location is denoted by an asterisk (*). The simulated zone is a square.

icicle hanging from your roof. The region in space occupied by ice has a boundary—the surface of the icicle. During the day, minute by minute, some of the ice may melt and drip off the icicle. As a result, the boundary of the icicle moves with passing time as it borders less and less ice.

The word "problem" means all kinds of things to different people. To mathematicians, "problem" may mean the task of formulating some real-life process in the language of mathematics, and saying something intelligent about the resulting mathematical "model" of the process. "Something intelligent" might include information or predictions about the process or identification of future experimental goals. Thus, moving boundary problems are mathematical problems in which moving boundaries play a role.

Up to the last decades of the nineteenth century, mathematicians were kept very busy with stationary boundary problems. An interesting problem of this kind is one in which a mathematician must predict the temperature of points at various depths in the ground over a period of time. What information must be given to do this? At the boundary between the air and the ground, we must determine what is happening to the temperature. This information, referred to as a "boundary condition," may be given in the form of specifying the temperature or the rate at which heat enters or leaves the earth at that point. Furthermore, those properties of the earth affecting the temperature must be known to

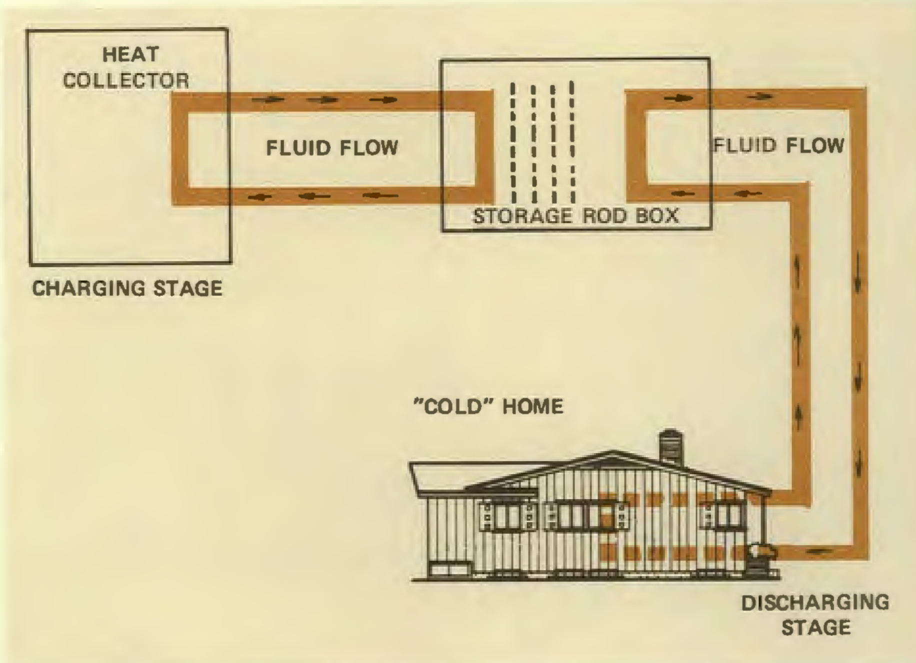
Ralph Deal at the two water tanks, one heated, the other at ambient city water temperature, with which he controls the surface temperature of the container of PCM in his experiment in the basement of Building 9204-1.



us. We can then use mathematical language to describe the temperature in terms of depth and time. Finally, we can attempt to compare our predictions with any available observations to check on the validity of our model. Why go through all of this? Because, once "verified," our model can be used as an additional tool in predicting the behavior of such processes.

In 1831, B. Clapeyon and G. Lame posed the problem of determining the thickness of the frozen crust of a liquid body formed by exposing its surface to a temperature below the freezing point. The boundary at this depth separates the liquid and solid phases of the same material. With the passage of time, this moving boundary does, indeed, intrude into the liquid. The essential difference between this freezing process and the earlier heat conduction process with a fixed boundary is the accompanying "latent-heat" effect at the moving boundary. A liquid freezes only when it reaches its freezing temperature (0°C for water) and gives up an additional amount of heat, its latent heat (80 calories/g for water), at that temperature. Translated into mathematical terms, this latent-heat effect imposes an additional "moving" boundary condition at the phase boundary.

The latent-heat thermal-energy-storage concept for a home. The heat collected from its source (possibly solar or waste heat) is transferred to the storage-rod box containing rods filled with phase-change material. When the "cold" home requires it, the heat is discharged from the storage unit and transferred to the home.

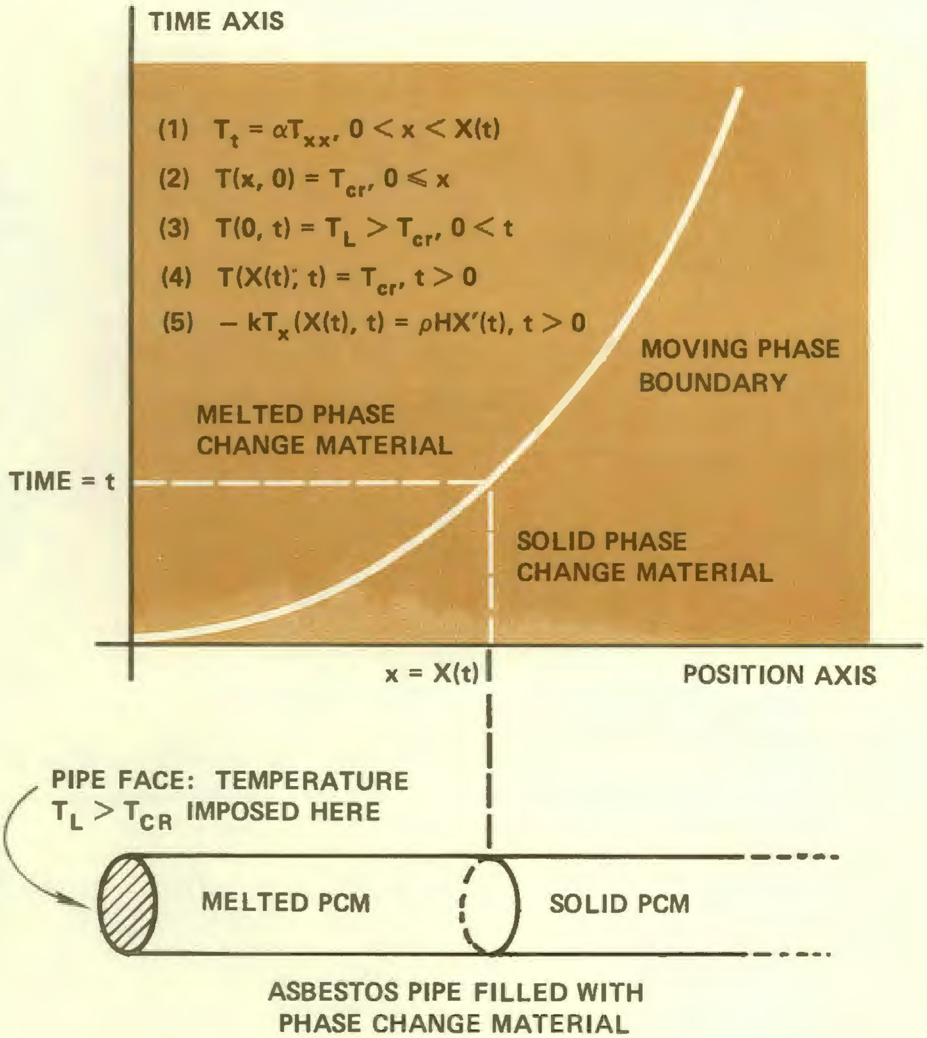


Recent Research

What have we done since 1889? We have identified important areas of application of moving boundary research. These include ablation problems (i.e., the wearing away of a surface by air or water), which we extensively studied in the 1950s; metal solidification and recrystallization, which is yet a vast open area; the freezing of ground, of crucial importance during the design and construction of the Trans-Alaskan pipeline; latent-heat thermal-energy-storage processes; and polymer solidification. These problems include such procedures as cryosurgery, the use of repeated freezing and thawing to kill unwanted tissues (e.g., brain tumors).

Motivated by these problems, we have formulated and studied moving boundary problems of increasing complexity and physical relevance, including diffusion processes arising in crystal growth, complex behavior at the phase-change front, radiation conditions at fixed and moving boundaries, anisotropic heat and mass transfer in solid-phase regions, natural convection in liquid-phase regions, and melting of transparent and semitransparent materials. We have uncovered processes in other areas whose mathematical formulations are similar to, if not identical with, the classical Stefan problem. We have developed numerous methods for obtaining at least approximate answers to many such problems. We have learned how, when all else fails, to apply computational methods to them.

In all of this work, however, we have as yet only scratched the surface. Two kinds of obstacles



Mathematical formulation of a moving boundary problem. Here we imagine a long asbestos pipe filled with a phase-change material. At one face of the pipe we can impose a desired temperature. Let us fill the pipe with solid material at its melting temperature T_{cr}*, and impose at the face the temperature* T_L *which is greater than* T_{cr}*. A melting process then ensues with a melting front progressing along the tube. Since the tube is of asbestos, the temperature of the material is uniform at any distance (x) from the tube face. The temperature of the material thus depends upon this depth and the time* t*, and can be denoted by* $T(x,t)$*. The equations (1) through (5) are merely the conditions that this quantity, and the phase-boundary depth* $X(t)$ *must obey. The constants* α, k, H *and* ζ *are the thermal diffusivity, conductivity, latent heat, and density of the material.*

have greatly limited our advances in recent years. The first is the lack of accurate physical and chemical data and knowledge of phase-changing materials and processes. The second is the limitation to our ability to deal with difficult mathematical problems. Thus, three-dimensional phase-change processes still stand defiantly behind a barricade of computing limitations and ignorance of mathematical foundations. The same can be said of most of the other areas described here.

Current work on moving boundary problems stresses the following activities: (1) strengthening our theoretical understanding of the various mathematical models, an essential step in all that follows, because it indicates physical relevance and points the way to solution procedures; (2) the study of combined heat- and mass-transfer phenomena; (3) two- and three-dimensional problems; (4) the development of closed form, or approximate relations, between the components of the problems; and (5) the development of effective numerical methods for such problems.

Work at ORNL

Here at ORNL we are engaged in a program of research on moving boundary problems that has two facets: mathematics research into models involving moving boundaries, and a comparison of the models with the real-world phenomena of melting and solidification.

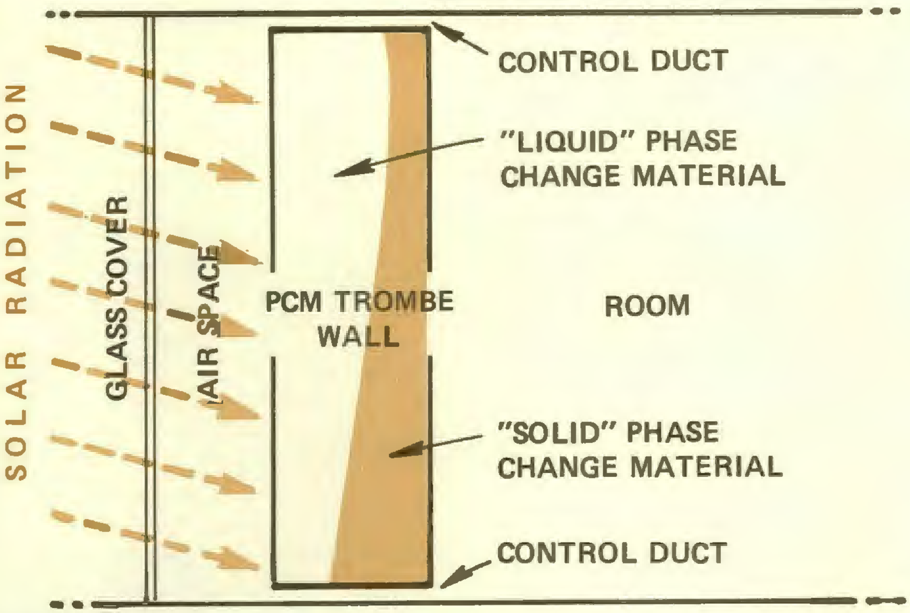
A mathematical model is usually in the form of a collection of equations relating known and unknown quantities. Generally, it is extremely difficult to infer useful information, such as how fast an icicle is melting, from this model. The derivation of such information is performed in several steps. The first step involves showing that the model "makes sense." For instance, does the model imply impossible

A wax-melting experiment. Initially the plexiglass box shown was filled with solid wax at a temperature below its melting point. Warm water was then pumped continuously through pipes on the horizontal aluminum face at the top of the box, inducing melting of the solid wax. The melt front, constituting the moving boundary of the process, is the (roughly) horizontal surface separating the transparent liquid wax (between it and the plate) and the solid wax below. The small hot plate on the lower right-hand side is one of the pieces of apparatus used to compensate for expansion of the wax under melting.

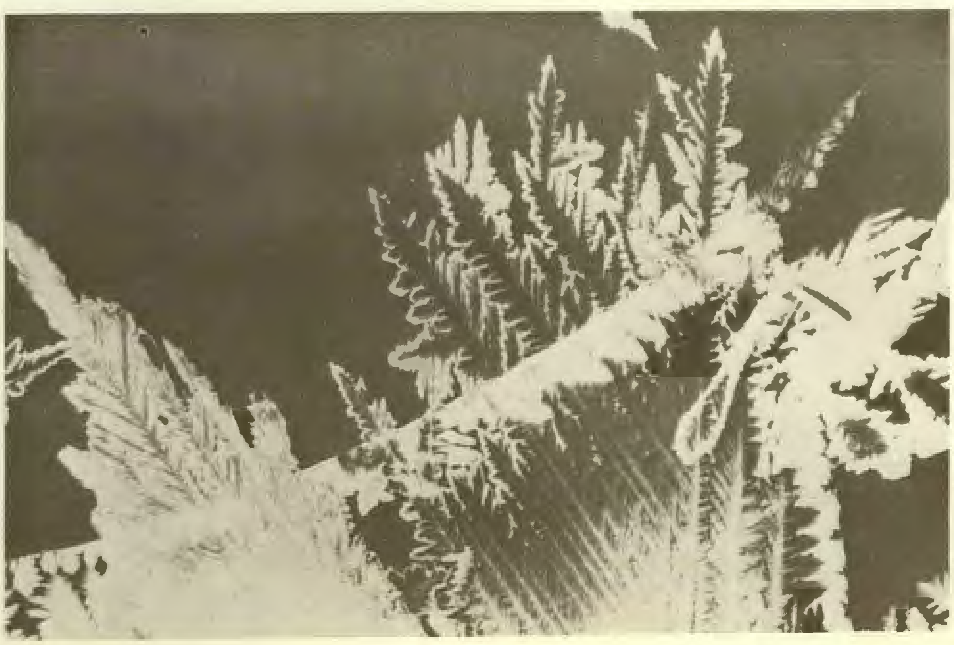
happenings, such as our icicle melting on a very cold day? Are relations that form our model self-contradictory? Can such questions as the speed at which an icicle forms be answered in principle by the model? The examination of whether a model "makes sense," or, in the words of the nineteenth century mathematician J. Hadamard, "whether the problems that we wish to solve with it are 'well-posed,' is central to the mathematical interest in the model. The importance of showing that a model makes sense is particularly great if we don't wish to waste computing time and money solving an unsolvable problem. One "well-posedness" result obtained recently by George Wilson of our mathematics research group relates to the solidification of a supercooled fluid—a fluid whose temperature is below its freezing point. If we mechanically disturb such a fluid at a point in its temperature drop, or "seed" it with an ice crystal, the fluid will freeze so that we see an expanding body of ice as the fluid freezes. Wilson was able to derive a quantitative condition under which it is impossible for the temperature at the ice–water moving boundary to reach the freezing temperature. Other results of this kind obtained at ORNL concern the behavior of rapidly joined solid and liquid phases of the same material.

After showing that a model makes sense, our next step is to seek qualitative information about it. Such information is, for example, a "lower bound" that we derive for the melting or freezing front arising in a "convective" heat-transfer process. Here, "lower bound" is simply a known boundary moving more slowly than the unknown phase-change front; we stress "unknown" because mathematical tools permit us to find such bounds *without* having to know where the exact boundary is. Of course, a convective heat-transfer process is simply one in which heat is passed to the melting material by a fluid flowing across its surface.

The third mathematical step is to seek answers to questions that we might pose. If you were to ask, "How fast does our icicle freeze?", we might search for a relation between time and the size of the icicle. If you were to ask, "What is the temperature at the base of the icicle when the icicle is 7 in. long?", your desired relation should link the temperature at this point to the icicle length. Sometimes, such relations can be found in "closed form" involving known familiar functions such as sine and e^x. More often, to our sorrow, they cannot. Nevertheless, sometimes by a combination of cunning and good mathemat-



The concept of a Trombe wall, containing phase-change material (PCM). Here solar radiation transmits heat to the PCM where it is stored primarily as latent heat of the phase change. When desired, the control ducts are opened to allow heat transfer into the room by natural convection as well as input (due to conduction) from the inner wall. The original concept, introduced in the 1950s by the French solar pioneer Felix Trombe, is in the form of a massive stone wall for storing sensible heat. It is very popular among solar enthusiasts because of its "passive" nature (no pumps are needed to move transfer fluids). The concept shows great promise under the right conditions.



Ice dendrites growing in supercooled water. To what extent can the tools of mathematics be developed to enable us to predict such complex and seemingly random processes, and how necessary is it that we do so? Perhaps continued and intensified research will tell us.

ics, close approximate relations can be found. Much of our work has involved finding such relations. In particular, we have obtained them for such questions as how long it takes objects of simple shapes (slab, cylinder, sphere, football) to melt totally, and whether the surface temperature of a melting material under convective heat transfer varies with time. In these days of programmable calculators, such relations may obviate the need for computing if very great accuracy is not needed.

If a model is sufficiently complex, or "realistic," we must turn to computational methods. But which methods? And how are they best applied? In our work, we have developed and studied a variety of computational methods for moving boundary problems. Among our recent results, we are most proud of methods for various kinds of heat-transfer modes at the surface of a melting body, a new kind of method for both two- and three-dimensional models, and results pertaining to the accuracy of computing methods.

The second facet of our work involves the testing of our results in the context of real-life, phase-change processes. We have been extremely fortunate to be part of an ongoing ORNL research program in Latent Heat Thermal Energy Storage (LHTES). This work, conducted in the Engineering Technology Division under the direction of David Eissenberg, with the aid of Ralph Deal (of Kalamazoo College), Herb Hoffman, and Robert Kedl, is aimed at developing methods for the storage of heat as the latent heat of a phase-change material (PCM), that is, one that can store heat over a significant length of time for later use. Let us illustrate this concept with two examples.

Two Examples

A south-facing wall is composed of a PCM-cement mixture. It is placed behind a glass frame. Due to the greenhouse effect (such as the intense heat buildup in your car on a sunny day), solar heat is trapped behind the glass during the day and is transferred to and stored in the wall as latent heat of the PCM. At night, it is passed on to the house, being given up by the now solidifying PCM.

In another example, aluminum beer cans are filled with a paraffin wax and placed on racks in a metal drum. The drum is attached to a solar collector and to the duct system of a home. When the sun is shining, latent heat of phase change is stored in the melting wax. When we wish to withdraw heat, the wax freezes, and the liberated heat is directed into the rooms of the house.

Our principal question is how these other energy-storage systems will actually perform—how fast can the system store and release heat? The key to this question is in the phase-change process of the PCM. How will the PCM in the can or in the cement behave when subjected to solar-heat input or the heating requirements of the house? The answer to this question comes only by studying the phase-change process in the PCM and it moving boundary problems. In an effort to link our mathematical "realities" to those of the engineer, extensive experimentation involving melting and freezing of a paraffin is now being performed by Ralph Deal. Current work includes an attempt to gain an understanding of the role of natural convection in the liquid phase, to estimate effective thermal properties of the PCM from the experiments, and to test models involving rapidly varying conditions.

A related effort is research being carried out on cryosurgical simulation. Cryosurgery is a procedure for killing unwanted tissue by repeated freezing and thawing via cold, liquid-nitrogen-filled probes. The conditions under which tissue actually dies is the subject of work by Peter Mazur of the Biology Division, who introduced us to this area. Moved by the hope that mathematical methodology can be applied to modeling the cryosurgical procedure, we have been examining how to model phase-change processes in two and three dimensions on a computer. By simulating the events that occur during cryosurgery, we hope to provide information to improve the surgeon's control and manipulation of the procedure. This work has led us to newer computing approaches, but it contains a number of potential mathematical pitfalls.

In this discussion, I, as a mathematician, have attempted to give you, a reader, a glimpse into a mathematical area of great beauty, challenge, and relevance. The word "beauty" is one perhaps not too often used by engineers for example, but translated to an engineering context, it might reflect the beauty of the shining new engines displayed proudly in the great expositions of the nineteenth century. "Challenge" is, of course, basic to the nature of legitimate scientific inquiry. As for "relevance," its meaning is, of course, the foundation from which the roots of our work draw sustenance. I have written no equations here, neither have I proved any theorems; but I hope that I have laid a basis for your appreciation and understanding of this particular branch of mathematics. ornl

letters

The article by Tom Wilbanks in your Spring 1979 issue was excellent. His articulation of the difficulties associated with communication between "hard" and "soft" scientists is outstanding. With your permission, I'm reproducing the article so that key people on our campus may have their own copy. Please send me three more copies of the *Review* to replace the copy that I cut up.

John C. Courtney
Assoc. Prof. of Nuclear Engineering
Louisiana State University
Baton Rouge, LA 70803

awards and appointments

The American Nuclear Society announces that the following ORNL staff members have been elected officers of its professional divisions: **N. A. Uckan,** secretary/treasurer, Controlled Nuclear Fusion; **Enzo Ricci,** vice chairman/chairman-elect, Isotopes and Radiation; **Ray Blanco,** chairman, Nuclear Fuel Cycle; **David Bartine,** treasurer, Radiation Protection and Shielding; **Helen Pfuderer,** treasurer, Environmental Sciences; and **John R. White,** vice chairman, Remote Systems Technology. **Ricci** has also been appointed to the society's National Planning Committee.

Charles Yust has been named a fellow of the American Ceramic Society.

The American Physical Society has chosen the following ORNL staff members as fellows: **Lee Berry, Julian Dunlap, O. B. Morgan, Jr., Masanori Murakami, Dieter Sigmar, Cheuk-Yin Wong, Jim Callen, Bill Appleton, Bob Hendricks, Carl Koch,** and **Herb Mook. Mike Wilkinson** has been elected to a two-year term on the advisory committee of the Solid State Division of APS.

Honored with the designation of Carbide Research Fellow were **Sam Hurst, Wally Koehler, Francis Perey,** and **Ralph Livingston.**

The East Tennessee Chapter of the Society for Technical Communication elected the following ORNL staff members to office: **David Armbruster,** first vice president; **Wes Robinson,** second vice president; and **Deborah Stevens,** recording secretary.

J. Michael Ramsey has been selected for a Eugene Wigner Fellowship and is currently assigned to the Analytical Chemistry Division.

A. L. Lotts has been designated director of the newly organized Nuclear Fuel and Waste Programs.

Director of the newly established national Materials and Structures Technology Management Center for DOE is **W. O. Harms.**

Reynold Berggren, Gene Goodwin, Robert Gray, Roy King, Gerald Slaughter, and **Jim Stiegler** have received the McKay-Helm Award of the American Welding Society, for their article in *Welding Journal* on Type 308 stainless-steel weld metal. **Goodwin** was also elected director-at-large of the society.

Wally Koehler has been notified by the president of the Scientific and Medical University of Grenoble that he has been given the honorary title Docteur Honoris Causa, by decision of the university's Scientific Council.

L. David Jackson, Plant Protection Division, was named one of the "Governor's 20," the top 20 "combat shooters" in Tennessee.

James D. Regan has been named a fellow of the Japan Society for the Promotion of Science, in which capacity he will spend three months of 1980 in research at the Mie State Medical School in Tsu, Japan.

Stanley I. Auerbach has been asked to serve as editor of the new journal, *Environment International.*

David Reichle has been named to the National Science Foundation's Advisory Subcommittee for the Applied Physical, Mathematical and Biological Section of the Division of Applied Research.

Charles C. Coutant was appointed to a three-year term on the editorial board of *Environmental Science and Technology.*

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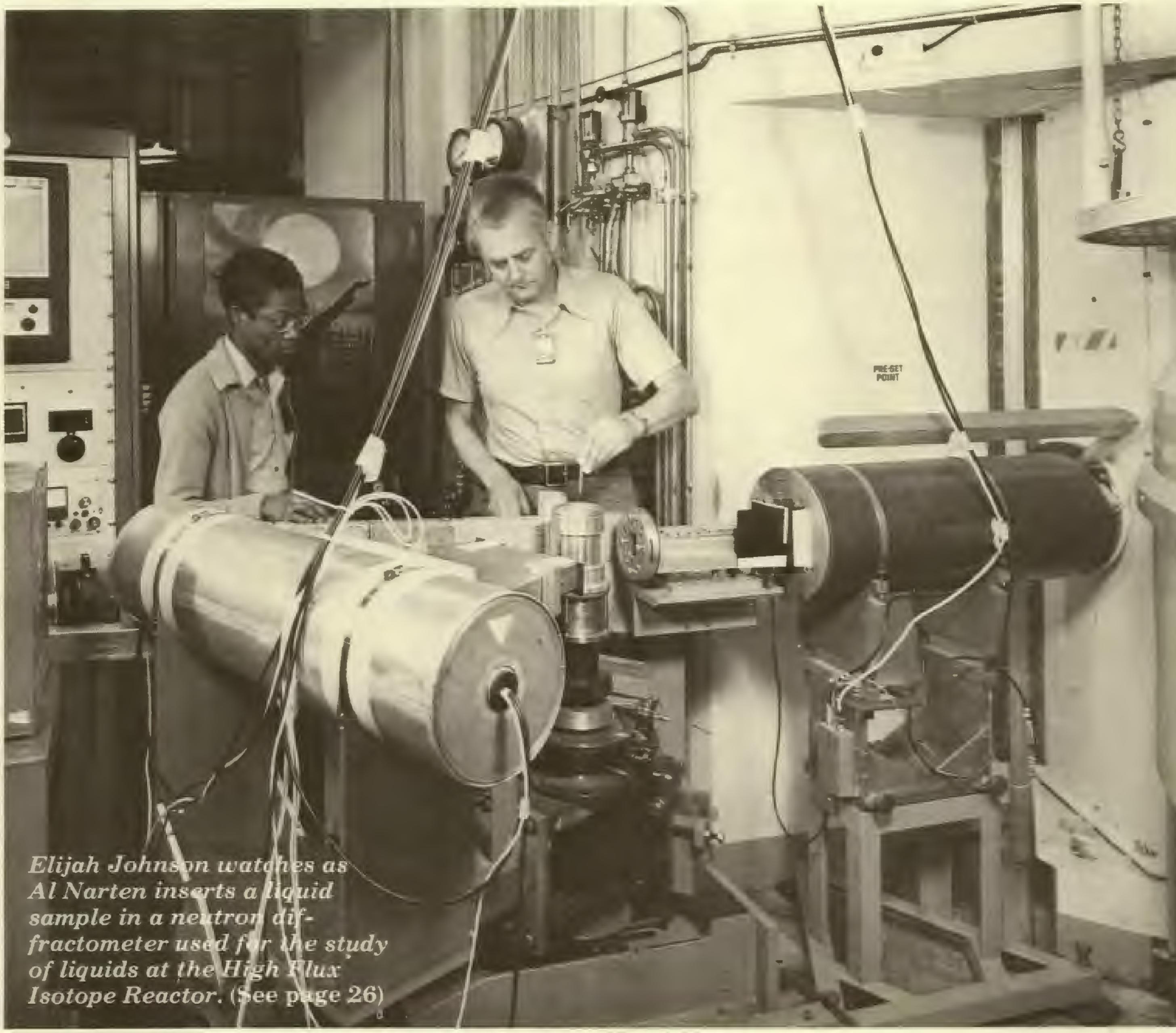

Elijah Johnson watches as Al Narten inserts a liquid sample in a neutron diffractometer used for the study of liquids at the High Flux Isotope Reactor. (See page 26)