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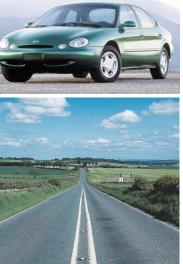
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Editorial: Putting East Tennessee on the Transportation Research Map

NTRC: Accelerating the Transportation Revolution

Toward a Cleaner Diesel Vehicle

6 An Emissions Mission: Solving the Sulfur Problem

7 New User Facility Has Old (But Excellent) Instruments

9

2

5

Truck Brake Tester Could Boost Highway Safety

10

Better Ways to Weigh Trucks

12

Carbon-Fiber Composites for Cars

13

Supercomputers Help Model Cars in Collisions

14

Power Electronics: Energy Manager for Hybrid Electric Vehicles

15

Is There a 'Green' Car in Your Future?

Biological Ways of Producing Ethanol

The new National Transportation Research Center (NTRC) in Knox County, Tennessee, is the home for advanced transportation studies by researchers from ORNL and the University of Tennessee. Some of the research at NTRC is featured in this special issue of the ORNL Review.

17

REVIEW Vol. 33, No. 3, 2000

ontents

Aviation Research Takes Off at ORNL

18 Packaging and Transporting Hazardous Materials

19 Transportation Planners Aided by GIS Research

20 Defense Transportation and Logistics Research

21 Software Tools Will Help Emergency Responders

22 E-Commerce's Impacts on Transportation

23 Learning Smart Ways to Use Intelligent Transportation Systems

24 UT Goal: Safer Trips

25 Mass Spectrometer Can Detect Weapons of Mass Destruction

26 ORNL's Graphite Foam May Aid Transportation

28

Microfocusing Mirrors May Advance Materials Science



Lee Riedinger

Editorial: Putting East Tennessee on the Transportation Research Map

utomobiles and airplanes have driven the U.S. economy for most of the 20th century. Mass-produced, affordable cars and trucks, combined with the U.S. highway system, created the American middle class and spurred the growth of cities and suburbs. U.S. fighter jets helped achieve many victories in world and regional conflicts, and U.S. aircraft stimulated the growth of American businesses and U.S.-based international corporations.

Although transportation helped bring Americans peace and prosperity in the 20th century, it threatens to impair our quality of life in the 21st century. As

gasoline prices rise, we are reminded of our growing dependence on foreign oil, a dependence that threatens our national security and economic health. Because the world's oil supplies may run out in 40 years, we must find ways to use gasoline more efficiently and rely on alternative fuels to ensure that the transportation needs of subsequent generations will still be met. Our transportation vehicles are responsible for one-third of our nation's energy use and carbon dioxide emissions, which could adversely affect the stability of our climate.

Because of a growing population, economic prosperity, and the resulting travel boom, congestion on our highways and at our airports is getting worse. Pollution from highway traffic is threatening air quality and health in our metropolitan areas and national parks. Additionally, we must continuously deal with threats to highway safety—ranging from cell phone use to defective tires—which are partly responsible for the 41,000 traffic accident deaths each year in the United States.

As President Clinton has noted, a competitive, growing economy requires a transportation system that can move people, goods, and services quickly, efficiently, reliably, and economically. Such a transportation system needs technological innovations to make it happen. A high-tech transportation system will increase fuel efficiency and safety and reduce air pollution, carbon dioxide emissions, and congestion.

The National Transportation Research Center, which opened in October 2000 in Knox County, Tennessee, is dedicated to helping develop and test advanced transportation systems and solve problems of the transportation industry. NTRC houses user facilities containing state-of-the-art equipment purchased by the Department of Energy. It has one of the largest concentrations of transportation researchers. It is expected to attract transportation research talent and businesses needing assistance. NTRC's 160 researchers—75% from Oak Ridge National Laboratory and 25% from the University of Tennessee at Knoxville—will make this center an important asset to the transportation community.

It is appropriate that transportation issues be studied in East Tennessee using world-class researchers and facilities. Tennessee ranks fourth in the nation in automotive manufacturing. Knox County has the second busiest truck weigh station in the nation, and the state of Tennessee ranks sixth in the United States in the number of trucks that pass through on the interstate.

This special issue presents the story of the birth of the NTRC, the transportation issues its researchers are addressing, and the research achievements and capabilities of many of its researchers. This issue features equipment and research plans for some of these NTRC labs: composites, infrastructure materials testing, human factors, geographic information systems, materials packaging, transportation policy analysis, vehicle and engine testing, commercial vehicle operations, intelligent transportation systems and traffic control, military transportation vehicle simulation, power electronics, and materials modeling and characterization. NTRC's state-of-the-art equipment includes a pad and bridge crane for package drop tests, a package vibrator, "weigh-in-motion" static truck scales, and several engine dynamometers. Two chassis dynamometers will be installed to measure the performance and emissions of cars and trucks.

This issue also highlights the most recent ORNL technologies that have won the prestigious R&D 100 award. All these winners are excellent examples of ORNL science and technology at their best, and one especially has a strong link to transportation. The development of a new type of carbon foam has opened the door to many areas for application of lightweight heat sink technology, including for automobiles.

The NTRC is an example of what a new facility can do to stimulate collaborative research and transfer technical knowledge by minimizing barriers, such as guarded fences. We hope this special issue will increase awareness of East Tennessee's new repository of transportation research expertise and equipment. It is hoped that NTRC will open up new avenues for investigation to help steer the U.S. transportation system in desirable directions.

See S. Riedinger, Deputy for Science and Technology at ORNL

REVIEW

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

NTRC:

NTRC researchers are addressing the nation's major transportation issues. Their expertise could be useful to local transportation companies.



E ast Tennessee is now a magnet for transportation researchers and businesses that should help propel the transportation revolution. The National Transportation Research Center (NTRC) recently opened its doors in northwest Knox County. NTRC brings together under one roof some 160 researchers—120 from Oak Ridge National Laboratory and 40 from the University of Tennessee. With the researchers combining their expertise and the center's stateof-the-art equipment, the NTRC should help solve complex national problems, make the U.S. transportation industry more competitive, and attract transportation-related firms and transportation research talent to the region.

On April 8, 1999, U.S. Transportation Secretary Rodney Slater and U.S. Rep. John J. Duncan, Jr., presided over the official groundbreaking of the \$15 million NTRC facility at the intersection of Pellissippi Parkway and Hardin Valley Road. "The National Transportation Research Center is a transportation solution

> The National Transportation Research Center in East Tennessee.

that will improve safety and service for the American people in the new century and the new millennium," said Secretary Slater. "Just as we created a blueprint for an interstate highway system that tied our nation together, the NTRC will help us create a 21st century blueprint for a hightech transportation system that saves lives, money, and time." Calling the NTRC one of his top priorities, Duncan said that the project "will greatly enhance the ability of the U.S. transportation industry to access the research and technological capabilities" of Oak Ridge National Laboratory.

The NTRC, a collaborative effort among the Department of Energy, ORNL, the University of Tennessee (UT), and The Development Corporation of Knox County (TDC), was built in less than two years on a six-acre site in the Pellissippi Corporate Center. TDC initiated the idea for building NTRC, Inc., and provided the site at a reduced price to the developer. Construction funds for the 83,000-square-foot facility came from Pellissippi Investors LLC, which will lease the facility to ORNL and UT separately. Major support for the facility comes from DOE's Office of Energy Efficiency and Renewable Energy. The Community Reuse Organization of East Tennessee (CROET) provided capital equip-

ment grants totaling nearly \$3 million.

BOLD NEW VENTURE

"Our emphasis will be on getting technology out to the private sector as quickly as possible," says Bob Honea, an ORNL manager named NTRC director. "The center represents a bold new venture that departs from the traditional ways in which government, industry, and the public sector have operated. For example, our transportation researchers from ORNL will no longer be behind a guarded fence, so they will be more accessible to private companies needing help with their transportation problems.

"Each collaborator brings important capabilities and assets to the facility, which we expect to attract the best talent available in transportation fields. The center and NTRC, Inc., will build upon and expand DOE's existing partnership with other federal agencies, such as the Department of Transportation and the Department of Defense."

David Greene, one of the ORNL researchers who has moved to the NTRC, believes that the existence of the center and NTRC, Inc., will open up new lines of research and sources of funding beyond what DOE offers. "We may have easier access to funding from the automakers, the oil companies, the National Science Foundation, and the Pew Charitable Trust," he says.

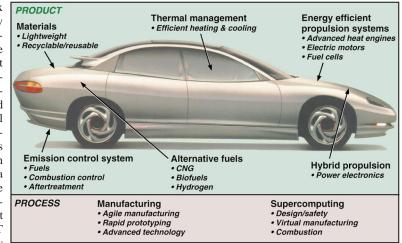
Researchers from industry, government, universities, and other laboratories around the country can call upon NTRC, Inc., for expertise in many different fields

of transportation. NTRC researchers are determining the energy efficiency of vehicles and engines and the effectiveness of their emissionscontrol systems. Some are looking at ways to improve road-paving materials. Others offer advice on packaging and transporting hazardous materials and high-value products. Research is being conducted on intelligent transportation systems, defense transportation and logistics, transportation manufacturing research, composite materials for vehicles, and geographic information systems used to identify alternative transportation routes around congestion. Computer simulations of car crashes and other research methods will be used to find ways to improve vehicle safety and to evaluate the performance of new lighter-weight materials. The NTRC will also house researchers doing planning and policy analysis concerning vehicle fuel efficiency and energy use in the transportation sector.

The UT Center for Transportation Research will be conducting research at NTRC on how to make car interiors safer and how to prevent injury to body extremities in car crashes. UT researchers will also be investigating better paving materials and improved bridge beam construction. (See article on p. 24.) UT brings to the NTRC several nationally recognized R&D programs in transportation logistics and advanced vehicle technologies, with a base funding approaching \$20 million. The Geographic Information Systems (GIS) laboratory at the NTRC, which is staffed mostly by UT researchers, is developing a map-based application that allows Tennessee Department of Transportation planners to identify roadway deficiencies and model recommended improvements to determine the costs and benefits of construction projects. The GIS group is also involved in a number of military logistics projects, such as identifying potential bridge and interchange deficiencies along convoy routes and prescribing alternate routes if necessary. (See pp. 19 and 20 to learn more about UT and ORNL research in the GIS and military logistics areas.) Specialized transportation research laboratories at NTRC and ORNL that have the best modern equipment will be available to users. DOE brings to the NTRC the scientific and technical capabilities of ORNL plus its existing funding base of nearly \$80 million in transportation research and development (R&D) from multiple sponsors.

ORIGINS OF NTRC

How did the NTRC begin? "It all began on September 10, 1993," Honea says. "A group of movers and shakers doing transportation research at ORNL decided at an off-site meeting at the Tellico Village Yacht Club that it would really be great to get together in one building. At that time we were scattered all over the Oak Ridge Complex and rarely saw each other except at off-site meetings. But when we got together, things really clicked and we found we all had a lot in common. So I was asked to begin looking for a building to house the group. Initially, we thought about asking UT if the university would be willing to build a facility



ORNL researchers are working on these transportation technologies.

to sublease to us, but UT's administrative management couldn't do that.

"We had almost given up when TDC expressed interest in helping us build the facility. Then TDC officials decided that their charter only allowed them to provide land, not construct buildings. Later, we evolved the idea of including in the building some transportation research labs as user facilities for outside researchers. In that way we were able to get DOE support. We talked to several private investors and looked at many sites before we settled on the Pellissippi Parkway site. Mr. Stan Roy, Mr. Milus Skidmore, and the Malicote family, who own Dixie Roofing, Inc. (whose president is Mike Malicote), formed a partnership called Pellissippi Investors to bid on the project using private funds to construct the building. We are now beginning to enjoy a fantastic facility."

HITTING TRANSPORTATION ISSUES HEAD-ON

The U.S. transportation system, which has long been a key to the success of our American economy, is a source of problems that could be partially solved by technology. Integrated technologies and appropriate policies could revolutionize the American transportation system so that its value to the economy is no longer undermined by its external costs. NTRC researchers are working on technological solutions to these transportation issues. Following is a look at some of these transportation issues and the solutions proposed by NTRC researchers.

• The American transportation system is responsible for one-third of the energy we use and onethird of our carbon dioxide emissions, which could contribute to unwanted climate changes.

One approach to solving these problems is to educate the public about the importance of buying cars and trucks that use fuel more efficiently so that less carbon dioxide is emitted. David Greene of ORNL's Energy Division is helping this effort through www.fueleconomy.gov, a Web site he manages and writes for DOE. The Web site, which was designed by UT's Janet Hopson, has been named "site of the day" by Yahoo (an Internet company) and USA TODAY. It gets 1000 visitors a day.

According to *Clean Energy for the 21st Century*, a document by DOE's Office of Energy Efficiency and Renewable Energy (EERE), which funds much of the research at NTRC, "DOE and six other federal agencies are working with the major U.S.-based auto makers in the Partnership for a New Generation of Vehicles (PNGV), which has the goal of creating by 2004 a full-size car that achieves 80 miles per gallon, without sacrificing safety, affordability, or other features we expect in an American car."

Using PNGV funds, ORNL researchers are studying better and cheaper ways to manufacture lightweight carbon-fiber composites to replace steel for body parts and other components of advanced vehicles; the lighter the vehicle, the less fuel it will require. They are also developing smaller electric motors and power electronics modules for hybrid vehicles, to make them more efficient. Hybrid vehicles use less gasoline or diesel fuel because they have an electric motor to help power the wheels during acceleration and stopping. (Some of the composites and electric motor researchers have their roots in the Oak Ridge gas centrifuge program of the early 1980s, which sought to develop a more efficient way to produce enriched uranium for nuclear power plants.) NTRC researchers will also be measuring the speed, power, and overall energy efficiency of engines and vehicles (especially foreign cars incorporating new technologies, to compare them with new American models). For this research, they will use engine dynamometers and a chassis dynamometer, which is like a treadmill for a car. One goal of this research is to help the U.S. automobile industry become more competitive in the world marketplace.

• Because of our growing transportation needs, half of the oil our nation uses is imported, jeopardizing our national security and economic health. According to www.fueleconomy.gov, "The vast majority of the world's oil reserves are concentrated in the Middle East (65% to 75%), and controlled by the members of the Organization of Petroleum Exporting Countries (OPEC) oil cartel. Transportation accounts for two-thirds of total U.S. petroleum use and nearly all of the high-value petroleum products, like gasoline and distillate fuel. In the past, dependence on oil has cost our economy dearly. Oil price shocks and price manipulation by the OPEC cartel from 1979 to 1991 cost the U.S. economy about \$4 trillion, almost as much as we spent on national defense over the same time period and more than the interest payments on the national debt. Each major price shock of the past three decades was followed by an economic recession in the United States. With growing U.S. imports and increasing world dependence on OPEC oil, future price shocks are possible and would be costly to the U.S. economy."

One possible solution to this problem is to encourage more people to buy and drive hybrid vehicles. ORNL and UT are working on this challenge. NTRC researchers are developing the smaller electric motors and power electronics modules required for hybrid cars and fuel-cell electric cars.

• Oil supplies are being gobbled up so fast that future generations may not have much fuel left for transportation. According to www.fueleconomy.gov, "It took more than 200 million years to form all of the oil beneath the surface of the earth. It has taken 200 years to consume half that endowment. If current rates of consumption were to continue, the world's remaining resources of conventional oil would be used up in 40 years."

One approach to sustaining future generations is to use alternative fuels from renewable sources, such as ethanol, to power cars and trucks. ORNL researchers are developing ways to produce more ethanol from corn and waste wood, using better enzymes and microorganisms. Other ORNL scientists are looking at ways to genetically alter hybrid poplar trees and switchgrass so that they hold more carbon as they grow, making them even better sources of ethanol.

As part of EERE's effort to expand the use of alternative fuel vehicles, which use ethanol, natural gas, methanol, or electricity, ORNL has a fleet of "green cars" that operate on E-85 fuel, which is 85% ethanol. EERE is also seeking to stimulate the development of a refueling station infrastructure throughout the nation.

• Partly because of transportation, air quality is declining in our metropolitan areas and national parks, aggravating the health of people with respiratory illnesses. ORNL researchers at the Advanced Propulsion Technology Center, a user facility that is being relocated to the NTRC, are studying the effects of high-sulfur and lowsulfur gasoline and diesel fuel on the emissions of vehicles with advanced emission control systems. Too much sulfur can poison advanced catalysts, making them gradually ineffective at removing nitrogen oxides, hydrocarbons, and particulates. Federal regulations call for reduced automotive emissions of these pollutants and the gradual use of ultra-low-sulfur fuels in vehicles. Increased traffic congestion and deteriorating roads, as well as congestion on our rivers and at our airports, are causing losses in productivity and profits. ORNL researchers have been developing computer models of traffic congestion on freeways, growing congestion of barge traffic on a major river, and airplane congestion en route to airports. These models are providing insights into how to reduce congestion. Software tools are being developed at NTRC to help emergency responders avoid streets that are closed or blocked. NTRC researchers are also developing weigh-in-motion methods to speed up the accurate weighing of trucks, to reduce highway congestion around weigh stations.

• More than 41,000 people die each year on U.S. highways. NTRC's development of tools to weigh trucks faster and comprehensively test their brakes and rollover stability could ultimately increase highway safety if the technology catches on. NTRC is also boosting highway safety through its evaluations that ensure that hazardous materials are properly packaged and transported along routes in less populated areas. In this way, packages are less likely to release their contents in case of an accident in transit and thus possibly expose a large population.

ORNL researchers are developing computer tools to help traffic management centers anticipate and avoid unnecessary congestion, which can lead to traffic accidents and waste fuel. They are also trying to determine whether car cell phones, PCs for e-mail and Web surfing, and navigational systems that guide drivers around heavy traffic and help them avoid accidents cause "information overload" that might undermine the technologies' contributions to safety. ORNL researchers are also using supercomputers to simulate collisions involving vehicles designed to use materials lighter than conventional steel, such as high-strength steel, aluminum, and carbonfiber composites. The purpose is to determine whether new, lighter cars will hold up in accidents as well as or better than today's heavier steel cars.

Patricia Hu, director of ORNL's Center for Transportation Analysis (CTA), is studying older driver safety. In research conducted for General Motors, Hu and her colleagues at CTA project that highway fatalities of drivers over 65 years old will almost triple by the year 2025, compared with the number for the same age group in 1995. This increase is due to the expected increase in the number of older people in the general population and, subsequently, on the highway, coupled with the increase in traffic. CTA's research shows that some older women often stop driving prematurely (for example, after their first stroke) whereas some older men tend to drive until they have had a second stroke. Older men who have impaired vision and limited motor skills and use anti-depressants are at a greater risk of being involved in highway crashes than other older male drivers.

However, Hu says that the expected increase in highway crashes will be partially offset by a decrease in the crash risk as a result of currently evolving technologies (e.g., airbags and intelligent transportation systems). The CTA study suggests that new technologies could reduce the crash risk even more.

Thanks to new technology development and policy analysis occurring with support from NTRC, Inc., ORNL, and UT, beneficial results of the transportation revolution may be just down the road. @

Traffic congestion causes losses in productivity and profits.



Toward a Cleaner Diesel

Vehicle

A t the University of Tennessee at Knoxville, a diesel car spins its wheels on a treadmill called a chassis dynamometer. It looks like a patient having heart surgery. It is highly instrumented to provide on-line measurements of its engine's speed, power, and fuel use and the ability of its exhaust treatment system to remove harmful constituents.

Researchers in ORNL's Engineering Technology Division (ETD) take measurements on this car, as well as on engines at the four stationary engine dynamometers at DOE's Advanced Propulsion Technology Center (APTC). These dynamometers will eventually be moved from this user facility at ORNL to the National Transportation Research Center, which will also acquire chassis dynamometers. ORNL research on





Brian West checks a Mercedes A170 diesel engine, which is being tested to determine the efficiency of its emissions control system in removing nitrogen oxides and particulate matter from its exhaust. The engine is run on an ORNL stationary engine dynamometer, which applies the same resistance to the engine as the road would if the engine were connected to wheels. Top photo enhanced by Gail Sweeden.

ORNL researchers are helping to evaluate and improve the effectiveness of new emissions control systems for diesel engines. They are also determining the makeup of exhaust constituents.

machines is guiding the development of effective emissions control systems for next-generation vehicles.

The heart of the lean, clean car of the future proposed by the U.S. Partnership for a New Generation of Vehicles (PNGV) is likely to be a compression-ignition, direct-injection diesel engine that uses 40% less fuel per mile than do today's typical gasoline-burning cars. If the diesel engine is combined with an electric motor in a hybrid car, it could come close to meeting the PNGV goal of 80 miles per gallon for a familysized sedan.

Unfortunately, the lean-burn operation of diesel engines is incompatible with today's catalytic converters used to eliminate 90% of the nitrogen oxides (NO_x) in gasoline car exhaust. In addition to producing NO_x , which contributes to acid rain and smog (which, in turn, creates a greenhouse effect), diesel engines also emit particulate matter—airborne soot particles that may

be hazardous to humans inhaling them because they are small enough to reach the lungs. To meet PNGV goals and the tough emissions standards mandated for 2006 by the Environmental Protection Agency (EPA), new exhaust treatment systems are being developed for diesel engines by catalyst companies and DOE national laboratories. The APTC, led by Ron Graves, Ralph McGill, and others in ETD, is playing a key role in evaluating these emissions control systems to help improve their effectiveness.

"We use an engine dynamometer to determine how well the engine, fuel system, and emissions control system work together," McGill says. "We measure the engine's speed and load, the fuel system's air-fuel ratio, and the concentration of constituents in the exhaust before and after treatment by the emissions control system. We are trying to determine and optimize the efficiency of the catalytic converter in reducing emissions."

"We are now conducting dynamometer experiments on seven engines—one gasoline and six diesel engines, plus two vehicles," Graves says. "This effort demonstrates the high level of interest in the diesel engine today and the challenge of solving the emissions problems with those engines." The ETD researchers are working with auto makers and diesel engine manufacturers through seven cooperative research and development agreements. Important results have emerged from these collaborations.

"We have developed methods and instruments to measure faster and more accurately the concentrations of a broad range of exhaust constituents," says Graves. "These constituents include nitrogen oxides, particulate matter, sulfur oxides, carbon monoxide, and hydrocarbons.

"We showed that advanced diesel vehicles could achieve 2006 emissions standards. We did some clever engineering to create a highly effective emissions control strategy for a diesel car. We determined the right mixture of hydrogen and carbon monoxide from unburned diesel fuel that could regenerate the NO_x adsorber and simulated this exhaust mixture with bottled gas. This mixture is injected at precise intervals and reacts with the nitrogen oxides, converting them to nitrogen, carbon dioxide, and water vapor."

John Storey and others in ETD developed an electrostatic method of capturing diesel particulates from engine exhaust so their structure and makeup can be studied. Doug Blom in the Metals and Ceramics Division is studying these samples of particulate matter using the Hitachi HF-2000 transmission electron microscope. He has found that the structure of these particles ranges from noncrystalline to semicrystallinethe atoms are lined up in layers that are oriented in different directions. Pete Reilly of ORNL's Chemical and Analytical Sciences Division has developed a laser-based ion trap mass spectrometer that can be used to determine the composition of particles measuring 1 to 100 nanometers in real time

"If the particles we measure are mostly sulfuric acid, then we must rethink whether they represent a health risk or are harmlessly diluted by water in the lungs," Graves says. "If they are a health problem, it could go away after fuel sulfur is lowered to meet EPA limits." (See the following article.) More precise information on the makeup of particulate matter could steer scientists to a better understanding of its health effects. ()

An PREMIUM Emissions Mission: Solving the Sulfur Problem

ORNL researchers are conducting studies related to the EPA's decision to reduce sulfur levels in gasoline and diesel fuel to ensure the effectiveness of emissions controls in advanced vehicles.

In 1998 the Big Three automakers pledged to put clean-burning cars on the road by 2001, beating the Clean Air Act Amendments mandate by five years. They declared that their gasoline-burning engines would emit 50% fewer nitrogen oxides (NO_x) and 70% fewer hydrocarbons, thanks to advanced catalytic converters. Shortly after this low-emission vehicle concept was announced, the U.S. Environmental Protection Agency (EPA) revealed its concern that these reductions might not be achievable if high-sulfur gasoline and diesel fuel continue to be used. The reason: Studies involving EPA and the automobile and oil industries showed that fuel sulfur atoms can bond with reactive sites on the catalyst surface, preventing catalyzed reactions needed to break down NO_x and hydrocarbons.

Because of its concern that high-sulfur gasoline could decrease the effectiveness of advanced catalytic converters, EPA mandates that by 2005 the nation's largest oil refiners must reduce the sulfur content of gasoline by 90%, from an average of 300 parts per million (ppm) to 30 ppm. EPA also calls for an equally large reduction in diesel fuel's sulfur levels (to 15 ppm) by mid-2006.

Diesel fuel is used mostly in trucks, but demand for it is expected to rise. Because they are 40% more efficient than gasoline-powered vehicles and produce less carbon dioxide, light-duty diesel vehicles, including sedans and sport utility vehicles, are being developed for the Partnership for a New Generation of Vehicles (PNGV). By combining the diesel engine with an electric motor in a hybrid car, the PNGV goal of 80 miles per gallon for a family-sized sedan might be met. Advanced emissions control devices are being designed for these diesel vehicles, to reduce their emissions of NO_x and particulate matter (PM) to regulated levels. According to the EPA, the combination of advanced emissions control devices and ultra-low-sulfur fuel in both gasoline and diesel engines could greatly reduce air pollution, which has been blamed for respiratory health problems, crop damage, acid rain, and low visibility.

ENTER ORNL

ORNL researchers have conducted several studies related to the EPA decision on fuel sulfur. For example, in a study for the Department of Energy (DOE), Jerry Hadder of ORNL's Energy Division used a refinery model to determine the impacts of low-sulfur gasoline production on petroleum refining operations and investments. "We estimated that the total refining industry investment to enable production of low-sulfur gasoline will be \$5 to \$10 billion," Hadder says. "Partly as a result of our study, DOE expressed concerns about the high degree of technical uncertainty surrounding refinery product quality and the potential consequences of rising costs for the refining industry and gasoline consumers." EPA set a schedule for introducing low-sulfur gasoline that was in line with DOE's recommendation to facilitate a smoother, more certain implementation. Based on ORNL's refining cost estimates, DOE recommended to EPA that ultra-low-sulfur diesel fuel be phased in according to the market demand for light-duty diesel vehicles with advanced emissions controls. If this recommendation is followed, diesel fuel production and distribution costs could be reduced by \$20 billion over a 10-year phase-in.

ORNL researchers in the Chemical Technology and Engineering Technology divisions have been involved in several projects concerning sulfur levels in automotive fuels. In one effort, properties of sulfurcontaining compounds in fuel samples from refineries and gas stations are being measured. In another, the effects of fuel sulfur on diesel emission controls are being determined experimentally. In a research project on biodesulfurization, genetically engineered microbes and a solvent have been tested to determine how well they remove sulfur from diesel fuel.

CHEMICAL PROPERTIES OF SULFUR-CONTAINING FUELS

At DOE's new Physical Properties Research Facility at ORNL (see sidebar), vintage instruments are being used for a DOE Fossil Energy Program project to help refineries meet EPA goals for sulfur in fuels. Chemical Technology Division researchers Bill Steele, Debra Bostick, Catherine Mattus, and Tom Schmidt, director of the new user facility, are measuring a range of thermochemical and thermophysical properties of sulfurcontaining compounds shown to exist in gasoline and diesel samples obtained from refineries and gas stations nationwide. Results from these measurements will aid in the design of either improvements in existing refining technology or in the conceptual testing of new processes (e.g., advanced catalysts and absorbers) for sulfur removal.

Petroleum refineries extract hydrogen from natural gas to produce plastics (e.g., polyethylene) and add the hydrogen to crude oil to make gasoline. To remove sulfur during gasoline production, hydrogen is added under pressure along with a catalyst to produce hydrogen sulfide, which is removed as a gas. To produce the maximum amount of gasoline from crude oil, the process of adding hydrogen must be run in a narrow temperature and pressure range. The catalyst used effectively removes most sulfurcontaining compounds.

"To get rid of the most difficult sulfur compounds, the refinery must operate at a lower temperature or higher hydrogen pressure, which will raise its fuel production costs," Schmidt says. "At a lower temperature, the reaction will go slower, so more refining capacity must be added and more crude oil must be used to produce the normal yield of gasoline. At a higher

New User Facility Has Old (But Excellent) Instruments



Debra Bostick measures properties of sulfur-containing compounds in gasoline and diesel samples obtained from refineries.

In the summer of 1999, Bill Steele left Oklahoma for a job at ORNL. In addition to chemical analysis expertise, he brought highly useful equipment to ORNL from the now defunct National Institute for Petroleum Energy Research, a DOE facility in Bartlesville, Oklahoma. The center, which from 1918 to 1975 had been operated by the Bureau of Mines in the U. S. Department of the Interior, was closed in November 1998. During its 80 years of existence, Bartlesville was the site of thermodynamic property measurements on a wide range of fuels and fuel components. In the 1960s and 1970s much work was focused on the development of rocket fuel including JP10, the propulsion fuel for cruise missiles used so effectively during the Persian Gulf conflict. Now the Bartlesville equipment will provide new insights in basic and applied research at DOE's new Physical Properties Research Facility at ORNL.

Tom Schmidt, facility director, believes that both chemical manufacturers and pharmaceutical companies may want to use DOE's new user facility at ORNL to obtain physical property measurements on intermediate chemicals used in their manufacturing processes. "PPRF is unique because it allows a whole range of precise property measurements to be performed under one roof on a small amount of sample,"

he says. "One of us can measure the heat released during manufacture of the chemical—information that a manufacturer needs to prevent runaway reactions and explosions. Down the corridor, another group member can make vapor pressure measurements that help researchers predict whether releases of the chemical during manufacture will exceed toxicity or environmental limits."

"Each piece of equipment is unique," Steele says. "One piece, an inclined rotating frictionless piston, is used to measure vapor pressure and to relate that property to the piston face area and the acceleration due to gravity at the exact position of the apparatus on the earth's surface. Another unique instrument, a rotating bomb calorimeter, was originally designed to precisely measure the energies of combustion of tetra-alkyl lead compounds when lead was used as an antiknock agent in gasoline." The full range of the equipment and details on each individual piece, including measurement type, range of property measurements, and application of results can be found at http://www.ornl.gov/divisions/ctd/pprf/ppgroup.htm.

pressure, the wall thickness of the refinery units must be doubled or tripled, which is a difficult and expensive engineering problem."

ORNL is providing petroleum companies such as Chevron, Phillips, Shell, and Texaco with information on the properties of thiophene, benzyl thiophene, and dibenzyl thiophene (model sulfur-containing compounds in crude oil) to aid in the design of an improved refinery process for removing a higher fraction of the sulfur in the oil. By using precise data from ORNL, the companies will be less likely to overdesign their refinery equipment and raise their costs more than necessary.

ORNL data help refineries determine the temperatures and pressures required to reduce sulfur levels in gasoline to the EPA limit. "We can tell them what percentage of sulfur compounds will be removed by operation at a specific temperature or pressure," Bill Steele says. "We might inform them that if they change the temperature or pressure by a certain amount, the best they can get is 50 ppm sulfur, which is short of the goal of 30 ppm."

FUEL SULFUR AND EMISSIONS CONTROL

What are the effects of fuel sulfur on advanced emissions control systems for diesel engines? Researchers in ORNL's Engineering Technology Division—John Storey, Brian West, Norberto Domingo, Scott Sluder, Ralph McGill, and Ron Graves—are directing and conducting research to help answer this question. This work is part of the Diesel Emission Control-Sulfur Effects (DECSE) program, a joint effort of DOE's Office of Transportation Technology, two national laboratories, and manufacturers of diesel engines and emissions control systems. Some of the work is being conducted at the Advanced Propulsion Technology Center, another new DOE user facility at ORNL that will eventually be located at the National Transportation Research Center.

One purpose of the DECSE program is to conduct research to determine the impact of fuel sulfur on exhaust emissions control systems designed to lower tail pipe emissions of NO_x and particulate matter (PM) from diesel engines. The ultimate goal of the program is to determine the types of diesel fuel, engines, and exhaust emissions control systems that, working together, will enable diesel-powered vehicles to meet the stricter new regulations.

EPA's new Tier 2 light-duty emissions standards will phase in from 2004 to 2009. Under Tier 2, vehicle emissions are categorized into "bins," with NO emissions ranging from 0 to 0.2 grams per mile (g/mi), with a fleet average of 0.07 g/mi. The PM standards for these bins range from 0 to 0.02 g/mi. Unlike current Tier 1 emissions standards, the same Tier 2 standards apply to all passenger vehicles regardless of engine type, fuel type, or vehicle mass. Under the current Tier 1





The effects of low-sulfur fuel on a diesel engine's emissions control system (top) were studied by ORNL researchers using this Mercedes diesel car on a University of Tennessee chassis dynamometer (bottom). ORNL's Scott Sluder is in the car.

Transportation Research

standards, diesels and larger vehicles have less stringent standards than do gasoline-powered passenger cars. Current NO_x emissions standards range from 0.4 to 1.5 g/mi, and PM emissions standards range from 0.08 to 0.12 g/mi.

"Sulfur from fuel or lube oil can have detrimental effects on emissions and emission controls," West says. "Sulfur can poison catalysts such as NO_x adsorbers and contribute significantly to sulfate PM emissions. While lower sulfur fuel is needed, the maximum tolerable level is still unknown. If we can design emission controls that are less sensitive to sulfur, then diesel engines have the potential for emissions that are on par with gasoline engines, without having to mandate a zero-sulfur fuel." Current diesel fuel is regulated to below 500 ppm sulfur, but EPA recently mandated a 15 ppm sulfur cap on diesel fuel by 2006.

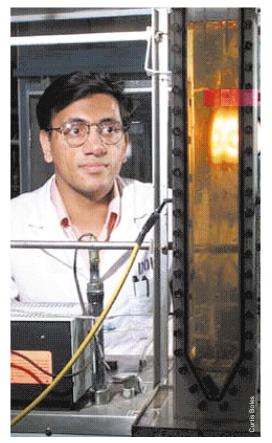
Using prototype emissions control equipment, ORNL researchers recently demonstrated that diesel vehicles have the potential to meet EPA Tier 2 emission requirements. The researchers achieved 0.05 g/mi NO, and 0.005 g/mi PM on the federal test procedure by fitting a lightduty diesel vehicle with a prototype NO. adsorber and catalyzed diesel particulate filter. These advanced emissions controls reduced the vehicle's NO and PM emissions by more than 90% from its baseline levels when 3 ppm sulfur fuel was used. However, after only 3000 miles of equivalent aging with 30 ppm sulfur fuel, the NO₂ adsorber was severely poisoned, resulting in only 80% NO, reduction. Under Tier 2, vehicles must be in emissions compliance for 120,000 to 150,000 miles, so more work is needed to solve this problem. Fortunately, the diesel particulate filter appears to be less sensitive to sulfur, although lower-sulfur fuel is still needed to prevent production of sulfate PM.

The durability of these emissions reduction systems has not yet been shown. But the results indicate that efficient diesel engines operating on ultra-low-sulfur fuel have the potential to power future cars and trucks, while emitting no more pollution than their gasoline counterparts.

"Some people believe that the new Tier 2 regulations will 'outlaw' the diesel engine in the light-duty sector," West says. "Although much more research is needed to make these systems commercially viable, the results of our laboratory experiments are promising, suggesting that diesel engines can have emissions comparable to those of gasoline engines, but with much better fuel economy."

SULFUR-REMOVING BIOTECH PROCESS

A novel chemical-biological process for removing sulfur from gasoline and diesel fuel has been developed by Abhijeet Borole, Catherine



Abhijeet Borole checks the operation of a bioreactor that uses suspended bacteria to remove sulfur from petroleum feedstocks.

Cheng, Eric Kaufman, and Brian H. Davison, all of ORNL's Chemical Technology Division, in collaboration with Petro Star, a small refinery in Anchorage, Alaska, and Travis/Peterson Consulting, Inc., also of Anchorage. Petro Star, which funded ORNL's biodesulfurization research, has developed a chemical process that adds oxygen to sulfur compounds in the diesel fuel to allow their selective removal using a solvent. As a result of this oxidation-extraction process, a desulfurized fuel and a high-sulfur extract are produced. The extract is about 10% of the original fuel and has recoverable hydrocarbons, the fuel's energy source. During the research project, this extract was sent to the ORNL group, whose job was to use bacteria to remove the sulfur from the extract and recover its fuel value.

"Biological processes may not be fast enough alone to give commercially economic rates of desulfurization," Borole says. "So, Petro Star's chemical process is being studied as an initial step because it is believed that oxidized sulfur species are more soluble in water where the bacteria reside, making it easier for the microbes to act on the sulfur. Our studies have indicated that this is the case."

For the research project, the ORNL group used genetically engineered *Pseudomonas* bac-

teria obtained from a Spanish molecular biology organization (Consejo Superior de Investigaciones Científicas of Madrid). Each microbe carries an inserted gene from another bacterium that breaks the carbon-sulfur bond by adding two oxygen atoms, converting each sulfur species to a sulfate (SO_4^{-2}) . The *Pseudomonas* bacteria were selected to carry this gene for two reasons. They have a high tolerance of the oil in which the sulfur compounds and hydrocarbons are present. In addition, because they can potentially produce biosurfactants, they can increase the contact between the oil and the water in which they reside. This increased mixing reduces mass transfer limitations and speeds up the biological oxidation reaction by which dibenzothiophene sulfone (an organic sulfur compound in diesel fuel) is converted to sulfate and sulfur-free hydrocarbons. In addition, the newly formed sulfate is soluble in the water phase, which naturally separates from the oil. The hydrocarbon-rich oil that remains can be used as a fuel.

"We measured the amount of energy the bacteria require for biodesulfurization, and we studied how well and how fast they remove sulfur from the diesel extract," Borole says. "It was not as fast as we'd like. We need to do more research to determine the best way for the bacteria to get more energy for desulfurization through metabolism of carbon sources. We need to find ways to increase the reaction rate to speed up the biological process for sulfur separation."

Borole notes that biodesulfurization is a potentially economical process because it can be performed at room temperature. Conventional refinery techniques for sulfur removal, which add hydrogen to crude oil, gasoline, and diesel to produce hydrogen sulfide gas, require temperatures as high as 300°C. "Biodesulfurization," Borole says, "may ultimately cost less because it will use much less energy."

The ORNL group is now doing research on modifying bacterial enzymes to make them more stable in an oil environment so they can react more readily with polyaromatic hydrocarbon (PAH) compounds, and later sulfur-containing PAHs, to upgrade crude oil. For example, the appropriate enzyme could make oil flow more easily at the production site or refinery. "We are proposing to use directed evolution to produce an enzyme that is not only stable in oil but also highly versatile," Borole says. "It would attack hundreds of sulfur compounds, not just a few dozen, in crude oil, gasoline, and diesel fuel."

The high concentration of sulfur in transportation fuels and the ability of sulfur to poison catalysts used in emissions controls are threats to the environment. It is hoped that research at ORNL and elsewhere will find economic ways to solve the sulfur problem.

Truck Brake Tester Could Boost Highway Safety

A new truck-testing technology that quickly and accurately weighs trucks, inspects their brakes, and predicts their chances of rolling over could save lives if widely used.

A fully loaded, 18-wheeler truck rolls into a weigh station. Its weight is measured in less than five minutes, but its brakes are not inspected thoroughly. The weight satisfies regulations, but the tendency of the truck's brakes to grab is not detected. The condition of the tractor-trailer rig's brakes increases the chances that the driver could lose control, causing an accident by jack-knifing or running into the wrong lane or off the road.

"Faulty brakes contribute to about one-third of truck-caused crashes in the United States," says Scott Stevens, a researcher in ORNL's Energy Division. "Current methods for brake inspection require too much time and labor and are subject to error, so only a small fraction of the trucks on the road are regularly checked."

Rollovers are another kind of traffic accident that can prove deadly for truck drivers. In the United States some 15,000 trucks a year roll over when drivers approach a curve at too high a speed for the load being carried. According to Stevens, "Truck rollover crashes are responsible for at least \$3 billion a year in losses associated with death and injuries, property damage, lost productivity, and lost time because of traffic backups."

Stevens and his colleagues offer a partial solution: a truck testing technology that quickly and accurately weighs trucks, inspects their brakes, and predicts their chances of rolling over under various conditions. Stevens has been working with University of Tennessee researchers Jeff Hodgson, Steve Richards, and Matt Cate to design, build, and operate a prototype advanced truck-testing facility. They believe that operation of this facility will demonstrate that this technology, if widely used, could greatly reduce the number of serious traffic accidents involving tractor-trailer trucks.

The facility, called the Multi-Plate Performance-Based Brake Tester, is being tested for use by the commercial vehicle operations and vehicle and engine research laboratories of the National Transportation Research Center (NTRC). The goal is to show that, compared with conventional weigh-station capabilities, this testing technology can weigh trucks more quickly and provide faster and more accurate information on the condition of truck brakes. "If this technology is used at most truck weigh stations," Stevens says, "state safety personnel can comprehensively check the brakes of many more trucks without hiring more staff. Our technology should be a credible deterrent to truck drivers who delay getting their brakes checked and repaired. They will not want to be caught with faulty brakes, which is a violation of the law, because they don't want to be put out of service."

The testing facility consists of a platform over which a tractor-trailer rig can be driven so that it can be weighed in a few seconds. To test the brakes, the driver is asked to drive the truck onto the platform at 10 to 20 miles per hour and brake sharply before leaving it.

The platform, which is 24 m long (80 ft), consists of 48 steel plates laid down in pairs, each of which measures about 1 m by 1.2 m (3 ft × 4 ft). Underneath each steel plate are sensor rods with transducers that convert the mechanical forces of the moving truck to corresponding electrical signals. As a truck rolls over the platform, the sensors measure the weight (vertical force due to gravity) and horizontal force on each plate as the wheels come to a stop. The braking force is related to the pressure exerted on the plates by

each truck wheel during deceleration and stopping. Four computers process the digitized measurements of braking force to determine whether the truck's brakes are working well or failing.

The new NTRC facility can also be used to determine the probability that a truck will roll over at different speeds, based on its weight and load characteristics. To test a loaded truck's rollover stability, the platform on which the truck sits will be tilted to measure sideways forces, simulating the effects of gravity on a truck winding around a curve. "Using this facility," Stevens says, "we will simulate the transfer of truck weight as a result of lateral forces and calculate the effect of this shift on rollover probability."

The researchers think the results that will roll out of NTRC's truck testing facility will show the value of its life-saving technologies. (*)

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Model truck and representation of a truck scale and brake tester to be installed at NTRC.

A Rollover Warning System for Trucks?

Scott Stevens and his colleagues have been gathering data from three trucks they instrumented that travel along the winding highway of Interstate 75. These "smart" trucks have global positioning systems and instruments that measure lateral acceleration for each position on a curve, whose characteristics are broadcast to each truck from a roadside beacon set up by the researchers. The smart trucks provide data that improve the researchers' ability to estimate the risk of rollover.

Results from the road tests and the facility experiments will be given to interested industrial firms to enable them to devise a rollover warning system for truck drivers. Such a system would sound an alarm if a driver is approaching a curve too fast, allowing time for corrective action to avoid rollover.

Better Ways to Weigh Trucks

ORNL researchers are developing "weigh-in-motion" techniques that will measure truck weights faster and more accurately.

J oe steers his company's tractor-trailer rig to an interstate weigh station in Knox County, Tennessee, for the required weight measurement and safety inspection. As with his other three stops on weigh station scales that day, his truck idles for about five minutes, wasting diesel fuel and precious time. But his truck weight is once again found to be below the legal limit, so he knows his company won't be ticketed and fined.

Joe's truck is one of 500,000 carriers on the nation's highways that are checked four times each day in the never-ending search for vehicles that are overloaded and otherwise unsafe. The cost to the motor carrier industry and, subsequently, to consumers of these mandated truck stops is estimated to be over \$15 million daily. In addition, because weight enforcement activities are slow and cumbersome, weigh stations are often overcrowded. Law enforcement officials often face two choices that together can create unsafe conditions. They can allow vehicles to back up in long lines near weigh station entrance ramps. Or they can let carriers bypass stations without being weighed or inspected.

Because the Knox County weigh station, which is near the I-75/I-40 junction, is the second busiest in the nation, about 70% of the 14,000 to 20,000 carriers traveling toward it daily are allowed to bypass it. In the past, Joe has been one of these. Some of these carriers legally bypass this station when truck lines are short because their weight is considered acceptable when they roll over an advanced, high-speed, weighin-motion (WIM) system in the westbound lanes of I-75. This is one of more than 75 commercial WIM systems embedded in the nation's highways that screen out commercial vehicles that may be overweight. Each driver who participates in the high-speed WIM program has a radiofrequency transponder for communication with the weigh station. If the truck weight is near the allowable limit, the driver is advised to stop at the upcoming weigh station for a more accurate weighing of the vehicle.

The Knox County system for weighing vehicles at high speeds is part of the National High-Speed WIM Test Facility. With support from the Federal Highway Administration and the Tennessee Departments of Transportation and Safety, this facility was developed by ORNL's Engineering Technology Division (ETD) in a cooperative research and development agreement with International Road Dynamics (IRD), Inc., of Saskatchewan, Canada.

The prototype advanced WIM system for I-75 was designed, installed, and tested by IRD and ORNL researchers David Beshears, Jeff Muhs, Matt Scudiere, and others in ETD. The ORNL group developed an improved system for acquiring and processing data from IRD's WIM hardware, which includes strain gauges and transducers that measure how much the plates they're attached to bend under the weight of truck tires, and then send corresponding electrical signals to the data acquisition system. The researchers also installed a small lab by I-75 for data collection and analysis. For the lab's computer, which receives digitized signals from the WIM signalprocessing unit, they developed an advanced weight-determining algorithm. As a result, the advanced system has an error rate that is 30% less than that of a standard commercial WIM system for high-speed weight monitoring.

Commercial high-speed WIM systems pose several problems. "Installation of these systems is expensive and requires extended lane closures, causing traffic jams," Beshears says. "Furthermore, these WIM systems are only 80 to 94% accurate. That's not accurate enough for law enforcement, so the use of static scales is required at weigh stations. Unless you get a truck weight that is better than 99% accurate, you can't legally issue a citation for a weight violation to a trucking company."

"We are now developing a 'weight enforcement on the fly' technology that will weigh trucks much more accurately at high speeds," Muhs says. "Its error rate will be less than 1%. When used with a license plate reader and wireless technology, this system will electronically identify and

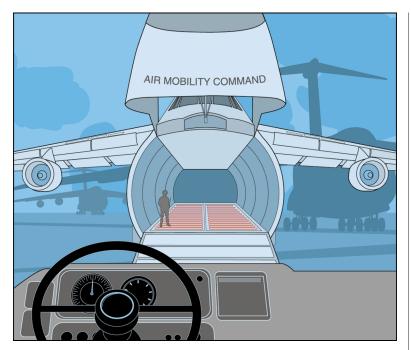
ticket overweight trucks passing by without making them stop at weigh stations."

In the meantime, the ORNL group is proposing that weigh station operators consider converting static scales to low-speed WIM systems. Working with the Tennessee Department of Safety



Gary Capps, leader of the Transportation Technology Development and Demonstration Team in ORNL's Engineering Technology Division, chats with Ralph Long, retired Exxon-Mobil truck driver, while the tractor (minus its trailer) is being weighed on the static weigh-in-motion scale at the NTRC. Inset: The weight of the tractor (22,100 pounds) is displayed on the scale meter.

Curtis Bole



ORNL researchers and Air Force officials have envisioned a WIM system for automatically weighing, marking, and loading an entire battalion of military vehicles onto a military aircraft. This system integrates wireless technology with load-planning software. Each vehicle has a distinctive radiofrequency (rf) signature, which is identified by an rf reader as the vehicle passes over a WIM scale. The vehicle's weight and center of balance are measured and transmitted with its rf identification to a computer, which has load-planning software. The computer decides where on the aircraft each vehicle should go to give the aircraft the proper center of balance so it can take off safely. The driver of each vehicle (see above) follows computer-controlled guide lights on the aircraft that tell him where to park the vehicle.



Members of the Tennessee Air National Guard at McGhee-Tyson Airport (including Colonel Fred Forster, right front) test ORNL's portable weigh-inmotion system for the U.S. Air Force. This automated system uses plates, strain gauges, and an advanced data acquisition system and algorithm to weigh and determine the center of balance of military vehicles in motion before they are loaded onto cargo aircraft for rapid deployment.

and the Carlton Scale Company and using funding from the Defense Advanced Research Projects Agency, the researchers have shown that it is feasible to convert the static scales at the Knox County weigh station into a high-accuracy, low-speed WIM system. This system was recognized as an emerging technology at the American Museum of Science and Energy's Tribute to Tennessee Technology Awards ceremony in 2000.

"By using a static scale platform that is 40 feet long, we have a large enough area and a long enough time to sample the weight of the truck," Muhs says. "We developed an algorithm that averages out the bounciness, or oscillations, of truck tires as they alternately press heavily and lightly on the platform of the scale. The algorithm allows us to weigh a truck moving at 30 miles per hour with an error rate less than 1%, which is required for law enforcement."

Besides increasing enforcement efficiency, this approach will let trucks go through weigh stations faster but allow inspectors time to determine whether a vehicle should be pulled out of line and checked for brake problems or additional safety violations. Traffic simulations of ORNL's low-speed WIM system indicate the average delay for a motor carrier can be reduced by a factor of seven, from 280 seconds to 40 seconds, eliminating traffic bottlenecks that cause trucks to bypass weigh stations. Such a system also could be used to weigh trucks as they enter and leave depot areas, such as grain elevators and landfills.

A low-speed WIM system using a static scale is located at the NTRC. The ORNL group is using it for research and demonstrations.

Muhs spearheaded the development of a fiber-optic WIM in 1989, but the project was abandoned a few years later because the fiber used by the ORNL group was no longer being fabricated. So the group focused on a different WIM technology. In 1996 in partnership with the Tennessee Air National Guard, the ORNL group developed, tested, and evaluated a portable WIM system for the U.S. Air Force. The system was demonstrated at McGhee-Tyson Airport in Knoxville and at two military bases.

This automated vehicle data acquisition (AVDAC) system, which uses plates and strain gauges, weighs and determines the center of balance of trucks, tanks, and other military vehicles in motion for rapid deployment by aircraft into and out of a theater of operation. The goal is to make sure that military aircraft and their cargo arrive safely and on schedule to help meet a humanitarian need, provide assistance during a regional conflict, or help protect the national security.

"If the center of balance of the aircraft is not in the right zone, it cannot take off safely," Beshears says. "That's why military vehicles must be weighed so it can be determined where to put them and how best to distribute the load in the cargo plane." The AVDAC system, which has been licensed to Intercomp, Inc., in Minnesota, combines a weight-determining algorithm and an electronic data acquisition system developed by ORNL with hardware that converts tire forces into electrical signals. It could replace the manual method of using small portable scales, a calculator, and a tape measure to determine number of axles, axle weight, axle spacing, gross weight, and center of balance. Because the AVDAC system is fully automated, it is not subject to operator error and it is safer to use.

"Our AVDAC system cut the error rate in half for WIM systems," Beshears says. "It greatly simplifies the weighing operation and increases productivity by 500%, saving 40 minutes per aircraft. Over 10 years this technology could save the Air Force \$45 million and prevent the loss of at least one \$200 million C-17 cargo aircraft."

Saving time and money is not just a whim, but it may be a benefit of tomorrow's WIM systems. 0

ORNL researchers are seeking ways to reduce the costs of making lightweight carbon-fiber composites for use in advanced vehicles. Composites for Cars

To make a vehicle that gets 80 miles per gallon of gasoline to satisfy one goal of the U.S. Partnership for a New Generation of Vehicles (PNGV), the automobile industry is seeking a lighter structural material. Steel is the material of choice today because of its strength and low cost. But steel is heavy, so the industry is starting to use lighter materials instead. Fiberglass has long been used extensively in the Chevrolet Corvette and more recently in some body panels of the Saturn car. Audi's A8 automobile and the hood and engine parts of the Ford F150 pickup are made of aluminum.

To meet the ultimate PNGV mileage goal, one potentially enabling technology is to use carbon-fiber composites, which form the structure of U.S. fighter jets. Carbon-fiber composites weigh about one-fifth as much as steel, but can be comparable or better in terms of stiffness and strength, depending on fiber grade and orientation. These composites do not rust or corrode like steel or aluminum. Perhaps most important, they could reduce vehicle weight by as much as 60%, significantly increasing vehicle fuel economy.

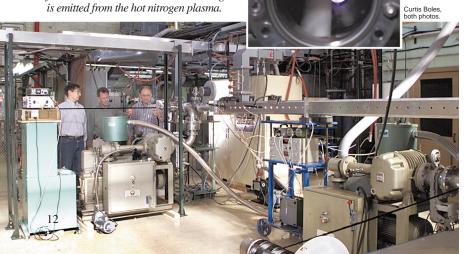
The problem is that carbon-fiber composites cost at least 20 times as much as steel, and the automobile industry is not interested in using them until the price of carbon fiber drops from \$8 to \$5 (and preferably \$3) a pound. Production of carbon fibers is too expensive and slow. The raw material is typically pitch, or polyacrylonitrile (PAN) precursor. It is converted to carbon fibers using thermal pyrolysis, a slow, energy-consuming process that is combined with stressing to achieve the right properties. The precursor, the energy needed to heat it to make fibers, and the large ovens and other capital equipment required in the process contribute to the high cost. As a result, carbon-fiber composites cannot compete economically with steel in the auto industry.

Researchers Alicia Compere and Bill Griffith in ORNL's Chemical and Analytical Sciences Division and several industrial teams are exploring alternative precursors to reduce carbon fiber raw material costs. One promising candidate is lignin, a waste produced during pulping to make paper. This is one project in a joint program of research between ORNL and North Carolina State University (NCSU). The program was recently formalized in a memorandum of understanding between the UT-Battelle management team and NCSU, one of the team's six core universities.

The Composite Materials Technology Group in ORNL's Engineering Technology Division (ETD) is collaborating with the automobile industry to improve the processes of manufacturing and characterizing carbon-fiber composites under program manager Dave Warren. This group, led by Bob Norris, is also developing materials for NASA's Advanced Space Transportation Pro-

Terry White (left), Ken Yarborough, and Felix Paulauskas examine carbon fiber produced rapidly by the microwave/plasma processing device they developed. A carbon-containing, stabilized or partially stabilized polyacrylonitrile (PAN)

precursor fiber is fed into a large tube containing nitrogen gas. When heated by microwaves from the generator in the background, the gas becomes a hot plasma that burns away all the PAN fiber's constituents except carbon, producing the carbonized fiber shown below. Inset: Ultraviolet light is emitted from the hot nitrogen plasma.



gram, armor protection for Army aviation and the Federal Aviation Administration, and high-temperature shafting for the Comanche helicopter. Felix

Paulauskas is leading a team of ETD and Fusion Energy Division investigators and industrial collaborators who are working to demonstrate that microwave heating of PAN precursor in a plasma instead of using less-energy-efficient thermal processing increases the speed and reduces the cost of producing carbon fibers. The project showed that a properly designed and implemented microwave-assisted plasma energy delivery system might quadruple production speed and reduce energy needs and fiber price by up to 20%.

Several methods for fabricating carbonfiber composites have been developed by ORNL researchers and others. For most automotive composite applications, carbon fibers are aligned into a preform, which is placed in a mold. The resin is then injected into a mold and preform and heated to activate and cure the resin. As a result, the fibers are glued together, providing tremendous strength. ETD researchers are working with the auto industry to develop techniques that will automatically align fibers for the preform and will infuse resin effectively into the preform to create finished composites.

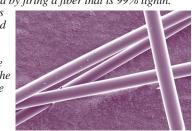
Several ETD mechanical test machines will be moved to the National Transportation Research Center. One device being built by ETD specifically for this program is an intermediate strain rate test machine. The device requirements were developed by ETD's Ray Boeman in collaboration with the automobile industry. In this machine, samples will be compressed at a very fast rate, and measurements will be made to determine the effect of the speed of deformation on the material's properties.

"It's like silly putty," says Dick Ziegler, manager of ORNL's Transportation Technology Program. "If you pull it in two directions slowly, it simply stretches. If you pull it fast, it breaks." The data from this device will be valuable for computer simulations of crashes involving cars made of carbonfiber composites. (See the article on p. 13.)

Because of their high strength, carbonfiber composites could make cars safer. But they won't be used in cars until ways are found to reduce this low-weight material's high cost. ()

Photomicrograph of a carbon fiber precursor produced by firing a fiber that is 99% lignin.

Lignin is dissolved out of wood to separate it from the cellulose used to make paper.



Supercomputers Help Model Cars in Collisions

ORNL researchers are building computer models of vehicles made of regular steel, highstrength steel, aluminum, and carbon-fiber composites. This research could lead to safer cars.

S rdan Simunovic takes an empty beverage can and squeezes it until it folds and collapses like an accordion. "This is what you want to happen to a car during a collision with a rigid barrier or another car," he says. "Metals tend to bend and deform as they absorb the energy of the impact rather than fragment into numerous pieces, as fiber-reinforced composites do. It is this simple plasticity of metals in response to sudden impacts that we can simulate using our materials modeling codes." The codes are run on the IBM RS/6000 SP supercomputer at ORNL.

Simunovic and the six researchers in the group he leads—the Computational Material

Sciences Group in ORNL's Computer Science and Mathematics Division-have developed computer models of vehicles whose bodies are made of regular steel, high-strength steel, and aluminum. With funding from the National Highway Traffic Safety Administration (NHTSA), the group recently developed detailed computer models of the Ford Explorer. These models have been included on ORNL's external Web site, which has received a number of hits because of growing interest in the causes of rollover accidents involving this sport utility vehicle.

The models were built after disassembling a Ford Explorer and scanning in the parts. Each finite-element impact

model, which divides the vehicle into hundreds of small sections, includes a materials model that predicts how the car body material will behave as the vehicle collides from different directions, with a rigid barrier, at 35 miles per hour (mph).

"We are also working on the computational analysis of a concept car made of highstrength steel," Simunovic says. "We use the models to predict the effects on new advanced materials of various collisions, such as two cars colliding with each other. Because these new steel alloys have such high strength, less steel is needed for the body of the car, making it lighter. We found that the ability of the high-strength steel vehicles to hold up in a crash can be even better than that of today's heavier steel vehicles."

In addition, the group has modeled an allaluminum Audi A8 car crashing against a rigid barrier at 35 mph. The data used to improve the model came from NHTSA tests of both an Audi A8 car and its space frame (without the interior, doors, and fender) crashing against a barrier. "We needed crash data on the space frame," Simunovic says, "so we could predict the extent of deformation more accurately." "We are developing constitutive models to predict how the material will behave during an impact at 35 mph," Simunovic says. Referring to the crushed beverage can on his desk, he notes that metals tend to dissipate energy by bending and deforming plastically in response to a blow, whereas composites, which are lighter than steel and have higher specific strength, tend to be stiff, making them less likely to give as easily.

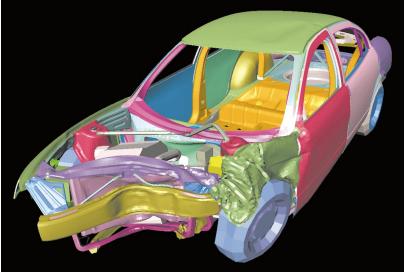
"The impact could cause fibers to break away, or debond, from the polymer matrix," Simunovic says. "The goal is to develop a composite that exhibits controlled progressive fracture during impact. Such a material can dissi-

pate a large amount of impact energy and gradually decelerate the vehicle. We must learn how to model these effects and accurately predict how they change the ability of the material to resist breaking catastrophically in a crash."

For computer simulations of crashes involving cars made of carbon-fiber composites, the ORNL group will use data from the intermediates strain rate crush test station, which will be installed in 2001 at the National Transportation Research Center (NTRC). The station will compress samples at speeds up to 15 mph, providing information on changes in the number of small and long cracks produced as the impact velocity varies.

Members of the Computational Material Sciences Group include J. D. Allen, Jr.; G. A. Aramayo; C. O. Beasley, Jr.; H. K. Lee; B. Radhakrishnan, and G. B. Sarma. A collaborator is A. Bobrek of the University of Tennessee at Knoxville.

"Our goal," Simunovic says, "is to provide the material models and computational tools that designers need to develop highly efficient, low-emission, lightweight vehicles that have improved safety features."



Computational visualization of a high-strength steel automobile body after crashing into a rigid barrier. An NTRC computer will be used for crash modeling.

For Simunovic an even bigger challenge is modeling fiber-reinforced polymer composites, a project he has been working on since 1993. These composites consist of glass or carbon fibers embedded in a polymer matrix. Advanced carbon-fiber composites are made by the P4 process. P4 stands for the programmable powder preform process, in which robots spray fibers of different lengths in a desired orientation on a wire mesh before the fibers are glued together in a mold by means of an activated resin.

Power Electronics: Energy Manager for Hybrid Electric Vehicles

Researchers are improving power electronic modules and electric motors to help hybrid cars squeeze every last mile out of a gallon of gasoline or diesel fuel.

When you drive the next-generation car, advanced electronics will be in charge of the vehicle's energy use. Some people are already driving hybrid vehicles designed in Japan, such as the Toyota Prius and Honda Insight. But the next-generation car likely to come out of Detroit by 2004 will get 80 miles per gallon, while maintaining the size, comfort, and performance of today's family sedan. Because less fuel is burned per mile and the energy is used more efficiently, this car will also emit less carbon dioxide and other pollutants. Power electronics, which controls the flow of electrical energy, will be the key to making the car high in efficiency and low in emissions, meeting the goals of the U.S. Partnership for a New Generation of Vehicles (PNGV).

Each car company has its own unique approach to vehicle design and power control. Generally, the American hybrid car will have a smaller gasoline or diesel engine, sized to meet the average power requirement rather than the peak power required in normal driving. Electric motors powered by batteries will provide extra power to the wheels when needed to accelerate the car or help it climb a hill.

When you step on the brakes, the kinetic energy of the car won't be completely dissipated as heat. Instead, in what is called regenerative braking, the electric motor will act as a generator, capturing energy from the wheels and charging the batteries.

How and when fuel and electricity are used in hybrid cars will be dictated by a computer aided by power electronics. An inverter will convert direct current (dc) from the car's batteries to alternating current (ac) to drive the electric motor that provides power to the wheels. The inverter also converts ac to dc when it takes power from the generator to recharge the batteries.

Don Adams, leader of the Power Electronics and Electric Machinery Research Group in ORNL's Engineering Technology Division (ETD), is spearheading an effort to reduce the sizes, weights, and costs and to increase the efficiencies and useful life of automotive electric motors and inverters. Using Department of Energy funding, he and his colleagues are collaborating with researchers in the U.S. automobile industry to reach these technical targets.

"We are trying to reduce the electric motor to about one-third the volume and onehalf the weight of today's motors," says Adams. "So we have developed a series of highly

efficient electric motors. Another goal is to develop the right materials and manufacturing techniques to reduce the cost of inverters from \$200/kilowatt to \$7/kilowatt. The industry knows how to achieve cost, size, or performance goals, but not all three simultaneously."

The ETD group has already developed an evolving series of "soft-switching inverters" that are more efficient, more compact, and more reliable than conventional inverters. Leon Tolbert, a member of the ETD group and a University of Tennessee professor, says, "To meet PNGV goals, we are trying to reduce the size and cost of the new inverter module by developing circuits that are more efficient so that the heat sink can be made smaller. Our inverter is a strong candidate for electric cars and buses, partly because its lighter weight will increase vehicle energy efficiency."

"Far more electrical power will be required in new vehicles than in today's automobiles," Adams says. "We must make sure that there is enough electricity to operate the wheels, air conditioning, power steering, lights, and information

inverters. Using One of Chattanooga's electric buses has an ORNL-developed soft-switching Department of inverter (shown here) that makes the vehicle lighter and more energy efficient. This Energy funding, inverter also eliminates the problems of voltage spikes, waste heat, and electromagnetic interference that can disrupt operations of other electronic devices.



systems, such as the auto PC and displays of navigational informa-

tion. We must ensure that these systems work well together. We're doing all this work hand-in-hand with the auto companies and their suppliers. Furthermore, we help DOE decide the appropriate direction of the research and assess the progress toward the goals."

At the National Transportation Research Center, researchers are charging ahead with power electronics projects that may help make future cars cleaner, more efficient, and affordable. In the not-too-distant future, that fossil-fueldriven engine will be replaced by a fuel cell. When that happens, the role of power electronics and electric motors will become even more prominent. @

ORNL and UT are working with various organizations to promote vehicles that use less energy and emit less carbon dioxide. Car in Your Future?

G etting people to switch from a gasguzzling sport utility vehicle to a fuel-saving two-seater may seem like a stretch, but anything's possible in an age of rising gasoline prices and concerns about our climate's stability. Look at the Ford Motor Company. It dropped out of a coalition that opposed increasing technology efficiency to avoid climate change. The auto maker then vowed it would voluntarily improve the efficiency of the Ford Escape, its next light truck model, by 25%.

ORNL's Center for Transportation Analysis (CTA) in the Energy Division is actively involved in an effort to persuade more consumers to buy and drive "green" cars and trucks, which use less fuel per mile and emit less carbon dioxide. In 2000 CTA and the University of Tennessee held a Green Vehicle Workshop involving representatives of the U.S. Environmental Protection Agency (EPA), DOE, state and federal agencies, environmental groups, U.S. auto makers, and oil companies. As a result of the workshop, UT and ORNL are forming an industry-government coalition to promote green vehicles through an advertising campaign. In addition, UT and ORNL will work with EPA to develop a rating system that shows which cars emit the most carbon dioxide and pollutants and which ones discharge the least.

"We will expand our efforts with UT to promote green vehicles, such as electric and hybrid vehicles," says David Greene, a CTA researcher based at the National Transportation Research Center and lead author of the transportation chapter for an upcoming report of the Intergovernmental Panel on Climate Change. Greene concedes the goal will not be easy to achieve.

"Hybrid cars are remarkable technical achievements," he says. "They work well and improve fuel economy a lot. The problem is that the Toyota Prius looks like a Toyota Echo but it costs \$5000 more. That extra \$5000 won't be covered by fuel savings over the lifetime of this hybrid car in the United States, but it would be in Tokyo. The Honda Insight costs \$18,000, which is awfully expensive for a two-seater." But, he notes, many people are willing to pay more to drive a car. "The value to most people of owning and driving a car exceeds the price," Greene says. "For example, Europeans are driving more cars even though their fuel price is four times the U.S. cost of gas."



This green truck is part of the ORNL fleet that operates on ethanol fuel.



The flexible-fuel Ford Taurus can run on fuel that is 15% gasoline and 85% alcohol (methanol or ethanol).



Toyota hybrid vehicles have been mass produced since December 1997.

The hope is that more Americans will buy expensive green cars because they value technologies that help protect the environment and preserve fuel supplies for future generations.

"Paul Leiby of ORNL and I are studying the alternative fuel market," Greene says. "We

are evaluating how well existing technologies are doing—such as ethanol, methanol, LPG, compressed natural gas, battery electric, and hybrid cars. These cars are mostly owned by government agencies and big corporations, which are required by the Alternative Motor Fuels Act to operate large fleets of cars that use alternative fuels. For example, ORNL has an ethanol fleet. Our analysis indicates that even with the private alternative-fuel fleets and government subsidies to support refueling stations, the market for alternative-fuel cars and new technologies such as hybrid cars is not going to take off.

"The costs of the car and fuel are too high. Most rational persons will not pay more than \$3000 to have a car that is twice as efficient as what they have now. Hybrid cars must be made much cheaper. But it is possible with advanced technology to bring this cost down."

Greene cites the NECAR, the fuelcell car designed by Mercedes and now being produced and marketed by Daimler Chrysler. "In five years," he says, "the cost of the NECAR came down to one-tenth its original price."

Because diesel cars are 40% more efficient than gasoline cars, Greene sees a good future for diesel cars in the United States if they are sold here by several auto makers. "Diesel cars have improved," says Greene, "The newer ones accelerate better than the older cars, and they don't smell and rattle anymore. They do emit nitrogen oxides and particulates, so diesel cars will have advanced catalytic converters to remove these air pollutants. To keep the catalysts from being poisoned, the new cars will use diesel fuel that has much lower levels of sulfur."

If the diesel car becomes an affordable green car, many more Americans may be willing to spend their greenbacks on it. ()

Biological Ways of Producing Ethanol



This bus in Peoria, Greater Peoria Mass Itansu District, Courtesy of DOE/NREL Illinois runs on fuel made mostly of ethanol produced from corn.

ORNL researchers are investigating ways to reduce the costs of *mostly of ethanol produce* **producing ethanol to make the automotive fuel more competitive with gasoline.**

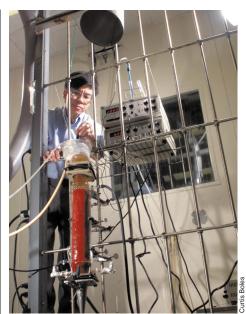
t's easy to get carried away with the advantages of ethanol as a transportation fuel. It is a clean-burning, renewable, domestically produced product made from fermented agricultural products, such as corn. The use of ethanol does not contribute the amount of noxious fumes and volatile organic compounds that standard gasoline spews into the air. Ethanol contains oxygen, which provides a cleaner and more efficient burn of the fuel. In E-85 fuel, made of 85% ethanol and 15% gasoline, ethanol lowers emissions of unhealthy carbon monoxide by 30% and carbon dioxide by 27%. Although ethanol emits carbon dioxide when burned, much of this greenhouse gas is absorbed, or recycled, by the types of crops from which the ethanol was made. As a result, burning ethanol contributes very little net carbon dioxide to the atmosphere.

In terms of cost, however, E-85 doesn't compete with gasoline yet. Dick Ziegler, manager of ORNL's Transportation Technology Program, who often drives one of ORNL's green ethanol cars, says, "On one of my trips to Detroit, when gasoline cost \$1.34 a gallon, E-85 fuel cost \$2.26 a gallon. A 50 cent per gallon tax credit would be required to make ethanol cost the same as the wholesale price of gasoline."

Several ORNL researchers are working on lowering the cost of ethanol production. In the first step of this process, cellulose from waste wood and paper or harvested corn, switchgrass, or hybrid poplars is pretreated with enzymes and acids at the appropriate pressures and temperatures. Cellulose is a polysaccharide containing chains of 6-carbon sugars. Jonathan Woodward and his colleagues in ORNL's Chemical Technology Division (CTD) are trying to find a more efficient, cost-effective enzyme that can split cellulose into individual sugar molecules, such as glucose and xylose, for direct conversion to ethanol.

The next step is fermentation—converting sugar into ethanol using microorganisms. Researchers Nhuan Nghiem, Brian Davison, and Tanya Kuritz, all of CTD, are working on lowering the cost of this step.

Nghiem and Davison are experimenting with a syrup of simple sugars, called lignocellulosic hydrolyzate, supplied to them by Arkenol Inc. They pump the syrup up through a fluidized-bed bioreactor (FBR) containing gel beads stuffed with



Nhuan Nghiem checks the bioreactor in which microorganisms stuffed into gel beads convert sugar (from enzyme-degraded cellulose) to ethanol for use as fuel.

Zymomonas mobilis bacteria. The bacteria eat the sugars and excrete ethanol, which comes out of the top of the bioreactor looking like beer froth.

"By using immobilized biocatalysts in an FBR, we produce ethanol 10 to 20

times faster than do traditional batch processes using suspended bacteria in stirred tank bioreactors," Nghiem says. "If our technique were widely used to produce ethanol, the cost of the fuel could be lowered by 3 to 6 cents per gallon."

To reduce costs further, the researchers envision a single system for using both cellulose-degrading enzymes and microbes that ferment the resulting syrup to produce ethanol (which would then be distilled to yield a transportation fuel). The problem is that *Zymomonas mobilis* bacteria prefer a temperature of 35°C and cannot tolerate the 55°C temperature at which the enzymes work best. "Tanya Kuritz and I are trying to genetically engineer two candidate sugar-eating microbes that thrive at 55° C," says Nghiem. "We will add the genes that make the two key enzymes that produce ethanol as the desired final product, which is a waste product of the bacteria. We will knock out the genes responsible for the excretion of other products, to maximize ethanol production."

DOE's Bioenergy Feedstock Development Program, which is managed at ORNL by Janet Cushman and Lynn Wright, is using genetic manipulation in a quest to maximize carbon production in hybrid poplar trees and switchgrass, a native perennial prairie grass. One goal is to increase the yield of ethanol from these plants.

Sandy McLaughlin of ORNL's Environmental Sciences Division and Marie Walsh of the Energy Division are studying the economics of using switchgrass to produce ethanol. They are evaluating the soil and water quality and farm income benefits that result from producing switchgrass in place of corn, wheat, and other annual crops. They are also comparing the greenhouse gas emissions that result from producing and using ethanol made from switchgrass with those from the use of gasoline and other alternative transportation fuels. Inclusion of environmental and social benefits into the market price of transportation fuels has the potential to alter significantly the relative economics of the different fuels. (2)



Janet Cushman, co-manager of DOE's Bioenergy Feedstock Development Program at ORNL, examines species of fast-growing switchgrass.

Aviation Research Takes Off at ORNL

ORNL researchers are studying ways to improve air traffic management and safety.

L ate landings. Canceled flights. Airplanes idling on runways as pilots or the signal to depart. For the second it summer, passengers flying on U.S. airndured an increasing number of flight depometimes having to miss scheduled events to p overnight in air terminals. Why is air approaching gridlock? Reasons given are reasing number of passengers and flights

west Airlines and assisted by Lockheed Martin Management and Data Systems, Simon Rose, Rome, and Lee performed a cost-benefit study for NASA to determine whether the airline might save money by swapping landing slots among its own flights. During the final descent phase of flight, planes can speed up or slow down by as much as 10 minutes to enable these swaps.

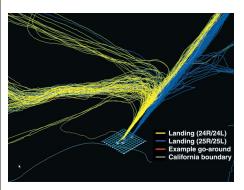
"Moving a flight a few minutes can mean the difference between lots of missed connections and just a few missed connections involving both passengers and crew members," Rome says. "Changing a flight from 30 minutes late to 20 minutes late can remove delay costs entirely."

For the study, cost models and an optimum resequencing algorithm were developed. Using the results of the study, the ORNL researchers concluded that the U.S. airline industry would save \$75 million a year if this strategy were operationally feasible. About 30% more would be saved if unused landing slots were employed.

To increase their numbers of daily flights (airport capacity), many airports used the controversial practice of allowing one aircraft to land on one runway and stop short of a second, intersecting runway, permitting another plane to simultaneously land on or take off from that runway. In 1999 the Airline Pilots Association (ALPA) opposed this practice as being potentially unsafe and threatened a boycott unless the safety margins were increased. Berry recently provided a better estimate of the cost of eliminating the procedure and, thus, allowing fewer flights. This estimate improved the basis for making decisions about trade offs between increased safety margins and reduced airport capacity. The arguments were presented to the major airlines' operations managers, ALPA, and the FAA. FAA and ALPA worked out a compromise that both improved safety margins of such simultaneous operations and retained much of the increased capacity.

Aviation safety is being studied by ORNL researchers Joe Cletcher, Gary Mays, Mike Poore, and Simon Rose. They are applying techniques developed for the nuclear industry to aviation. The goal is to identify accident precursors by coding the chains of events that contribute to aviation accidents and incidents.

In another safety analysis study for the FAA, Berry worked with Austin Digital, Inc., to identify situations that could lead to safety problems, such as missed approaches to runways (e.g., an airplane coming in too fast at the wrong angle). The collaborators modified digital flight data analysis software (used for "black box" data) so that it could analyze radar data. They demonstrated its use to high FAA officials in March 2000. "This tool," Rose says, "is the first to use radar data for safety analyses." ()



This sample of airplane landings at Los Angeles International Airport shows an example go-around flight that occurs when a pilot is informed that the airplane is coming in too fast at the wrong angle—what is known as a "missed approach."

planes idling on runways as pilots wait for the signal to depart. For the second straight summer, passengers flying on U.S. airlines endured an increasing number of flight delays, sometimes having to miss scheduled events or sleep overnight in air terminals. Why is air traffic approaching gridlock? Reasons given are the increasing number of passengers and flights as a result of lower fares, severe thunderstorms, insufficient runway space, airline employee strikes, and an antiquated air traffic management system. Yet, the national air system has excelled in keeping big jets from flying into one another.

In 1991, when Lee Berry, Jim Rome, and other ORNL researchers began analyzing air traffic operations for the Federal Aviation Administration (FAA), they predicted that the worst air congestion at the end of the decade would occur over the Cleveland, Ohio, area. "That has proven to be the case," says Teresa Rose, program manager for aviation research at the National Transportation Research Center.

According to Rose, the ORNL group hopes to help the FAA reduce "en route airline congestion" by developing a computer model. Berry, Rome, and Ron Lee have received FAA funding to develop a model to predict the probability of airplane delays for different sectors of air space.

"We will look at ways to avoid delayed landings caused when airplanes are forced to take a longer route to better space out planes headed for the airport," Rose says. "The model will take into account severe weather, flight delays, and increased spacing of plane arrivals and departures to allow air traffic controllers time to adjust to upgraded equipment. Our model should help airlines select better flight times and routes to reduce en route delays."

ORNL researchers have completed several studies of air traffic congestion. With American Airlines, they modeled delay propagation by simulating delays and introducing the concept of

Packaging and Transporting Hazardous Materials



O n May 11, 1996, ValuJet Flight 592 crashed shortly after takeoff in the Everglades near Miami, Florida, killing all 105 passengers and 5 crew members. The National Transportation Safety Board determined that the probable cause of the accident was a fire in the airplane's cargo compartment that was started by the activation of at least one of the oxygen generators being improperly carried as cargo. This crash is a vivid example of the potential for tragedy that can result from the transport of undeclared "dangerous goods."

The expired but unexpended oxygen generators were identified as "airplane parts," instead of being properly classified as hazardous materials and specially packaged and handled to mitigate the hazards. "Proper classification, labeling, and packaging are important to safety," says Scott Ludwig, leader of the Transportation Technologies Group in ORNL's Chemical Technology Division. The group is located at the National Transportation Research Center (NTRC).

Rick Rawl, one of the group's members, has spearheaded the development of the Hazardous Materials Transport Expert System, which tells users what type of package is required for a product, as well as how to properly classify, label, and ship the package to meet regulations. "If a user wants to know how to safely package, label, and ship a substance—even an unusual mixture of substances such as a combination of acetone and hydrochloric acid—our software can provide the answers," Rawl says.

Since 1960 the Transportation Technologies Group has been evaluating the ability of packages to protect their contents from damage and prevent the contents from escaping in case of accidents. The researchers have focused on containers of radioactive materials, including spent nuclear fuel. To meet federal regulations, any container for transporting a significant quantity of radioactive materials must be designed so that none of the material escapes, even if the container is involved in a rail or truck accident.

The ORNL group has conducted drop tests of packages of various designs to determine which ones best contain and protect their contents following a severe impact. Casks and other containers have been dropped 200 feet from ORNL's Tower Shielding Facility and, more recently, 30 feet from a mobile crane onto a specially designed, unyielding steel-and-concrete pad. The dropped packages and their contents are photographed and evaluated to determine the extent of damage and the potential for leaks of radioactivity.

"There have been very few transportation accidents involving radioactive materials," Ludwig notes. "One accident happened on December 8, 1972, in nearby Lake City, Tennessee, when a truck rolled over and a cask of spent fuel fell to the ground. Unfortunately, the driver was killed. But the cask was not damaged, and no radioactivity was released to the environment." "We will continue drop tests at the NTRC."

says Larry Shappert, who has been conducting drop tests of packages for 40 years. "We have the capability at the NTRC to drop 10,000-pound packages from 30 feet onto a newly designed impact pad. We also have an impact pad inside the packaging lab which can be used to test small packages."

To guide designers and shippers of casks of radioactive materials, Shappert in 1998 prepared the *Radioactive Materials Packaging Handbook*, 350 copies of which have been published. It provides information on shielding, criticality, heat transfer, testing, and operation, as well as Department of Transportation and Nuclear Regulatory Commission regulations.

Shappert currently advises the Defense Logistics Agency on what needs to be done to properly package and ship 55-gal. drums of radioactive materials and special chemicals that could be sold. He also tests the effectiveness of special materials designed to cushion the contents against the shock of an impact by absorbing its energy. These materials, called impact limiters, are usually made of steel honeycomb, redwood, or balsa wood.

"At the NTRC, our program will be expanded to test packages for hazardous chemicals and high-value commodities, such as television sets and other electronic devices," Ludwig says. "We hope to offer packaging advice to local companies."

"In the NTRC lab we will have a vibration table to shake packages and a compression testing device to squeeze them," Rawl says. "For example, the vibration table will allow us to shake a TV set until it breaks. In this way, we'll know the level of vibration the package should be designed for to protect the TV against transportation-related damage."

The group's computer center at the NTRC provides information that will help shippers minimize the effects of transportation accidents, although rare, involving radioactive materials. Users can access an NTRC server that hosts Transportation Routing Analysis Geographic Information Systems (TRAGIS). This software package selects interstate and state-preferred routes for radioactive materials carriers that avoid heavily populated areas. The computer service, which provides the latest census information, is used in conjunction with risk codes such as RADTRAN. Thus, users can calculate the potential total radiation exposure of all drivers and the public who live within a half mile of the truck, rail, or waterway route taken by the vehicle carrying radioactive materials. The information is useful for environmental impact statements and other risk assessments.

So, if you're looking for a useful transportation-related software package or a package test, you may find it at the NTRC. O

Transportation Planners Aided By GIS Research

Most people rely on paper maps to guide them to a destination, but some researchers use geographic information systems (GIS) tools to make maps to improve transportation. GIS is a computer system that assembles, stores, manipulates, and displays data identified according to their geographic locations. GIS technology can be used for scientific investigations, resource management, and development planning.

At ORNL's Center for Transportation Analysis (CTA) in the Energy Division, Bruce Peterson and Frank Southworth have developed a GIS-based research tool used by the U.S. Department of Transportation (DOT), state DOTs, private companies, and universities. It is called the North American Intermodal Freight Network Model. ORNL researchers have used the model to estimate the annual ton-miles of freight on U.S. roads, waterways, and rail lines in support of the U.S. Census Bureau's 1997 Commodity Flow Survey.

For this project, Peterson developed algorithms that calculate the shortest route and the least costly combination of modes (truck, barge, rail car) for moving freight rapidly and economically from one zip code area to another in the United States. Some 5 million such routes were simulated in support of the 1997 Commodity Flow Survey.

"Separate truck, rail, and waterway networks have existed for a long time," Peterson says. "We have come up with a unified network that models the U.S. transportation infrastructure by including all freight-carrying modes."

"State departments of transportation could use the network to simulate the flow of traffic over their major highways, rail lines, and waterways," Southworth says. "These flow patterns might then be used to estimate the need for new investments in transportation infrastructure."

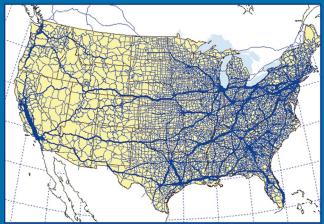
S. M. Chin of CTA uses GIS tools to study the movement of freight between airports; truck and rail terminals; and sea, lake, and river ports. He identifies bottlenecks where freight changes hands from one mode of transportation to another, such as the traffic congestion around Los Angeles International Airport. Displays of data on GIS maps suggest where resources should be invested to reduce congestion and eliminate bottlenecks to expedite truck-air, truck-rail, truck-water, and rail-water transfers of freight.

Some of ORNL's GIS researchers may move to the GIS laboratory at the National Transportation Research Center. The director of the laboratory is Don Alvic of the University of Tennessee (UT), and the laboratory is staffed by UT researchers. One project under way there is to use data from county departments of transportation to determine the best places to locate proposed new roads. The UT researchers examine the characteristics of the current highway system, interchange accessibility, bridge weight limitations, and landuse considerations before recommending possible locations for new routes.

"Our GIS lab produces data similar to the Internet maps from search engines, but these maps are more complicated," Alvic says. "Our software will find the shortest, fastest route between two points. Military transportation planners, for example, may

want the best highway route that allows them to avoid travel through some cities and over certain bridges. If they are shipping biological and chemical warfare materials for disposal, they may want to find a route that passes through areas of very low population, to minimize the chances of accidental exposures."

GIS studies by ORNL and UT researchers are helping to put East Tennessee on the transportation research map.



This GIS map shows areas of the United States where truck traffic is particularly heavy (denoted by thickness of colored lines).

Defense Transportation and Logistics Research

Better ways to deploy military troops, manage military supply chains, and minimize river barge congestion may result from ORNL-UT teamwork.

On the large "video wall" of the National Transportation Research Center's (NTRC's) Operations Center, ORNL and University of Tennessee (UT) researchers will demonstrate to current and potential sponsors their latest computer programs for coordinating the actions of personnel and the deliveries of supplies. In this way, they can simulate an actual operations center or provide needed training.

In the early 1990s, this facility could have come in handy for demonstrating the Airlift Deployment Analysis System (ADANS). The system was developed partly by Glen Harrison, Mike Hilliard, Cheng Liu, Ingrid Busch, and Charlie Davis, all of the Center for Transportation Analysis (CTA) in ORNL's Energy Division, and several UT researchers, who are all now working at NTRC's Operations Center. ADANS is a series of scheduling algorithms and tools that enabled the Air Mobility Command of the U.S. Air Force to deploy troops and equipment to the Persian Gulf in 1990 and 1991 more rapidly and more efficiently than had been done before. Since then, ADANS has been used for all major U.S. deployments, including Somalia, Haiti, Rwanda, Bosnia, and Kosovo.

ADANS is now being maintained by an Air Force subcontractor. However, Davis and Busch still provide assistance as consultants, and the CTA group still helps with improving the scheduling algorithm.

CTA, which has provided analytical and operational support to the defense transportation community for more than 15 years, will continue to do so at NTRC through its Defense Transportation and Logistics Program. It is developing innovative, practical tools and techniques that will be used to analyze and manage military transportation and logistics systems.

Working with Robert Russell and other staff from UT's Transportation Management and Logistics Program and private consultants, Harrison, Hilliard, Liu, Rekah Pillai, and Angela Sexton (Computational Physics and Engineering Division) are evaluating the Defense Logistic Agency's (DLA) management of its supply chain from cradle to grave. DLA's mission includes managing over four million consumable items and processing 83% of all Department of Defense requisitions.

"If the military forces fight with it, wear

it, eat it, burn it as fuel, or otherwise use it, DLA probably provides it and then arranges for its reuse after the consumer no longer needs it," Hilliard says. "We examine the flow of consumables for DLA to see if they can be transported efficiently but at lower cost. Currently, many items are sent across the country by Federal Express or other premium shipping options, which is expensive. "We look at how

the services acquire items by purchasing them from vendors, where they are stored in depots, and how they are distributed to end users. The major storage depots are in California and Pennsylvania, with 20 local depots in between. We are studying the use of third-party logistics providers and information technology, to minimize the cost of storage and transportation of goods."

Another transportation-related logistics project involving the CTA group is the development and testing of the Ohio River Navigation Investment Model for the U.S. Army Corps of Engineers. Each year, more than 260 million tons of cargo move across the 2400 miles of the Ohio River system. The river is economically attractive as an alternative to rail and highway transportation of heavy bulk cargo such as coal, grains, and building materials if travel times are reasonable. However, as travel times increase because of congestion at the river's locks, the additional cost of operating a tow boat and barges cuts into the transportation savings.

The ORNL-UT computer model examines the economics of shipping goods by barge on the Ohio River over the next 70 years as barge traffic increases. The model calculates the risks of lock closures that could result from failures in lock components, maintenance activities, and blockages caused by, say, barge collisions and floating logs.

"Our model will determine what investments should be made by the Army Corps of Engineers to expand, repair, or replace locks to maximize the flow of barge traffic and yield maximum economic benefits to the nation," Hilliard says. "We evaluate the economics of various options at each lock. One option is to replace the electrical system and other components early to prevent lock failures. Another option at the smaller locks is to double lock size to allow a tow boat pushing 15 barges to get through without having to stop, break apart some barges, and push only half as many through the lock at one time. Of course, lock construction and other options, such as shifting some cargo to trucks and trains during the work, have a cost."

The ORNL-UT model could help the Army Corps of Engineers improve its operations on the nation's river systems. (9)



Fifteen barge tows head downstream from Belleville Locks and down the Ohio River. Construction on the far side of the dam is a hydro electric power plant. Belleville Lock and Dam is located on West Virginia and Ohio shores and was completed in 1968.

Software Tools Will Help Emergency Responders

The nerve gas sarin is surreptitiously released into the unprotected airconditioning vent of a Knoxville, Tennessee, high school. Some 500 students and teachers are affected. Many vomit and cough violently. Others complain of headache, nausea, blurred vision, and muscle weakness. Paramedics are rushed to the scene to begin treatment. Some 400 victims are taken to local hospitals, and all but two survive this terrorist attack.

Then a week later, at a Tennessee Vols football game attended by 108,000 people, terrorists release anthrax bacteria in Neyland Stadium. An anonymous letter from the terrorist group to a local newspaper claims responsibility for exposing unsuspecting football fans to a biological warfare agent. As a result of the publicity, thousands of people flood Knoxville hospi-

tal emergency rooms, demanding treatment. Physicians are brought in from other Tennessee cities and other states to assist local doctors in determining which patients inhaled the anthrax bacteria and need immediate treatment with an antibiotic. Additional medical supplies are provided from around the country to save the lives of the victims.

These fictitious scenarios are in the minds of the developers of the Responder Assets Management System (RAMS), a suite of software tools for assisting "first responders"—police, fire, medical, and city emergency personnel. RAMS is designed to help responders deal more quickly with daily emergencies, such as fires. It also, however, will better enable emergency personnel to respond to mass casualty incidents, such as earthquakes and re-

leases of chemical and biological weapons by terrorists.

RAMS is being developed for the U.S. Army's Soldier and Biological Chemical Command by Bob Hunter and Amy King, both of ORNL's Computational Physics and Engineering Division; Scott McKenney of BWXT Y-12, LLC; and several University of Tennessee researchers, all of whom are based at the Operations Center of the National Transportation Re**ORNL** and **UT** have developed software tools to assist police, fire, medical, and city emergency personnel.

search Center. Scheduled for completion by July 2001, RAMS is being revised using recommendations from first responders in Atlanta, Georgia; Baltimore, Maryland; Knoxville; Salt Lake City, Utah; and Wichita, Kansas.

"The responders tell us what information they need and we tell them what is possible with the technology," Hunter says. "We have expertise in redefining problems normally solved on expensive workstations so they can be handled by low-cost, easy-to-use personal computers. We developed a PC-based command and control system for the Atlanta police that was used for the RAMS should help responders with PCs deal more effectively with traffic flow problems, thanks to its tools for managing street status information. Responders will be able to electronically share information in a Web browser. They can send or read messages that tell which streets are flooded out, impassible due to an accident or downed power lines and tree limbs, or turned into one-way lanes to aid traffic flow (e.g., after a big sports event or in an evacuation in response to hurricane warnings).

RAMS also has a street management tool that might be used to help responders plan for an

event such as the 2002 Winter Olympics Games in Salt Lake City. All the traffic management information comes together in an integrated "situation display"—an interactive geographic information systems map on a big screen that shows what's happening any place in the city at any time.

A most useful RAMS tool is the Response Options Generator (ROG), a decision support tool that enables commanders to better understand and manage a crisis situation, such as a release of a chemical or biological agent. RAMS displays the location and status of hospitals, satellite clinics, and medical equipment. It gives the symptoms of exposure to various agents, tells whom to notify, and provides links to state and federal emergency management resources.

"As you enter data to profile the situation, ROG identifies the optimal response, which you can modify," Hunter says. "ROG then automatically generates a schedule for responders to follow and identifies resource shortfalls. For example, it tells you how many more medical personnel and medical supplies you will need brought in to treat the victims of a terrorist attack."

RAMS allows responders to strike fast, turning scary events into opportunities to save lives. (*)



RAMS software tools will help police, fire, medical, and city emergency personnel respond more quickly to mass casualty incidents.

1996 Summer Olympic Games. Because PCs are cheap and newly hired responders are often computer literate, now is the time to automate responders' jobs throughout the nation."

Many of the RAMS tools will help public safety agencies carry out routine daily functions, such as timekeeping, scheduling, dispatch analysis to find trends, personnel training, and equipment tracking. Some of these tools are already being used by the Atlanta police.

E-Commerce's Impacts on Transportation

In some ways, electronic commerce could reduce transportation needs, but in other ways, it could increase them.

magine that you have a computerized home business that tracks truck routes and auctions off truck space to various companies that need help delivering their products all over the nation. You feel good about your business because it increases transportation efficiency. It puts on the road a larger number of fully loaded trucks and fewer half-empty ones. You also feel good because you do your banking online and download most of the books, videos, and music that you want from the Internet. That means you are not driving to your bank and several stores; instead you're saving fuel and reducing emissions of carbon dioxide and other pollutants. Nevertheless, you are ordering groceries, clothes, and household items online, so you're partly responsible for the increase in delivery truck traffic in what used to be a quiet neighborhood.

Now, multiply yourself many times over and you can see why ORNL's Center for Trans-

portation Analysis (CTA) and the Transportation Research Board co-sponsored a workshop on the "Impacts of the New Digital Economy on Transportation: Developing Research and Data Needs." As a result of the workshop held September 14 and 15, 2000, in Washington, D.C., Pat Hu, director of CTA, is developing a research agenda and identifying the data needed to allow accurate predictions of the effects of the digital economy on transportation with respect to planning, land use, safety, the environment, and energy use.

Mike Hilliard, Frank Southworth, Rekha Pillai, and David Middendorf, all of the CTA in ORNL's Energy Division, recently published a white paper entitled Potential Effects of the Digital Economy on Transportation, which was distributed at the

workshop. They evaluated business-to-business, business-to-consumer, and consumer-toconsumer electronic commerce, as well as telecommuting.

"We tried to identify how e-commerce will change the demand for transportation," Hilliard says. "Because information can be transmitted electronically, it may be unnecessary in the future to ship as many books, videotapes, and music CDs by Federal Express, United Parcel Service, or the U.S. Post Office. Banking can be done online so people won't have to drive to the bank so often. So the effect of e-commerce could be a reduction in the driving of cars."

On the other hand, Hilliard notes, if an increasing number of people do online shopping and order groceries and other items from large discount stores online, there will be increased demand for deliveries by truck and increased truck traffic in residential neighborhoods, threatening the safety of pedestrians and pets.

An increase in telecommuting could create its share of altered traffic patterns, as well. "If more people telecommute, they may move farther from their workplace in the city," Hilliard says. "But when they do commute to their business for occasional meetings, they will drive farther."

Transportation needs could be reduced if community work centers networked to multiple employers were established for telecommuters throughout the nation. "You drive a short distance to a center that has up-to-date computer equipment leased by your company," Hilliard says. "You do your work at the center for your company whose headquarters are far away."

Hilliard says that the digital economy could impact land use. "How will the digital economy change our cities 20 years from now?" he asks. "Will the large, multi-purpose shopping malls of today remain popular in 20 years, or will e-commerce make them as uncommon as they were only 40 years ago?"

Current planning to meet future transportation needs is complicated by our inability to predict the effects of e-commerce on those needs. According to ORNL's white paper: "With the competing forces at work in this system, it will be challenging to determine the net effect of the changes, particularly as the digital economy continues to



Because information, entertainment products, and money can be transmitted electronically and shopping can be done online, electronic commerce is expected to affect transportation needs. Photo collage by Gail Sweeden.

Learning Smart Ways to **Use Intelligent Transportation Systems**

ORNL-developed tools may help traffic management centers reduce congestion. Researchers will determine if intelligent transportation systems in cars cause information overload.

Intelligent transportation could be seen as a high-tech search for the road less traveled. It strives for improved traffic flow to ensure safer, quicker, less expensive, and moreenergy-efficient travel.

Many intelligent transportation systems (ITS) are being designed to better manage traffic on well-traveled roads to reduce congestion and achieve these goals. Inside cars, navigational systems with display panels are intended to guide drivers around heavy traffic and help them avoid accidents. Traffic management technologies are designed to communicate with drivers on busy interstate highways through navigational systems and variable message signs.

The Federal Highway Administration (FHWA) initiated a Dynamic Traffic Assignment (DTA) research project to develop advanced software tools that will be used to address complex traffic control and management issues in the information-based, dynamic ITS environment. Under the DTA project, Rekha Pillai, Cheng Liu, Ingrid Busch, and Charlie Davis, all of ORNL's Energy Division, along with researchers at both the University of Texas at Austin and the Massachusetts Institute of Technology, are developing real-time Traffic Estimation and Prediction System (TrEPS) software tools. The goal is to help traffic management centers (TMCs) anticipate and avert traffic congestion.

TrEPS uses traffic surveillance data in conjunction with advanced traffic models to estimate and predict traffic network conditions and to generate guidance for travelers. In addition, it can interact with advanced ITS-based traffic control systems to produce proactive traffic control actions to reduce congestion.

TrEPS will eventually be used by TMCs in urban areas. For example, TrEPS can provide input to traffic managers who decide where and when to post specific messages on variable message signs, such as AVOID CONGESTION-EXIT HERE FOR ALTERNATE ROUTE.

"The typical operations of traffic management centers tend to be relatively reactive in nature," says Bill Knéé, ORNL program manager for intelligent transportation systems at the National Transportation Research Center (NTRC). "Using real-time traffic data from road sensors monitoring the number of cars and their speed, TrEPS predicts traffic conditions in the near future. Thus, it could help TMCs become more proactive by alerting them to control measures that lead to poor traffic flow. TrEPS also allows traffic managers to predict how traffic flow patterns will change under what-if scenarios, such as adding a lane or building a bridge."

Knoxville will soon establish one of the first TMCs in Tennessee. Video cameras, road sensors, and variable message signs will be placed along interstate routes.

"We hope NTRC will be a site for the Knox County Traffic Operations Center because we can collect data and do research using TrEPS and be partners in improving operations at the center," Knéé says. "We can use this center to showcase advanced traffic systems technologies and traffic management strategies."

ORNL's Energy Division researchers became interested in doing research on ITS because

these information systems could potentially save energy by allowing drivers to avoid congestion (unless the technologies entice people to do more driving). But Dan Tufano and Phil Spelt, two researchers in ORNL's Computer Science and Mathematics Division who once studied the human factors of nuclear reactor operations, are interested in the behavioral aspects associated with driving cars equipped with these technologies. They want to know to what extent drivers are distracted, startled, or annoved by information overload as a result of ITS in cars. These technologies include cell phones, navigational systems with map displays, voice messages, collision avoidance warning systems, and electronic mail from the auto PC (which can also be used for Web surfing).

At NTRC, Tufano and Spelt will be studying people's reactions on a driving simulator, which features a driving buck (the forward portion of a car body, with a steering wheel, accelerator, and ITS technologies) and a screen showing the car being driven along a computer-generated road in the presence of both other computergenerated cars and pedestrians. They also plan to measure reactions of drivers of DOE's research vehicle, a 1999 Dodge Intrepid that is outfitted with ITS. The researchers may measure and compare brain-wave patterns, heartbeat rate, and muscle tension of each volunteer when driving a traditional car and then the research vehicle.

Meanwhile, ITS researchers at ORNL are looking around the bend at new projects coming their way: integrating ITS in a Smart Truck for the military and participating in DOE's 21st Century Truck Program for developing trucks that have improved fuel efficiency, reduced emissions, and enhanced safety.

Fortunately, smart people are studying whether smart vehicles and smart highways are being used in the most intelligent way.



Dan Tufano (left) practices driving while Phil Spelt watches a simulator incorporating the car in a virtual road trip.

UT Goal: Safer Trips

Safer roads and safer rides are among the goals of some University of Tennessee (UT) researchers at the National Transportation Research Center (NTRC).

Mike Jackson, a UT professor, is paving the way for more durable roads. He is studying ways to improve highway pavement materials and systems. He notes that the design of pavement is currently based on design equations developed from performance tests completed in the late 1950s and early 1960s.

"Because of the ever-increasing traffic on our highways, we are experiencing an increasing frequency of pavement failure in the form of rutting, cracking, and—ultimately—potholes," Jackson says. "To reduce the public's exposure to reconstruction, rehabilitation, and maintenance activities, we are attempting to identify pavement systems in the laboratory that will last longer on the highway, increasing safety and minimizing costly delays to the traveling public."

Jackson and other researchers are currently evaluating new pavement performance tests in the NTRC's infrastructure materials laboratory. Jackson hopes to identify longer-lasting pavement materials for possible use on the road.

Jackson and his colleagues at the Tennessee Department of Transportation (TDOT) are also participating in the construction of a fullscale test track at the National Center for Asphalt Technology (NCAT) in Auburn, Alabama, to

evaluate different pavement materials and design principles.

Loaded trucks will be repeatedly run over pavement test sections at the NCAT test track. The results of this full-scale testing will be used by TDOT to further evaluate the performance of Tennessee's pavements.

Jackson will also test these pavement materials in the NTRC lab with special equipment, such as an asphalt pavement analyzer from Pavement Technology, Inc. This accelerated testing device will help researchers evaluate the anticipated performance of different aggregate and asphalt blends in the laboratory. Jackson hopes that once the NTRC lab is outfitted with this and other equipment, new avenues of external funding will open up. Tyler Kress, an assistant professor of industrial engineering at UT Knoxville, has made important contributions to improving the safety of automobile airbags and understanding injuries associated with personal watercraft.

Since the late 1990s, the U.S. government has required automobile manufacturers to install airbags in all passenger cars and trucks to protect occupants during an accident. Several manufacturers started using airbags as early as the late 1980s. Because the early "one size fits all" airbag design causes serious and sometimes fatal injuries to some children and adults during deployment, newer airbags have been designed to be "smarter." "To minimize injuries," Kress says, "some airbag systems have sensors that detect occupant size, use or nonuse of a seat belt, and crash severity, to determine how the airbags should be deployed."

Kress was one of the human factors researchers who gathered information for the engineers designing the newer airbag systems. He and his colleagues studied people's injuries resulting from airbag deployment and then tried to reproduce the injuries on cadavers and dummies in the lab. They subjected heads of cadavers and dummies to impacts from airbags made from different materials, folded in various ways, and deployed at different speeds. They measured the force, velocity, and pressure of the airbags and assessed the extent of the resulting "injuries."

In the mid-1990s Kress and his colleagues drew upon the results of their studies to suggest ways to improve airbags to make them safer and more effective. Kress and four researchers from other universities were invited to present their findings to the National Transportation Safety Board. Since then, he and his colleagues have noted improvements in the commercial airbag.

Kress's airbag research is not, however, limited to road vehicle safety. Last year, the Federal Aviation Administration announced a need for a regulation to improve safety features on commercial aircraft. Kress recently completed a paper with a colleague at BF Goodrich that discusses inflatable lap belts as a feasible protective alternative for certain applications.

At the human factors and biomechanical engineering laboratory at NTRC, Kress hopes to continue his work to understand how personal watercraft injuries occur. In his research with the personal watercraft industry, he has collected data on damaged jet skis, accident scenes, and actual injuries.

> Kress, who is also associate director of The Engineering Institute for Trauma and Injury Prevention, has created dummies with breakable "synthetic" bones for crash tests, to evaluate designs of products, such as outboard motor propeller guards in watercraft and motorcycle crash bars. He uses sled systems, drop towers, high-speed cameras, velocity detectors, and force and acceleration measurement devices to assess injury potential during "crashes." The goal is to collect information to be used to improve the design of vehicles to minimize injuries to occupants during collisions. (9)

(Wendy Bigham, a graduate student in the Science Communication Program of the University of Tennessee's School of Journalism, contributed information and photographs to this article.)



Tyler Kress measures the dimensions of a dummy head after subjecting it to airbag testing in a laboratory at Southern Impact Research Corporation.



Mike Jackson evaluates the anticipated performance of pavement samples in this testing device. He hopes to identify longer-lasting pavement materials.

Editor's note: The following three articles describe ORNL technology developments that won R&D 100 Awards in 2000. The awards are presented annually by R&D Magazine in recognition of the year's most significant technological innovations. ORNL's 107 R&D 100 awards place it first among DOE laboratories and second only to General Electric.

Mass Spectrometer CanDetect Weapons of MassORNL helped design the first portable massDestruction

reconnaissance soldier drives a A humvee through a field in enemy territory. His companion pushes a button on the display unit of a computerized instrument. Both soldiers are wearing protective gear. Their goal is to map out the area to determine which routes are safe for U.S. troops and which ones should be avoided. Eventually an alarm sounds. "Nerve gas VX has been detected," the soldier says to the driver, while checking the instrument. "We'd better take a different route." The soldiers drop warning markers and head in a new direction. An hour later, an alarm sounds again. This time the instrument has sniffed out another nearby threat: a cloud of anthrax spores. "Let's try another way," the driver says.

This scenario may play out in two or three years in a combat zone where soldiers will be able to use a vehicle-mounted Block II chemical biological mass spectrometer (CBMS), developed by ORNL and several partners. The CBMS, which received an R&D 100 Award in 2000, can detect both biological and chemical warfare agents in the midst of pollen; mold spores; engine exhaust; and fumes from fuels, lubricants, and fires, which would confound most detectors.

The CBMS can detect a biological warfare agent in about 5 minutes, much faster than the almost 15 minutes required by its nearest competitor. But it is unique in other ways, too.

"The CBMS is the only integrated system that can detect and identify chemical agents on the ground and in the air and biological agents in the air," says Wayne Griest, principal investigator for ORNL's project to develop the CBMS. "Compared with separate detectors, it is lighter, smaller, less power-intensive, and able to detect and identify more agents with improved sensitivity and reliability. It is tolerant to radiation, less expensive to use, and easier for soldiers to

operate and maintain."

The heart of the Block II CBMS is an ion trap mass spectrometer. It is an outgrowth of the ORNL-developed direct sampling ion trap mass spectrometer successfully deployed to identify and measure hazardous chemical pollutants in the field. Vapors of chemical warfare agents (e.g., the nerve agent VX or blister agent HD) are drawn through a capillary line and routed to the ion trap analyzer cell by a sampling mode valve and opensplit capillary interface. There, they are converted to ions by the chemical ionization reagent gas. The agents are identified from their unique product ions, which are split off from the parent ions in tandem mass spectrometry (MS/MS).

To detect biological warfare agents such as anthrax spores or

bacterial toxins, the CBMS bio-concentrator samples air and concentrates micron-sized respirable aerosol particles. These are heated and reacted with a derivatizing reagent that produces fatty acid esters and other biomarker molecules characteristic of a hazardous organism, toxin, or virus. The ratios of the detected biomarker molecules indicate the presence of a particular biological agent. In the spectrometer, the biomarker molecules are ionized and analyzed using MS/MS.

Sophisticated algorithms are being developed to identify biological agents present in a background that may also include naturally occurring microorganisms, pollen, mold, and fungus. These algorithms determine whether the biomarker ions detected by the CBMS in the field match those characteristic of each suspected biological warfare agent. A library of these spectra is being built through experiments at ORNL's Chem-Bio Facility.

The Block II CBMS Program Team includes ORNL, Orbital Sciences Corporation, MSP Corporation, and the Colorado School of Mines. Collaborators include Dugway Proving Ground, White Sands Missile Range, and the Armed Forces Institute of Pathology. The sponsor is the U.S. Army Soldier and Biological Chemical Command.

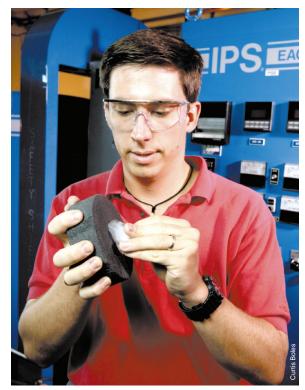
In the fourth year of the project, Orbital Sciences Corporation has built six pre-production CBMS units. The team has plans to build additional units in the next year. Over the next two years, the team will be adding new capabilities to the units to meet new Army requirements. By 2003, a large number of rugged CBMS units will be produced for use on the battlefield.

"The 35 people at ORNL who have worked with me say that the CBMS project has been the most technically demanding of their careers," Griest says. As a result of the challenge, several innovations have come out of ORNL and the rest of the team. And the project has been especially rewarding because the prize-winning detector should save many soldiers' lives. @



ORNL's Graphite Foam May Aid Transportation

ORNL's prize-winning graphite foam may improve the efficiency of future transportation vehicles.



James Klett shows that ice held against the graphite foam will melt quickly because the heat from the hand holding the foam is transferred rapidly through the foam. As a result, this hand feels the cold fast.

A rtificial diamonds. Buckyballs. Carbon foam with high thermal conductivity. These products are the results of serendipitous discoveries made by researchers working with carbon. Carbon foam was discovered in 1998 at ORNL by James W. Klett, a carbon researcher in ORNL's Metals and Ceramics Division. The foam received an R&D 100 Award in 2000 from R&D magazine for being one of 100 most significant innovations in the past year. In June 1999 a patented ORNL method for making this special graphite foam was licensed exclusively to Poco Graphite in Decatur, Texas, which calls the product PocoFoamTM (see www.pocofoam.com).

Currently, materials research on the carbon foam at ORNL is being funded by DOE's Office of Transportation Technologies. "This is a truly revolutionary material that will find uses in many applications," says Patrick Davis of the Office of Transportation Technologies. "Specifically, we believe carbon foam is an enabling technology that will solve critical heat rejection problems we must overcome before fuelcell and advanced power electronics technologies can be introduced into automobiles."

Klett says he made his fortunate discovery of graphite foam by accident while changing a fabrication process. "We had been making carbon-carbon composites, which are carbon fibers embedded in a carbon matrix," he explains. "Because of their heat transfer abilities, such composites show promise for making better brakes and heat shields. But we were trying to find a cheaper way to make the composites."

Klett was experimenting with a process he modified by eliminating a couple of steps. He noticed that a carbon foam had formed as a result.

"We usually heat treat a carbon material to very high temperatures to develop a graphite product," he says.

"I took the carbon foam and heat treated it to make it a graphite foam. I then noticed that it transferred heat remarkably fast. When I held the sample in the palm of one hand and pressed an ice cube in tweezers against the top, the heat from my hand caused the ice to melt quickly, cooling my hand.

"So Tim Burchell and I made more foam samples, ran heat conductivity tests on them, and confirmed they had a special property. We were the first to recognize that a carbon foam could be made that has unusually high thermal conductivity."

Klett and his colleagues found that the key to the foam's conductivity is its unusual graphite crystal structure. It has a skeletal structure full of air pockets, making it only 25% dense and lightweight. The network of ligaments in the foam wicks heat away from its source almost better than do high-performance graphite fibers. PocoFoamTM, which is three to nine times more thermally conductive than typical lightweight carbon foams, conducts heat better than aluminum but at one-fifth the weight. Moreover, the open porosity allows air, water, or some other fluid to pass through the foam. This property, combined with the high surface area, leads to very high heat transfer coefficients in heat exchangers made of PocoFoamTM.

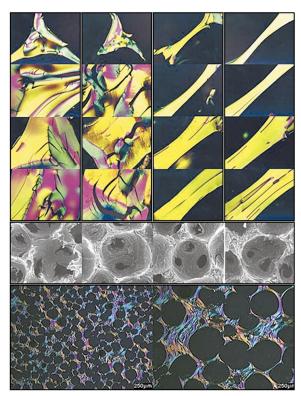
TRANSPORTATION APPLICATIONS

After the discovery, Klett and Burchell began thinking up applications for the foam. They determined that because the foam is lightweight and transfers heat rapidly, it could improve the efficiency of transportation vehicles. For example, the foam could be used to make a smaller, lighter car radiator that might be placed away from the front of a car to give it an energy-saving and less-polluting aerodynamic design. If the size of the front of the car is reduced, the car will not have to push as much air in its forward motion, allowing it to use fuel more efficiently. Because a smaller radiator can make a car lighter and faster since it allows a more aerodynamic design, automotive racing teams are interested in foam radiators.

This radiator would quickly transfer heat from the engine to air blowing through its foam components. In a heat sink made of the foam, hot air or water coolant may pass through a tube penetrating a foam block, and cold air or water would pass through the porous foam. Conversely, the foam can be machined into fins (vertical parallel plates) or vertical pins on a base, as in metal heat sinks.

"A subcontractor is now building car radiator prototypes from PocoFoamTM," Klett says. "Small radiators could remove heat from fuel cells that will be used to power electric cars and buildings." In cars, the heat from the car radiator could be transferred to warm the passenger compartment. In buildings the waste heat could be recaptured for additional power production.

The Department of Defense is interested in smaller radiators for personnel carriers, Klett says. A smaller radiator would present less of a



Colorful micrographs show skeletal structure and air pockets of $PocoFoam^{TM}$.

chip's temperature by 10°C (20°F)," Klett says, "a rule of thumb is that its lifetime will double before it fails."

The foam could also be used in pistons because it can withstand temperatures as high as 500°C in air. Robert Kirk, manager of DOE's Office of Advanced Automotive Technology, observes, "When I review the list of recurring areas of automotive interest, I see the thermally conductive carbon foam most frequently. I am pleased with this high level of industry interest because it provides convincing evidence that our research funds are well placed and effectively used."

There are other possible uses for foam heat sinks, as well. They may prove useful in protecting electronic components on space satellites from heat damage. Another possible application would be in evaporative cooling, in which the high specific surface area (>4 m^2/g) combines with the high thermal conductivity to produce very efficient cooling as water evaporates from the foam surfaces.

"The aerospace industry is interested in coating carbon foam with titanium to make a high-strength ma-

terial with high thermal conductivity," Klett says. "The Navy is considering using it for various components to make its boats lighter and smaller."

BAKE IT LIKE A CAKE

Klett compares the batch method he cultivated to produce graphite foam production to baking a cake. "You put the batter in a pan, stick

it in the oven, and heat it to the right temperature until you get a foam," he says, explaining that in essence a cake is a foam. "In our method, we put pitch-tar-in a vessel, pressurize it, heat it, and let it decompose. The gas evolved by decomposition during pyrolysis bubbles through the viscous heated pitch, producing a foam."

Klett looks forward to making more discoveries as he searches for "out-of-the-box" applications for PocoFoam[™]. ∅

James Klett holds a block of graphite foam. A prototype radiator in the background is made partly of this type of foam.

target to the enemy, making it less likely that it would be hit, effectively stopping the vehicle.

PocoFoamTM could be used also for cooling brakes (which develop hot spots), as well as oil and transmission fluid in automotive systems. It could find a place in lithium-ion batteries being developed to power electric cars. "Our preliminary studies show that carbon foam may work better than the typical carbon fibers in the anode of a lithium-ion battery," Klett says. "Our evidence suggests that a carbon foam anode would discharge ions to the electrolyte faster than a graphite fiber anode."

PocoFoamTM could be used to replace aluminum blocks as heat sinks to cool power electronic modules in hybrid vehicles now being developed in the United States. A hybrid vehicle has a gasoline engine and an electric motor/generator. The vehicle requires small, lightweight power electronic modules, such as inverters, to convert direct current (dc) from batteries to alternating current (ac) for use by the electric motor in accelerating the wheels. The electric motor becomes a generator when it captures energy from the wheels to slow or stop them. The inverter then converts ac to dc when it takes power from the generator to recharge the batteries.

At ORNL a heat sink with fins made of the special graphite foam has been cooling a Pentium 133 chip in a desktop computer since December 12, 1998. "If you reduce an electronic

Poco Graphite has an exclusive license to produce graphite foam using ORNL's patented batch method. The company has started pilot production of PocoFoam[™] in the form of sheets and blocks. In May 2000 the first PocoFoam[™] product was sold. Poco Graphite also has the machining capability to produce finished parts made of the foam.

The PocoFoamTM production process is expensive, but the manufacturer says the price of the product should come down as demand increases. "Remember VCRs" says Klett. "They cost more than \$1200 apiece when they first came out and now they're much less expensive." In the meantime, Klett, Burchell, Claudia Walls, Claudia Rawn, and Marie Williams (all part of the graphite foam development team at ORNL) are testing and evaluating another process in search of a cheaper production method.

"We're looking at methods that will allow continuous production of the foam," Klett says. "This approach should reduce production time and increase throughput."

Klett concedes that PocoFoamTM is not exceptionally strong; its tensile and compressive strength and its other mechanical properties are not as good as those of aluminum and copper. "But its compressive strength compares well with some aluminum honeycombs used for heat sinks," Klett says. "When we impregnated foam samples with epoxy resin, we found that the foam's compressive strength increased ten times. Nevertheless, we believe that if we tweak the fabrication process to improve the foam's mechanical properties, we would probably sacrifice its high thermal conductivity."

Meanwhile,

Microfocusing Mirrors Advance Materials Science

X-ray microfocusing mirrors conceived at ORNL can help scientists determine which manufacturing processes make more reliable electronic circuits and aluminum parts for cars.

new era of X-ray science is being ${
m A}$ ushered in by an advance in X-ray mirror technology in which an ORNL scientist played a key role. Gene Ice, leader of the X-ray Research and Application Group in ORNL's Metals and Ceramics Division, worked with Beamline Technology Corporation of Tucson, Arizona, to develop advanced X-ray microfocusing mirrors, which received an R&D 100 Award from R&D magazine in 2000. The new technology, combined with computer software to analyze X-ray patterns, opens a new frontier for materials scientists, permitting direct observation of the building blocks of most materials. The technology will allow scientists to characterize material defects down to less than a millionth of a meter (a micron). It will also help them determine which manufacturing processes make more reliable electronic circuits, more efficient materials for energy production, and stronger, lighter transportation materials-such as aluminum-for car bodies.

The building blocks of most materials are small, single-crystal grains packed together in a complicated network that includes intersections called grain boundaries. "Our 3D X-ray crystal microscope will allow researchers for the first time to see the three-dimensional crystal structure of each grain making up a material of interest," Ice says. "We will now be able to look at a grain's orientation, size, and shape. We can determine if a grain points in a different direction, becomes deformed, or breaks up into smaller subgrains as a result of internal forces induced by a manufacturing process. We can observe the changes in grains that cause the material to fail."

RESEARCH CHALLENGES

In the mid-1990s, Ice was traveling around the nation to try to win funding for materials research experiments that would use brilliant X rays from the Advanced Photon Source (APS), which began operating in 1997 at Argonne National Laboratory. During his visit to Bell Laboratories, he learned of an urgent technical challenge. A major factor in the reliability of computers and computer chips is strain in integrated-circuit wires. The tiny polycrystalline aluminum or copper wires in the integrated-circuit chips expand and shrink differently from the silicon bulk material as temperature changes during processing or computer operation. Together with the mechanical forces associated with current flow through the wires, this effect results in strain, which varies at the micron level because of distortion in individual crystalline grains. This strain can affect the mechanical evolution of the aluminum or copper interconnect wires during operation or even when a chip is made. Mechanical evolution is a change in the shape, size, rotation, and strain (internal stretching) of a grain. It is difficult to study strain, however, because the interconnect wires are buried under an amorphous silicon dioxide film. Today Ice and Ben Larson of the Solid State Division (SSD) and their ORNL colleagues are using the 3D X-ray crystal microscope at APS to study strain in integrated-circuit wires, as well as other materials science problems.

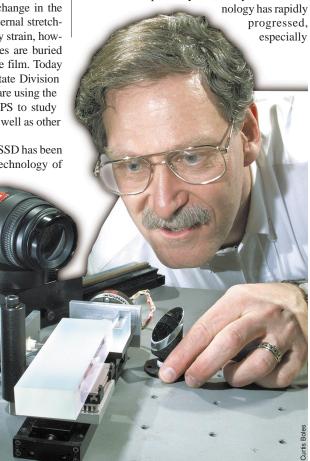
For example, John Budai of SSD has been leading an effort to advance the technology of

making effective hightemperature superconducting materials in which a thin superconducting singlecrystal film is deposited on a buffer layer that coats a metal substrate. In the best superconducting wires, the film grains are deposited on aligned metal substrates and actually increase their alignment as they grow so that most of the crystals point in the same direction. To determine which processes repeatedly produce superconducting materials with the best alignments, ORNL researchers are using the 3D X-ray crystal microscope to examine many different samples produced by various processes. Their results may help lead to the

development of commercial superconducting wires and devices.

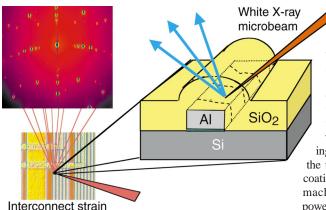
ORIGIN OF THE X-RAY MICROSCOPE

In the late 1940s and early 1950s, P. Kirkpatrick and Albert V. Baez (father of singer Joan Baez) demonstrated that two mirrors could be arranged to focus an X-ray beam at a small spot on a target material. Such "crossed mirrors" came to be known as Kirkpatrick-Baez mirrors. In the past 50 years, X-ray mirror tech-



Gene Ice inspects two advanced elliptical X-ray microfocusing mirrors used for focusing X rays to submicron spots. The mirrors received an R&D 100 award in 2000.

R&D 100 <u>Award Winner</u>



X-ray image of grains in aluminum interconnect wires in a silicon semiconductor chip used in a computer.

in the production of mirrors with flat and spherical surfaces. (A mirror with a spherical surface can be visualized as a small strip from a hollow glass sphere).

To focus the beam on a spot small enough to "observe" crystalline grains, it was necessary to fabricate and polish mirrors with elliptical surfaces. The ideal elliptical mirrors can be visualized as strips cut out of the surface of glass shaped like a symmetrical egg. However, the technology does not exist to polish an elliptical mirror to get the required X-ray quality. In recent years, flat mirrors have been elastically bent to produce elliptical surfaces. Although bent mirrors can produce beams that focus to a spot less than a micron in diameter, they are sensitive to mounting stresses and thermal loads.

In the 1990s, with the construction of the APS it was apparent that improved X-ray optics technologies would be needed to exploit the brilliant, laser-like X rays expected from the APS. Ice pushed for improvements in X-ray optics as early as 1990. His sense of urgency grew when he became part of a group that would have a dedicated beam line for experiments at APS, thanks to internal ORNL funding and a collaborative agreement in 1996 with Howard University, a historically black university. Ice called the X-ray optics experts he knew around the country. Eventually, he found a company willing to try making an elliptical mirror to his specifications.

The company, Beamline Technology Corporation of Tucson, Arizona, was interested in depositing a coating of varying thicknesses to build a mirror with the required shape. Andrew Lunt, general manager of Beamline Technology, told Ice that the company had already developed a differential deposition technology for use in correcting small shape defects in X-ray mirrors.

To make the desired elliptical mirror surface, a Beamline Technology team cut out a small strip from the surface of an X-ray-polished spherical mirror made of ultra-low-expansion glass or single-crystal silicon. Scientists at Argonne measured the surface shape, and Ice calculated the re-

quired deposition profile. Then a layer of chrome was deposited to bind the differentially deposited coating to the substrate. To build an elliptical surface in the shape specified by calculations, a thin layer of gold was differentially deposited on the chrome coating. Gold atoms were sputtered from a source using a computer-controlled machine; the thickness of the deposited gold coating was adjusted by changing the machine's power-the higher the power at any one point, the thicker the coating there. A final layer of palladium was deposited on the gold coating to make the mirror highly reflec-

tive of X rays up to 24,000 electron volts (24 keV).

Throughout the process, many measurements were made to determine the mirror shape. Beamline Technology sent samples to ORNL for Ice to test at APS. The differentially coated mirrors were also tested successfully by researchers at the National Synchrotron Light Source at Brookhaven National Laboratory, where Ice worked for five years. Based on feedback from the researchers, Beamline Technology perfected the differentially deposited mirror technology for the X-ray crystal microsope.

X-RAY MICROBEAMS AT APS

Ice, Larson, Budai, and their ORNL colleagues Jon Tischler, Eliot Specht, Jin-Seok Chung, Nobumichi Tamura, Wenge Yang, Ki-Sup Chung, and Mirang Yoon have performed experiments at the APS using the X-ray crystal microscope. Although the microscope is based on a

well-known X-rav diffraction technique called polychromatic Laue diffraction, no one had ever pushed the technology to obtain such detailed quantitative information. In fact, several years ago X-ray experts advised ORNL that the technology was not possible. The microscope is possible, Ice says, because of the availability of ultra-brilliant synchrotron radiation at the APS and three other major technical advances. One advance is novel achromatic focusing mirrors that allow the microscope to achieve high spatial resolution with broad spectrum X-ray beams. Another is an innovative X-ray

scanning monochromator built at Howard University that allows for the rapid measurement of absolute stresses (internal forces) in crystals. A third is specialized pattern analysis software that determines the type, orientation, and stress of individual grains from overlapping multi-grain X-ray scattering patterns.

The X-ray diffraction patterns are captured by a charge-coupled detector (CCD), which is carefully calibrated to determine the precise direction of the scattered X-rays. From the pattern on the CCD, the number, orientation, and distortions of the crystal grains can be determined. This information is essential to understanding the forces driving the evolution of the grains at the subgrain level. A complete description of the local forces that are deforming each grain can be measured using the Howard University micromonochromator.

Ice credits Jim Roberto, then director of SSD, for encouraging him and Ben Larson to apply successfully for internal funding from the Laboratory Directed Research and Development (LDRD) Program at ORNL to build an X-ray microprobe for mesocale studies.

With LDRD funding and through collaborations with Howard University scientists, Larson and Ice put together all the pieces for a working 3D X-ray crystal microscope. Early results provided essential support for a successful twopercent initiative proposal from ORNL to DOE's Office of Basic Energy Sciences.

In addition to winning an R&D 100 Award, the new elliptical mirrors have another claim to fame. They have beaten the bent mirror focus record $(0.8 \times 0.8 \text{ mm}^2)$ by achieving a focused spot size of ~ $0.4 \times 0.5 \text{ mm}^2$. Clearly, these achievements reflect well on the sponsors of the development of the 3D X-ray crystal microscope. (9)



The advantage of bombarding a material with the Advanced Photon Source's (above) high concentration of X rays of many different wavelengths is that it increases the chances of satisfying Bragg's Law, a statement of the conditions under which a crystal will reflect a beam of X rays with maximum intensity. Because the grains in a material may be pointing in different directions and because it is slow and impractical to rotate the sample, focusing a finely collimated beam of polychromatic X rays on each single-crystal grain should produce detailed information regardless of the grain orientation.

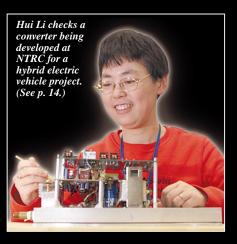
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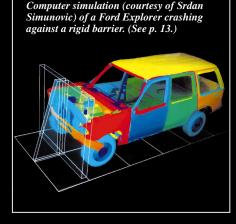
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Photos taken by Curtis Boles and enhanced by Jane Parrott and LeJean Hardin.





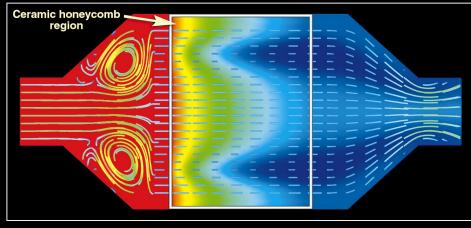






John Thomas checks a diesel engine on an eddy-current dynamometer for a shaft speed test. (See p. 5.)





In this computational visualization by ORNL's Engineering Technology and Computer Science and Mathematics divisions (courtesy of Ross Toedte), the temperature contours and flow streamlines represent the combined effects of exhaust gas flow, heat transport, and chemical reactions in a typical automotive catalytic converter during a cold start. Cold start performance is critical to reducing harmful emissions from automobiles.



Bill Partridge prepares to use a mass spectrometer to analyze the effectiveness of diesel fuel hydrocarbons in regenerating a catalyst used to remove nitrogen oxides from engine emissions. (See p. 5.)