DOE at UC

A REPORT ON
UNIVERSITY OF CALIFORNIA RESEARCH
FOR THE DEPARTMENT OF ENERGY

Office of Research, UC Office of the President   Winter 2000

The Department of Energy and UC Strive for a Greener Future

The DOE granted $66 million to nine University of California campuses in fiscal year 1999. The 163 grants span a wide variety of research topics in energy, the environment, and genetics. These DOE grants are awarded through competition with other universities and distinct from the funds UC is paid to manage three national laboratories (see story on page eight).

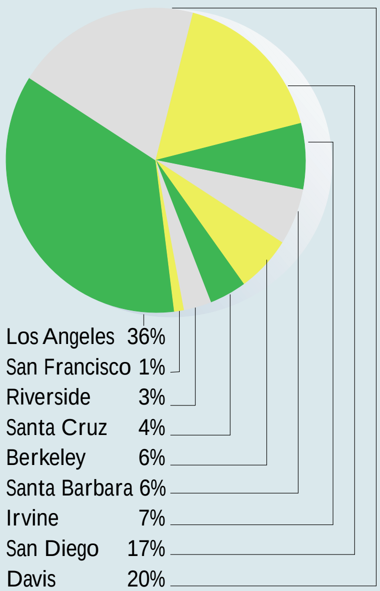
> *Our basic research aims to discover fundamentally new sources of energy, and processes and phenomena that are inherently more efficient and environmentally benign.*
>
> from DOE Office of Science Strategic Plan

Although almost two-thirds of the DOE-funded research at UC concentrated in the traditional disciplines of physics and engineering, DOE also funds research in environmental and climate studies and genomics and other life sciences. DOE is the third-largest government sponsor of basic research in the United States, and DOE and its predecessor agencies like the Atomic Energy Commission have supported the award-winning research of several Nobel Prize laureates.

In FY99, UC Los Angeles gathered more than one-third (36 percent) of all DOE funding to UC. These awards were based on strengths in two diverse areas – molecular biology and fusion physics. UC Davis was awarded 20 percent of the total, including $8 million for the National Institute for Global Environmental Change. At UC San Diego, strong physical science research helped capture 17 percent of total funding. The remaining 27 percent of DOE funding was split among UC Irvine (seven percent), UC Santa Barbara (six percent) and UC Berkeley (six percent), with slightly less going to the smaller campuses of UC Santa Cruz (four percent) and UC Riverside (three percent). The remaining one percent of funding was awarded to UC San Francisco, the only campus in the UC system dedicated entirely to the health sciences.

IN BRIEF

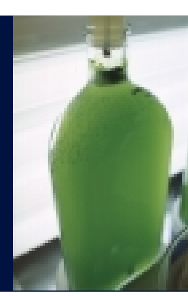
DOE Funding by Campus

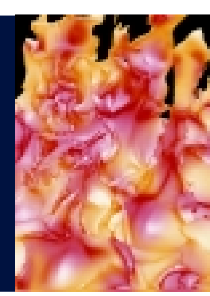


DOE Funding Facts

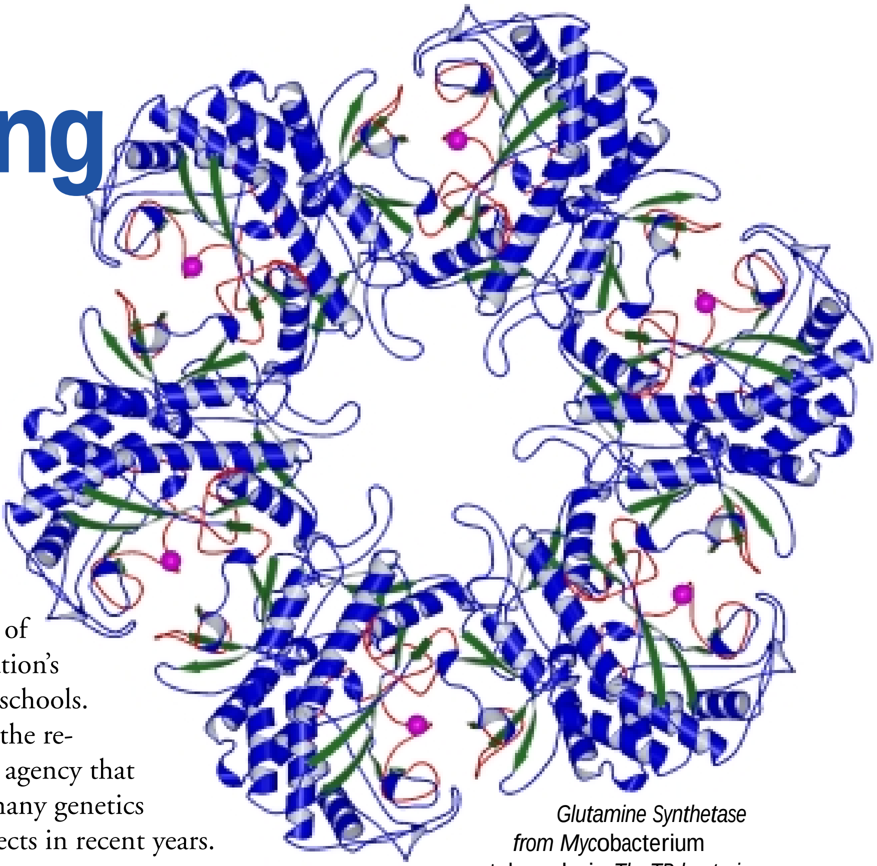
- DOE is the third-largest government sponsor of basic research.
- Nine UC campuses received 163 grants in FY99, worth $66 million.
- UC Los Angeles captured over $23 million in DOE funding.
- UC Davis gathered 20 percent of all DOE funding to UC, a large portion of it for the National Institute for Global Environmental Change.
- At UC Berkeley, Prof. Anastasios Melis has developed a new source of renewable hydrogen fuel.
- The UCLA-DOE Laboratory of Structural Biology and Molecular Medicine is laying the foundation for new tuberculosis drugs.
- At the Stanford Linear Accelerator, the UC Santa Cruz Institute for Particle Physics is exploring the fundamental nature of matter.

IN THIS ISSUE





Deconstructing Tuberculosis



Glutamine Synthetase from Mycobacterium tuberculosis. The TB bacterium secretes this enzyme during cell wall development, making it a good target for drug development. This model was built by Harindarpal Gill at the UCLA-DOE lab.

In the realm of genetics, the amino acids are the letters and proteins are the words of life. From observing their structure and context, you can determine the relationship between the proteins and derive a dictionary of protein functions.

That is the task of the UCLA-DOE Laboratory of Structural Biology and Molecular Medicine. Prof. David Eisenberg and colleagues are attempting to build such a dictionary and then use it to deconstruct the life processes of one of humanity's most deadly enemies, the tuberculosis baterium (TB).

Worldwide, *Mycobacterium tuberculosis* kills about two million people annually. TB has become epidemic in overcrowded, poorly ventilated Russian prisons. In Sub-Saharan Africa, HIV and chronic malaria ravage victims' immune systems, leaving TB to deal the death blow.

In the United States, the number of cases reported annually declined steadily for decades (from 84,304 in 1953 to 22,201 in 1985), but began to rise again as a consequence of the HIV epidemic and reductions in public health spending.

Although the rate of new infections in the U.S. once again is declining, in an era of rising globalization the U.S. will not be able to isolate itself from the international TB epidemic. New tools are needed in the fight against the disease, especially against its drug-resistant forms.

The UCLA-DOE lab has taken aim at TB with its sophisticated arsenal of structural and molecular biology tools. The lab is a collaboration between two powerful organizations. UCLA brings to the partnership the resources of one of the nation's best medical schools. DOE brings the resources of an agency that has funded many genetics research projects in recent years.

DOE's predecessor, the Atomic Energy Commission, began studying the genetic consequences of exposure to nuclear radiation in the 1940s. DOE was the lead federal agency in the early years of the human genome project, although it has been surpassed by the rapid growth of the National Institutes of Health.

Using techniques described in a recent article in *Nature* magazine, Eisenberg and the UCLA-DOE lab will identify 500 of some of the most important proteins of the 3,974 coded by the TB genome. In addition to determining their function, in collaboration with Los Alamos National Laboratory, UC Berkeley and other centers of structural biology the lab also will determine the shape and three-dimensional structure of the TB proteins.

The functions of these proteins can be determined by finding other proteins that have evolved in a similar fashion in other fully sequenced organisms. Eisenberg and his colleague, Prof. Todd Yeates, call this the method of phylogenetic profiles. Another technique, dubbed the Rosetta Stone method, links proteins by finding other organisms where the DNA code for the proteins has fused together on a single gene.

Once the dictionary of TB protein function has been built, this information will be used to deconstruct TB's life functions. The three-dimensional structures of the most important TB proteins will be determined. These structures will allow others to design drugs that will interact with the key proteins, drugs that will act as molecular monkey wrenches to jam the works of the TB bacteria.

The ultimate goal is a new arsenal of anti-TB drugs. Says Eisenberg, "At the UCLA-DOE lab, we are starting to understand how proteins work together. The goal is to understand tuberculosis and other organisms much better, and that will eventually lead to better drugs. We have high expectations."

Symmetry and the Standard Model

Why is there something, instead of nothing? What seems like an arcane philosophical question actually has profound implications for modern-day particle physics.

Researchers at the Santa Cruz Institute for Particle Physics are helping build the detectors for the BaBar project at SLAC.

In collaboration with DOE laboratories and with scientists from several different countries, the UC Santa Cruz Institute for Particle Physics (SCIPP) is taking part in a bold experiment to answer that question.

According to our current understanding of the origin of the universe, the big bang should have generated equal amounts of matter and its oppositely charged, mirror-image counterpart, known as anti-matter. If this were so, then in the instant after the big bang, particles of matter and anti-matter would have annihilated each other in countless bursts of energy. Yet we live in a universe dominated by matter. Somehow the universe must favor matter over anti-matter.

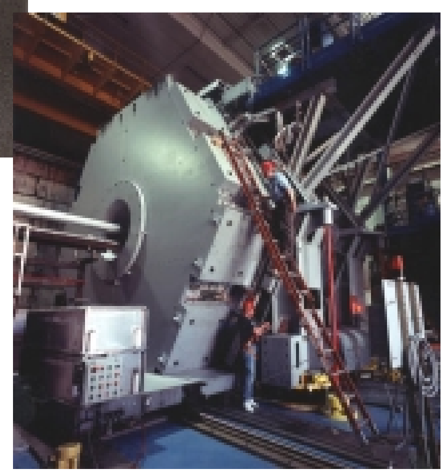
In the late 1960s, Russian physicist Andrei Sakharov pointed out the importance of this asymmetry, known as charge-parity (CP) violation. Ask a particle physicist why there is something instead of nothing and the answer likely will be "CP violation."

Unfortunately, this excess matter does not fit well with what physicists call the standard model, our basis for understanding phenomena from nuclear fusion to the radioactive decay of the isotopes used in medical imaging. Can the standard model be tuned-up to better account for CP violation, or does it need a complete overhaul?

Experiments at the DOE-funded Stanford Linear Accelerator Center (SLAC) already have begun to produce results and may tell us the answer within the next few years.

At SLAC, B-mesons are created at the facility known as the B-factory. To create B-mesons and their anti-matter counterparts, electrons are accelerated clockwise inside a 1.4-mile long circular ring. Positrons are accelerated counter-clockwise and with less energy inside a second ring lying on top of the first. At the right moment the two beams collide, leaving a splatter of subatomic particles. Just like two eggs rolled toward each other at different speeds, the splatter spreads out in the direction of the faster-moving particles.

With funding from the DOE, scientists from SCIPP helped to build the detector that tracks the resulting splatter of B-mesons and their anti-matter twins – denoted by a B with a bar on top, or "B-bar" mesons. The detector has been named BaBar, after the elephant in the children's books by Laurent de Brunhoff. Like its namesake, BaBar is big, gray, endearing (at least to scientists), and will produce results for many years.



Putting finishing touches on the BaBar B-meson particle detector.

Physicist Abraham Seiden has led UC Santa Cruz's efforts on the BaBar detector. "B-mesons and their anti-matter counterparts have lives measured in trillionths of seconds," he says, "But some B-mesons may survive just a bit longer than B-bar mesons. If we can measure and verify the difference, BaBar will provide experimental confirmation of CP violation."

The B-factory itself was the brainchild of Pier Oddone, deputy director of the UC-managed Lawrence Berkeley National Laboratory. The successful completion of the B-factory and BaBar demonstrate the value of collaboration between UC campuses and DOE laboratories.

Hydrogen A Renewable Fuel for a New Millennium

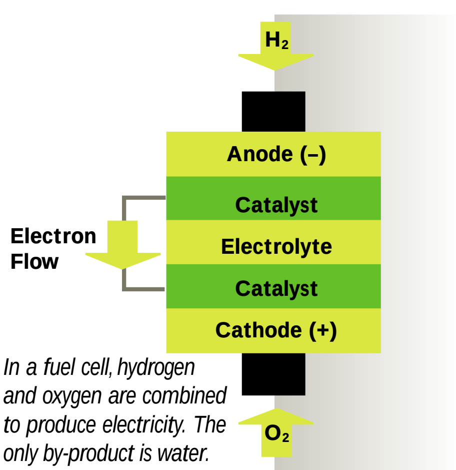
Neatly aligned alongside a bank of glowing fluorescent tubes, the bottles of translucent green fluid could be concentrated lemon-lime soda pop. But the bubbles inside the flask are not carbon dioxide but hydrogen, and the brew is a specially nurtured batch of green algae.

At UC Berkeley's plant and microbial biology department, Prof. Anastasios Melis has learned to turn on a metabolic switch in the algae. This switch throws the algae onto an alternative metabolic pathway, one that consumes sugars and other internal products and yields hydrogen.

Hydrogen is the cleanest-burning of all fuels. When burned in the atmosphere, it combines with oxygen to release energy. The by-product is water.

Hydrogen looks like a good energy bet because of the convergence of three technologies – fuel cells, hybrid cars, and now, renewal hydrogen production.

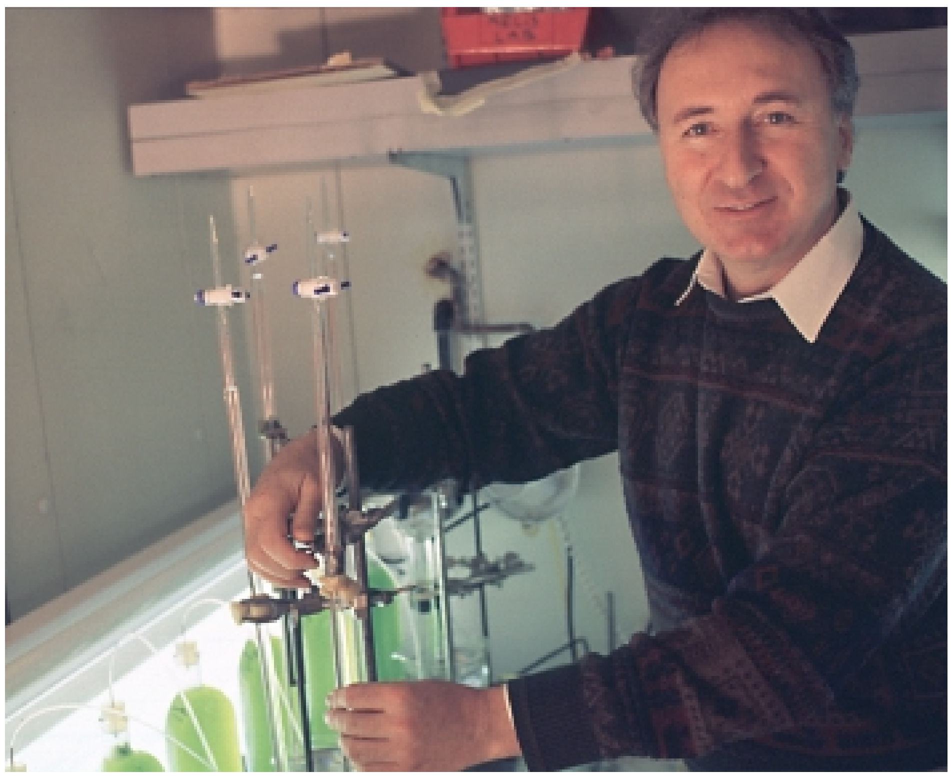
Automakers Toyota and Honda have developed hybrid cars – electric cars with lightweight batteries and a small engine/generator on-board to keep the batteries recharged. Canada's Ballard Power Systems already markets fuel cells for nonpolluting buses.



In a fuel cell, hydrogen and oxygen are combined to produce electricity. The only by-product is water.

The missing piece of the puzzle has been a clean, renewable source of hydrogen. At his Berkeley laboratory, Melis may have found this renewable source of hydrogen. Take a hybrid vehicle, add a fuel cell, and fill the tank with algae-produced hydrogen, and presto – a car that runs on photosynthesis.

This biological curiosity has remained a puzzle. During photosynthesis, plants use energy from the sun to convert carbon dioxide and water into sugars and oxygen, a by-product. But plants, like humans, also respire – they burn sugars in oxygen for energy, with water and carbon dioxide as by-products.


Prof. Anastasios Melis has discovered how to turn algae into a renewable source of hydrogen fuel.

How Melis, working in conjunction with the DOE National Renewable Energy Lab (NREL), accomplished this feat is a story of patience and persistence. Researchers have known since 1942 that the algae *Chlamydomonas reinhardtii* ("pond scum," in the words of NREL collaborator Michael Seibert) can produce minute quantities of hydrogen.

What is the source of the hydrogen? The first breakthrough came in the summer of 1997, when Melis was testing algae, a plant often used to study photosynthesis efficiency. He noticed that photosynthesis eventually shut down if sulfur is left out of the nutrient mix. Melis wondered if respiration shut down as well. If not, in a closed container, the algae would continue to respire, absorbing all the remaining oxygen in the culture. Then what?

Take a hybrid vehicle, add a fuel cell, fill the tank with algae-produced hydrogen, and presto – a car that runs on photosynthesis.

Melis and Seibert found out in the summer of 1998. Deprived of sulfur and placed in a sealed flask, first photosynthesis came to a halt, and the algae switched to respiration. But once the oxygen was exhausted – and the algae was unable to perform either photosynthesis or respiration – an alternative metabolic pathway was triggered that released far more hydrogen then previously observed. Explains Melis, "The algae utilizes stored compounds and exhales hydrogen just to survive. It's probably an alternative form of breathing, an ancient strategy that the organism developed to live in sulfur-poor anaerobic conditions."

Melis estimates that when the process is refined and commercialized, a small pond could produce enough hydrogen to fuel a dozen automobiles. Experiments in scaled-up production have begun at the University of Hawaii. UC Berkeley and DOE's NREL have applied for a patent on its procedure.

A recent NREL report states "there are no technical showstoppers to implementing a near-term hydrogen fuel infrastructure for direct hydrogen fuel cell vehicles." But it noted there are problems with timing and coordination of capital investments. Automakers won't produce hydrogen-powered vehicles unless hydrogen filling stations exist. Yet fuel producers won't build the filling stations until the vehicles exist.

In California, this Catch-22 is being tackled by a joint public-private venture, the California Fuel Cell Partnership. Members include gasoline producers, automakers, a fuel cell manufacturer, and state agencies. The partnership has been developing strategies for resolving fueling infrastructure issues.

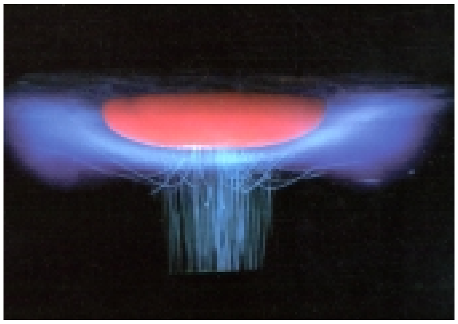
Hydrogen bubbles forming inside a flask of sulfur- and oxygen-deprived green algae.

Algae hydrogen production requires raw materials that are abundant – water, sunlight, algae, and a small amount of nitrogen fertilizer and other nutrients. Less developed countries could produce their own hydrogen and reduce their dependence on imported fuels.

Urban dwellers worldwide would benefit. "Think of the reduction in respiratory and other ailments caused by pollution, and the benefits to society that would come from switching to hydrogen," says Melis. "We may be on the verge of a new era, the era of hydrogen."

With research into hydrogen production, fuel cells, and other technologies, UC and DOE's National Renewable Energy Laboratory are helping to chart a course to a cleaner, healthier future.

Making Diesel Engines Cleaner



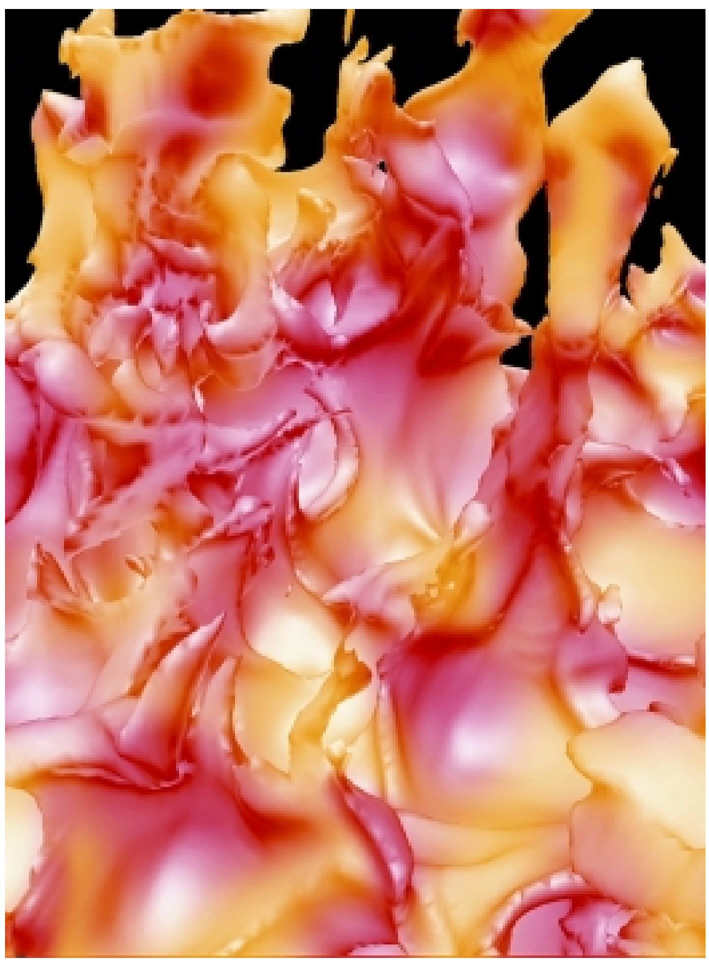
In the UCSD combustion lab, water droplets impinge upon a stainless steel plate heated by a methane flame.

Diesel engines get great gas mileage but emit high levels of polluting NO_X, or oxides of nitrogen (see next page for the effects of NO_X). With funding from DOE, UC San Diego's Center for Energy and Combustion Research has been looking for ways to make diesel engines run more cleanly.

Center director Forman A. Williams and colleagues have been studying the complexities of spray combustion. In a gasoline engine, the fuel-air mixture is drawn or injected into the cylinder and ignited by a spark plug. In a diesel engine, the fuel is sprayed directly into the cylinder, where it ignites due to residual heat.

Understanding and modeling spray combustion – how fuel droplets impinge on a hot surface, atomize and burn – is extremely complicated. Yet to minimize the NO_X produced by diesel combustion, we must comprehend what happens during spray combustion to thousands of fuel droplets, some only 40 millionths of an inch in diameter.

To determine this, Williams and colleagues Shui-Chi Li and Paul A. Libby heat a stainless steel plate with an air-methane flame. Then they impinge various mixtures of air, methane, and water spray upon the plate. The spread and velocity of the droplets are measured with the laser beams of a phase doppler particle analyzer.



Computer simulation of the flame front. Turbulence can accelerate combustion, improving efficiency and reducing pollution. Courtesy of the National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory.

Williams, Li and Libby showed that fairly simple theory can produce good agreement with experimental observations on droplet behavior. The researchers are using these results to reduce NO_X emissions from burning fuels.

Scientists generally agree that NO_X is formed when nitrogen and oxygen in the air combine at temperatures as high as 1700 degrees Centigrade. To date, most engineering efforts to reduce NO_X emissions have concentrated on blocking this high temperature reaction.

Through studies on the basics of NO_X production, however, Williams and colleagues are finding that a different reaction may be responsible for significant vehicle emissions. NO_X can also be formed when hydrocarbons react with nitrogen in the air. Hydrocarbons don't require much heat to initiate this reaction so NO_X can be formed in the very early stages of combustion. The UCSD researchers believe that interrupting this reaction is key to reducing NO_X emissions.

To fight NO_X production the researchers use a two-staged approach. In the first stage, the fuel mixture is kept rich, reducing the temperature and converting the hydrocarbons to energy before they have a chance to react with nitrogen to form NO_X. In the second stage, water is sprayed on the flame, cooling it and binding with the remaining hydrocarbon atoms, blocking NO_X formation again.

Cleaner-burning diesels will reduce NO_X emissions and will help lead to the day when an ugly brown haze will no longer hang over many communities. DOE and UCSD are working to make that day a reality.

Good Ozone/Bad Ozone

Ozone is the Dr. Jeckyll and Mr. Hyde of atmospheric gases. In the stratosphere (10 to 30 miles up), ozone is good, and protects the earth from harmful ultraviolet (UV-B) rays. But in the troposphere (0-10 miles up), ozone is bad.

A highly reactive form of oxygen, ozone combines three oxygen atoms into a single molecule (O_3) instead of the usual two (O_2). As an ingredient of urban smog, ozone can irritate and damage the lungs, leaving city-dwellers more susceptible to other pollutants. It damages plants and reduces crop yields. It may be implicated in the epidemic rise of asthma in the U.S.

Prof. Barbara Finlayson-Pitts

With help from a DOE grant, UC Irvine atmospheric chemist Barbara Finlayson-Pitts is trying to unravel the complex chemistry of ozone in the lower atmosphere.

"Surface concentrations of O_3 in remote areas of the world have risen to 30 to 40 parts per billion (ppb)," says Finlayson-Pitts, "as compared with 10 to 15 ppb in preindustrial times. We need to better understand why this is happening."

The allowable limit of ozone exposure is 80 ppb for eight hours, according to the Environmental Protection Agency, a limit that is often exceeded in urban areas.

The distribution and burning of fossil fuels is the main culprit in ozone pollution. Since the early 1950s, researchers have known that ozone is the result of chemical reactions involving volatile organic chemicals (VOC) and oxides of nitrogen (NO_X). The main source of VOCs are vapors of gasoline, lighter fluid, and solvents. NO_X is a by-product of burning fossil fuels.

"But we still don't understand the role of halogens in ozone pollution," says Finlayson-Pitts. The main source of halogens (chlorine and its related elements, fluorine, bromine, and iodine) is sea salt spray, which can migrate up to 500 miles inland. Since many of the world's most polluted cities are in coastal regions, the interaction of salt spray, VOCs and NO_X might be critical for understanding and reducing ozone levels.

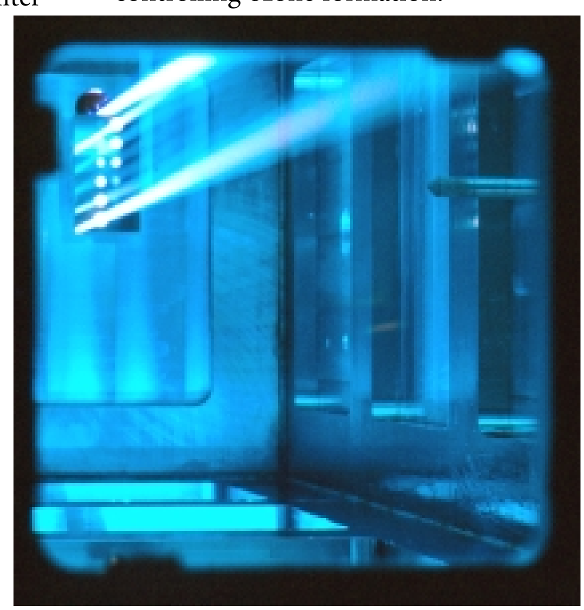
At UC Irvine, Finlayson-Pitts works among a distinguished group of atmospheric chemists that includes Nobel laureate F. Sherwood Rowland and UCI Chancellor Ralph J. Cicerone. She has constructed a 560-liter aerosol chamber to collect experimental data on halogens and other atmospheric gases.

The chemical interactions are so complex that under different concentrations of NO_X and VOCs, halogens might either reinforce the creation of ozone or they might interact with ozone and destroy it. Evidence gathered from monitoring arctic ozone levels at the beginning of the long polar day have shown that bromine might actually reduce ozone concentrations under those conditions.

Ozone plays another role in the atmosphere – as a greenhouse gas that also indirectly affects other greenhouse gases, such as methane. To accurately model regional and global climates, ozone concentrations and interactions must be accurately predicted. Working with Prof. Donald Dabdub of UCI's mechanical and aeronautical engineering department, her colleagues in the chemistry department, and researchers from the Academy of Science of the Czech Republic, Finlayson-Pitts is trying to understand ozone and particle pollution at the macro scale.

"Clearly, understanding the chemistry of halogens in the troposphere is critical to quantifying the relation between emissions of VOCs and NO_X and the formation of ozone," Finlayson-Pitts says. "The issue has attracted national interest because of its potential health- and climate-related impacts."

With help from DOE, Finlayson-Pitts and UC Irvine will continue to find ways of understanding and controlling ozone formation.



Light beams passing back and forth through the new aerosol chamber in the Finlayson-Pitts laboratory are used to measure gases such as ozone during their reactions with sea salt particles.

UC and the DOE National Laboratories

In addition to competing for and performing research for DOE on a grant-by-grant basis, the University of California also manages three of the DOE's national laboratories – Lawrence Berkeley National Laboratory (LBNL) and Lawrence Livermore National Laboratory (LLNL) in California, and Los Alamos National Laboratory (LANL) in New Mexico.

LBNL, originally E.O. Lawrence's laboratory on the Berkeley campus, was designated by the UC Regents as "The Radiation Laboratory" in 1936. The Berkeley Laboratory is acknowledged to be the prototype of the big, interdisciplinary, national science laboratories in this country and abroad. Its scientific expertise was used in the development of the atomic bomb during World War II. The laboratory now conducts only unclassified basic and applied research across a spectrum of disciplines and specializes in development and operation of unique national experimental facilities.

Located 35 miles northwest of Santa Fe, NM, on a plateau high in the Jemez Mountains, LANL developed the first nuclear weapon under the leadership of Berkeley physicist J. Robert Oppenheimer and a cadre of scientists. While national security remains a central part of its mission, the laboratory's research ranges from innovative biological investigation to modeling global climate, and from novel methods for examining material properties to helping explore the outer reaches of the solar system.

LLNL, located in Livermore, CA, was founded by Lawrence and Edward Teller with the mission to advance nuclear weapons research and development and to explore nuclear energy for peaceful purposes. Today, LLNL's mission is to apply science and technology in the national interest, with a focus on global security, worldwide ecology, and bioscience, and to work with industrial and academic partners to increase national economic competitiveness and to improve science education.

The Los Alamos and Livermore laboratories continue their work in national security through the Science-Based Stockpile Stewardship Program. This program is designed to ensure the safety and reliability of the enduring stockpile in an era of no nuclear testing.

For more information about DOE awards at UC campuses, contact:

Michael Barnes
Office of Research
UC Office of the President
1111 Franklin St., 11th Floor
Oakland, CA 94607-5200
voice: (510) 987-9492
fax: (510) 987-9456

In Washington, D.C. contact:

Matt Peterson
UC Office of Federal Governmental Relations
1523 New Hampshire Ave. NW
Washington, D. C. 20036
voice: (202) 588-0002
fax: (202) 785-2669

For more information about research programs at the UC-managed DOE laboratories, contact:

Rulon Linford
Associate Vice Provost
Office of Research
UC Office of the President
1111 Franklin St., 11th Floor
Oakland, CA 94607-5200
voice: (510) 987-9405
fax: (510) 987-9412

Office of Research
Publication Web site:
www.ucop.edu/research/profiles.html