Innovation for Our Nation

NNSA LABORATORY DIRECTED RESEARCH & DEVELOPMENT PROGRAM

2008 SYMPOSIUM
FOCUS ON ENERGY SECURITY

SEPTEMBER 18, 2008

LDRD
Laboratory Directed Research and Development

NNSA
National Nuclear Security Administration

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

SEPTEMBER 2008

LLNL-PROC-406572

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Welcome to the NNSA
Laboratory Directed Research and Development Program 2008 Symposium Focus on Energy Security

The Laboratory Directed Research and Development (LDRD) Program was authorized by Congress in 1991 to fund leading-edge research and development central to the national laboratories' core missions. LDRD anticipates and engages in projects on the forefront of science and engineering at the Department of Energy (DOE) national laboratories, and has a long history of addressing pressing national security needs at the National Nuclear Security Administration (NNSA) laboratories. LDRD has been a scientific success story, where projects continue to win national recognition for excellence through prestigious awards, papers published and cited in peer-reviewed journals, mainstream media coverage, and patents granted. The LDRD Program is also a powerful means to attract and retain top researchers from around the world, to foster collaborations with other prominent scientific and technological institutions, and to leverage some of the world's most technologically advanced assets. This enables the LDRD Program to invest in high-risk and potentially high-payoff research that creates innovative technical solutions for some of our nation's most difficult challenges.

Worldwide energy demand is growing at an alarming rate, as developing nations continue to expand their industrial and economic base on the back of limited global resources. The resulting international conflicts and environmental consequences pose serious challenges not only to this nation, but to the international community as well. The NNSA and its national security laboratories have been increasingly called upon to devote their scientific and technological capabilities to help address issues that are not limited solely to the historic nuclear weapons core mission, but are more expansive and encompass a spectrum of national security missions, including energy security.

This year's symposium highlights some of the exciting areas of research in alternative fuels and technology, nuclear power, carbon sequestration, energy efficiency, and other energy security research projects that are being conducted under the LDRD Program at the DOE/NNSA national laboratories and under the Site Directed Research and Development Program (SDRD) at the Nevada Test Site. Speakers from DOE/NNSA, other federal agencies, the NNSA laboratories, and the private sector will provide their insights into the national security implications of emerging energy and environmental issues, and the LDRD investments in energy security at the national laboratories.

Please take this opportunity to reflect upon the science and engineering needs of our country's energy demands, including those issues posed by climate change, paying attention to the innovative contributions that LDRD is providing to the nation.

Jamileh Soudah
Director, Office of Institutional and Joint Programs
National Nuclear Security Administration

Speakers

Michael Aimone

Assistant Deputy Chief of Staff for Logistics, Installations, and Mission Support
U.S. Air Force

As Assistant Deputy Chief of Staff for Logistics, Installations, and Mission Support at the U.S. Air Force Headquarters in Washington, D.C., Michael Aimone leads, manages, and integrates Air Force civil engineering, logistics readiness, supply, transportation, and aircraft and missile maintenance. He is also responsible for setting policy and preparing budget estimates that reflect enhancements to productivity, combat readiness, and quality of life for Air Force people.

Mr. Aimone entered the Air Force in 1970 and served in numerous field and staff engineering assignments. After leaving active duty and serving in the Air Force Reserve from 1979 to 1997, Mr. Aimone was recalled to extended active duty to command the 819th Red Horse Squadron at Malmstrom Air Force Base from July 1997 through December 1998.

Mr. Aimone joined the Federal service in 1980 as a project electrical engineer with U.S. Air Force Headquarters. He served in various supervisory positions within the Department of the Air Force and the Office of the Secretary of Defense until leaving federal service in 1993. From 1993 until his recall to active duty in 1997, Mr. Aimone was vice president of an electrical engineering software development company. He returned to Federal service in January 1999.

Mr. Aimone has a bachelor of science degree in electrical engineering from Michigan Technological University and a master of science degree in electrical engineering from the University of Florida, Gainesville, and is a professional engineer registered in Virginia, California, Wisconsin, and Ohio. His awards include a Legion of Merit, Bronze Star Medal, a Meritorious Service Medal with four oak leaf clusters, and a 2007 Presidential Award for Leadership in Federal Energy Management.

Paul P. Bollinger, Jr.

Deputy Assistant Secretary of the Army for Privatization and Partnerships
(Installations and Environment)

Paul P. Bollinger, Jr. was sworn in on April 3, 2008 as the Deputy Assistant Secretary of the Army for Privatization and Partnerships. He has responsibility for and oversight of Army installation privatization initiatives, including energy initiatives. He previously served as Special Assistant to the Assistant Secretary of the Air Force for Installations, Environment and Logistics, responsible for the management of the alternative fuels program. His efforts in alternative energy include the creation of the U.S. Government Inter-Agency Working Group on Alternative Fuels. Mr. Bollinger also serves as the Department of Defense (DoD) representative on the Strategic Unconventional Fuels Task Force. In addition, he was the DoD representative on the Western Governor's Association Coal-to-Liquids Task Force and the Environmental Protection Agency's Advanced Coal Technology Working Group. Mr. Bollinger also ran the successful U.S. Air Force Energy Forums I and II, held in 2007 and 2008.

A native of Kentucky, Mr. Bollinger graduated from the University of Kentucky with a bachelor's degree in aviation and business. He earned a graduate certificate from George Washington University. He is also a licensed U.S. Coast Guard Captain. In 1979, he came to Washington, D.C., to serve as assistant director of the American Association of Airport Executives. He started Bollinger & Associates in 1988 and was the first executive director of the Airport Consultants Council. Subsequently, he became the senior vice president of the Airports Council International–North America and then vice president of DMJM Aviation in Philadelphia. He returned to Washington, D.C., as vice president of aviation for HNTB Corporation. He is also a past president of the Air Traffic Control Association.

Mr. Bollinger is the founder of the Greater Washington Aviation Open—the largest aviation charity event in Washington, D.C.—and serves on the board of directors of the Corporate Angel Network, the tournament beneficiary, which arranges for cancer patients to fly on business aircraft to treatment facilities across the country.

Thomas P. D'Agostino

Undersecretary for Nuclear Security
Department of Energy, and
Administrator
National Nuclear Security
Administration

Thomas P. D'Agostino is Undersecretary for Nuclear Security at DOE and Administrator for the NNSA. He was sworn in by the Secretary of Energy on August 30, 2007. Previously, as Deputy Administrator for Defense Programs at NNSA, Mr. D'Agostino directed the Stockpile Stewardship Program (SSP). Prior to that, as Assistant Deputy Administrator for Program Integration, Mr. D'Agostino directed the formulation of the programs, plans, and budget for the SSP. As Deputy Director of the Nuclear Weapons Research, Development, and Simulation Program, he directed the formulation of the programs and budget for the research and development program that supports the SSP. From 1989 to 1996, Mr. D'Agostino worked in numerous assignments in the federal government in starting up tritium production reactors and at the Naval Sea Systems Command as a program manager for the Seawolf submarine propulsion system.

Mr. D'Agostino achieved the rank of captain in the U.S. Naval Reserves, where he has served with the Navy Inspector General and the Deputy Chief of Naval Operations for Submarine Warfare in developing concepts for new attack submarine propulsion systems. He also served with the Deputy Chief of Naval Operations for Plans, Policy, and Operations in the Navy Command Center in the Pentagon. In this capacity, he was the French Desk Officer for the Chief of Naval Operations responsible for all politico-military interactions with the French Navy and served as the Duty Captain at the Navy Command Center.

His eight years of active duty in the Navy as a submarine officer included assignments aboard the U.S.S. *Skipjack* and with the Board of Inspection and Survey as the main propulsion and nuclear reactor inspector. In this position, he performed nuclear reactor and propulsion engineering inspections for over 65 submarines and nuclear-powered ships in the Atlantic and Pacific Fleets.

Mr. D'Agostino's awards include the Navy Commendation Medal with Gold Stars, Navy Achievement Medal, Navy Expeditionary Medal, Meritorious Unit Commendation, National Defense Service Medal, Presidential Rank Meritorious Executive Award, and many others. His most recent degree is a master's of science in national security studies from the Naval War College.

Tomás Díaz de la Rubia

Associate Director for Chemistry,
Materials, Earth, and Life Sciences
Lawrence Livermore National
Laboratory

Tomás Díaz de la Rubia joined Lawrence Livermore National Laboratory (LLNL) as a postdoctoral researcher in 1989 after completing his Ph.D. in physics at the State University of New York at Albany. He carried out his thesis research in the Materials Science Division at Argonne National Laboratory and in the Materials Science Department at University of Illinois at Urbana–Champaign. The focus of his scientific work has been the investigation, via large-scale computer simulation, of defects, diffusion, and microstructure evolution in extreme environments.

At LLNL he first worked on materials issues for the fusion program and then joined the Chemistry and Materials Science Directorate in 1994. Between 1994 and 1996, he focused his research activities around the development of physics-based predictive models of ion implantation and thin film growth for semiconductor processing in collaboration with Bell Labs, Intel, Applied Materials, IBM, and other semiconductor firms. Between 1994 and 2002, he was also involved in the development of multiscale models of materials strength and aging in irradiation environments and worked in the Advanced Simulation and Computing Program developing models of materials strength.

In 1999 he became group leader for Computational Materials Science and helped build and lead an international recognized effort in computational materials science at LLNL. Between 2000 and 2002, he served as the Chemistry and Materials Science Materials Program Leader for the National Ignition Facility, where he focused on optical materials and target development.

Mr. Díaz de la Rubia was selected as the Associate Director for Chemistry and Materials Science in 2002 and currently leads the Chemistry, Materials, Earth, and Life Sciences Directorate, formed in 2007.

Mr. Díaz de la Rubia has published more than 140 peer-reviewed articles in scientific literature, has chaired numerous international conferences and workshops, and has edited several conference proceedings and special journal issues. He belongs to the editorial board of five major scientific journals and continues to serve in numerous national and international panels. He was elected a fellow of the American Physical Society in 2002 and is currently the vice chair (chair elect) of the Division of Computational Physics. He is a fellow of the American Association for the Advancement of Science and served as an elected member of the board of directors of the Materials Research Society between 2002 and 2005.

Raymond Lee Orbach

Undersecretary for Science
Department of Energy

As DOE's Under-secretary for Science, Raymond Lee Orbach serves as the Secretary's advisor on science policy and on the scientific aspects of all of DOE's operations, from basic research to nuclear energy, defense programs, and the environmental cleanup of Cold War legacy sites. Mr. Orbach is also responsible for planning, coordinating, and overseeing DOE's research and development programs, its 17 national laboratories, and its scientific and engineering education activities.

Secretary Bodman has tasked Mr. Orbach with implementing the President's American Competitiveness Initiative, which will help drive continued American economic growth. As Technology Transfer Coordinator and chair of the Technology Transfer Policy Board, he is also responsible for leading efforts to transfer technologies from DOE's national laboratories and facilities to the global marketplace. Since 2002, Mr. Orbach has also served as Director of the Office of Science.

With a Ph.D. in physics from the University of California (UC) at Berkeley, Mr. Orbach has conducted research in theoretical and experimental physics, the results of which are described in more than 240 published scientific papers. His numerous honors include two Alfred P. Sloan Foundation fellowships, a National Science Foundation senior postdoctoral fellowship at Oxford University, and a John Simon Guggenheim Memorial Foundation fellowship at Tel Aviv University. He is a fellow of the American Physical Society and the American Association for the Advancement of Science and has also held numerous visiting professorships at universities around the world, including the Imperial College of Science and Technology in London.

Mr. Orbach entered academia in 1960 as a postdoctoral fellow at Oxford University. He became an assistant professor of applied physics at Harvard University in 1961 and joined the faculty of UCLA two years later as an associate professor, becoming a full professor in 1966. He served as provost of the UCLA College of Letters and Science from 1982 to 1992 and as chancellor of UC Riverside from 1992 to 2002.

Terry A. Michalske

Director for Energy Innovation Initiatives
Sandia National Laboratories

As Director for Energy Innovation Initiatives, Terry A. Michalske is responsible for focusing Laboratory-wide resources and partnerships on key national security issues involving our nation's energy. While on this special assignment, he is on leave from his duties as Director for Biological and Energy Sciences, which includes his role as Director for the DOE Combustion Research Facility, an international user facility providing scientific and technical tools for understanding and predicting complex chemical and combustion systems. Mr. Michalske is the founding director of the DOE Center for Integrated Nanotechnologies (CINT), one of five DOE nanoscale science research centers. As CINT Director, he oversaw the design and construction of the $75M research facility and established CINT's unique role as integrator of nanoscience discoveries with the microscale and macroscale worlds of devices and real-world applications. He has made numerous technical accomplishments in the areas of materials science, surface and interfacial phenomena, nanoscale properties of materials, and integrated microsystems. His research on the stress corrosion fracture of silica has been recognized by several international awards, including the Ross Coffin Purdy Award (1985) and the Weyl International Glass Science Award (1989). He is co-recipient of an R&D 100 Award (1994) for development of the interfacial force microscope. Mr. Michalske has organized numerous international meetings and symposia, and he has managed several technical organizations at Sandia, including Surface Science, Biomolecular Materials, and Nanotechnologies. He is a fellow of the American Vacuum Society and of the American Ceramic Society. Mr. Michalske has testified before the U.S. Senate and the California and New Mexico state legislatures on the topics of nanoscience and energy. He currently serves as a trustee of Alfred University, chairs the Board of Directors for the Joint BioEnergy Institute, and participates in a number of external advisory boards for university and government programs and initiatives in energy, nanoscience, and biotechnology.

Alan R. Shaffer

Principal Deputy Director for Defense Research and Engineering
Department of Defense

As the Department of Defense's (DoD's) Principal Deputy Director for Defense Research and Engineering, Alan R. Shaffer is responsible for formulating, budgeting for, planning, and reviewing the DoD's research, development, testing, and evaluation programs. He reviews the maturity of technology as part of the acquisition cycle and develops options to reduce the DoD's overall technology development risk.

Prior to entering the federal government, Mr. Shaffer served in the U.S. Air Force for 24 years, with assignments in weather, intelligence, science and technology management, acquisition oversight, and programming. During Operation Desert Storm, he was responsible for deploying a 500-person theater weather force. Other assignments include Wing Weather Officer supporting the 320th Bombardment Wing at Mather Air Force Base and intelligence officer in the Foreign Technology Division at Wright Patterson Air Force Base.

After retiring from the Air Force in 2000, Mr. Shaffer was appointed as the Director of Multidisciplinary Systems in the Office of the Deputy Undersecretary of Defense for Science and Technology. In 2001, he became Director for Plans and Programs, Defense Research and Engineering—a capacity he has continued until the present while serving as the Principal Deputy Director—and as such is responsible for oversight of the DoD's science and technology portfolio of over $10.5 billion. Mr. Shaffer has served as executive director of several senior task forces, including the DoD Energy Security Task Force in 2007 and, most recently, the Mine-Resistant Ambush Protection Task Force.

Mr. Shaffer earned a bachelor of science degree in mathematics from the University of Vermont, a bachelor of science degree in meteorology from the University of Utah, a master of science in meteorology from the Naval Postgraduate School, and a master of science in national resource strategy from the Industrial College of the Armed Forces. He has been awarded the Distinguished Executive Presidential Rank Award in 2007 and the Meritorious Executive Presidential Rank Award in 2004.

Jamileh Soudah

Director
Office of Institutional and Joint Programs
National Nuclear Security Administration

As director of the Office of Institutional and Joint Programs, Jamileh Soudah oversees more than $2 billion of research and development, Work for Others, and technical partnership projects across the nuclear complex. Ms. Soudah began her career as a teaching and research assistant at Kuwait University, leading computer-simulated radar systems development and teaching radar and communication theories to senior engineering students. At the IBM Research Center at Kuwait University, she worked on signal-processing techniques and conducted intensive research on jamming and antijamming technologies.

Ms. Soudah joined the Department of Defense Contract Management Agency (DCMA) in 1992 as a software engineer for the Army Digital Topographic Support System program. Since then, she has held various positions as an information technology professional, program integrator, project manager, and team leader for various command and control systems and countermeasures, including F-15 simulators, Bradley A3 enhancements, and the Intensive R&D Rapid Advanced Signal Processing Project for the Defense Advanced Research Projects Agency. She has led various tiger teams assessing major acquisition systems for the National Aeronautics and Space Administration and the Department of the Air Force; was instrumental in developing the DCMA software quality management training program, which serves more than 300 software professionals; and has led many technical evaluations and negotiations on critical engineering change controls. Ms. Soudah joined NNSA in 2001 to lead verification and validation activities across the national laboratories. In 2004 she became acting director for the readiness program, overseeing the development of new and enhanced processes, technologies, and capabilities to meet current and future nuclear weapon design and production needs across the complex.

Ms. Soudah has a bachelor of science in electrical engineering from Kuwait University, a master of science in electrical engineering from the University of Wisconsin, DoD level III certification as engineer, and project management certification from the Project Management Institute and under the Defense Acquisition Workforce Improvement Act.

Terry C. Wallace, Jr.

Principal Associate Director
of Science, Technology, and Engineering
Los Alamos National Laboratory

As Principal Associate Director of Science, Technology, and Engineering, Terry C. Wallace, Jr. is responsible for all basic science programs at Los Alamos National Laboratory (LANL) and coordinates the activities of the four science and engineering directorates. Mr. Wallace brings strong science credentials and a track record as an effective science manager at LANL. From 2005 to 2006, he was Associate Director of Strategic Research, which encompassed LANL's science program offices and the five line divisions that implemented those programs and supported LANL's nuclear weapons, threat reduction, and energy security missions. He was also responsible for LANL's non-NNSA DOE programs, including basic science, energy technology, and environmental technology.

Raised in Los Alamos, Arizona, Mr. Wallace returned there in 2003 after 20 years as a professor of geosciences and an associate in the applied mathematics program at the University of Arizona, in Tucson. In addition to teaching, he carried out research on global threat reduction, nonproliferation verification, and computational geophysics. During his academic career, he collaborated with LANL on nuclear test monitoring and threat reduction, with an emphasis on interpreting the indications of nuclear testing by a foreign government. He has an international reputation in geosciences as applied to national security issues.

Mr. Wallace holds Ph.D. and M.S. degrees in geophysics from the California Institute of Technology and B.S. degrees in geophysics and mathematics from the New Mexico Institute of Mining and Technology. He is the author or coauthor of more than 80 peer-reviewed publications on seismology and tectonics, including ground-based nuclear explosion monitoring and forensic seismology. He also wrote a widely used textbook on seismology. Mr. Wallace is a fellow of the American Geophysical Union (AGU) and in 1992 he received the AGU's Macelwane Medal. He has served as president of the Seismological Society of America, chairman of the Incorporated Institutions for Research in Seismology, and authored the AGU's position paper on the verifiability of a comprehensive test ban treaty. He has testified before Congress on the comprehensive test ban and participated in numerous National Academy panels, including ones on research in support of comprehensive test ban monitoring. Wallace chaired the National Research Council's Committee on Seismology and Geodynamics from 2000 to 2006.

R. James Woolsey

Venture Partner, VantagePoint Venture Partners
Former Director of Central Intelligence

In addition to working as a venture partner at VantagePoint Venture Partners of San Bruno, California, R. James Woolsey also chairs the Strategic Advisory Group of the Paladin Capital Group, is a senior executive advisor to Booz Allen Hamilton, and is counsel to the Washington, D.C., office of the Boston-based law firm Goodwin Procter. In these capacities, he specializes in a range of alternative energy and security issues.

Mr. Woolsey has served the U.S. government for a total of 12 years, most recently as Director of Central Intelligence (1993–95). Prior to that, he was Ambassador to the Negotiation on Conventional Armed Forces in Europe (1989–1991), Undersecretary of the Navy (1977–79), and General Counsel to the U.S. Senate Committee on Armed Services (1970–73). He was also a delegate-at-large to the U.S.–Soviet Strategic Arms Reduction Talks and Nuclear and Space Arms Talks (1983–86). As an officer in the U.S. Army, he was an adviser on the U.S. delegation to the Strategic Arms Limitation Talks (1969–70).

Mr. Woolsey currently serves on or chairs a wide range of government, corporate, and nonprofit advisory boards, including that of ExecutiveAction, LLC; serves on the National Commission on Energy Policy; co-chairs (with former Secretary of State George Shultz) the Committee on the Present Danger; chairs the Advisory Boards of the Clean Fuels Foundation and the New Uses Council; and is a trustee of the Center for Strategic and International Studies and the Center for Strategic and Budgetary Assessments.

Previously he chaired the Executive Committee of the Board of Regents of The Smithsonian Institution, was a trustee of Stanford University, and was a member of the National Commission on Terrorism, the Commission to Assess the Ballistic Missile Threat to the U.S. (Rumsfeld Commission), the President's Commission on Federal Ethics Law Reform, the President's Blue Ribbon Commission on Defense Management (Packard Commission), and the President's Commission on Strategic Forces (Scowcroft Commission).

Mr. Woolsey has a B.A. degree from Stanford University (1963), an M.A. degree from Oxford University (1965), and an LL.B. from Yale Law School (1968).

Presenters

Keith S. Bradley
Program Leader, Nuclear Fuel Cycles
Global Security Principal Directorate
Lawrence Livermore National Laboratory

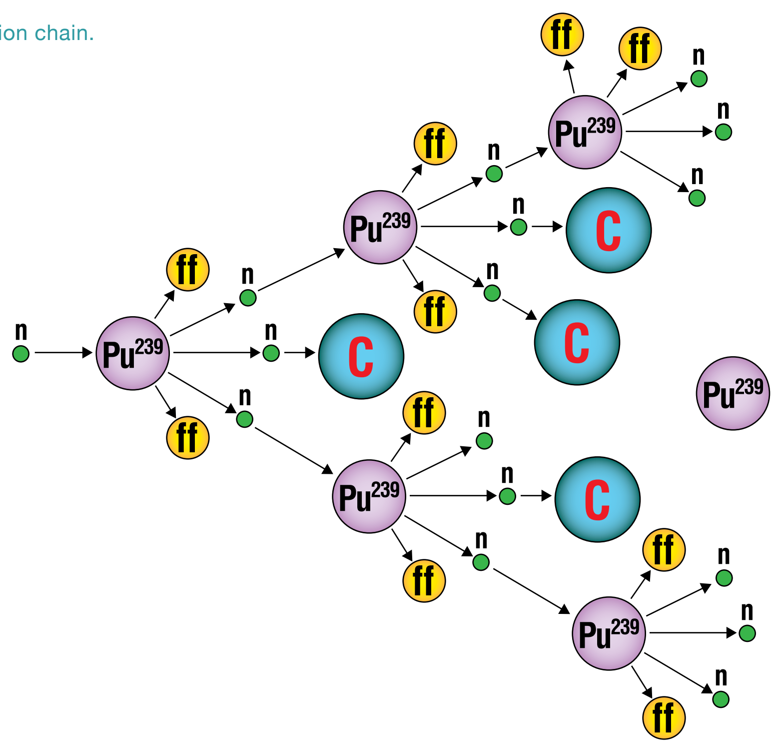
Toward More Intrinsically Secure Nuclear Fuel Cycles

Global dependence on nuclear power is widely predicted to at least triple in the next 40 years. While there are clear benefits to reducing dependence upon fossil fuels, such dramatic growth in nuclear power will exacerbate challenges such as waste management and proliferation and may also introduce new challenges, such as the depletion of uranium ore and other raw materials used to produce nuclear fuel. Consequently, we must enable that growth in a way that optimizes the benefits while minimizing undesirable consequences.

One possible approach is to close the nuclear fuel cycle. Since the late 1970s, the U.S. has eschewed such approaches because of the proliferation risks associated with reprocessing spent nuclear fuel. The past few years, however, have seen the emergence of a policy to promote closure of the fuel cycle in a proliferation-resistant manner. Although dozens of novel fuel cycles have been proposed claiming to reduce the risk of nuclear proliferation, the basis of those claims rarely rest upon true expertise in nuclear weapons physics, design, and performance.

This project is leveraging expertise and methodologies originally developed to design and maintain the U.S. nuclear arsenal to assess the utility of proposed nuclear fuel cycles and the materials mixtures generated therein for use by adversaries as nuclear explosives. We are also extending that expertise to explore novel means of degrading the utility of such materials to discourage their misuse. We will describe our methodologies, report current results, and highlight some of the enduring challenges that deserve greater attention.

The plutonium-239 fission chain.



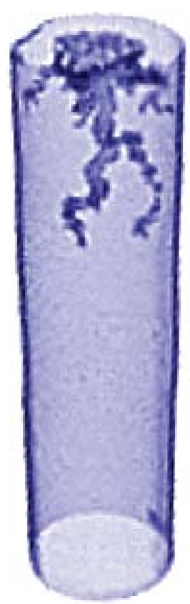
Bill Carey
Earth and Planetary Materials Team Leader
Earth and Environmental Sciences Division
Los Alamos National Laboratory
Harvard University

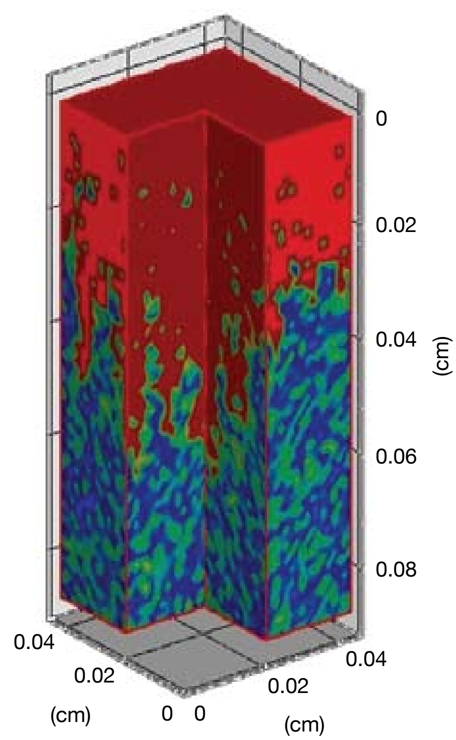
Science of Geological Carbon Sequestration: Integration of Experimentation and Simulation

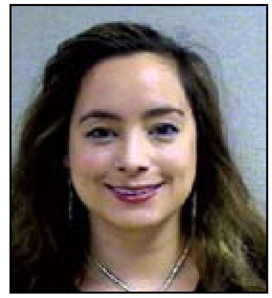
A broad consensus now exists in the scientific community that increased levels of carbon dioxide and other greenhouse gases are driving global warming and dramatic changes in weather patterns. In 2002, President Bush announced the Global Climate Change Initiative, committing the nation to cut greenhouse gas intensity. As highlighted in the Initiative, sequestering carbon dioxide in geologic formations represents one of the most promising near-term solutions for the development of carbon-neutral industrial processes.

The goal of our LDRD project was to develop an integrated experimentation–modeling approach to address the most significant technical issues associated with carbon dioxide sequestration. The carbon dioxide problem is complex because the system is multiphase, with partly miscible fluids, and system performance depends entirely on microscopic details of carbon dioxide brine–rock interactions. Our research was organized around four key issues in carbon sequestration: injectivity, storage capacity, leak rate, and reservoir-scale distribution of carbon dioxide. We examined these issues through a combination of experimental studies of multiphase flow in reservoir and wellbore systems, phase equilibria studies of carbonate mineralization, tomographic imaging of pore-scale processes, development and enhancement of pore-scale and continuum-scale modeling (parallelization, multiphase capability, and reactive chemistry), and development of upscaling methods to integrate pore-scale processes in large-scale models. Our research results have provided new insights into fundamental carbon dioxide brine–rock interactions and have yielded significant advances in the computational representation of carbon dioxide storage processes.

Left: Neutron tomography image of experimentally induced worm-hole formation in limestone following injection of carbon dioxide. Right: Pore-network numerical simulation of carbon dioxide–induced dissolution of limestone.







Whitney Colella
Truman Research Fellow
Sandia National Laboratories

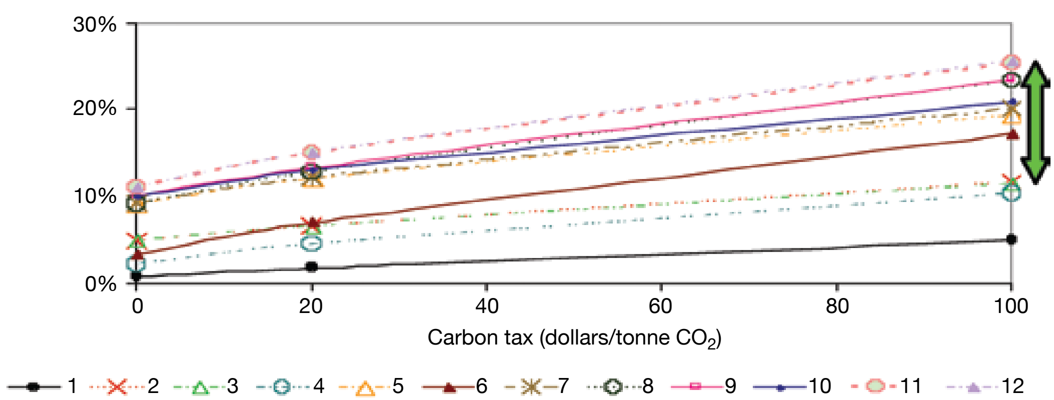
Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

We are developing computer models to examine novel designs of stationary fuel-cell power plants tuned to the energy-demand curves of the buildings they could serve. These models evaluate energy supply by fuel cell systems (FCSs) and distributed energy devices relative to the energy demand in surrounding buildings. Novel design, installation, and control strategies for FCSs are examined with the goals of reducing energy costs to building owners and mitigating carbon dioxide emissions. Because optimal strategies are unique for different climates, economic environments, and building load curves, simulation studies are crucial for identifying optimal strategies for a given installation.

We are investigating novel strategies not typically pursued by industry. Conventionally, FCSs are installed as stand-alone, non-load-following systems with a fixed heat-to-power ratio and producing only electricity. However, we are evaluating novel approaches such as networking, electricity load following, heat load following, variable heat-to-power ratios, heating and cooling recovery, and combinations of these approaches.

Our simulations have already shown that for the load curves examined, FCSs always achieve significantly higher energy cost savings when networked rather than as stand-alone devices. Furthermore, a networked system with a variable heat-to-power ratio—and either with or without load following, depending on the load curve shape—has been shown to be most economical. Finally, FCSs coupled with absorption chillers can convert recoverable heat to cooling power and, when networked, may be more cost competitive and have lower carbon dioxide emissions than conventional cooling power.

A computer model predicts that combining a carbon tax with novel strategies can augment the tax's impact on energy cost savings and installed capacity (the quantity of fuel cell systems installed in buildings).

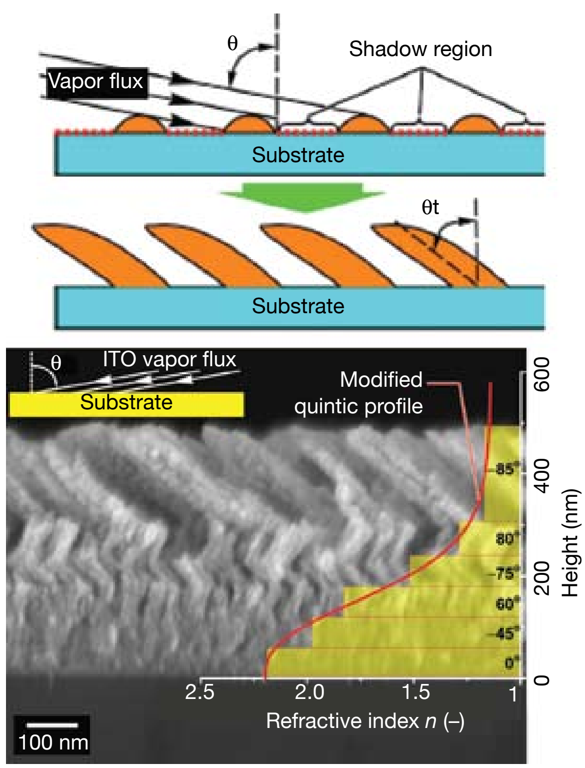


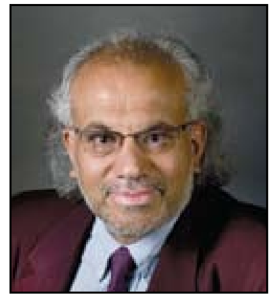
Mary H. Crawford
Distinguished Member of the Technical Staff
Semiconductor Material and Device
Sciences Department
Sandia National Laboratories

Nanoengineering for Solid-State Lighting

Solid-state lighting (SSL) based on light-emitting diodes (LEDs) has the potential to have a dramatic global impact. If LED electrical-to-optical energy conversion efficiency goals of 50% or greater can be achieved, worldwide electricity consumption due to lighting could be decreased by more than 50%, and total consumption of electricity could be decreased by more than 10%. However, to realize this future benefit we must overcome significant technical challenges. This project seeks to address those challenges by developing and applying, in collaboration with Rensselaer Polytechnic Institute, innovative concepts to achieve energy-efficient SSL by the enhancing optical efficiency of LED materials in two ways: (1) nanoscale engineering of dielectric and metallic coatings for enhanced light extraction and (2) study and manipulation of nanoscale properties of semiconductor light-emitting materials to fundamentally understand and improve LED internal quantum efficiency. Our light-extraction efforts include developing and applying novel dielectric graded-index nanorod coatings that will increase LED efficiency by 28%. Our semiconductor material studies have already yielded insight into the impact of crystalline defects on LED efficiency and the mechanisms that presently limit LED efficiencies at the high current densities required for illumination applications.

Novel graded refractive-index materials were developed and used to obliquely coat nanorods for improved light extraction from light-emitting diodes.





Manvendra Dubey
Geochemistry Team Leader
Earth Environmental Science Division
Los Alamos National Laboratory
Harvard University

Quantifying Aerosol Radiative Forcing to Constrain Climate Sensitivity for Optimal Transition to a Carbon-Neutral and Clean-Air World

Climate sensitivity—the ratio of warming to radiative forcing—determines the vulnerability of our Earth system to human activity and natural variability. Climate sensitivity is, however, currently uncertain by a factor of two to four: Although forcing by greenhouse gases is well quantified, our knowledge of forcing by aerosols is incomplete. Accurate determination of this parameter is essential to inform energy policy as we transition to a carbon-neutral economy. Quantifying the role of aerosols poses a challenge because of their complex composition, short lifetime, heterogeneous distributions, ability to absorb and scatter solar and terrestrial radiation, and their effects on clouds. Furthermore, aerosol-induced weakening of the hydrological cycle is a key water sustainability issue for the 21st century. Our project created a confluence of observational (satellite-based and in situ), modeling (cloud-resolving and global), and laboratory (single-particle and bulk) research on the microphysics, dynamics, and optics of aerosol–cloud interactions to quantify their climatic effects. We made quantum leaps in aerosol–cloud modeling, optical instrumentation, and satellite inversion algorithms. These advances were successfully integrated to glean process-level information about aerosol physical–chemical transformations in the atmosphere as they age and effect clouds. Our poster highlights the following results from field campaigns.

Measurements of pollution over Barrow, Alaska, made during research on indirect and semidirect aerosol effects on clouds (April 2008). Absorption and scattering of light at three wavelengths in the blue (405 nm), green (532 nm) and red (532 nm) spectrum were measured by the world's first three-laser photoacoustic instrument.

In California, we observed a dark aerosol plume in a marine stratus cloud. Analysis showed that soot, when mixed with sulfate, is effectively scavenged by cloud drops, which alters cloud reflectivity—a phenomenon that had not been incorporated into climate models. When measuring diurnal profiles of aerosol absorption and scattering in Mexico City, we discovered large photochemical production of organic aerosols in the afternoon—which are also missing in current models. We integrated a wealth of data to estimate the net radiative forcing by pollutants and greenhouse gases for a mega-city, a new metric to guide policy. In Houston, Texas, we discovered that cloud-processed aerosols are darker above Houston. This could result from selective scavenging of sulfate or from reduction in the size of aerosol particles. Finally, in the Arctic we interrogated pollution by deploying the world's first three-laser photoacoustic instrument. We measured extreme pollution above the Arctic from Chinese dust, Siberian fires, and fossil energy sources. Our analysis implicated Arctic haze in the rapid melting of Arctic ice.

Our research has allowed us to quantify aerosol effects on climate and develop novel approaches to determine climate sensitivity from observations, which will enable an optimal transition to a carbon-neutral and clean-air world.

Masood Hadi
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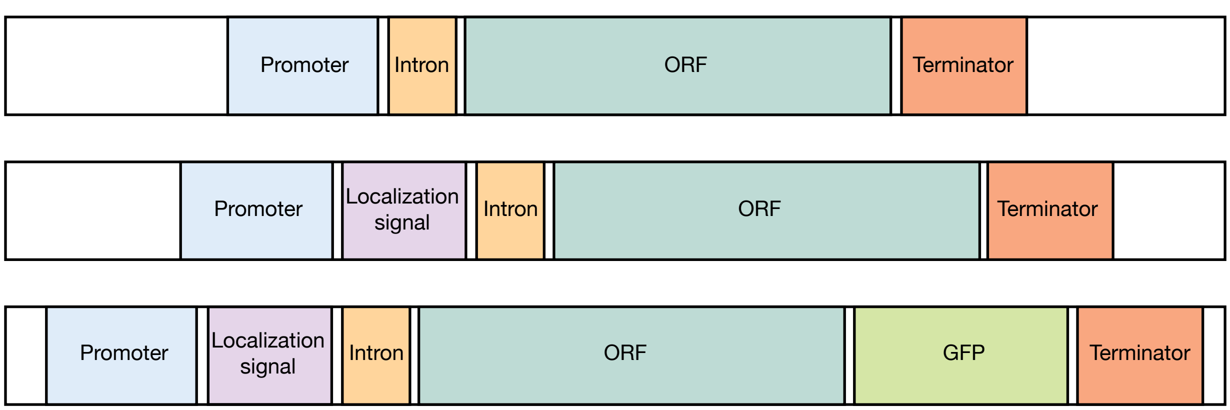
Director of Technologies Division
Joint Bioenergy Institute

“Trojan Horse” Strategy for the Deconstruction of Biomass for Biofuels Production

The production of renewable biofuels to displace fossil fuels currently consumed in the transportation sector is a pressing multiagency national priority. Currently, nearly all fuel ethanol is produced from corn-derived starch. Dedicated “energy crops” and agricultural waste are the preferred long-term solutions for renewable, inexpensive, and globally available biofuels because they avoid some of the market pressures and secondary greenhouse gas emissions of corn ethanol. These sources of lignocellulosic biomass are converted to fermentable sugars using a variety of chemical and thermochemical pretreatments, which disrupt cellulose and lignin cross-links, allowing exogenously added recombinant microbial enzymes to more efficiently hydrolyze the cellulose for deconstruction into glucose. However, this process is plagued with inefficiencies, primarily due to the recalcitrance of cellulosic biomass, mass transfer issues during deconstruction, and low activity of recombinant deconstruction enzymes. In addition, costs are high because of the required enzymes and reagents and the energy-intensive and cumbersome pretreatment steps.

One potential solution to these problems is found in synthetic biology. This project proposes to engineer plants that self-produce a suite of cellulase enzymes targeted to the apoplast for cleaving the linkages between lignin and cellulosic fibers. The genes encoding the degradation enzymes, also known as cellulases, are obtained from extremophilic organisms that grow at high temperatures (60–100°C) and acidic pH levels (<5). These enzymes will remain inactive during the life cycle of the plant but become active during hydrothermal pretreatment; that is, elevated temperatures. Deconstruction can be integrated into a one-step process, thereby increasing efficiency (cellulose–cellulase mass-transfer rates) and reducing costs. Our proposed disruptive technologies address biomass deconstruction processes by developing transgenic plants encoding a suite of enzymes used in cellulosic deconstruction. The unique aspects of this technology are the rationally engineered, highly productive extremophilic enzymes, targeted to specific cellular locations (apoplast) and their dormancy during normal plant proliferation, which become “Trojan horses” during pretreatment conditions. We are leveraging established Sandia enzyme engineering and imaging capabilities. Our technical approach not only targets the recalcitrance and mass-transfer problem during biomass degradation, but also eliminates the costs associated with the industrial-scale production of microbial enzymes added during processing.

Recombinant-DNA actuator constructs used to engineer archaeal extremophile cellulase and endoglucanase enzymes for ultimate expression in specific plant tissues after genetic transformation.



Ronald Justin
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Special Technologies Laboratory
SDRD, Nevada Test Site

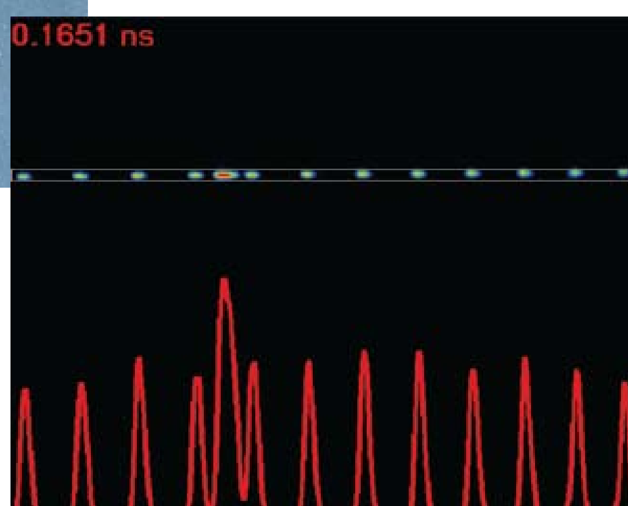
Optical Comb Generation for Streak Camera Calibration for Inertial Confinement Fusion Experiments

The National Ignition Facility at Lawrence Livermore National Laboratory is coming online to support physics experimentation for DOE programs in inertial confinement fusion and stockpile stewardship. Optical streak cameras are an integral part of the experimental diagnostics instrumentation at the National Ignition Facility. To accurately reduce streak camera data, a highly accurate temporal calibration is required. This poster describes a technique for simultaneously generating a precise 2-ps optical marker pulse (fiducial reference) and trains of precisely timed, short-duration optical pulses (called “comb” pulse trains) that are suitable for the timing calibrations.

These optical pulse generators are used with Livermore’s optical streak cameras. These small, portable light sources can produce a series of temporally short, uniformly spaced optical pulses using a laser diode source. Comb generators have been produced with pulse-train repetition rates up to 10 GHz at 780 nm and somewhat lower frequencies at 664 nm. Individual pulses can be as short as 25 ps (full width at half maximum). Signals are output via a fiberoptic connector on the front panel of the generator box. The optical signal is transported from comb generator to streak camera through multimode, graded-index optical fiber.

A comb/marker generator.

Streak camera image of a 2-GHz comb with fiducial marker superimposed.



Raymond P. Keegan
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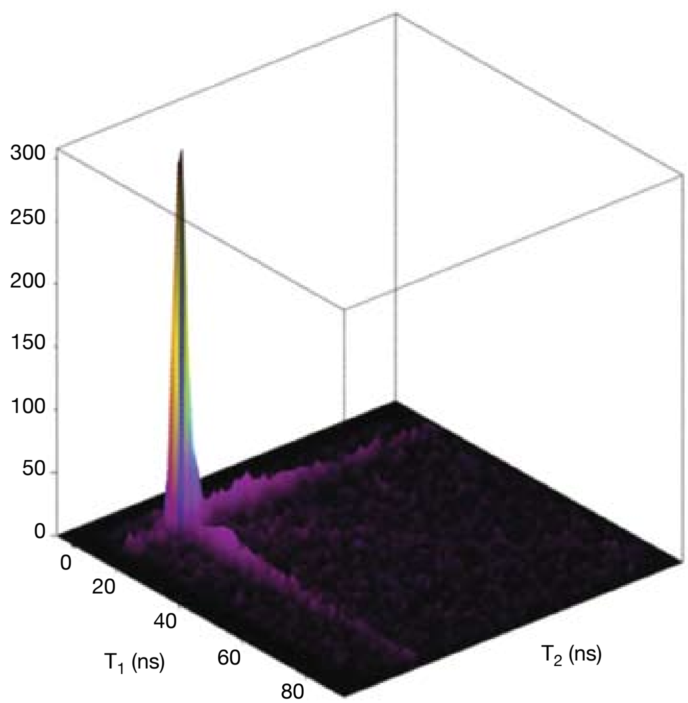
Remote Sensing Laboratory, Las Vegas
SDRD, Nevada Test Site

Fission Detection Using the Associated Particle Technique

In this project, a beam of tagged 14-MeV neutrons from the deuterium–tritium reaction is used to induce fission in a target composed of depleted uranium. The generator yield is 107 neutrons per second radiated into a 4π solid angle. Two 4-inch-square sodium iodide detectors are used for gamma-ray detection. The fission process is known to produce multiple gamma-rays and neutrons. Triple coincidences (alpha–gamma–gamma) are measured as a function of neutron flight time up to 90 ns after fission, where the alpha particle arises from the denterium–tritium reaction. A sudden increase in the triple coincidence rate at the location of the material is used to localize and detect fission in the interrogated target. Comparisons are made with experiment runs where lead, tungsten, and iron were used as target materials. The triple coincidence response profile from depleted uranium is shown to be different to those observed from the other target materials. The response from interrogation targets composed of fissile material is anticipated to be even more unique than that observed from depleted uranium.

The triple-coincidence technique for detecting depleted uranium demonstrates a sensitivity equivalent to detecting 1.56 kg of plutonium-239 or 1.8 kg of uranium-235 at 60 cm.



Julie K. Lundquist
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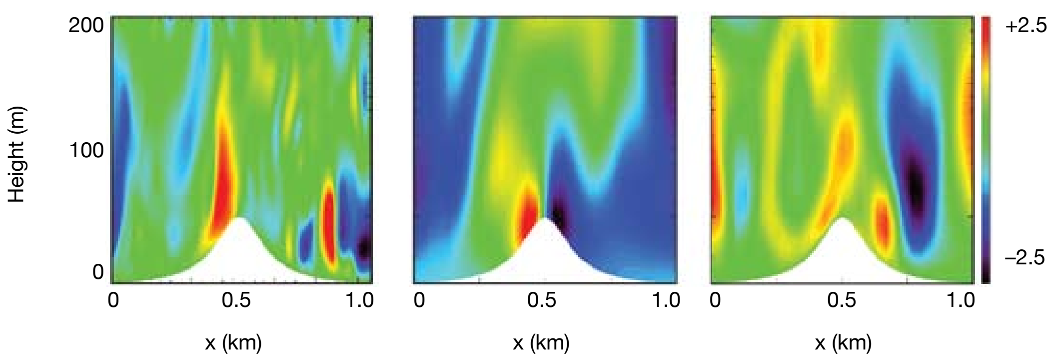
Chemistry, Materials, Environmental, and Life
Sciences Directorate
Lawrence Livermore National Laboratory

Atmospheric Turbulence Modeling for Energy Security and National Security Applications

Urban areas and regions of complex topography affect atmospheric flow, channeling winds and generating turbulence. Accurate simulations of these flows are required for important applications such as predicting how wind will spread radiological, biological, or chemical contaminant plumes and predicting the energy that can be generated from wind turbines. Wind forecasts must account for complexities of microclimates, using very high horizontal spatial resolution (i.e., grid cells with horizontal resolution on the order of 10 to 400 m) and vertical resolution of approximately 2 m near the surface. Such high-resolution simulations are more complicated than conventional weather forecasts because existing parameterizations—designed for coarser-resolution simulations—fail at such high resolution. This LDRD project, in collaboration with the University of California at Berkeley, has incorporated very-high-resolution turbulence parameterizations into the community numerical weather prediction model WRF. These parameterizations have been validated for the range of atmospheric stabilities expected over a daily cycle. Furthermore, this new capability can capture the relevant physics for flows in complex terrain at coarser resolution than with other turbulence parameterizations. This efficiency can save two orders of magnitude or more on computational time.

These instantaneous snapshots from simulations of flow over a hill compare the ability of models to capture recirculation patterns in the lee of a hill. Contours of vertical velocity for three different simulations are shown; flow is from the left in all cases. At left, simulated with expensive high resolution (8-m grid cells), the simulation shows the expected recirculation (updrafts and downdrafts) in the lee. At center, WRF's native subgrid turbulence parameterizations at 32-m resolution fail to capture the recirculation, showing only downdrafts in the lee. At right, Livermore's new parameterizations at 32-m resolution capture the recirculations expected in the lee, at roughly one-fourth the computational expense of the simulation at far left. (Because these images are snapshots in time, exact matches between the models are not expected.)



Richard Maurer
Deputy Chief Science Officer
Remote Sensing Laboratory
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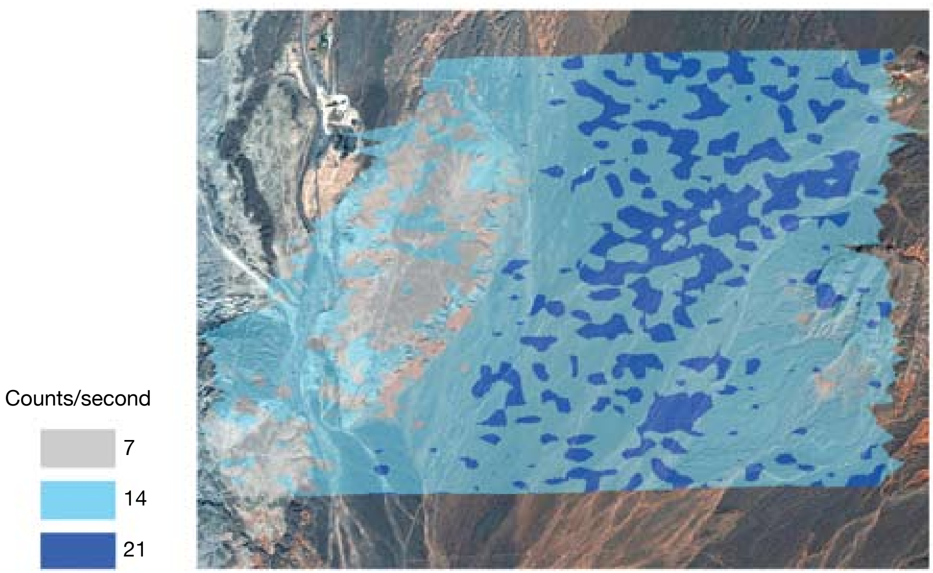
SDRD, Nevada Test Site

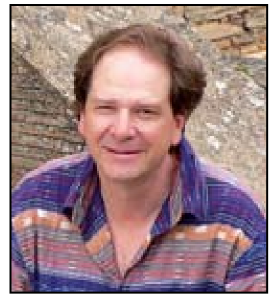
Aerial Neutron Detection of Cosmic-Ray Interactions with the Earth's Surface

We have demonstrated the ability to use aerial neutron detection to measure the neutron flux produced by cosmic rays interacting with nuclei in the ground surface. High-energy cosmic rays (primarily muons with gigaelectronvolt energies) interact with the nuclei in the ground surface and produce energetic neutrons via spallation. At the air–surface interface, the neutrons produced by spallation either scatter within the surface material, become thermalized and reabsorbed, or are emitted into the air. The mean free path of energetic neutrons in the air can be hundreds of feet, as opposed to only a few feet in dense materials. Consequently, the flux of neutrons escaping into the air provides a measure of surface nuclei composition. We have demonstrated that this effect can be measured at long range using neutron detectors on low-flying helicopters.

We conducted radiological survey measurements in the Government Wash area of Las Vegas, Nevada, which has a very unique geology, spanning a wide of nuclide mixtures and formations. These measurements have shown that the neutron background from cosmic ray–soil interactions is repeatable and directly correlated to geological data. The results of our preliminary measurements are presented in the poster.

Neutron flux measured over Government Wash (Las Vegas, Nevada) using our cosmic ray-based technique.





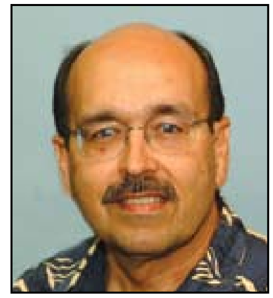
James E. Miller
Advanced Materials Laboratory
Sandia National Laboratories

Direct Approaches for Recycling Carbon Dioxide into Synthetic Fuel

The national security implications of our dependence upon foreign oil, as well as the dangers of climate change resulting from greenhouse gas emissions, prompt a search for alternative sources of liquid fuels. Despite the decades-long availability of synthetic fuel (synfuel) technologies, the large capital cost and expense of manufacturing synthesis gas (a mixture of carbon monoxide and hydrogen) has largely limited their impact. Furthermore, coal-to-liquid and other similar approaches will increase the carbon dioxide footprint of our transportation infrastructure relative to petroleum. The "hydrogen economy" is a newer alternative, but it poses countless technical and infrastructure challenges. However, by integrating carbon dioxide capture and utilization into the hydrogen economy, a new alternative emerges that realizes the benefits of hydrogen while capitalizing on much of the existing fuel infrastructure.

A solar furnace will be the initial source of concentrated heat for the counter-rotating-ring receiver/reactor/recuperator employed to split carbon dioxide, yielding carbon monoxide for subsequent production of synthetic fuels.

Current approaches to carbon dioxide utilization generally opt for "re-energizing" carbon dioxide through a sacrificial reaction with an energetic molecule. Typically, carbon dioxide is reacted with hydrogen to form carbon monoxide and water, and then further reactions with water yield synfuel or synfuel intermediates. The project aims to identify and validate potentially more energetically efficient thermochemical processes for directly splitting carbon dioxide into carbon monoxide and oxygen as the basis for synfuel production. We have already demonstrated the cyclic thermochemical production of carbon monoxide from carbon dioxide using both iron- and ceria-based active materials fabricated into robust monolithic parts, and have made significant progress towards understanding the working metal oxides. The project will culminate with the demonstration of carbon dioxide splitting in a novel solar-driven continuous reactor designed to maximize thermal efficiency.



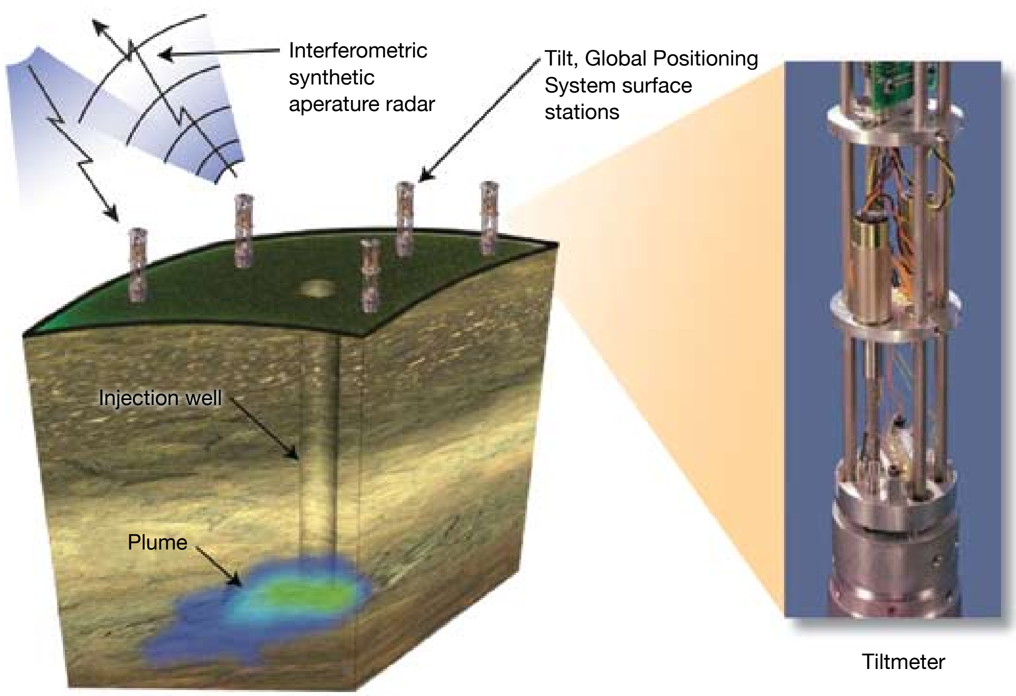
A. L. Ramirez
Atmospheric Earth and Energy Department
Chemistry, Materials, Environmental, and Life Sciences Directorate
Lawrence Livermore National Laboratory

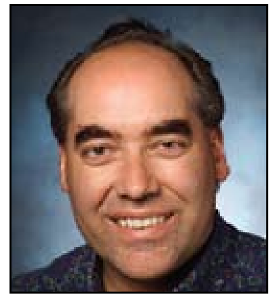
Joint Reconstructions of Subsurface Injection and Production Processes Using Stochastic Inversion

Effective oil reservoir management requires accurate models of subsurface process zones such as those associated with enhanced oil recovery and the geological sequestration of carbon dioxide. Fluid injection creates subsurface plumes and process zones that are often complex and difficult to reconstruct. For instance, steam moving along a high-permeability path such as a fracture zone will bypass most of the oil in the reservoir. Carbon dioxide escaping along a fault zone or abandoned well can create hazardous conditions at the surface. As plumes become increasingly complex, accurate reconstruction of plumes and process zones requires the collection and integration of multiple geological, geophysical, and geochemical data sets.

We have developed a computational tool that jointly reconstructs different types of data and produces more accurate models of subsurface fluid plumes and of the reservoirs that contain them. The tool produces images that are consistent with disparate data types such as reservoir permeability models, measurements of injected fluid volume, ground deformation measurements (using the Global Positioning System, tiltmeters, or interferometric synthetic aperture radar), and cross-borehole electrical resistivity measurements. Importantly, our approach formally integrates available data and identifies alternative plume models that are consistent with the data. Our approach also quantifies solution uncertainties stemming from unknown reservoir properties, measurement error, or poor sensitivity of geophysical techniques. We use Bayesian inference and the Markov chain Monte Carlo technique to sample the space of possible plume models, including the shape, location, and fluid saturation of the plume.

We use various types of measurements to reconstruct subsurface plumes created by injection and extraction processes.





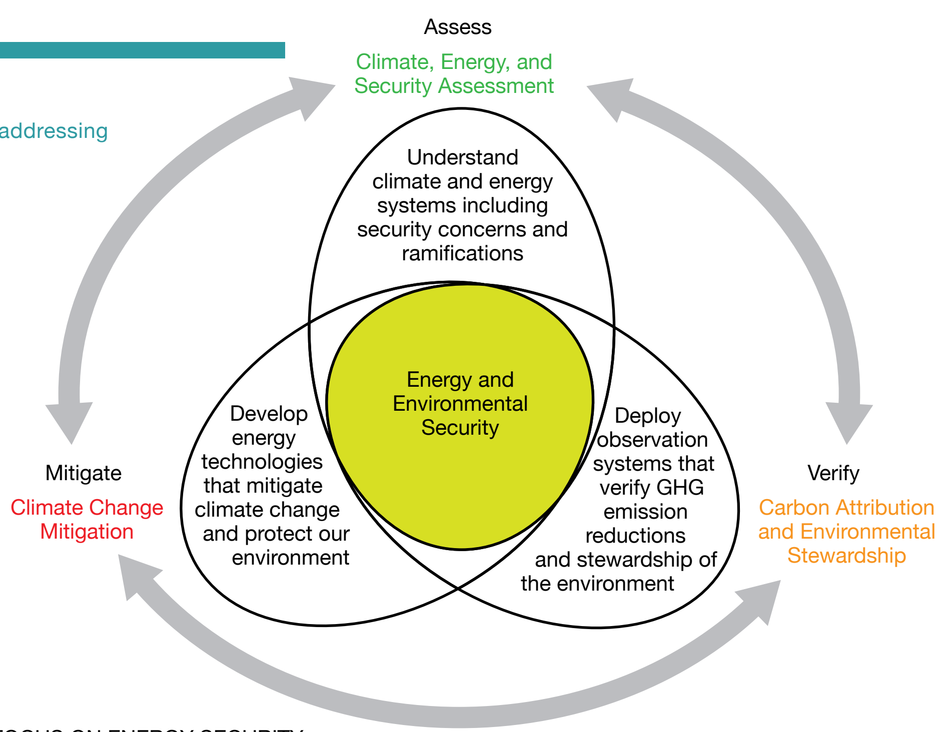
Doug Rotman
Director
Energy and Environmental Security Program
Global Security Principal Directorate
Lawrence Livermore National Laboratory

Confronting Climate Change: A U.S. National Security Challenge

Addressing climate change while simultaneously meeting the accelerating demand for energy and water is perhaps the greatest challenge ever faced by mankind. The use of fossil fuel-based energy, particularly over the last century, has led to a 30% increase in atmospheric carbon dioxide, which is driving climate change, with dramatic global, regional, and local implications. Experts believe that global warming will cause impacts to our environmental systems that may alter the national security posture of the United States. Increasing population (estimated to be eight billion by 2050), combined with continued economic development across the globe, will result in energy demands that are double of those today, approaching 25 terawatts. Increasing competition for energy resources—especially our nation's reliance on foreign oil—places the U.S. in a vulnerable security position.

Cross-cutting both energy and climate is water: Climate change is expected to reduce the availability of fresh water, which in turn will increase global instability. Confronting this challenge is a matter of national and global security and requires a three-pronged strategy to (1) assess the drivers and ramifications of climate change and energy security, (2) mitigate future climate change by developing advanced energy technologies, and (3) verify mitigation technology performance and environmental stewardship through comprehensive observation systems.

With LDRD support, LLNL is conducting research and development in each of these areas, and the poster presented gives an example from each. To assess climate change, we are performing climate simulations at very high resolutions to determine regional impact, with a focus on analysis and projections of water availability. To mitigate future climate change, we are developing technologies for underground coal gasification that can expand our nation's secure supply of fossil energy, produce power at lower costs using less water, and—when used along with carbon capture and sequestration—avoid carbon emissions. To verify our stewardship of the environment, we are applying monitoring and modeling capabilities that will ensure safe groundwater supplies during the deployment and operation of underground coal gasification and carbon sequestration capabilities.



A three-phase strategy for addressing climate change.

Richard Schaller
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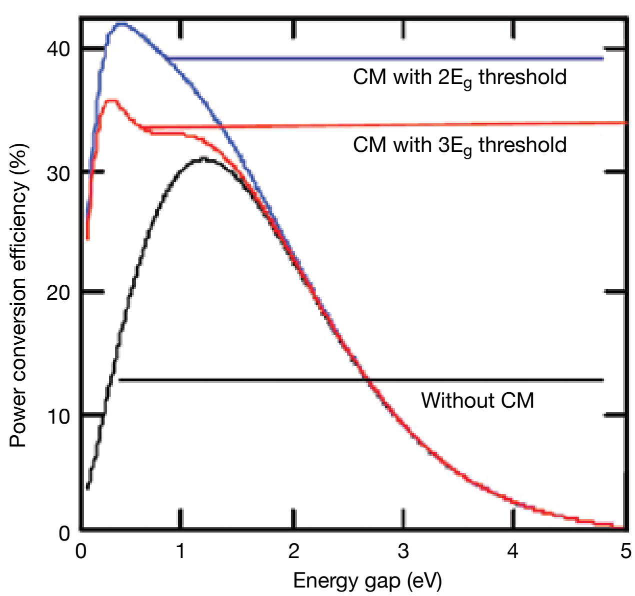
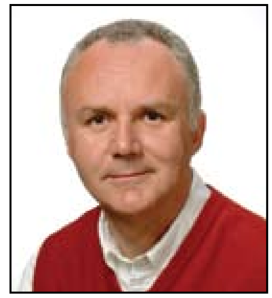
Los Alamos National Laboratory
University of California, Berkeley

Carrier Multiplication in Nanoscale Semiconductors for High-Efficiency, Third-Generation Photovoltaics

The solution to the global energy challenge requires revolutionary breakthroughs in areas such as the conversion of solar energy into electrical power. One such breakthrough is the high-efficiency generation of multiple electron-hole pairs (excitons) from absorption of single photons, a phenomenon known as carrier multiplication. For more than 20 years it has been recognized that theoretically such a process has the potential to significantly increase the power conversion efficiency of photovoltaic devices by delivering more current at the same voltage. In 2004, using a novel experimental approach, it was discovered that semiconductor nanocrystals—in distinction from bulk materials—generate excitons very efficiently under sunlight. In this LDRD project, we are theoretically and experimentally studying the fundamental physics of carrier multiplication and relevant phenomena (e.g., charge and exciton extraction from nanocrystals) with the aim of developing novel principles, materials, and architectures to utilize this process in practical photovoltaic technologies. Specifically, to identify the factors that control the energy onset and the efficiency of multiple exciton generation, we are performing detailed studies of the carrier-multiplication mechanism. We are also studying the carrier-multiplication performance of elongated nanocrystals (i.e., quantum rods) and quantum wires because these two types of nanostructures have good transport properties and are readily incorporated into devices, which could simplify practical realization of photovoltaics utilizing multiple-exciton generation. Finally, we are investigating energy- and charge-transfer processes in engineered energy-gradient structures in the context of extracting multiple charges produced via carrier multiplication from nanocrystals.

Calculated power conversion efficiencies of a single-junction solar cell with and without carrier multiplication (CM) for two different energetic onsets [as a function of semiconductor energy gap (E_g)]. Delay of CM onset leads to increased power conversion efficiencies. If CM onset occurs at $2E_g$ (the theoretical limit), maximum solar cell efficiency is 42%, as compared to 31% without CM.



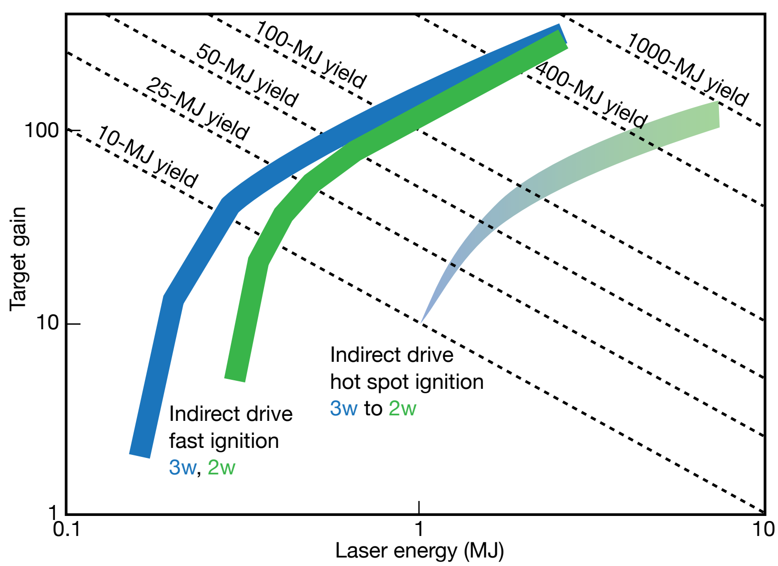


Richard Town
AX Division
Weapons and Complex Integration Principal Directorate
Lawrence Livermore National Laboratory

Fast Ignition and Its Role in Future Energy Production

The campaign to achieve fusion ignition and propagating burn with inertial confinement fusion targets will begin in 2010 at the National Ignition Facility. Early experiments to demonstrate ignition and gain will use central hot spot ignition, which relies on the simultaneous compression and ignition of a spherical fuel capsule in an implosion. Fast ignition is an alternative approach that promises higher gain, lower ignition thresholds, and relaxed symmetry requirements than central hot spot ignition. The relaxed requirements of fast ignition are accomplished by separating compression from the ignition phase: In fast ignition, x rays generated by the interaction of the laser with the hohlraum wall are used to compress deuterium–tritium fuel to a uniform density. Then, a short-pulse, high-intensity laser sparks ignition in the fuel. The relaxed requirements, along with the improved performance, also make fast ignition a more attractive energy source, not only as a pure inertial fusion energy program but also as a driver for proliferation-resistant fusion and fission options. For example, fast ignition's reduced symmetry requirements could allow two-sided illumination, simplifying target chamber design, while its lower peak density means less stressful requirements on the compression laser. Furthermore, its higher gain would allow lower energy compression lasers. However, the physics basis of fast ignition is not as mature as that of central hot spot. In particular, the coupling efficiency from the short-pulse laser to the fast ignition hot spot is a critical parameter dependent on very challenging and novel physics. Multiple LDRD projects have illuminated basic theoretical and experimental physics in this area, including a definitive experiment on the National Ignition Facility to determine the short-pulse laser energy required for ignition. This poster gives an overview of fast ignition—emphasizing how it can be used to improve the overall system engineering of a power plant—and also presents a proposed power plant design.

Gain curves for indirect drive fast ignition and central hotspot ignition approaches to inertial confinement fusion showing the higher gain and lower ignition threshold for fast ignition.



Blas Uberuaga
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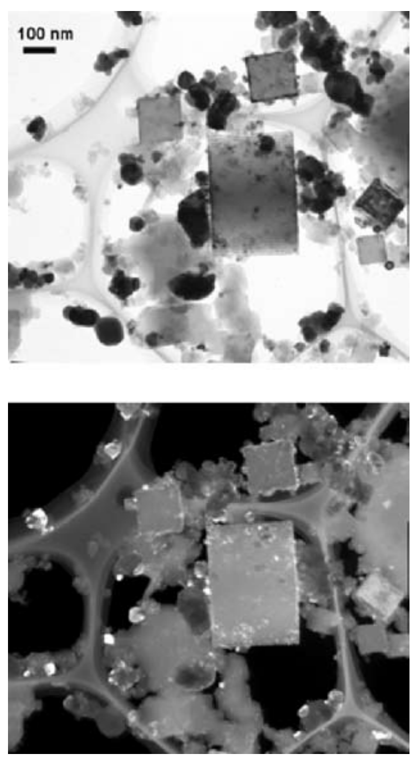
Los Alamos National Laboratory
University of Washington

Advanced Nuclear Fuel Forms with Microstructures Tailored to Naturally Induce Fission Product Separation During Service

As the world enters a nuclear renaissance, more will be demanded of the materials used in nuclear reactors. Materials with enhanced properties—including radiation tolerance and ease of separation—need to be developed. In particular, a closed nuclear fuel cycle, in which fuel is preprocessed and reused in a nuclear reactor, requires a highly efficient and cost-effective separation strategy. This project's objective is to investigate the key scientific and technological issues underpinning the design of a revolutionary type of nuclear fuel possessing the desirable attributes of conventional nuclear fuel (uranium oxide or magnesium oxide) but with a tailored microstructure that radically eases the separation of fission products, drastically reduces separation costs, and substantially mitigates the proliferation risks of the separated material. Our advanced nuclear fuel design is based on a dispersion (two-phase composite) nuclear fuel concept. The goal of this project is not to develop a licensable form of nuclear fuel but rather to develop the underpinning science to facilitate more rapid evaluation and acceptance of new fuel forms. This project promotes a designed merger of two aspects of the nuclear fuel cycle—burning and reprocessing—that ordinarily are managed independently.

We expect to determine if we can create a two-component nuclear fuel that eases the complexities associated with spent fuel chemical separation. This fuel form must not only be easy to separate chemically, but during service it must exhibit both robust and predictable behavior. We will test our advanced materials to ensure that they possess the necessary physical and chemical stabilities. The natural, in-service chemical separations strategy of our novel approach will greatly reduce both technological challenges and costs compared to conventional reprocessing.

Transmission electron microscopy images, in both light-field and dark-field conditions, of a composite powder before formation of a compact pellet. The upper image shows the high-symmetry, square-shaped magnesium oxide crystallites that appear lighter in contrast than the dark, irregular-shaped hafnium oxide lower-symmetry crystallites. This powder is used as the basis for a set of experiments on one nanocrystalline form of a dispersion fuel.



Pat Unkefer
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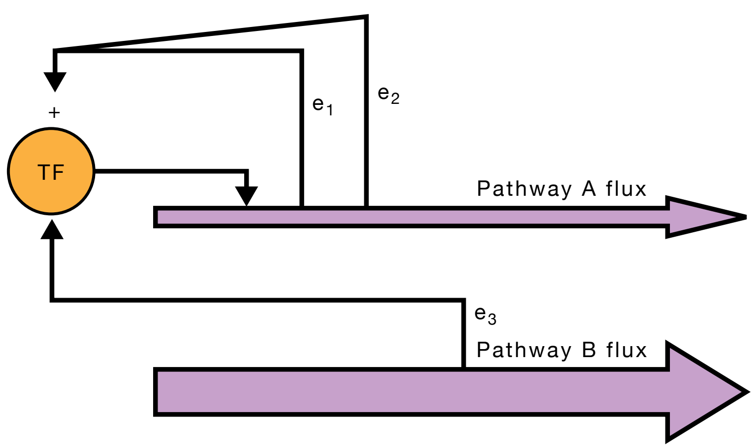
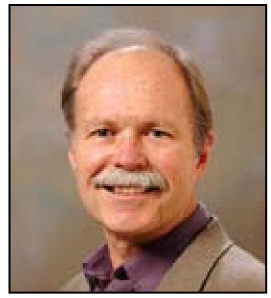
Los Alamos National Laboratory
Texas A&M University

Distributed Metabolic Regulation: The Key to Synthetic Biology for Carbon-Neutral Fuels

To achieve the DOE goal of exploiting biological systems for renewable energy production and carbon sequestration, we must understand how control processes are integrated in cellular control networks. Transcription factors (TF) are proteins that regulate gene transcription and are central to control networks. They regulate gene expression by binding small-molecule effectors and specific DNA sequences. The conventional view of TF–effector complexes is that they are "on/off" switches, whereas our recent discoveries suggest that TFs are sophisticated signal processors. We hypothesize that metabolic control relies on the integration of many signals, of which TF–effector complexes are the focal point. Understanding metabolic control will ultimately lead to capabilities in harnessing biological systems. Two recent technical advances in examining TF binding events enable our success. First, we developed a frontal affinity chromatography mass spectrometry approach at Los Alamos National Laboratory that rapidly identifies TF effectors and quantifies their binding to TFs. Second, our collaborator at Harvard developed a technique to identify TF-bound regulatory DNA sequences. After identifying effectors and DNA regulatory sequences, we will use quantitative flow cytometry assays to measure TF–DNA affinity. Constants of TF–effector and TF–DNA affinity will be the basis for transcription regulatory network models. Integration of metabolism and gene regulation into dynamical models is unique to this project. We will develop regulatory models of carbon utilization pathways in the bacterium *Burkholderia xenovorans*. Only with a clear understanding of cellular regulation processes can we manipulate carbon-cycling pathways to maximize carbon sequestration or optimize organisms for biofuels production.

In this transcription factor (TF) and effector complex, carbon and energy are wasted by undesired pathway A because of integrated metabolic regulation. Pathway A is turned on by metabolite effector e_3 (made in pathway B) and by metabolite effectors e_1 and e_2, which are produced in pathway A.





Steven A. Wright
Advanced Energy Concepts Department
Sandia National Laboratories

Supercritical Carbon Dioxide Brayton Cycle Test-Loop Development, Controls, Testing, and Model

Research, development, and demonstration of more-efficient and more-compact electrical power conversion concepts is an essential element in maximizing the energy efficiency and cost effectiveness of next-generation nuclear power plants. The supercritical carbon dioxide Brayton cycle is considered one of the most promising power conversion cycles because it can achieve very high efficiency (40–50%) at relatively low reactor coolant exit temperatures (<600°C). The cycle involves compression near the critical point of carbon dioxide to achieve a significant efficiency increase over other Brayton cycles. The nonlinear behavior in this region and the effect on compressor control and stability must be understood and demonstrated before development of this more-efficient cycle can occur. Although no demonstration of the supercritical carbon dioxide Brayton cycle and compression near the critical point has been done, recent advancements in the development of turbo-machinery, gas foil bearings, high-speed alternators, compact high-pressure heat exchangers, and advanced inexpensive power electronics make it possible, for the first time, to affordably evaluate and experimentally demonstrate this essential technology on an appropriate scale. This project aims to (1) develop the world's first supercritical carbon dioxide Brayton cycle test-loop to study these critical point compression issues; (2) operate the loop to study the coupling of reactors with supercritical carbon dioxide power conversion systems, test and understand control methods associated with supercritical phenomena, and study the scalability to larger systems; and (3) develop integrated dynamic simulation models for supercritical compression and Brayton cycles to support the development of effective control methods.

Sandia's new supercritical carbon dioxide Brayton cycle test loop (~300 kWe).