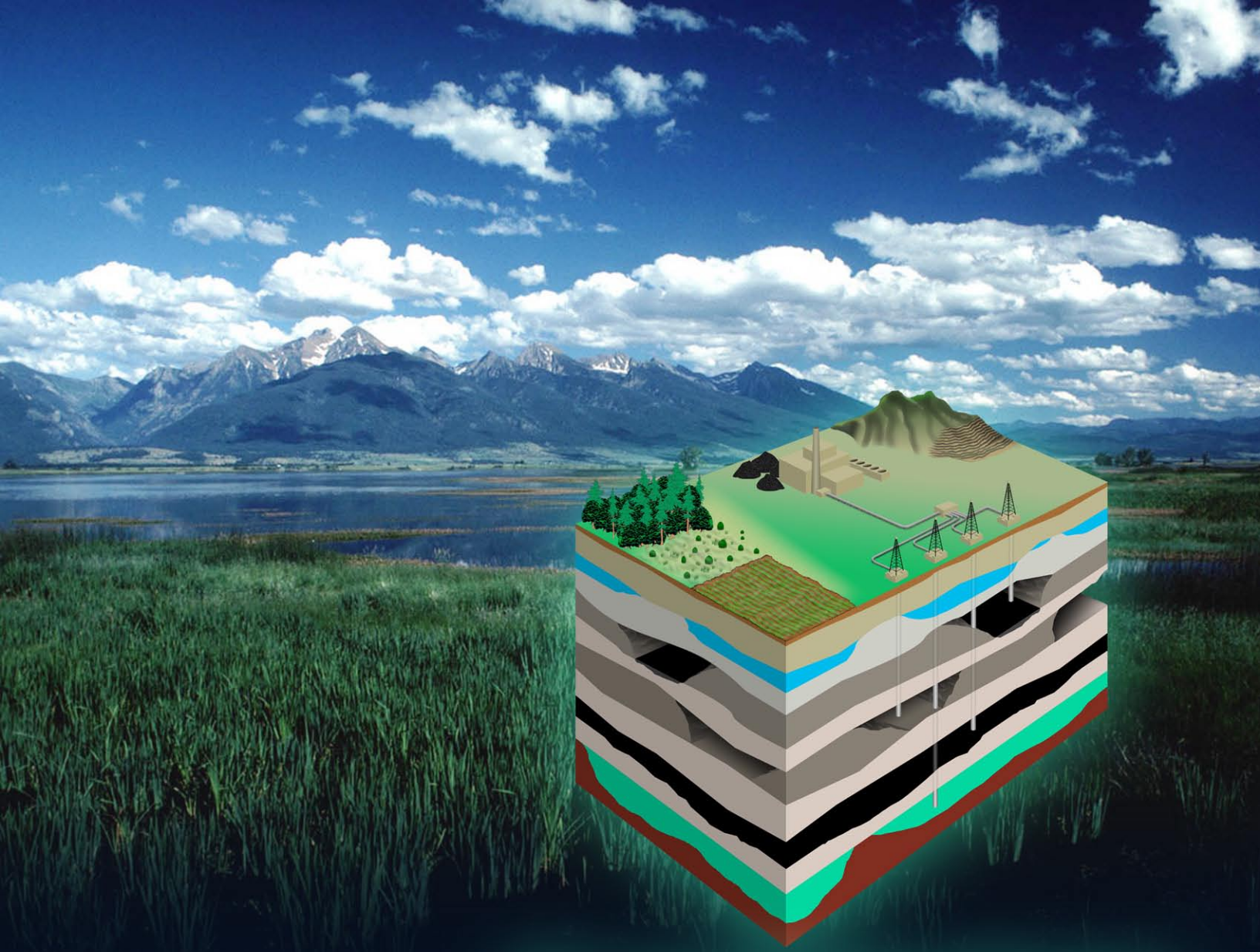

CARBON

Energy and Environment Compendium

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CARBON

Energy and Environment Compendium

This book is part of Los Alamos National Laboratory's Energy and Environment Compendium series. Other books in this series:

CLIMATE
HYDROGEN
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Carbon Fuel Cycle Research at Los Alamos National Laboratory

Fossil fuels represent an abundant and cheap domestic resource for energy, yet increasing levels of atmospheric carbon dioxide (CO_2, which is by volume the largest by-product of fossil-fuel combustion) are challenging their continued use.

Early in 2002, the President announced the need for a "new environmental approach" to the use of fossil fuels, recognizing the challenge of reducing the intensity of greenhouse gas emissions (particularly carbon dioxide) while sustaining economic growth. To meet this challenge, Los Alamos National Laboratory is leveraging a range of theoretical and experimental capabilities to identify new approaches to improving the efficiency of the carbon fuel cycle and minimizing its environmental impact.

The Los Alamos effort is focused on integration of all components of the carbon fuel cycle, including

- Extraction of fossil fuels (oil, gas, coal, hydrates) from the earth;
- Utilization of fossil fuels to produce electricity or to produce a carbon-free energy carrier (e.g., hydrogen);
- Distribution of the electricity/energy carrier to the end user;
- Separation of mixed gases (e.g., from synthesis gases or flue gases);
- Transportation of gas via pipelines; and
- Storage of produced carbon dioxide in a safe and environmentally sound manner.

In addition to the anthropogenic carbon fuel cycle, natural carbon cycles actively move carbon between various earth compartments, such as between the atmosphere and ocean or between terrestrial systems and the atmosphere. These cycles can provide important insights into possible engineered approaches. Moreover, any engineered solution must factor in the coupling between anthropogenic and natural carbon cycles. Los Alamos efforts are focused on understanding both anthropogenic and natural carbon cycles as well as their coupling. For example, the Los Alamos Parallel Ocean Program is being used to understand the impact that biogeochemical carbon cycling in the ocean has on ocean-atmosphere dynamics.

Current Scientific Challenges in Carbon Fuel Cycle Research

To effectively manage the carbon fuel cycle, we must overcome significant technical and scientific challenges, including

- Storing large volumes of carbon dioxide safely and permanently with minimal environmental impact;
- Separating carbon dioxide from mixed-gas streams;
- Improving the efficiency of energy production/conversion;
- Elucidating the complex interplay between carbon cycles and climate; and
- Expanding U.S. fossil fuel reserves.

Los Alamos's Capability Areas in Carbon Fuel Cycle Research

To support its core-mission activities, Los Alamos has developed a suite of unique capabilities that are now being applied to carbon fuel cycle issues. These capabilities fall into several broad categories:

- Monitoring and measurement,
- Catalysis,
- Theory,
- Advanced concepts,
- Separations, and
- Science-based prediction for engineered geological systems.

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Seismic and Acoustic Methods to Improve Subsurface Imaging

The Challenge: Imaging Complex Subsurface Structures

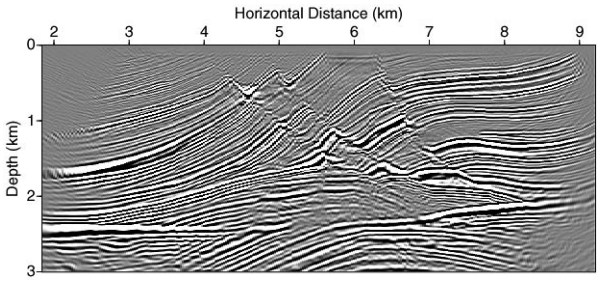
The petroleum industry's primary technique to determine where to drill for oil and gas exploration is seismic imaging. Today, new oil and gas exploration targets are in geologies that are increasingly difficult to characterize, and drilling costs are rising. With current methods and technologies, less than 2% of the 7,000 trillion cubic feet of natural gas in the Rocky Mountains' low permeability or "tight" reservoirs can be economically produced. Innovations in acoustic and seismic imaging technologies and methods are vital to future oil and gas extraction.

Los Alamos Innovation: Novel Application of Theory and Interpretation

Los Alamos has developed expertise in characterizing structures in the Earth's subsurface, including (1) seismic modeling and imaging, and (2) monitoring and interpreting seismicity induced by fluid injections. Los Alamos and its partners have produced several breakthroughs:

- Seismic imaging based on wave equations;
- Patented methods for imaging and characterizing materials using nonlinear effects in wave propagation;
- Numerical datasets for testing imaging and characterization methods;
- Application of time-reversed acoustics to characterize elastic materials;
- New methods for measuring and analyzing seismic events induced by changes in volume and fluid pressure;
- More realistic models for petroleum-reservoir geology.

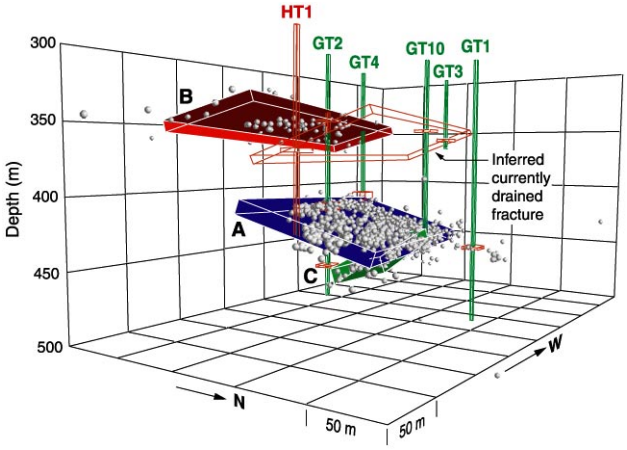
In the future, Los Alamos researchers may be able to yield further breakthroughs in (1) imaging and characterization; (2) understanding and mapping flow paths for fluids in reservoirs (including the effects of induced seismicity); and (3) improved information from images.



Innovative approaches to theory (wave-equation migration shown above) and practice (high-precision arrival time shown below) can lead to dramatic improvements in seismic imaging.

The Impact: Increasing Oil and Gas Production

These Los Alamos projects can enhance productivity from oil and gas reservoirs by (1) reducing the risk of drilling dry wells; (2) extracting more oil and gas from permeable rock; and (3) increasing production from existing oil and gas fields. By investigating, testing, validating success, and transferring new technology to the petroleum industry, Los Alamos can help open up substantial new oil and gas resources.



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Seismic Stimulation to Recover More Oil and Gas

The Challenge: Maximizing Oil and Gas Extraction

At the average U.S. oil and gas site, about 60% of the oil and gas remains in the ground after primary production. There are compelling reasons to break through current limits to affordable and effective Enhanced Oil Recovery (EOR) methods and technologies, which now rely heavily on water and CO_2 flooding. Seismic stimulation has the potential to meet this need, but is currently unreliable. Results have varied from field to field, and scientists cannot yet predict where it will work and where it will not. The mechanisms involved in seismic stimulation must be far better understood.

Los Alamos Innovation: Seismically Stimulating Fluid Flow

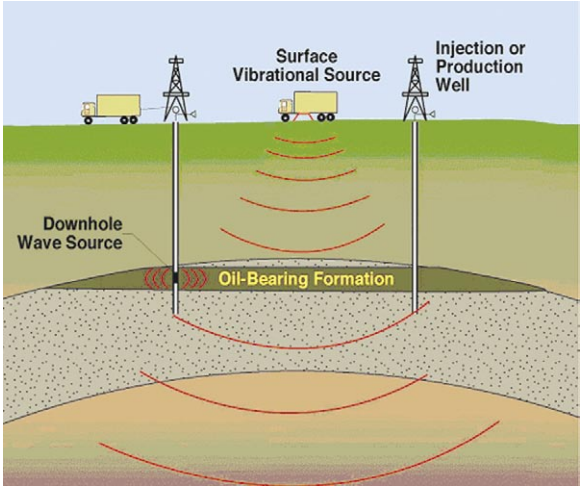
Work on seismic stimulation began with an innovative concept—that low-amplitude, low-frequency (1–500 Hz) seismic stress waves can cause large changes in porous fluid flow in the Earth. Prior to 1992, field tests in the Soviet Union indicated that seismic stimulation could increase oil production rates by 50% or more.

Los Alamos became the first major U.S. research laboratory to investigate seismic stimulation. Los Alamos designed and built a laboratory facility that allows dynamic stress effects on multi-phase fluid flow to be quantified during bench-top experiments on porous core samples. The capabilities of this facility are believed to be unique in the world.

Via experiments performed at its Core Stimulation Facility, Los Alamos is beginning to identify possible guidelines for where and how to apply seismic stimulation effectively. These include (1) using sources that couple energy directly to the core fluids (rather than the solid matrix of the formation) and (2) choosing to stimulate significantly oil-wet (rather than water-wet) reservoirs. Future experiments with field core samples will further quantify these guidelines and help establish additional guidelines.

Los Alamos has also initiated industry field tests for developing seismic stimulation sources, and has established numerous collaborations with the oil and gas industry, universities, and other national laboratories. These efforts have increased the credibility of the technology and international scientific interest in the subject.

Early experiments show that stress stimulation can enhance the extraction of Dense Non-Aqueous-Phase Liquid (DNAPL) contaminants from groundwater aquifers. Scientists have also recently identified possible mechanisms coupling stress waves to porous flow.



Seismic stimulation can be used to drive fluids in the subsurface.

The Impact: Recovering More Oil and Gas

More research and testing could convert seismic stimulation into an application technology. If so, this capability may (1) allow a greater share of the 60% of oil and gas not recovered at U.S. sites to be recovered and produced; (2) reduce U.S. reliance on foreign oil sources; (3) prevent or delay potential future energy crises; and (4) extend the life of the world's oil and gas supply.

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Fuel Decarbonization and Catalysis to Reduce Fossil-Fuel Emissions

The Challenge: Reducing Emissions from Fossil Fuel Use

It is well known that producing energy by burning fossil fuels produces carbon dioxide (CO_2), which is widely regarded as a leading greenhouse gas. Government decision-makers struggle with how to reduce emissions of carbon dioxide, particularly in the transportation sector, without putting economic vitality at risk. Solutions are needed to lower the amount of CO_2 produced per unit of energy.

Los Alamos Innovation: More Efficient Catalysis Processes

Advances in energy production technologies could yield such solutions. Since 1995, Los Alamos has brought its expertise, capabilities, and multidisciplinary technical approaches to bear in its carbon-focused Fuel Decarbonization and Catalysis project. First with internal funding and then with funding from the Department of Energy (Office of Science and Office of Energy Efficiency and Renewable Energy) and various chemical and energy industry partners, Los Alamos has investigated carbon catalysis. With both heterogeneous and homogeneous efforts, Los Alamos scientists have built on advantages unique to Los Alamos to achieve the following advances:

- Selectively oxidizing alkanes in heterogeneous catalysis;
- Converting methane to methanol in homogeneous catalysis;
- Using lean nitrogen oxide (NOx) reduction catalysis to enable more fuel-efficient, "lean-burn" engine technologies.

In the future, Los Alamos's efforts can open up a broad range of applications in energy conversion and utilization, including (1) easier conversion and transportation of stranded natural carbon, (2) more affordable carbon conversion and transportation, (3) portable units converting stranded natural gas to a liquid suitable for fuel cell and vehicle use, and (4) further advances in carbon-reduction technology at Los Alamos and elsewhere.

Rapid throughput energy containment reactor boosts catalyst discovery and testing rates.

The Impact: Cleaner, More Efficient Energy

Los Alamos's efforts in this field can (1) increase the efficiency of energy production, (2) reduce fuel consumption in the transportation sector, and (3) reduce greenhouse gas and other emissions.

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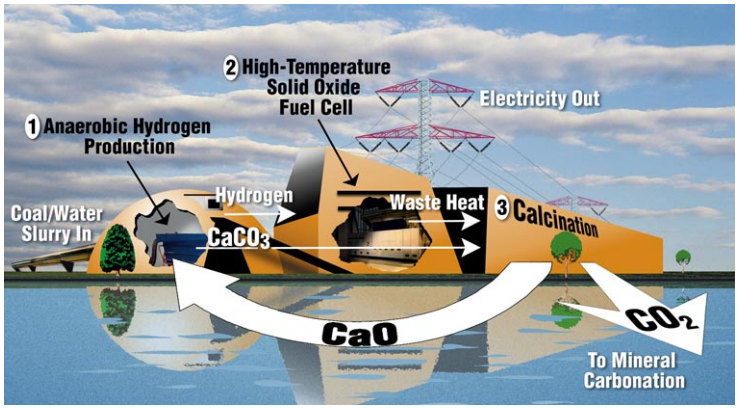
Integrated CO_2 Capture and Energy Conversion to Reduce Coal and Other Fossil-Fuel Emissions

The Challenge: Reducing Emissions in the Energy Sector

Coal is by far the most abundant fossil fuel for the U.S. and the world. However, current methods for using coal to generate energy produce CO_2 and other by-products, creating a variety of environmental challenges. Current approaches to these challenges have evolved largely from modifications to existing technologies and practices. Conventional approaches to purification of CO_2 and its capture focus on upstream separation of oxygen.



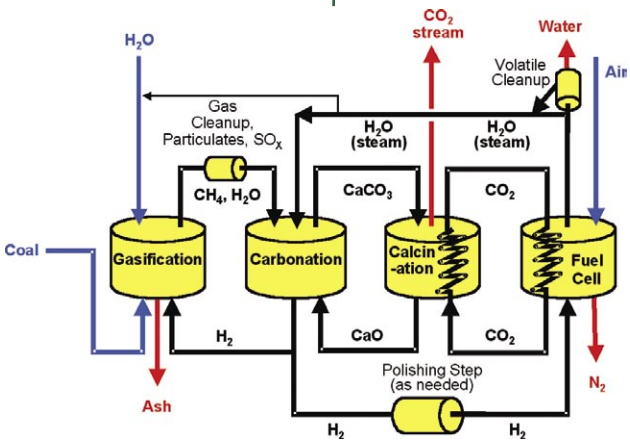
Los Alamos Innovation: Integrated CO_2 Separation and Energy Conversion

New environmental challenges provide a driver for considering novel approaches to efficient energy production via coal and other fossil fuels. As part of its portfolio in technologies related to zero-emissions energy production from fossil fuels, Los Alamos has developed a process to improve the efficiency of power production by explicitly integrating the separation and capture of CO_2. This process—often referred to as the ZEC (Zero-Emission Coal) Process—reuses waste heat and includes a lime-CO_2 separation step. Los Alamos's ZEC Process has very high theoretical efficiencies (averaging 70% in one independent evaluation) in purifying CO_2.

Before the ZEC Process is ready for implementation on the pilot scale, critical technical obstacles must be overcome, including (1) development of high-temperature fuel cells that operate at 900°C and higher and (2) integration of the process elements into a seamless operation. Los Alamos has begun researching these obstacles using internal funding and is currently seeking partners and funding to expand this research and development.

Applications derived from Los Alamos's work on the ZEC Process also include (1) coal-compatible fuel cells, (2) novel trace-element clean-up cycles, and (3) CO_2 mineralization. In the future, the ZEC Process can be combined with a variety of CO_2 storage options. With modifications to various clean-up steps, the ZEC Process can be applied not only to coal but to any fossil fuel or carbon-containing fuel.

Integration of CO_2 capture with energy conversion could lead to new highly efficient methods for production of hydrogen and electricity from coal. For example, the Zero Emission Coal Process uses lime to shuttle waste heat from high-temperature fuel cells to the shift reaction while separating CO_2 from the gas stream.



The Impact: Abundant, Clean, and Low-Cost Energy

Using the ZEC Process with biomass and a sequestration process, excess CO_2 could actually be removed from the atmosphere. The ZEC Process appears highly promising, and may lead to energy production with zero airborne emissions. If so, the ZEC Process may help secure a sufficient supply of clean, low-cost energy for the U.S. and the world.

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Thermally Optimized Membranes to Separate Gases at High Temperatures

The Challenge: Separating Carbon Dioxide from Mixed Gas

Separating carbon dioxide from mixed-gas streams is the first step in carbon sequestration. To be viable, the separation method must apply to relevant gas streams (including flue gases and synthesis gases) and be able to handle large volumes. The effectiveness of current technologies for separating CO_2 is limited. Amine-based technologies work only at low temperatures. Pressure-swing absorption and cryogenic distillation have significant energy penalties (up to 35%).

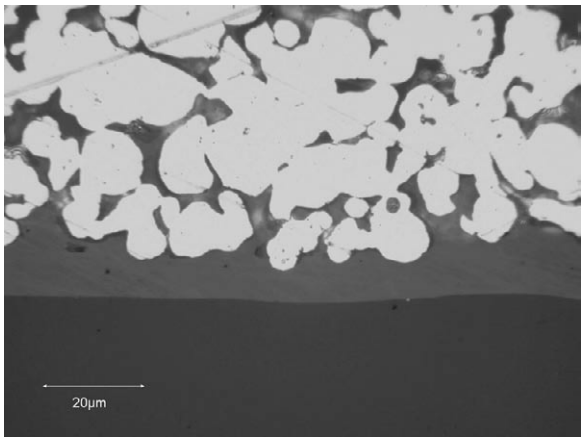
Los Alamos Innovation: A Polymeric-Metallic Composite Membrane

Los Alamos, along with partners, is developing polymeric-metallic composite membranes. These membranes function at significantly higher temperatures (>400°C) than commercially available polymeric membranes (<150°C).

To develop and test this membrane system, Los Alamos has exploited its capabilities in materials synthesis, materials characterization, fabrication techniques, and high-temperature membrane testing. To date, Los Alamos and its partners have produced

- The first polymeric-metallic membrane that is selective from room temperature to 400°C;
- The first polybenzamidizole silicate molecular composites;
- A unique approach to optimizing long-term membrane performance under challenging operating conditions;
- The first-ever simultaneous measurements of gas permeation and membrane compaction at elevated temperatures.

In the future, this project will provide a membrane technology that can be used in a variety of gas separation applications.



Scanning electron microscope image of a polymer-metal composite membrane. Bright spots are metal and the lighter gray is polymer.

The Impact: Less Energy Use in Separating Gases

Polymeric-metallic composite membrane separation is promising. Applications of this technology will reduce energy penalties during the separation process.

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Acoustic Phase Separator to Separate CO_2 from Mixed Gases

The Challenge: Separating CO_2 from Mixed Gases

Carbon sequestration requires separation of CO_2 from mixed-gas streams. Current methods and technologies for separating CO_2 have considerable disadvantages, including (1) high energy penalties (up to 35%), (2) degradation in high-temperature gas streams, and (3) high levels of operative maintenance.

Los Alamos Innovation: The Acoustic Phase Separator

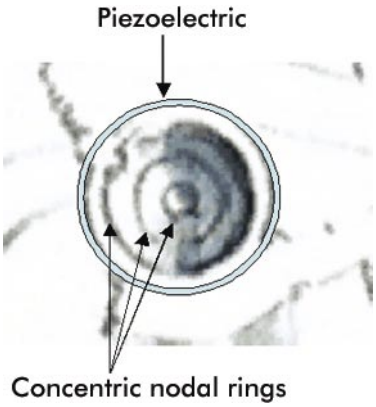
Gases with different properties can be separated using acoustic methods. An acoustic phase separator takes advantage of the sound pressure gradient in a standing wave field in a cylindrical resonance chamber. Los Alamos has patented this novel method, with a second patent pending.

The U.S. Department of Defense has used an acoustic particle concentrator to enhance existing particle counters. The petroleum industry has used acoustic methods and technologies to separate multi-phase liquids.

Los Alamos's acoustic phase separator offers safe, rugged, and ambient operation. The separator is all solid-state with no moving parts, requires no maintenance, and is highly energy-efficient. The temperature of the gas has no effect on operational efficiency. The system is scalable, and multiple units can be stacked together to provide higher throughput. The entire system can be made extremely compact. The separator can be used to separate not only CO_2 but a variety of gases. It can also be used to agglomerate suspended particles in gases and separate those from the gas stream.

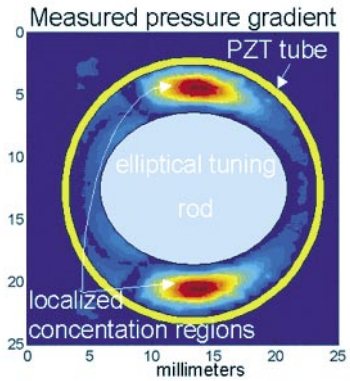
The Impact: Safe and Efficient Separation of Gases

The acoustic phase separator offers a safe, energy-efficient, and cost-effective way to separate mixed gases at high temperatures. The separator uses no cryogen or other chemicals, and it will reduce the cost of the separation process significantly.



Above: Particulate matter in air concentrates at the circular nodal regions of an acoustic standing wave set up inside a piezoelectric hollow cylinder through which the air is flowing.

Below: By breaking the circular symmetry of the cylindrical cavity of the piezoelectric cylinder using an elliptical cross-section insert, the concentration regions can be localized into two spots instead of rings.



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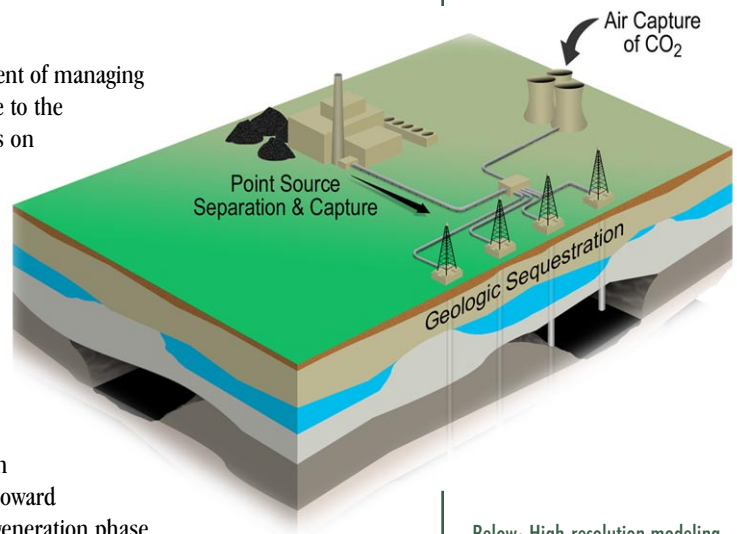
Total Management of CO_2 Through Air Extraction

Air extraction of CO_2 prior to sequestration could complement direct capture from large point sources.



The Challenge: Managing Carbon from All Sources

The control of atmospheric CO_2 levels will likely be an essential component of managing environmental risks associated with the sustained use of fossil fuels. Due to the difficulties of collecting CO_2, current strategies to control emissions focus on capture from large point emitters such as power plants. This strategy neglects past emissions and current emissions from small sources such as automobiles.

Los Alamos Innovation: Directly Extracting CO_2 from the Air

Los Alamos recently proposed the unique concept of directly extracting CO_2 from the atmosphere. This approach focuses on reducing actual atmospheric CO_2 levels rather than reducing just future emissions, which is the idea behind most CO_2 mitigation approaches (including the drive toward renewable sources like wind and solar power). By separating the power generation phase from the CO_2 capture phase, carbon from all sources can be managed without the need for immediate and costly renovations of the infrastructure. Los Alamos's efforts include

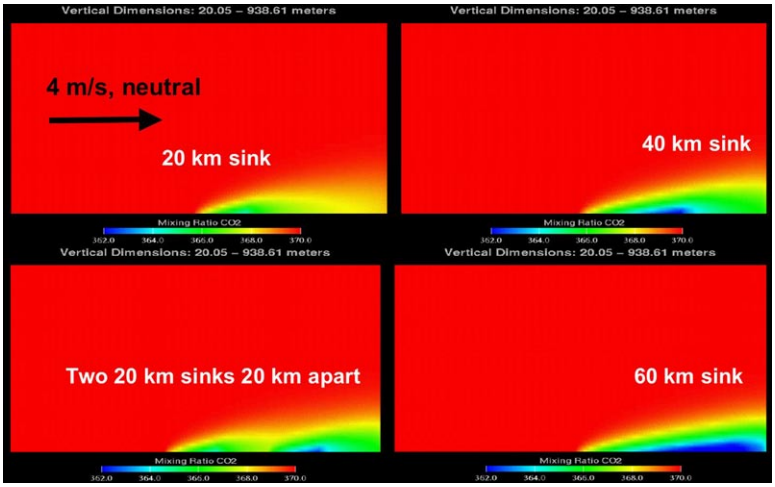
- Demonstrating rapid and large fractional removal of CO_2 from an air stream at gram-scale using alkaline solutions;
- Applying global scale and high-resolution atmospheric modeling to understand scale and scope;
- Examining the implications of direct air capture with respect to required scale;
- Estimating how the cost of capture justifies further research and development;
- Publicizing the concept to engage members of the research community.

The Impact: Restoring the Atmosphere

Direct extraction of CO_2 from the air may prevent an increase in atmospheric carbon dioxide, and could possibly restore atmospheric CO_2 to pre-industrial levels. Direct air extraction of CO_2 also offers the following potential benefits:

- Controlling emissions from the myriad small CO_2 emitters that account for a significant share of global emissions;
- Providing purified carbon dioxide for use with a variety of storage options;
- Completely separating power generation and CO_2 capture processes in both space and time;
- Controlling CO_2 emissions from the transportation and home sectors without restructuring;
- Eliminating the need for extensive pipeline infrastructure to transport CO_2 from the source to the eventual sequestration sites.

Below: High-resolution modeling of CO_2 uptake flux as a function of sink size and separation. The panels show CO_2 levels as function of height and length for various size CO_2 sinks. The vertical scale is about 1 km and the horizontal scale is on the order of 100 km. The background atmospheric CO_2 levels are in red (370 ppm) and the losses caused by the sink are evident in the CO_2 distributions (blue indicates 362 ppm; green, 365 ppm; yellow, 368 ppm).



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Integrated Approaches to Managing Terrestrial Carbon

The Challenge: Measuring and Mitigating Depletion of Terrestrial Carbon Pools

Managing terrestrial systems is a critical component of carbon management. Over the decades, terrestrial carbon pools have been depleted. The largest terrestrial carbon fluxes into and out of the atmosphere are caused by photosynthesis and respiration. Drought, fire, and other disturbances often result in large, rapid losses of terrestrial carbon. Current global carbon assessments do not quantitatively include such losses, and a scientific basis for doing so is lacking.

Los Alamos Innovation: New Approaches to Prediction and Management

To account for these losses, and to assess options for their mitigation where feasible, Los Alamos is using an integrated set of approaches. Los Alamos's assets include (1) advanced soil carbon measurement technology (Laser-Induced Breakdown Spectroscopy or "LIBS" and microbial biochemistry); (2) the CENTURY ecosystem modeling program; (3) field experimentation, including drought effects; (4) long-term monitoring; and (5) advanced carbon flux assessments.

Additional Los Alamos advantages in performing research on carbon in terrestrial ecosystems include

- The world's most instrumented semi-arid woodland site with the longest soil moisture data;
- A unique experimental facility for assessing drought impacts;
- Multi-tower assessment for estimates of high-resolution carbon fluxes while in progress;
- Detailed physiological data relating plant growth and mortality to soil and water;
- Linkages between vegetation pattern and soil erosion;
- A study facility with the world's most rapid change in an ecotone boundary (forest to woodland).

Combined with advances in soil carbon instrumentation, Los Alamos will have the ability to conduct rapid assessments and projections of carbon dynamics for different sites.

The Impact: Improved Ecosystem Management

Improving predictive capabilities and management strategies for carbon in terrestrial ecosystems could have far-reaching effects. Professionals in the field will be far better at predicting when plant mortality is likely to occur, how much erosion may result, what the impacts for carbon reserves will be, and how alternative management strategies would impact carbon stores. Terrestrial carbon pools could serve as important repositories for storing carbon and may help decrease carbon dioxide concentrations in the atmosphere.

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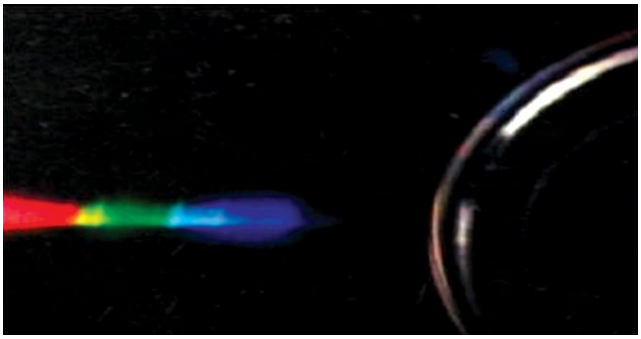
LIBS Analysis of Terrestrial Systems to Improve Carbon Management

The Challenge: Measuring Terrestrial Carbon Rapidly

Carbon fluxes into and out of terrestrial systems make up a significant share of the global carbon budget. Carbon management will likely soon include terrestrial sequestration, altering these carbon fluxes through active management of plant growth in forests, croplands, and woodlands. Tradable credits for sequestration are heightening interest in this approach. The key to market-based trading in terrestrial carbon sequestration is the ability to measure the quantity of carbon stored in soils, plants, and trees across diverse areas. There are drawbacks to current efforts to measure carbon in terrestrial systems; it remains both time consuming and costly.



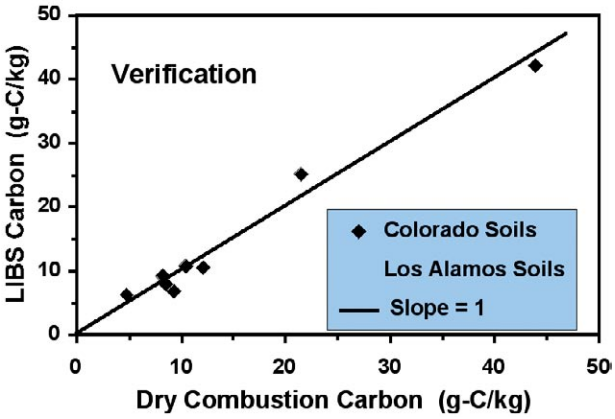
Los Alamos Innovation: Laser-Induced Breakdown Spectroscopy

Los Alamos originally developed Laser-Induced Breakdown Spectroscopy (LIBS) to analyze light elements in solids. Researchers have recently adapted this technique to the analysis of carbon in soils. LIBS analysis is particularly amenable to field-based carbon determination and to scenarios requiring rapid, almost instantaneous, measurement results at minimal cost. This instrumentation provides new analytical capabilities, including

- Rapid analysis (<1 minute per sample);
- Surface and subsurface measurements using a cone penetrometer system;
- *In situ* measurement with little or no sample preparation;
- Good sensitivity for carbon detection, with accuracy and precision rivaling laboratory methods;
- Simultaneous detection of other elements of interest.

Laboratory efforts are now focused on applying LIBS to the rapid determination of carbon *in situ*. LIBS can be deployed in a number of analysis scenarios. Two transportable units are used to analyze discrete soil samples and to map in depth the carbon concentration in core samples. One unit is deployed at Los Alamos to monitor changes in soil carbon in ongoing programs, and a second unit is undergoing a nationwide U.S. Department of Agriculture testing program. Two-person portable units are in development to provide optimal field deployability for (1) verifying efficiency of sequestration protocols through direct soil analysis and (2) improving measurement (respecting both performance and cost) of soil carbon to elucidate heterogeneity in distribution.

With Laser Induced Breakdown Spectroscopy (LIBS), a laser produces a plasma which generates a color spectrum (above) characteristic of the elemental composition of the sample. This spectrum can be analyzed to determine carbon content, using conventional analysis methods to develop a calibration curve (below).



The Impact: Improved Carbon Management

LIBS appears on its way to upgrading the measurment of carbon in terrestrial systems (particularly the speed and affordability) and strengthening programs for tradable credits in carbon sequestration. LIBS can play a key role in improving global carbon management.

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Microbial Signatures to Monitor Soil Carbon

The Challenge: Detecting Early Changes in Terrestrial Ecosystems

Both the energy and agriculture industries could benefit from advanced tools for monitoring changes in soil carbon. The energy industry will need inexpensive carbon sequestration options, such as terrestrial sequestration, that will rely on carbon monitoring. Managing soil carbon is also critical to improving the efficiency of food production.

Los Alamos Innovation: Microbial Signatures for Soil Carbon

Los Alamos has initiated a project to use soil microbes as indicators of the status of soil carbon content and has succeeded in identifying the first set of microbial signatures of increasing, decreasing, and static soil carbon content. The size and diversity of microbial populations make them difficult to characterize. To simplify the problem, Los Alamos is focusing on specific genes in the microbial population and is creating modern DNA-based assays to examine the microbes in carefully selected target soils. Key Los Alamos efforts are directed toward (1) calibrating the microbial indicators on a few select soils and (2) testing several parameters for impact on the microbial population.

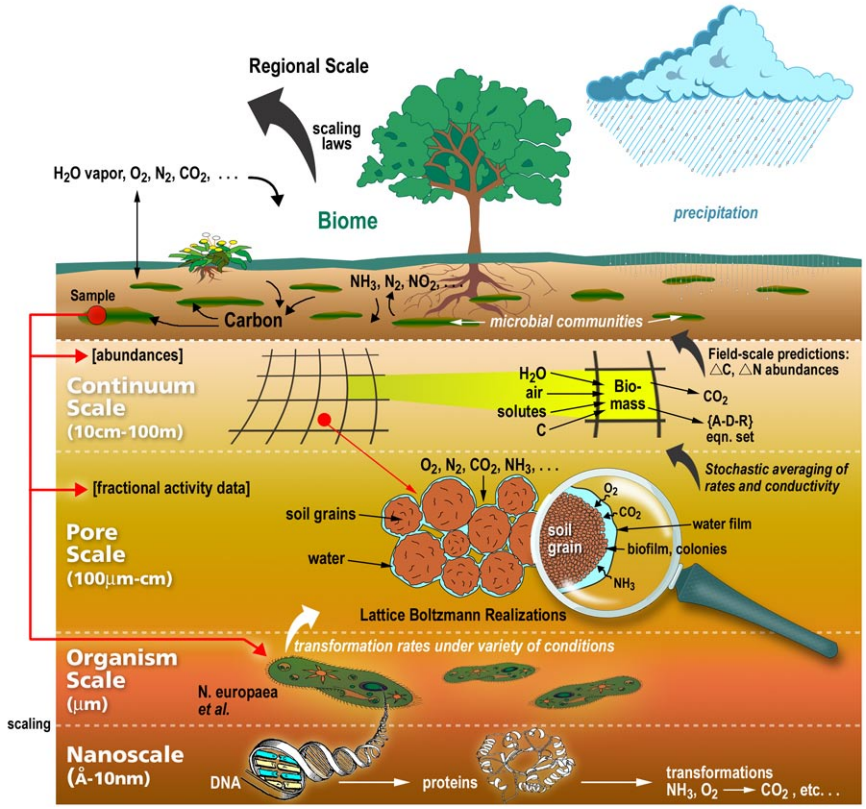
Microbial populations are integral components of the nanoscale systems that underpin terrestrial ecosystems.

Building on initial success, the ultimate goal is to develop the microbial indicators into practical commercial tools for soil carbon monitoring. These tools could be applied to

- Detect increases in soil carbon early as an inexpensive assay;
- Forecast the permanence of carbon storage in soils by providing model data; and
- Assess soil productivity by providing data to parameterize models.

The Impact: More Effective Terrestrial Carbon Management

Microbial indicators can be a valuable part of the suite of new monitoring technologies needed to indicate change in terrestrial ecosystems. Microbial signatures promise early, consistent, affordable, and highly predictive soil carbon monitoring. With these tools, the energy industry can meet higher environmental standards, and the agriculture industry can become more efficient and productive.



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An Integrated, Automated System to Process and Analyze Soil, Air, and Water

The Challenge: Effective Analyses of Soil, Air, and Water

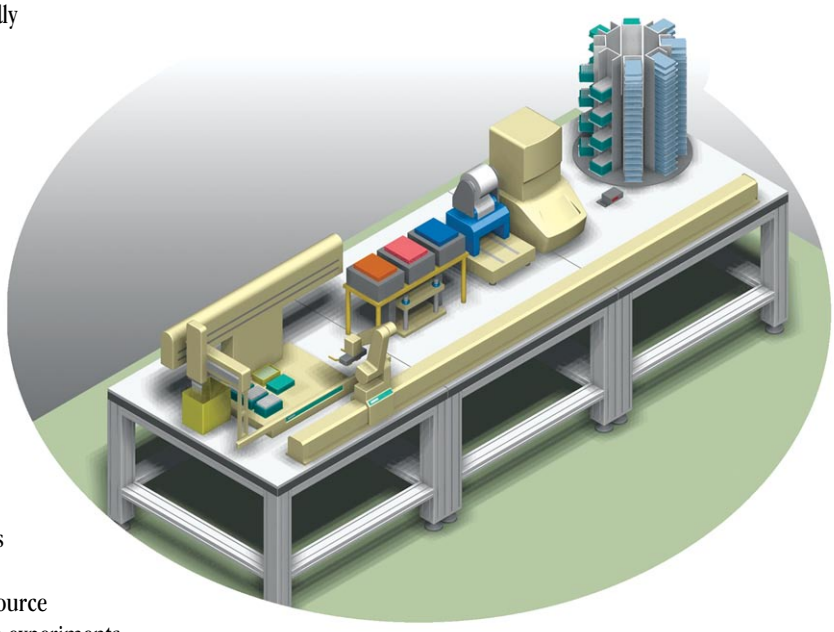
To improve understanding of the carbon life cycle, analysis of large numbers of samples is needed. Traditional approaches to sample collection, tracking, preparation, and analysis are very labor- and time-intensive, and conventional techniques do not scale very well. A new system is needed to perform high-volume, rapid, reliable, and repetitious analyses of soil, air, and water.

Los Alamos Innovation: Integrated and Automated Sample Analysis

The best way to achieve efficient, high-throughput sampling is by using an automated, highly-integrated sample processing and analysis system. To achieve this end, Los Alamos has formed a multidisciplinary team of biologists, chemists, mechanical engineers, software engineers, electrical engineers, and technicians. This team has considerable expertise in developing laboratory automation systems and custom instrumentation.

Working with industrial partners, other government agencies, and NIST, ASTM, and other standardization organizations, the Los Alamos team has developed equipment controls, interfacing standards, and systems that can be rapidly developed and deployed.

In the future, soil-sample processing systems could automatically separate, dry, pulverize, repackage, barcode, and weigh inhomogeneous soil samples. In addition to actively managing the sample material flow, this processing system would automate the information flow between all system components, thus enabling sample tracking and audit trailing.



An automated sample analysis system, which integrates sample processing, analysis, and tracking.

The Impact: Better Carbon Management

This system could be used to support soil sampling efforts ongoing at the U.S. Department of Agriculture and other research institutions. The benefits of automation technologies in carbon fuel cycle research and other research programs include (1) higher throughput, (2) lower costs, (3) more resource sharing, (4) automated result validation, (4) more repeatable experiments, (5) less potential for human errors, (6) more accurate results, (7) tracking, system monitoring, and reporting in real-time, and (8) reduced (possibly to zero) human exposure to potentially hazardous material environments. Processing samples automatically will reduce soil analysis costs and allow sufficient characterization of terrestrial systems for carbon management.

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Biophysical Principles and Models to Predict Biophysical Behavior

The Challenge: Predicting Biophysical Behavior

Predicting dynamics of terrestrial carbon systems and of biological systems generally is difficult but important. We lack a powerful underlying theory, and few universal biophysical principles are known beyond the genetic code and the evolutionary process. Across the size range from microbes to the biosphere, all life uses the same chemical constituents and reactions. All life functions by transforming energy from physical or chemical sources to build, maintain, and reproduce complex, organized structures and processes. How do we find the universal principles governing this immense variety of dynamic living forms, functions, and behavior?

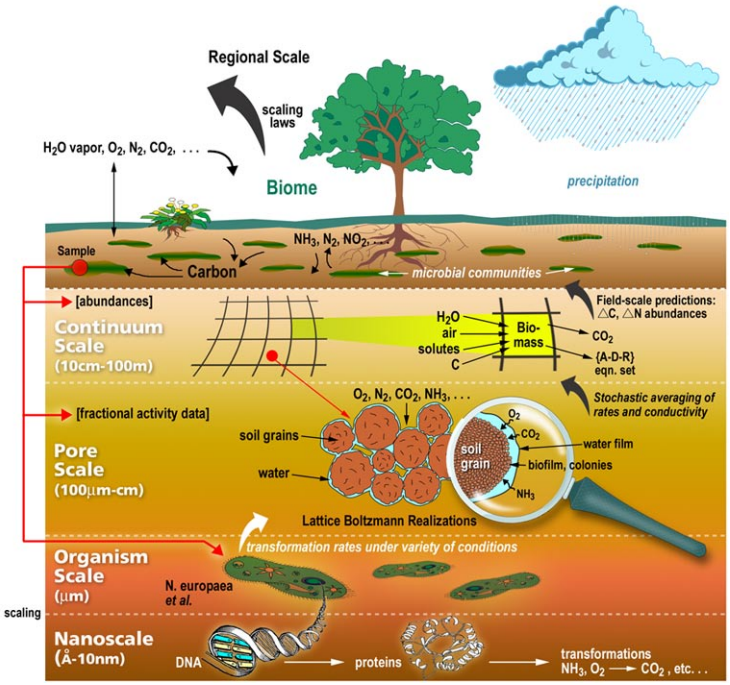
Los Alamos Innovation: Predictive Biophysical Models

Los Alamos is addressing these issues and beginning to provide a quantitative basis for exploring biological systems and predicting their behavior. By extending current theory, conducting macro-ecological analyses, and conducting advanced experimental and observational testing, Los Alamos is producing and applying an integrated scientific capability.

Los Alamos scientists and collaborators have developed a model based on allometric scaling laws, which relate size to measurable biological quantities. This model quantitatively predicts and describes how energy production is constrained by the transport of resources in biological systems. So far, the theory has provided fundamental new insights related to terrestrial carbon, including in these five areas:

- Tree growth rates among diverse species;
- Above-ground vs. below-ground biomass;
- Biophysical constraints limiting tree size;
- Plant-spacing relationships; and
- Ecosystem photosynthesis, respiration, and associated carbon flux rates.

Terrestrial ecosystems consist of processes and subsystems that function on scales ranging from the nanoscale to the biome scale.



The Impact: Understanding Life at All Levels

Results suggest that this powerful new theory may be extended to offer a robust predictive and explanatory understanding of how biological energetics provides the basis for scaling, from molecules to the biosphere, and linking many attributes of biological structure, function, and diversity. The new theory will allow (1) broad-scale analysis of terrestrial carbon pools and dynamics across diverse ecosystems; (2) cost-effective assessments of terrestrial carbon sequestration options; and (3) improved predictive capability of trajectories of terrestrial carbon in a given system.

Understanding biophysical principles will not only improve carbon management, it will help us predict fundamental relationships and behaviors in biological systems. It can lead to understanding the nature of life at all levels.

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GENIE Software to Monitor All Stages of the Carbon Cycle

The Challenge: Monitoring All Stages of the Carbon Cycle

Monitoring all stages of the carbon cycle—both natural and anthropogenic, and at various scales—is a continental-scale challenge. Monitoring includes detecting and measuring emissions from processing and storage facilities, and monitoring environmental state-of-health at natural and managed terrestrial sequestration sites. Remote sensing techniques (using both spacecraft and aircraft) are available, but involve mostly manual analysis. Traditional techniques are overburdened trying to keep pace with the flood of data from instrument platforms.

Los Alamos Innovation: GENIE Software to Assemble Remote-Sensing Tools

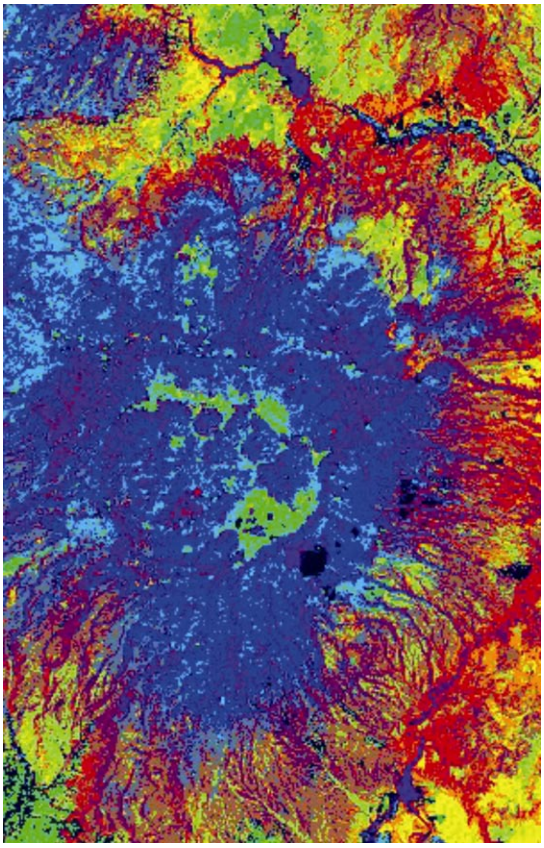
The solution: automated analysis techniques via modern machine learning methods providing adaptive, robust algorithms. The Los Alamos GENIE machine-learning software system uses a genetic algorithm.

GENIE assembles automated remote sensing tools from low-level image operators. Each assembled tool is evaluated against training data provided by the user, and the best tools in each generation are allowed to reproduce to build new tools. The population of tools evolves until it converges to a solution or reaches a minimum level of performance specified by the user.

GENIE provides the capability to build a suite of robust, adaptive tools to detect and analyze problems at production and storage facilities and terrestrial sequestration sites. In the future, GENIE will be used to rapidly prototype and field remote-sensing algorithms customized for automated monitoring. Tools will be developed capable of fusing and exploiting new and archival data from satellite and aircraft instruments (including advanced sensors such as multi-spectral and synthetic aperture radar imagers).

The Impact: Mapping Effects of Disasters and Carbon Cycle Monitoring

Already GENIE has been applied to a range of real-world problems. GENIE mapped the effects of the 42,000-acre Cerro Grande wildfire in Los Alamos in May 2000. And, using satellite and aircraft optical and multi-spectral imagery, GENIE helped detect ash, debris, and the plume from the terrorist attack in New York City on September 11, 2001. In the future, GENIE will be used to develop tools for many more real-world applications. GENIE promises to help achieve monitoring of all stages of the carbon cycle.



GENIE land-cover map for the Jemez Mountains, NM, using a Landsat satellite image. GENIE was trained to find trees, grasslands, and bare soil using a small, manually produced map, and then asked to automatically remap an area hundreds of times larger. These results support forest state-of-health monitoring, wildlife habitat assessment, and wildfire emergency response planning.

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Microhole Drilling and Diagnostics to Contain Subsurface CO_2

The Challenge: Ensuring Containment of Subsurface CO_2

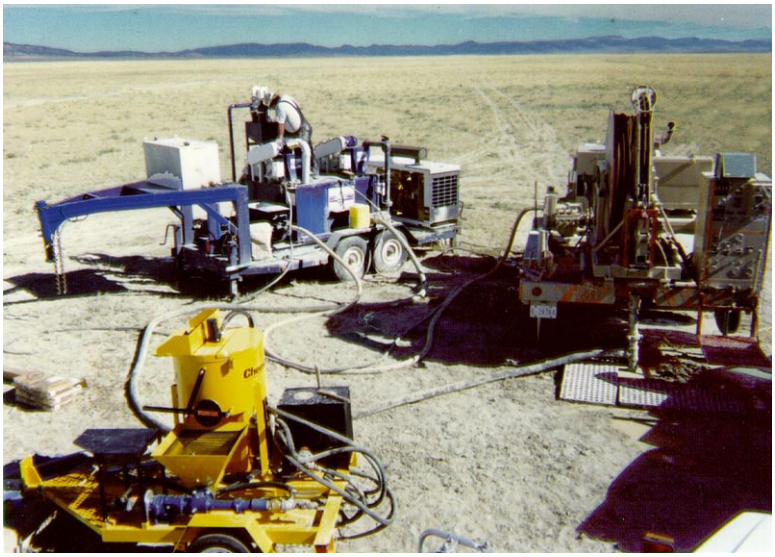
Ensuring that CO_2 is contained is a critical aspect of geologic sequestration. With conventional drilling, it is considered cost prohibitive to deploy sufficient instruments to adequately monitor sequestration processes.

CO_2 containment is ensured by measuring chemical and physical processes in the subsurface rock surrounding the new CO_2 reservoirs. To place the measuring instruments in the subsurface requires drilling. Contemporary deep boreholes have relatively large diameters. Advances in electronics and sensor miniaturization in the past decade have made new instrument packages with small diameters possible and increasingly affordable. These instrument packages, however, are poorly suited for large boreholes. Advanced drilling technologies are required to drill small-diameter boreholes primarily for deploying subsurface instrumentation.

Los Alamos Innovation: Microhole Drilling and Diagnostics

Los Alamos is developing microhole technologies for use in boreholes. These coiled-tubing technologies eliminate handling of segmented large-diameter drill pipes. Microholes with diameters of 2-3/8 and 1-3/4 inch are currently being drilled. With decreased size and use of materials to drill and complete microholes for instrumentation, savings of nearly 60% (discounting labor savings) will be realized.

Borehole instruments with 7/8-inch-diameter housings have also been developed and successfully deployed in microholes. To date, most of the advances in instrumentation have been in the area of microseismic instrumentation, used to detect subtle movements in fracture-dominated rock masses. Exploratory studies have revealed no engineering impediments to developing electrical-resistivity or nuclear-fluid monitoring tools for deployment in these wells.



Microhole coiled-tubing drilling rig deployed in central Nevada for drilling cased 1.25-inch diameter microholes for emplacement of seismic instrumentation. The tan equipment is the coiled tubing drilling rig, the blue is a mud conditioning system, and the yellow is a PVC casing grouting system.

The Impact: Better CO_2 Containment at Lower Cost

Microhole technology can reduce the cost of deploying instruments in the subsurface while improving measurement quality. This can greatly enhance safe CO_2 containment at geologic sequestration sites.

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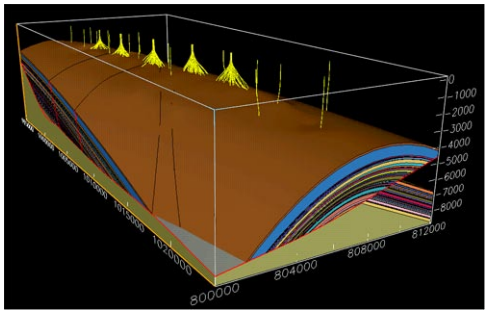
Investigative Modeling to Predict the Fate of Injected CO_2

The Challenge: Safely Storing CO_2 in Geologic Reservoirs

Large volumes of CO_2 can be sequestered in depleted oil and gas reservoirs, deep saline aquifers, deep unmineable coal seams, and similar geologic sites. Long-term storage of CO_2 in geologic formations would result in reactions between the CO_2, groundwater, and the geologic media. The reactions would change properties of the storage environment. This could affect the integrity of the natural barriers and could result in release of CO_2 to the accessible environment, adversely impacting health and safety.

Enhanced oil recovery methods have shown that large amounts of CO_2 can be injected into depleted oil reservoirs, but these methods have a short application history (about 50 years). Only with the capability to verify geologic sequestration methods with accurate predictive modeling tools will such long-term storage of CO_2 be possible.



Predicting the fate of CO_2 in the subsurface over time requires integrating reservoir-scale models (above) with detailed simulations of physical and chemical processes at the pore scale (below).

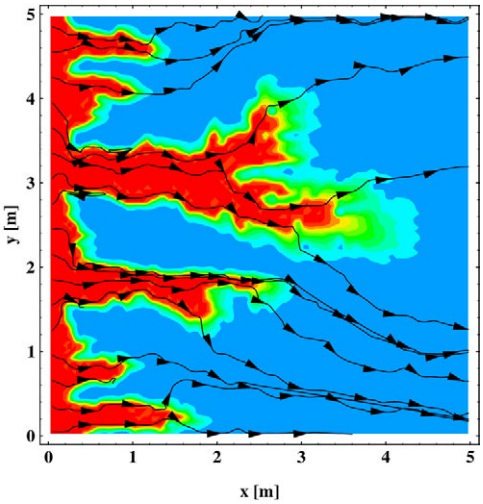
Los Alamos Innovation: Investigative Modeling of Injected CO_2

With new models, especially those coupling earth processes, it is possible to assess the fate of CO_2 injected into geologic formations. Los Alamos's numerical codes can be used to model the multiple, complex interactions of CO_2 and minerals in geologic media. While studying geothermal energy reservoirs, Los Alamos researchers developed numerical models for coupled heat-flow-mass transfer problems. These models have since evolved to study flow and reactive transport of contaminants in aquifers. Key abilities of these models include

- Coupling the heat-flow-mass transfer approach;
- Modeling problems that result in reactions with porous media; and
- Integrating EOS and reaction table data with an extensive thermodynamic application range.

The Impact: Predicting the Long-Term Fate of CO_2

Predicting the geologic fate of CO_2 has many applications, particularly in predicting CO_2's fate in sites considered for carbon sequestration. These models have been extensively applied to determine the fate of contaminants for a large number of contaminated sites in the vicinity of Los Alamos. In addition, they have been used to determine the long-term safety of the Yucca Mountain high-level nuclear waste repository. Long-term dynamic simulations could be used to understand how CO_2 and geologic media would interact over geologic time frames. Ultimately, it may be possible to predict how storage of CO_2 will affect the geologic media and the long-term safety and feasibility of geologic sequestration.



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Magnesium-Silicate Mineralization for Permanent Storage of Carbon Dioxide

The Challenge: Long-Term Storage of CO_2 Emissions

Each year, fossil-fuel use in the U.S. produces twenty tons of CO_2 per person. Worldwide, total emissions now exceed twenty billion tons per year—5 cubic miles in liquid form. By the year 2099, these emissions could easily increase by a factor of 5 to 10 times. These enormous volumes will impose significant constraints on potential storage options.

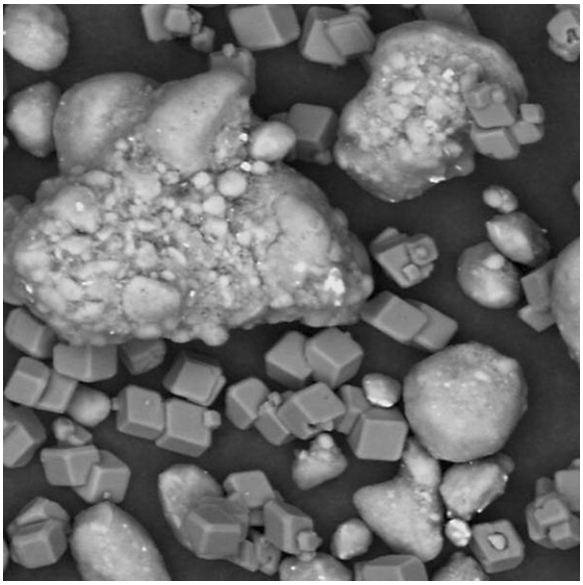
Los Alamos Innovation: Converting CO_2 to a Solid Carbonate

The ability to store large volumes of CO_2 safely for extended periods of time (thousands of years) is critical. Most of the CO_2 that once dominated the Earth's atmosphere has been removed by a natural process that weathered silicate materials to produce dissolved carbonates, clay minerals, and solid carbonates. Through this process, nature has safely stored much more CO_2 than could be produced by all of the world's fossil fuels.

Los Alamos researchers proposed an analogous approach to store anthropogenic CO_2 as a stable solid. Los Alamos proposed that serpentinites and other magnesium-rich silicate deposits could be reacted industrially with CO_2 to form silica and magnesium carbonate, resulting in a safe and immobile long-term storage medium for carbon dioxide.

In an effort funded by the National Energy Technology Laboratory (NETL), Los Alamos has partnered with several organizations to understand the conditions necessary for CO_2 mineralization and the processes that control its rate. The emphasis of the research is to identify a process that will allow CO_2 mineralization at a rate and cost that make it competitive with more conventional approaches to CO_2 sequestration.

Conversion is possible in an aqueous process, but sufficient rates are only achievable with limited olivine-rich ores and extensive (and costly) mineral preparation (mechanical grinding or heat treatment). Los Alamos's current process is most rapid at elevated CO_2 pressures (>1000 PSI), but pressures as low as 150 PSI appear encouraging.



Scanning electron microscope image of magnesite (rhombs) formed by reacting supercritical carbon dioxide with the magnesium silicate serpentine.

The Impact: Safe Permanent CO_2 Storage

Benefits of this process include

- Safety—magnesium carbonate is benign and has no negative impacts on the environment;
- Immobility—solid magnesium carbonate requires no long term monitoring and provides easy verification of storage volumes; and
- Valuable by-products—serpentinites and many other magnesium-rich rocks are enriched in platinum group elements and other valuable metals.

If a feasible, economic process can be developed, CO_2 mineralization could be implemented with any capture process that provides a relatively pure CO_2 stream.

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Ocean Simulations to Predict Effects of Carbon Management Plans

The Challenge: Understanding How Iron Affects the Ocean

The deep ocean is the largest potential CO_2 reservoir accessible from the Earth's surface. Over the next few centuries, the ocean will serve as a natural sink for atmospheric greenhouse gas. It is thought that engineering changes in micro-nutrient iron supply to oceanic plankton would significantly effect concentrations of atmospheric CO_2. Implementing large-scale iron fertilization to alleviate greenhouse gas is fast approaching economic viability. However, the fate and effects of this injected material would influence the ecology of the ocean. To understand the potential risks, advanced new tools are needed.

Los Alamos Innovation: Simulating Oceanic Carbon Cycles

A detailed ocean biogeochemistry model has been under development at Los Alamos. It includes many nutrients, tracers, and other metrics that influence the carbon cycle. The simulations are built into and based on the global general circulation models for which the Laboratory's climate team has become well known. Los Alamos codes can produce high resolution of biological and elemental cycling while supporting full biogeochemistry. Carbon related issues being addressed in the model include

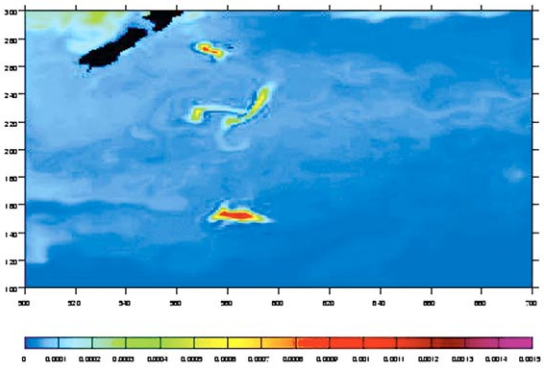
- Observing the impact of El Niño/La Niña events on marine ecosystems;
- Mimicking the behavior of patches created during the Southern Ocean Iron (Fe) experiments (SOFeX);
- Identifying oceanic regions where sequestered CO_2 might return to the surface rapidly; and
- Performing detailed simulations of the behavior of proposed iron fertilization of the oceans for carbon sequestration.

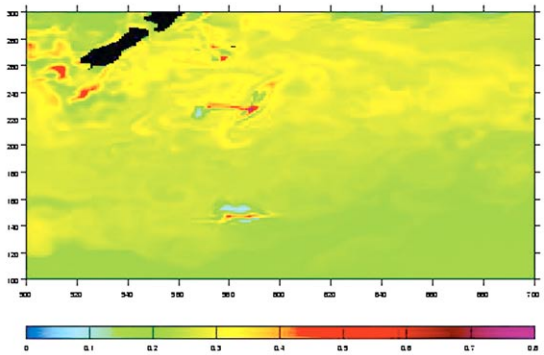
In the future, Los Alamos will investigate (1) how spatial and temporal dispersion of sequestered carbon can be predicted after perturbation; (2) how adding micro-nutrient iron to the surface ocean would stimulate marine organic carbon production; (3) how much organic carbon will sink to the deep ocean and to what extent it will be replaced by atmospheric CO_2; and (4) how iron fertilization changes physical and chemical conditions (both on the surface and mid-water).

The Impact: Knowing If Iron Can Safely Reduce Greenhouse Gas

Los Alamos's ocean-carbon sequestration studies will show how proposed marine carbon management plans affect the long-term fate of ocean environments. Enabling evaluation of various ocean sequestration strategies could have major implications for environmental management. If it is found that fertilizing the ocean with iron will have minimal effect on ocean ecosystems, policymakers may decide this is a viable solution for reducing or alleviating greenhouse gas, holes in the ozone, and global warming.

Biogeochemical model of three iron-enrichment patches introduced south of New Zealand. Iron is introduced in the model as roughly one-nanomolar iron injections over three square areas, each approximately 100 km on a side. The top image shows the resulting distribution of iron after one month of processing by surface ocean biology transport. The second image is the corresponding phytoplankton distribution (units of micromolar plant nitrogen content). Strong biological growth is apparent in the fertilized areas.





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