APRIL ISSUE 1998

LOS ALAMOS NATIONAL LABORATORY
WHERE SCIENCE MAKES A DIFFERENCE

DATELINE
LOS ALAMOS

NANOSPONGES SOAK UP CONTAMINANTS AND CUT CLEANUP COSTS

POLYMER COULD BECOME A NATURAL EXTENSION OF EVERY DRINKING FAUCET IN THE WORLD

← Chemist DeQuan Li (left) and graduate student Min Ma have developed a new polymer that can absorb and trap organic contaminants in water.

Los Alamos National Laboratory researchers have developed reusable nanosponges, a polymer-based material that forms nanometer-sized pores that can absorb and trap organic contaminants in water, which are proving highly effective in cleaning up organic contaminants in an industrial setting.

A nanometer is one-billionth of a meter.

The nanosponge polymer could become a natural extension of every drinking faucet in the world, according to Los Alamos polymer chemist DeQuan Li.

The polymer also could be used to clean up organic explosives, remediate underground water and clean up oil or organic chemical

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spills, especially in water — all while decreasing cleanup costs associated with current technologies.

Conventional processes using either activated carbon or zeolites are inefficient in reducing low-concentration contaminants in water and are totally ineffective in removing organic compounds from water down to the parts-per-trillion level, Li said.

The molecular binding between organic contaminants and the polymer is 100,000 times greater than with activated charcoal and the process is 100 percent reversible.

Activated carbon is made from material burnt in a super-heated, oxygen-rich atmosphere creating small holes throughout the grain of charcoal that effectively increases the carbon's surface area, making it more reactive.

Zeolites are a group of crystalline aluminosilicates with three-dimensional frameworks that form uniform surface pores enclosing internal cavities and channels and are used commercially as molecular sieves, mostly for gas separations.

The shape and size of the surface pores and internal cavities physically or chemically trap large chemical molecules within their lattice, breaking them into smaller ones.

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A MONTHLY PUBLICATION OF THE PUBLIC AFFAIRS OFFICE OF LOS ALAMOS NATIONAL LABORATORY

LOS ALAMOS NATIONAL LABORATORY, AN AFFIRMATIVE ACTION / EQUAL OPPORTUNITY EMPLOYER, IS OPERATED BY THE UNIVERSITY OF CALIFORNIA FOR THE U.S. DEPARTMENT OF ENERGY UNDER CONTRACT NO. W-7405-ENG-36

EDITOR
Kathy DeLucas

MANAGING EDITOR
Meredith Coonley

STAFF WRITER
Theresa Salazar

Send comments/questions to dateline@lanl.gov

CONTRIBUTING WRITER
Steve Sandoval

CONTRIBUTING PHOTOGRAPHER
John Bass

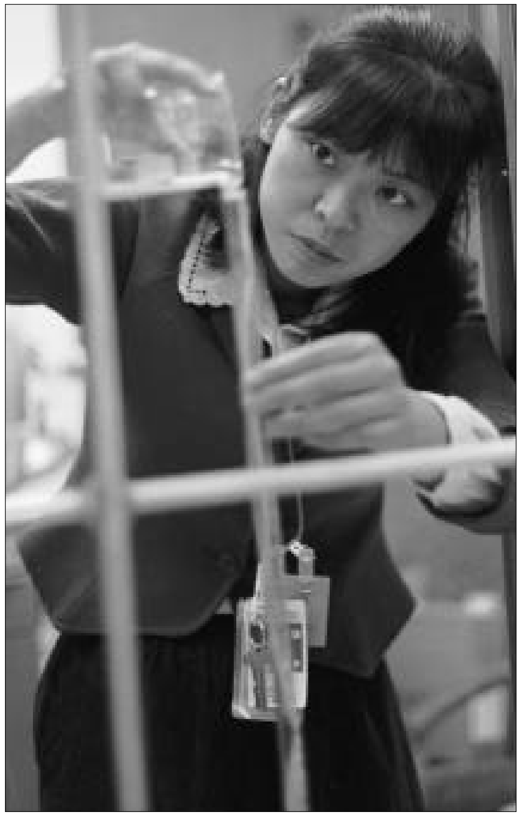
PRINTING COORDINATOR
G.D. Archuleta

LOS ALAMOS NATIONAL LABORATORY
PUBLIC AFFAIRS OFFICE, MS P355
LOS ALAMOS, NM 87545

But both activated charcoal and zeolites have drawbacks in water purification: They are easily deactivated by moisture in the air and cannot function effectively once they are completely saturated with water.

Zeolites, for example, are good for absorbing water from organics but not vice versa.

Discovered by Li and graduate student Min Ma, the newly developed material is made of polymeric building blocks called cyclodextrins that form cylindrical cages to trap organics.



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Graduate student Min Ma begins an experiment by pouring contaminated fluid into a burette — a glass tube with a tap on the end of it.

The nanosponge has a love-hate relationship with water. The polymer's cages have hydrophilic sites that have an affinity for water and hydrophobic sites that are repelled by water. This characteristic makes them useful in water yet able to attract organics.

The hydrophobic sites prefer the organic contaminant over the water. The water actually drives the organic compound into the polymer's cage-like structure. Researchers rinse the saturated polymer with ethanol to release the trapped contaminants and the nanosponge can be reused.

So far the research team has developed polymers to bind with trichloroethylene, toluene, phenol derivatives and a number of dye compounds. Li can fabricate the nanosponge material into granular solids, powders and optical-quality thin films.

Such flexibility enables users to customize the polymer for multiple applications and formats accommodating different water-treatment configurations and needs, Li said. For example, a polymer designed as a membrane could be placed on a household water faucet. This

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Decontaminated water drips into a beaker after passing through the nanosponge polymer. The nanosponge can be removed from the filtration device, rinsed with ethanol to release the contaminants, and reused.

membrane could purify water much like conventional filters do to soften it.

The only difference is that water softeners introduce sodium ions in exchange for the calcium ions that make the water hard; the polymers add nothing to the treated water.

Another advantage the polymers have is that the polymers are relatively cheap to manufacture; they are one step away from a commercially available product: cyclodextrins in starch.

The conversion is 100 percent effective; all the starch cyclodextrins are converted completely to polymer products. Mass production may bring down the cost below the current price of activated carbon or zeolites, Li said.

Unlike carbon and zeolites, the porous polymers remain effective in air and do not absorb moisture from the air. Activated carbon and zeolites must be "activated" before use or they lose their effectiveness to remove contaminants. But the polymers require no activation and can be placed immediately into the contaminated medium for *in situ* treatment.

The tiny sponge-like polymer can be readily incorporated into industrial and municipal online water purification systems, Li said.

CONTACT: DEQUAN LI
BIOSCIENCE AND BIOTECHNOLOGY
(505) 665-1158 • E-mail: dequan@lanl.gov

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FINDING BETTER WAYS TO TRAVEL

SIMULATION SYSTEM EXAMINES NEW APPROACHES FOR GETTING PEOPLE WHERE THEY WANT TO GO

A new transportation forecasting tool soon will help metropolitan planners design future roads and transit systems.

In a recent study conducted in the Dallas-Fort Worth area, Los Alamos researchers used the Transportation Analysis and Simulation System, or TRANSIMS, to create a virtual metropolitan region with a complete representation of the region's residents, their activities and the transportation infrastructure.

TRANSIMS is a set of integrated analytical and simulation models and supporting data bases that examines alternatives which help commuters and other travelers reach their destinations with less hassle and grief.

The computational system represents thousands of roadway and transit segments, intersection signals and signs, traveler origins and destinations and possibly millions of people and vehicles.

Metropolitan planners must plan the growth of their cities according to the stringent transportation system planning requirements of the Intermodal Surface Transportation Efficiency Act of 1991 and the Clean Air Act Amendments of 1990.

PRESIDENT BRIEFED ON TRANSIMS

President Clinton (second from left) and Secretary of Energy Federico Peña (left) receive a first-hand demonstration by Laboratory Director John Browne on TRANSIMS, a new transportation forecasting tool developed to assist metropolitan planners in the design of future roads and transit systems. The demonstration was part of a briefing the president received on Los Alamos supercomputing initiatives, which also included global ocean modeling. The Feb. 3 visit was the president's second to the Laboratory in five years. During his three-hour visit to Los Alamos, the president addressed a gathering of Laboratory employees and their families, and made a quick stop at the local high school, where the band serenaded him with "Louie, Louie."

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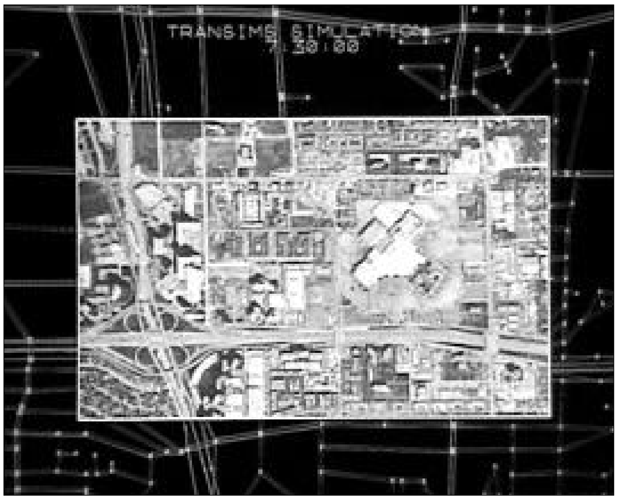

The microsimulation of the Dallas-Fort Worth area covers a 25 square-mile region that includes freeways, arterials and local streets near two major shopping malls — the Galleria and Valley View.

These laws require each state and its metropolitan areas to work together to develop 3-year and 20-year transportation improvement plans that estimate future transportation needs and evaluate ways to manage and reduce congestion. The plans also must examine the effectiveness of building new roads and transit systems and limit the environmental impact of the various strategies.

Accurate planning requires an analytical capability that properly accounts for travel demand, human behavior, traffic and transit operations, major investments and environmental effects.

Existing planning tools that are based on methods developed in the 1950s use lumped information and representative behavior to predict average response and average usage of transportation facilities. They don't account for individual traveler response to the transportation environment.

TRANSIMS, however, emphasizes the complex nature of individuals interacting with the transportation system. It generates a synthetic population and places households and individuals within the metropolitan area. The demographic makeup and spatial distribution of the artificial population comes from census data and matches that of the region's real population.

Based on survey data, TRANSIMS then builds a model of household and individual activities that might occur at home, work, school or shopping centers. Trip plans that include departure times, travel modes and specific routes are created for each individual to reach his or her daily activities.

TRANSIMS simulates the movement of individuals by executing their trip plans throughout the transportation network. The simulation also includes individuals' use of vehicles such as cars or buses, on a second-by-second basis.

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This virtual world of travelers mimics the traveling and driving behavior of real people. The interactions of individual vehicles produce realistic traffic dynamics from which analysts use TRANSIMS to estimate vehicle emissions and judge the overall performance of the transportation system.

In this context, a complete transportation system includes travelers, freight, vehicles, roadways, sidewalks, paths, intersections, transit schedules and even policies.

Los Alamos researchers are developing and implementing computer models that imitate situations, for example, where travelers choose various routes as opposed to others due to traffic congestion or when travelers change from car to bus or vice versa which in turn affect a transportation system's performance.

The executed route and mode travel times of individuals obviously differs from the information that was used to plan each trip in the first place. So, these travel times are gathered from the travel simulation, used to replan the individuals' activities and trips, and the travel simulation is run again.

This iteration between the planning model and travel simulation is repeated until the trip plans and simulated travel do not change significantly between runs. Thus, a complete study may involve numerous cases and may require hundreds of executions of the activity-demand model, trip-planning model and the travel simulation.

TRANSIMS' virtual world mimics the traveling and driving behavior of real people. ↓

To address the computational demands, Los Alamos researchers apply methods that simplify the modeling of the individual traveler's interactions with the transportation system but produce appropriate dynamic behavior of the transportation system as a whole.

For instance, quick-running, simple models were created in which vehicles hopping along the roadway generate realistic traffic flow and congestion.

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← The top computer-generated image simulates the present-day traffic flow near the Galleria and the I-635 and Dallas North Tollway interchange. The TRANSIMS simulation indicates slow, congested traffic on the tollway and a major arterial street. The lower image shows reduced congestion and improved traffic flow for a TRANSIMS simulation with improvements to several arterial streets.

The researchers study procedures that rapidly select the nearest location for a traveler's activity and that find the travel modes and routes that are the shortest or quickest between locations.

The Dallas-Fort Worth study emphasized an initial TRANSIMS capability for evaluating traffic flow dependence on roadway alternatives. The microsimulation covered a 25-square-mile region that included freeways, arterials and local streets. The region's center is at the intersection of two major roadways — Interstate 635 and the Dallas North Tollway — located near two major shopping malls — Galleria and Valley View.

Two alternative roadway improvements were evaluated for improved access through the region, to the Galleria and to other locations in the region. A freeway change added another lane to I-635 in both directions. An arterial change included additional lanes on four major arterials, additional frontage roads to improve traffic flow and Galleria access and several redesigned major intersections.

Los Alamos researchers found that TRANSIMS provides new ways of measuring the effectiveness of transportation system changes. To demonstrate, individual travel times can be grouped in five-minute intervals according to the trip starting time. Statistical properties of each group can be calculated.

So, in addition to comparing the traditional average travel time during the peak period of traffic congestion, the time dependence and the range of travel times can be compared between cases. The Dallas-Fort Worth study successfully demonstrated the TRANSIMS interim operational capability and indicated various ways in which it can be used to evaluate transportation alternatives.

The next phase in TRANSIMS development focuses primarily on the interaction between the planning models and the travel simulation, but also will incorporate activity demand and the capability for emissions predictions. This case study will be conducted in Portland, Ore.

Researchers anticipate that once TRANSIMS is developed, it will be used in every city where congestion and pollution are major concerns.

CONTACT: LARON SMITH
TECHNOLOGY AND SAFETY ASSESSMENT
(505) 665-1286 • E-MAIL: llsmith@lanl.gov

An aerial view of the roads near the Galleria and Valley View malls.

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RESEARCHERS AWARDED $5 MILLION

INNOVATIVE PROJECTS WILL SPEED UP ENVIRONMENTAL CLEANUP

Eight Los Alamos projects have received grants from the Department of Energy for innovative projects aimed speeding up environmental cleanup. This research program focuses on the fundamental science needed to develop technologies that reduce costs and risks to the environment, workers and communities. The program takes advantage of laboratory and university expertise to carry out long-term research.

←

Before and after photos of site remediation at Material Disposal Area M.

The projects, which were awarded nearly $5.5 million, range from studying fundamental chemistry to how radioactive contaminants move through the environment to aging effects in waste-storage tanks.

DOE awarded $46 million in grants for 66 projects nationwide at national laboratories, universities and private institutions for the 1998 fiscal year, which began Oct. 1, 1997. The grants from DOE's Environmental Management Science Program fund basic research projects that make DOE's environmental cleanup efforts more cost-effective and efficient.

The Los Alamos projects, which will be funded over three years, are:

• An investigation of the fundamental chemistry of technetium, a radioactive byproduct of uranium decay. The $900,000 grant was awarded in partnership with Lawrence Berkeley National Laboratory. The principal investigator is Carol Burns of Chemical and Environmental Research and Development.

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• A study of electrochemistry mechanisms to help develop more robust and less expensive methods for stabilizing plutonium- and uranium-bearing residue materials at DOE sites. The grant is for $750,000 and the principal investigator is David Morris of Bioscience and Biotechnology.

• Basic research in chemistry intended to aid development of new ways to simulate the complex ingredients in high-level radioactive waste tanks on DOE sites, which in turn can help lead to better treatment techniques. The grant is for $550,000 and the principal investigator is Rebecca Chamberlin of Nuclear and Radiochemistry.

• Materials science research aimed at improving the durability of the waste forms proposed for long-term disposal of DOE radioactive wastes, focusing on the thermodynamics of actinide-bearing mineral waste forms. The grant is for $1,150,000 and the principal investigator is Mark Williamson of Advanced Technology.

• Research aimed at a better understanding of the chemical behavior of technetium, including how technetium complexes behave in wastes at DOE's facility at Hanford, Wash. The grant is for $730,000 and the principal investigator is Norman Schroeder of Nuclear and Radiochemistry.

• An environmental science study into how local conditions can affect the movement of contaminants, such as plutonium, in soils on DOE sites. The grant is for $900,000 and the principal investigator is David Breshears of Environmental Science.

• A study of the chemical behavior of plutonium in contaminated soils on DOE sites to understand risks to the public and the environment and to develop appropriate cleanup methods. The grant is for $750,000 and the principal investigator is Mary Neu of Nuclear and Radiochemistry.

• Basic research into instrumentation that can determine the chemistry of complex mixtures such as the large volumes of mixed radioactive and hazardous waste on DOE sites. The grant is for $655,000 and the principal investigator is Phillip Hemberger of Environmental Science and Waste Technology.

CONTACT: BRUCE R. ERDAL
ENVIRONMENTAL MANAGEMENT
(505) 667-5338 • E-MAIL: erdal@lanl.gov

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BRIEFLY ...

THE LABORATORY AND NEW MEXICO STATE UNIVERSITY HAVE ESTABLISHED A PARTNERSHIP that will help attract new researchers to the Los Alamos Neutron Science Center and create a high-quality physics-research program at the university. "The agreement between the Laboratory and NMSU will broaden and strengthen cooperation between the two institutions," said newly appointed LANSCE Director Roger Pynn. Professor Heinrich Nakotte has been chosen to hold a joint position between NMSU and LANSCE devoting half-time to each position. The agreement spans six years or until Nakotte achieves a tenured position in NMSU's Physics Department. Congressman Joe Skeen (R-N.M.) and incoming Laboratory Director John Browne formalized the agreement at Skeen's Washington office.

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DATELINE LOS ALAMOS

A Monthly Publication of the Public Affairs Office of Los Alamos National Laboratory

Nonprofit Organization
U.S. Postage Paid
Albuquerque, NM
Permit No. 532

LALP-98-1-4

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