On the Leading Edge of Atmospheric Predictions

Computational tools developed at the National Atmospheric Release Advisory Center predict the spread of airborne hazards from toxic chemical spills, fires, and other atmospheric releases.

SENSORS detect an airborne hazardous material, and authorities quickly contact the National Atmospheric Release Advisory Center (NARAC) at Lawrence Livermore. Within 15 minutes, NARAC's suite of Web-based software produces fully automated, three-dimensional (3D) predictions that show which areas will be exposed to toxic levels of the airborne plume and provide protective action guidelines for emergency responders. The center's operations staff, which is on duty or on call around the clock, follows up with refined models calibrated with field measurements of airborne and surface concentrations of the toxic material.

Newly acquired data are included in computer simulations to better predict the plume's direction and its likely source. The revised projections give emergency responders and decision makers valuable information about hazard areas, potential health effects, populations at risk, and recommended protective actions. This hypothetical incident illustrates the services that NARAC provides dozens of times each year.

A toxic airborne release, whether intentional or accidental, can quickly affect a large population. To better protect the nation from such hazards, the Department of Energy (DOE) established NARAC in 1979 in the wake of the Three Mile Island nuclear power plant accident. The center's purpose is to respond to such events by predicting and mapping the probable spread of hazardous materials released into the atmosphere. Livermore scientists provide support during emergencies involving many kinds of potential atmospheric hazards—toxic industrial chemical spills, fires, biological and chemical agent releases, radiological dispersal devices, improvised nuclear weapons, and nuclear power plant accidents.

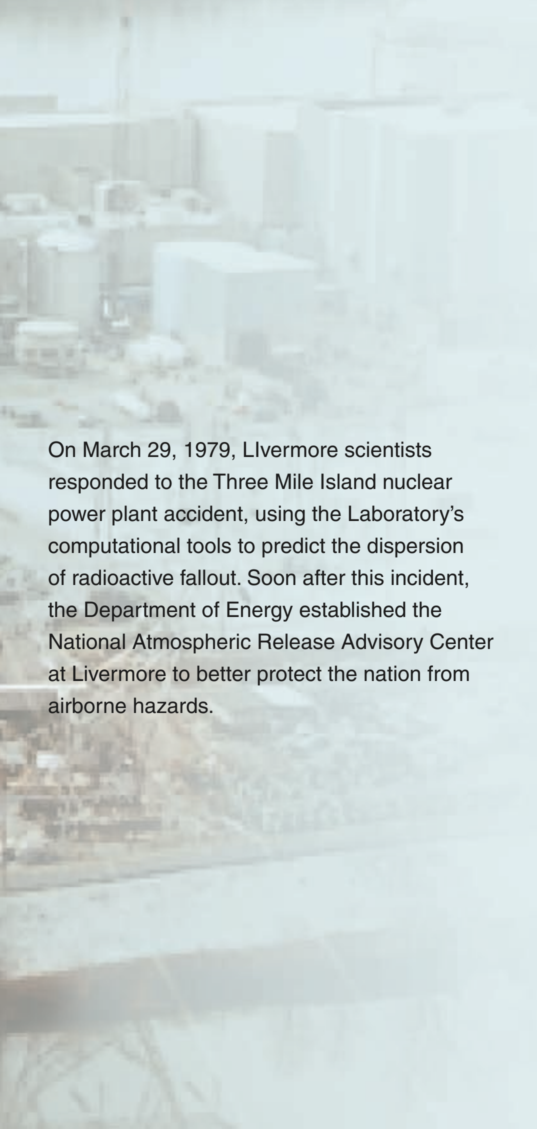
In 2004, the Homeland Security Council named NARAC as the interim provider of capabilities for the new Interagency Modeling and Atmospheric Assessment Center (IMAAC), which is led by the Department of Homeland Security (DHS). Under the U.S. National Response Plan, IMAAC coordinates dispersion modeling and disseminates hazard predictions for actual or potential incidents that require federal coordination.

NARAC receives real-time observations and weather forecast data feeds from the National Weather Service's National Centers for Environmental Prediction, the U.S. Navy and Air Force, and many other sources around the world. The center collects more than one million meteorological observations per day. By combining this information with the center's databases of maps, terrain, land use, population, material properties, and release mechanisms, the operations staff can use NARAC computer models to generate predictions that focus on almost any area, whether the scale is urban, regional, or global.

To provide integrated emergency response support, NARAC collaborates with more than 300 federal, state, and local agencies and emergency operations centers. The center's operational system responds to about 7,000 requests per year and has over 1,800 online users. An easy-to-use geographic information system (GIS) displays plume predictions and can export results to other GIS tools. Predictions can be requested and distributed with user-friendly Internet- and Web-based software, and access is available via dial-up, satellite, Ethernet, and wireless networks.

Staying on the Leading Edge

Gayle Sugiyama, who leads the NARAC/IMAAC Program in Livermore's Energy and Environment Directorate, ensures that models and codes are continually updated to incorporate the latest computational and scientific capabilities. "NARAC's operational needs drive our research and development, which in turn directly benefit the operations team and its clients," she says.



On March 29, 1979, LIvermore scientists responded to the Three Mile Island nuclear power plant accident, using the Laboratory's computational tools to predict the dispersion of radioactive fallout. Soon after this incident, the Department of Energy established the National Atmospheric Release Advisory Center at Livermore to better protect the nation from airborne hazards.

Currently, one-third of the center's staff is devoted to model and system research. Other staff members analyze airborne hazards or maintain the hardware and software systems. NARAC scientists routinely collaborate with other Laboratory engineers and scientists and with researchers at various institutions.

The center's current projects encompass a variety of prediction capabilities. New research areas include simulating releases in complex urban environments and developing probabilistic methods that use field measurements to reconstruct atmospheric release events and determine an unknown source. In other projects, scientists are incorporating new capabilities into existing dispersion models, including the effects of high-altitude releases, rain, atmospheric chemistry, and surface roughness. The center is also making significant improvements in its models of nuclear fallout, dense gases, and the resuspension of particles.

Simulating the Urban Scene

Cities represent a challenge for airborne flow and dispersion modeling. Buildings, sidewalks, and streets capture heat, creating urban heat islands. Structures and vegetation complicate the flow patterns, for example, channeling dispersion down the street canyons formed by high-rise buildings and causing wake zones and eddies to form. All of these surface features significantly affect the movement of an airborne plume. An indoor exposure to material released outdoors differs significantly from an outdoor exposure. Buildings "leak," and ventilation systems move contamination in or out of buildings. People and traffic carry contaminants with them, increasing the size of the hazard area.

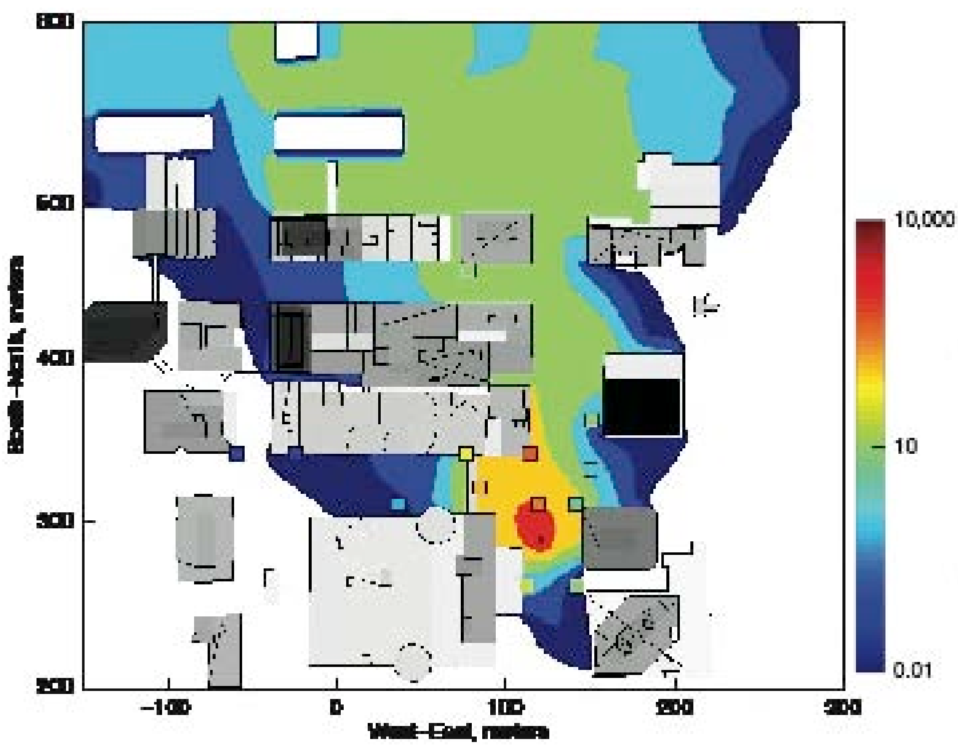
NARAC has long been a leader in developing urban modeling techniques. As computing power increases, scientists have improved the center's atmospheric flow and dispersion models to encompass higher spatial and temporal resolutions as well as more complex physical processes. This computational capability is particularly important for national security because cities are potential targets for weapons of mass destruction.

To better predict dispersion in an urban environment, NARAC scientists have developed a computational fluid dynamics (CFD) code called FEM3MP. (See *S&TR*, October 2001, pp. 16–19.) FEM3MP is a massively parallel code that generates accurate predictions of wind fields and dispersed concentrations. The code has been extensively tested against data obtained from wind-tunnel and field experiments, such as Urban 2000 in Salt Lake City, Utah, and Joint Urban 2003 in Oklahoma City. Livermore physicist Stevens Chan is responsible for ongoing development of FEM3MP.

FEM3MP is an excellent tool for the detailed site studies so crucial for emergency response planning and postevent analysis. It is, however, computationally intensive and is too slow for real-time predictions. A major roadblock to using FEM3MP and similar CFD codes in an emergency situation is the time required to generate the grids used in calculations.

To address this problem, scientists from NARAC and Livermore's Computation Directorate are incorporating FEM3MP's capabilities into the Adaptive Urban Dispersion Model (AUDIM). AUDIM uses adaptive mesh refinement to automate and integrate the steps in simulating dispersion in an urban environment, from grid generation to flow and transport prediction. AUDIM's grid-generation program can use raw lidar data from aerial surveys as well as "shape files" of building footprints and heights to generate 3D surface meshes in minutes.

A faster method for simulating an urban airborne dispersal is the Urban Dispersion Model (UDM), developed by the United Kingdom's Ministry of Defence

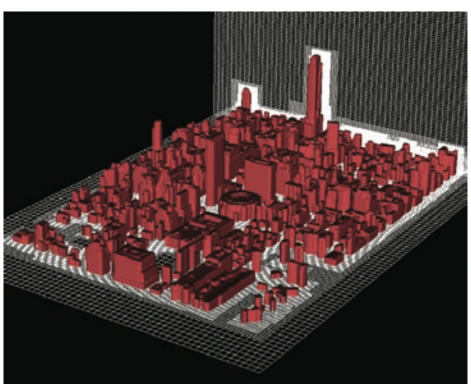


These concentration predictions, which were made by the computational fluid dynamics code FEM3MP, compared well with data collected during the Joint Urban 2003 field experiment.

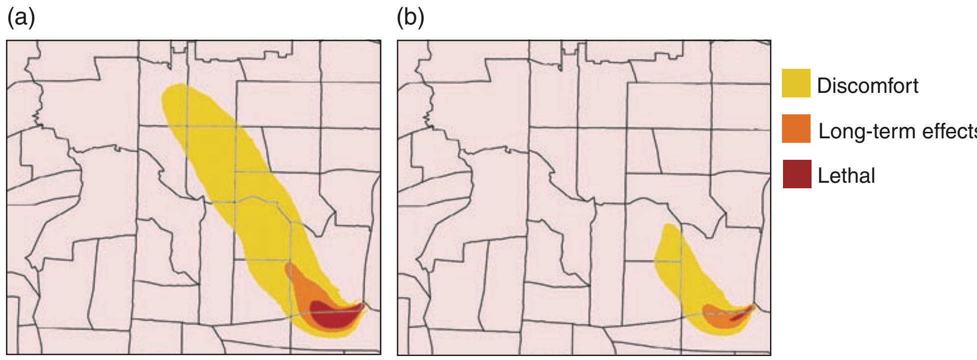
at the Defence Science and Technology Laboratory. UDM fills a gap between highly detailed CFD simulations and larger-scale urban canopy models, which use area-averaged data that do not resolve individual buildings. UDM empirically incorporates the effects of buildings on airborne transport. A joint project with the Defence Science and Technology Laboratory has completed a pilot integration of UDM into the NARAC operational system.

In another effort, Livermore physicists Lee Glascoe and Gwen Loosmore are working with computer scientist Hoyt Walker to address indoor exposure from an outdoor release. Their effort is based on building infiltration (leakiness) models developed by Lawrence Berkeley National Laboratory. "Building leakiness affects the dose to which an indoor population may be exposed during an airborne release," says Glascoe. "Understanding building infiltration leads to better decisions about evacuation versus sheltering in place."

Leakiness varies with the type of structure as well as with local weather conditions. For example, houses in California leak more than houses in colder Minnesota. Homes in economically disadvantaged communities also tend to have higher leakiness factors. With



The Adaptive Urban Dispersion Model (AUDIM) automatically produces large, high-resolution computational grids for complex urban environments. AUDIM created this detailed grid of lower Manhattan in less than 10 minutes.



(a) Modeling results show that the atmospheric release of a toxic agent would affect several counties in a region, as winds carried the materials northwest. (b) People who remained sheltered inside buildings would be better protected from the release.

Evaluating Model Performance

Scientists at the National Atmospheric Release Advisory Center (NARAC) test new simulation techniques and operational systems extensively to ensure that all of the center's tools perform as designed. Comparing predictions with analytic solutions is one method of testing models to measure how well new tools perform. Real events, such as the 2004 chemical fires in Cincinnati, Ohio, and Conyers, Georgia, make excellent operational test cases.

Another test method is field experiments. Livermore has participated in several field studies, including Urban 2000 in Salt Lake City, Utah, and Joint Urban 2003 in Oklahoma City. These experiments were collaborations of Department of Energy (DOE) national laboratories, other federal agencies, and universities to collect field data for testing urban flow and dispersion models. Urban 2000, funded by DOE, studied nocturnal releases under relatively light wind conditions. Joint Urban 2003 was the largest and most complex urban field experiment performed to date. Funded by the Department of Homeland Security and the Defense Threat Reduction Agency, this experiment consisted of daytime and nighttime releases of sulfur hexafluoride under moderate to strong winds.

Results from such experiments help researchers improve their modeling efforts. For example, observations at Joint Urban 2003 influenced NARAC's work on urban atmospheric turbulence for the Weather Research and Forecasting model. Conventional approximations of turbulence cannot account for the concentrations of sulfur hexafluoride measured during the exercise. Incorporating turbulence more accurately in forecasting models could make all the difference.

NARAC provided operational support for officials in Ohio during a massive fire at an illegal chemical storage facility. (Photograph courtesy of WCPO-TV, Cincinnati, Ohio.)

commercial buildings, leakiness depends on a structure's footprint, height, and geographic location. To improve simulations of indoor exposures, the Livermore team used census tract data to develop estimates of residential leakiness throughout the U.S. The team, which includes researchers from Lawrence Berkeley, recently completed a prototype code that can predict exposures to an outdoor chemical gas release for occupants of a commercial building. The team is working on a similar code to model aerosol release exposures.

Physicist Julie Lundquist is working with scientists from the University of California at Berkeley to incorporate the effects of the urban landscape—factors such as turbulence and heating—in the next-generation weather forecasting program, known as the Weather Research and Forecasting (WRF) model. WRF, which is being developed by the National Center for Atmospheric Research and many other institutions, will be a valuable resource both for weather forecasting and scientific research. Livermore is modifying WRF for use in detailed, urban dispersal simulations. (See the box on p. 15.)

Reconstructing a Release

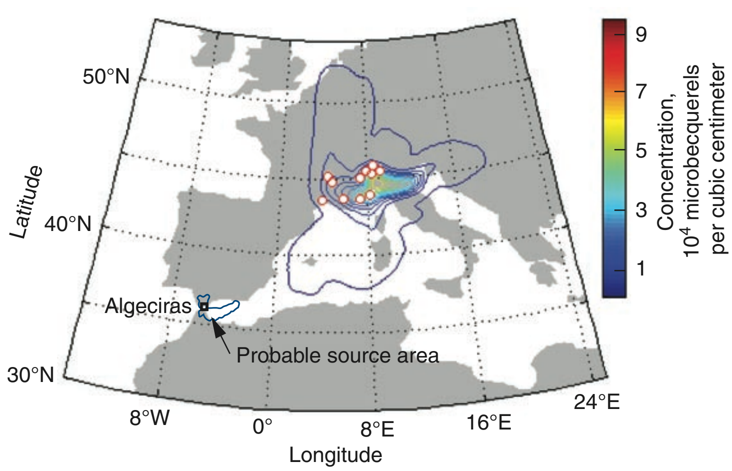
During many events, the greatest unknown factor is the source term: the data that define the physical and chemical properties of the airborne material, the quantity released, and the event's time and location. Fast answers about the source term can speed up emergency response, consequence management, and restoration activities. "The future for NARAC is improving the way we deal with unknown sources," says Livermore physicist Branko Kosovic.

Kosovic leads a team of NARAC researchers who are developing an event reconstruction methodology to estimate source terms and assess their likely impacts. Current methods for determining sources rely on first responders or analysts to estimate source characteristics, which are used as input to predictive models. (See the box on p. 17.) Because the variety and quantity of data available continue to increase during an airborne release, a high priority at NARAC is to develop a rigorous event reconstruction methodology that can take full advantage of incoming data.

The atmosphere is by nature chaotic. Sophisticated statistical sampling processes are required to model its unpredictable, nonlinear nature. Kosovic's team is developing an atmospheric event reconstruction framework based on a stochastic engine originally developed at Livermore to predict the behavior of subsurface contaminant plumes. (See *S&TR*, July/August 2002, pp. 21–23.) This methodology combines field measurements and model predictions via Bayesian inferencing and stochastic sampling to produce probabilistic estimates of unknown parameters. The development project was funded by the Laboratory Directed Research and Development (LDRD) Program and incorporated expertise from four Laboratory directorates.

This event reconstruction framework allows the use of multiple stochastic sampling algorithms and predictive models. In tests of the methodology, former postdoctoral researcher Tina Chow used FEM3MP and data collected during the Joint Urban 2003 field experiment in Oklahoma City to accurately reconstruct the source term and contaminant plume. With no prior information about the source location, the probabilistic computer calculations—called Markov chains—quickly focused on a half-block region containing the actual source location, as shown in the figure on p. 17, while simultaneously determining the approximate release amount. These results have been used to construct a "composite" plume showing the 90-percent probability level that concentrations exceed a given amount. Graduate student Stephanie Neumann and her colleagues performed a similar reconstruction using UDM.

The reconstruction methodology also was applied to an actual event involving a continental-scale release of radioactivity. On May 30, 1998, a piece of medical equipment containing cesium-137 was accidentally melted in a steel mill near Algeciras, Spain. The incident was first detected on June 1 and 2 by sensors in France and Italy. On June 9, the Swiss government announced that its national monitoring network had detected radiation levels up to 1,000 times background values. Because winds from the west drove the plume over the Mediterranean Sea, no Spanish sensors recorded the increased radioactivity. On June 10, the steel mill finally notified the Spanish Nuclear Security Agency that radiation had been detected in the mill's stack filters. Fortunately, none of the



With only a few measurements (red circles) from sensors more than 1,000 kilometers downwind from a 1998 cesium release, an event reconstruction model accurately predicts that the incident occurred at a steel-mill accident near Algeciras, Spain.

radioactivity levels recorded in Europe or near the source were sufficient to adversely affect the health of people or the environment.

In reconstructing this event, Livermore physicist Luca Delle Monache started with a possible accident domain that reached from northern Africa to well north of Scotland, an area extending 1,800 kilometers east to west and 3,600 kilometers north to south. The predicted source locations defined by the NARAC simulation cluster near the actual source. Says Delle Monache, "If these tools had been available in 1998, we could have provided predictions to authorities three days after the accident and helped pinpoint the release."

Upping the Physics Ante

Several NARAC projects focus on increasing the accuracy of physical models in existing dispersion codes. In a major DOE initiative, NARAC/IMAAC associate program leader John Nasstrom is working with physicists Kevin Foster and Ted Harvey to develop a nuclear fallout model that accounts for the complex patterns of wind flow and terrain. The model

Operational Event Reconstruction

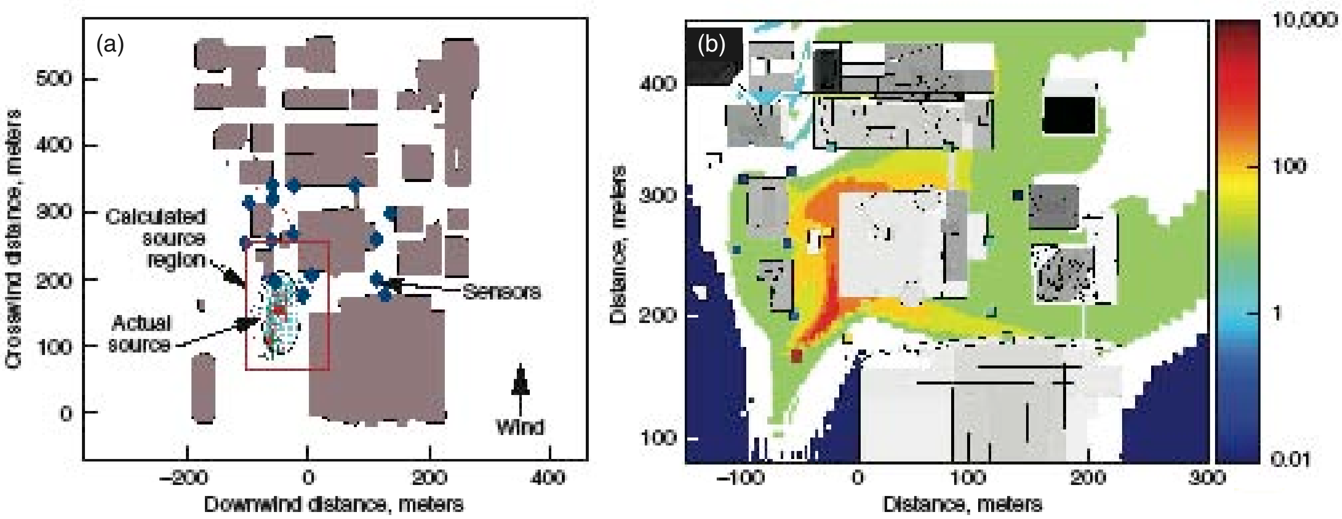
Gayle Sugiyama, the program leader at the National Atmospheric Release Advisory Center (NARAC), is particularly proud of her team's performance at the most recent Top Officials (TOPOFF) Field Exercise. The TOPOFF3 exercise, held in April 2006 at the New London City Pier in Connecticut, involved more than 10,000 participants representing over 200 federal, state, local, tribal, private sector, and international organizations as well as volunteer groups—all responding to multiple simulated large-scale terrorist attacks.

TOPOFF3 started on April 4 with the simulated explosion of a truck bomb near a large public gathering at the pier. Twenty minutes after the explosion, the Department of Homeland Security's Interagency Modeling and Atmospheric Assessment Center (IMAAC) was asked to analyze the source for the release. Mustard gas was used as a possible release agent, based on intelligence reports that terrorists might be developing chemical agents in the New England area.

As additional information on the size of the bomb arrived, Livermore team members concluded that the explosion was so large, it would have destroyed most of the mustard gas carried by a truck. However, reports from the field cited casualties with symptoms for a blister agent. In looking for other potential sources, analysts found that a low-flying plane had been observed over the pier more than two hours before the truck bomb.

The NARAC team generated a new analysis for IMAAC showing that the amount of material a small plane could carry was consistent with the number of casualties. Just before nightfall, IMAAC received an initial set of deposition measurements, and the NARAC team used these data to predict the plane's flight path and the amount of material released.

"That night and the next day, we were continually given misleading information," says Sugiyama. "Several agencies insisted the truck bomb was the source for the blister agent. But our analysis confirmed that a release from the aircraft was the only plausible source. Our scientists stood by their analysis." On day 3, a full set of field measurements confirmed the team's conclusions and showed that predictions made on day 1 were within 10 percent of the correct quantity.



A stochastic algorithm and the computational fluid dynamics code FEM3MP are being used together for event reconstruction. To test the model's accuracy, researchers ran simulations using data from the Joint Urban 2003 exercise in Oklahoma City. The model (a) successfully identified the half-block area (black oval) that included the actual source location (red square) and (b) produced the composite plume showing concentrations with a 90-percent probability of occurrence.

predicts not only gross radioactivity but also specific nuclides, and it can simulate multiple weapon bursts as well as global transport of radioactive materials.

Another research effort incorporates the effects of rain on an atmospheric dispersion. Raindrops grab dispersed particles and deposit them on the ground, a process called precipitation scavenging. Scavenging creates hot spots of deposition, a phenomenon seen after the Chernobyl accident. NARAC's models now incorporate spatially varying precipitation based on weather forecast data and the intertwining effects of raindrop and particle size. Says Loosmore, "The next step for even greater accuracy will be to use precipitation data directly from a live weather radar feed, when it is available."

Until recently, NARAC's workhorse codes have been limited in their ability to model the interaction of chemical or biological agents with the atmosphere. For example, when the nerve gas sarin meets naturally occurring hydroxyl radicals (OH) in the atmosphere, OH grabs hydrogen atoms to create water (H_2O) and in the process destroys the sarin. Because the destruction is cumulative, the effect of the chemical reactions increases as the plume ages. The net effect could thus significantly decrease the area at risk. OH is not an abundant molecule in the atmosphere, but its high reactivity makes it an important component for atmospheric chemistry.

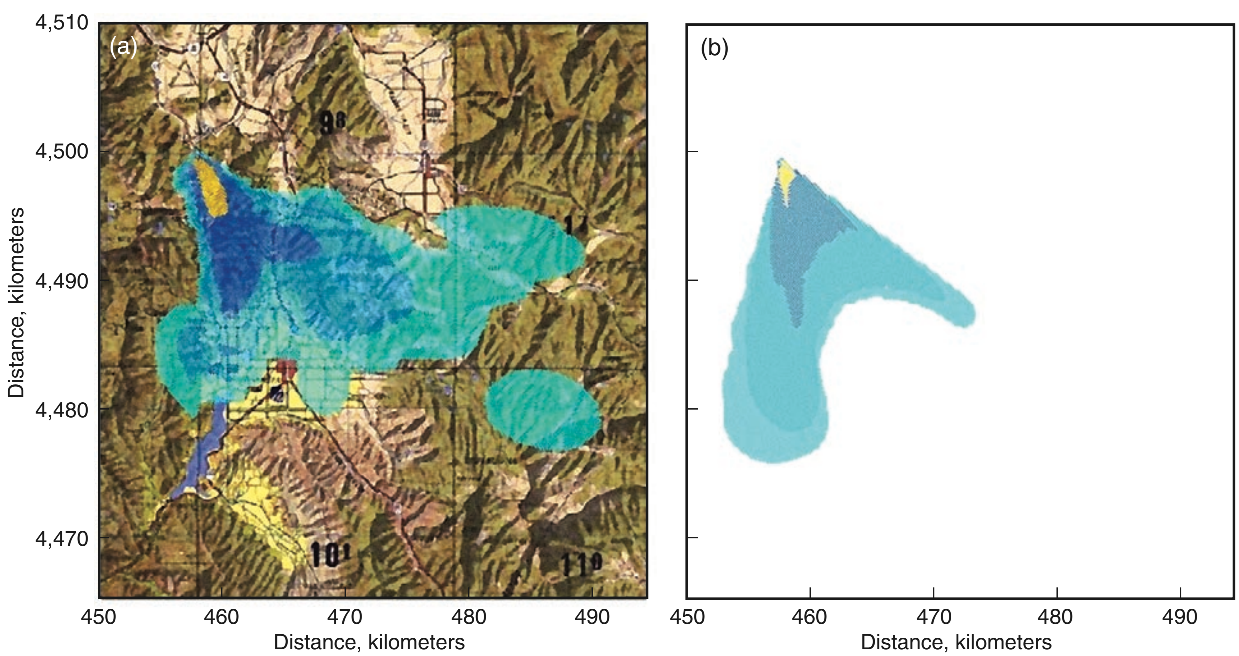
"Chemical changes during a dispersal are important for first responders," says atmospheric chemist Philip Cameron-Smith. "With more accurate plume predictions that consider atmospheric chemistry, the area to target with an antidote is much smaller."

Another project, which started with LDRD funding, is an effort to model high-altitude dispersion from a warhead carrying a biological or chemical weapon. Now funded by the Defense Threat Reduction Agency, this research is combining high-altitude weather data from the National Aeronautics and Space Administration (NASA) with NARAC's dispersal codes to improve the accuracy of the simulation results. The model also takes into consideration the rarefied physical environment at high altitudes.

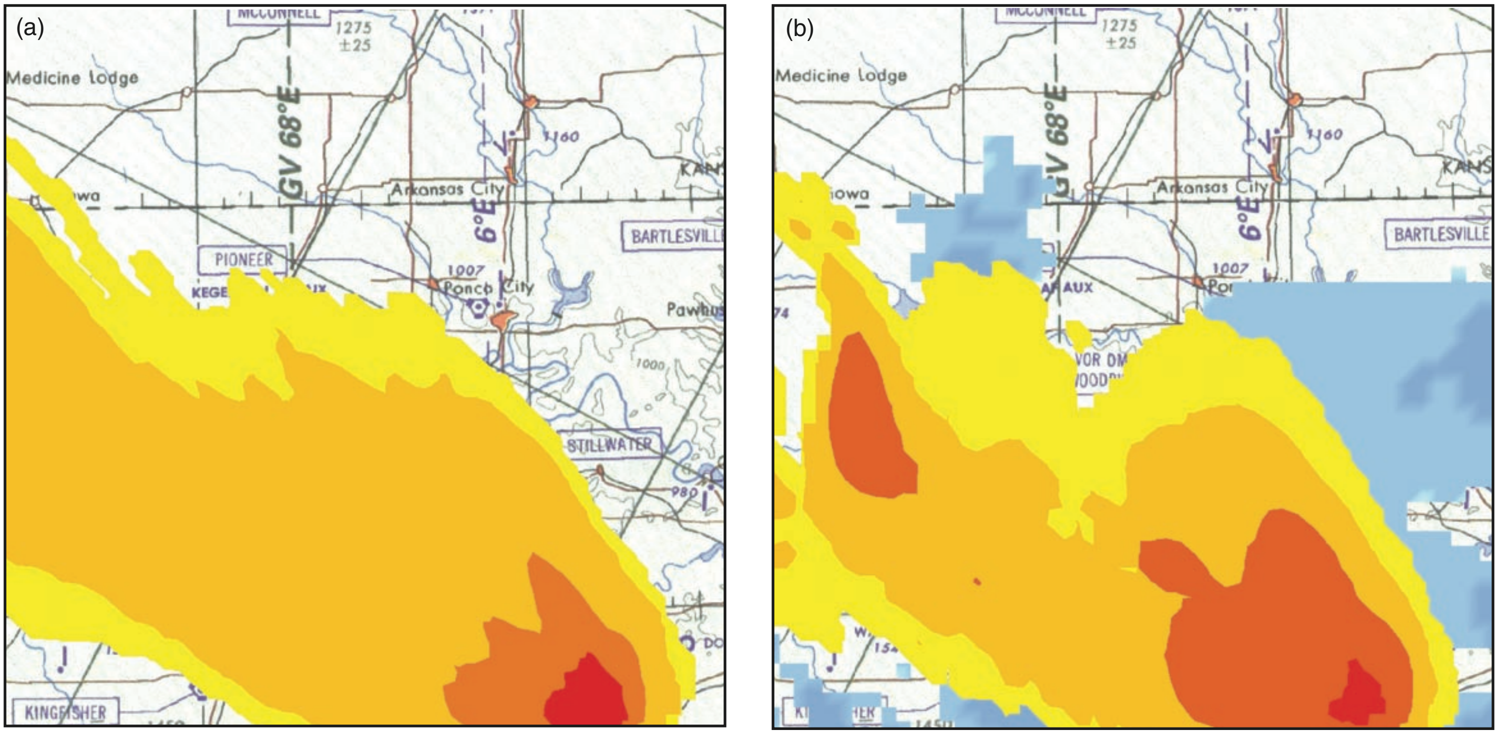
Future of NARAC Science

Several projects just getting started will improve NARAC predictions and the services provided to IMAAC. Lundquist will soon begin working with collaborators at NASA to obtain data from satellites about Earth's surface roughness. The land surface—grassy fields, a dense forest, small or large cities, lakes—significantly affects winds, turbulence, and plume dispersion. With improved roughness data, models can more accurately predict the spread and trajectory of hazardous plumes.

Loosmore is responsible for two new projects that will improve the center's operational codes. One effort involves the resuspension of particles. Biological agents and radioactive particles deposited on a surface may be returned to the atmosphere if, say, a car drives by. Resuspension can further spread contamination, resulting in new opportunities for exposure. The resuspension process is notoriously difficult to model because of the complex



(a) An updated model for fallout from nuclear explosions produces more accurate results than (b) the existing operational model.



Including precipitation data in dispersion models improves the accuracy of predictions. (a) With constant rainfall at 30 millimeters per hour, the model produces relatively uniform contours of the predicted ground deposition, which ranges from red (highest) to yellow (lowest). (b) When high-resolution precipitation data (blue) are included in the calculation, the model predicts that deposition hot spots will occur in several areas.

turbulence and chemistry that occur where particles meet the atmosphere.

Her second research effort is an LDRD project focused on incorporating the properties of heavier-than-air gases such as chlorine into FEM3MP simulations of dispersions in urban areas. "Dense gases typically reduce turbulence while buildings increase it," says Loosmore. "Our challenge is to determine how these competing effects work together."

A team of researchers is also enhancing FEM3MP to simulate how different material surfaces and sun versus shade affect bioaerosol degradation and viability. For example, particles will be quickly destroyed if they are deposited on a window in direct sunlight. In contrast, particles that stick to stucco in the shade will remain viable longer. To improve the nation's response capabilities, DHS needs models that accurately predict the sampling required to characterize the extent of contamination following a biological attack in complex urban environments. Such a capability would reduce the time and expense of restoration efforts.

NARAC models and the services provided for IMAAC are being incorporated into other operational systems for detection, warning, and incident characterization. In the future, researchers hope to couple operational models with epidemiological models and data on public health and water-borne hazards. As advances in these many projects are made, NARAC can only get better at protecting the public.

—Katie Walter

Key Words: airborne toxic release, atmospheric chemistry, computational fluid dynamics (CFD), event reconstruction, fallout model, FEM3MP, Interagency Modeling and Atmospheric Assessment Center (IMAAC), National Atmospheric Release Advisory Center (NARAC), precipitation scavenging, urban-scale dispersion model, Weather Research and Forecasting (WRF) model.

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