Dispersion of Biological Warfare Agents in Attack Zones

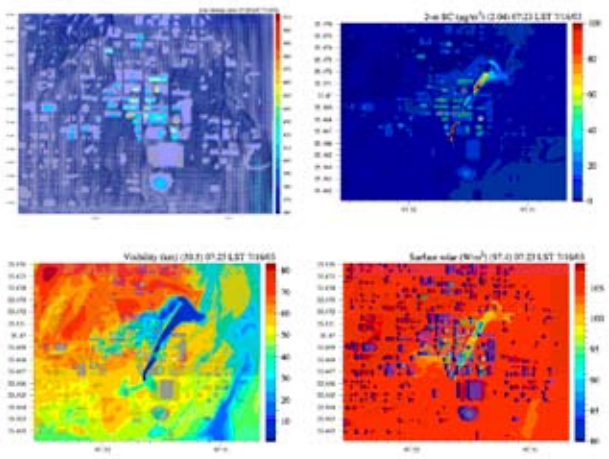
The alert call comes in at the emergency response center. A high concentration of an infectious virus has been detected in the air near a large urban area, possibly as the result of a deliberate hostile act. Which neighborhoods and how many should you evacuate, and how much time do you have? When your organization makes disaster response plans, how will you decide what medical supplies to stockpile and how much?

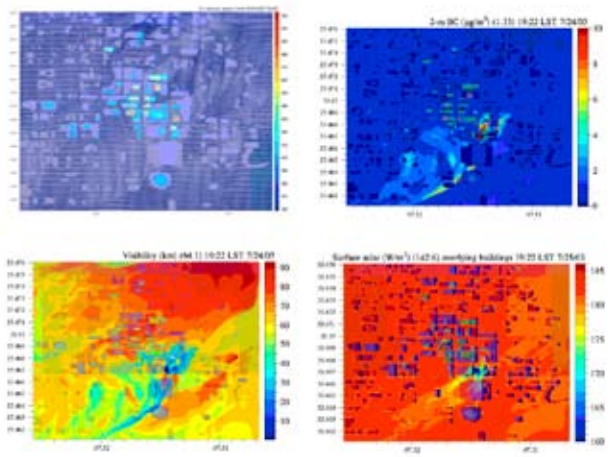
AHPCRC researchers from Stanford University are tackling these questions using high performance computing to create realistic simulations of hypothetical biological weapon agent (BWA) release scenarios. The team consists of Mark Jacobson (professor of civil and environmental engineering, professor by courtesy of energy resources engineering), Gianluca Iaccarino (assistant professor of mechanical engineering, Institute for Computational Mathematical Engineering), and Eric Shaqfeh (professor, chemical and mechanical engineering, ICME). Gerard Ketefian (postdoc under Jacobson), David Richter (Ph.D. student under Shaqfeh), and David Woodbury (undergraduate student under Iaccarino) also contribute to the research.

The Stanford team is developing a computational framework for modeling the dispersion of particles, from a few nanometers to more than 100 micrometers across, in a turbulent air flow. This computational framework will be used to predict the dispersion of aerosolized BWAs during various indoor or outdoor attack situations. The team has briefed several ARL scientists at the Natick Soldier Systems Center on their results to date. In addition, they have an ongoing interaction with researchers at the U.S. Army Edgewood Chemical and Biological Center and the Army Research Laboratory at Adelphi, Maryland.

Two Scales

Realistic large-scale or long-term release simulations using engineering models and incorporating motion at all scales is currently outside the reach of even the largest available computers. The team is addressing this problem by developing parallel DNS (direct numerical simulation) and LES (large eddy simulation) codes describing the dispersion of rod-like, flexible, or spherical particulate BWAs—including aerosolized organisms or protein toxins—in complex urban environments. Their models will simulate contaminants spreading through volumes of 30–50 cubic meters, about the size of a single room, to begin with. Subsequently, the additional integrated RANS (Reynolds-averaged Navier–Stokes) code will enable complete simulation, including atmospheric interactions, through large-scale spreading over 10–100 square kilometers.





Simulations for downtown Oklahoma City, 2003. Above, clockwise from top left: Wind velocity at 2m elevation, black carbon tracer concentration, surface solar radiation, and visibility for 07:23 LST, 16 July. Below: The same parameters for 19:22 LST, 24 July. All graphics courtesy M. Jacobson, G. Iaccarino, Stanford University.

The goal is to perform computations that include the details of the topographic map of the geographic region of interest, while preserving the small-scale motion and mixing in the region of the release. This multi-scale problem is being tackled using two main simulation codes. A large-scale atmospheric code, with resolution ranging from 10–50 m up to a global scale, is used to study the long-time and large-scale evolution of the plume and its interaction with atmospheric agents. A high-fidelity fluid-dynamic dispersion code predicts the dispersion dynamics in the vicinity of the release (0.1–50 m).

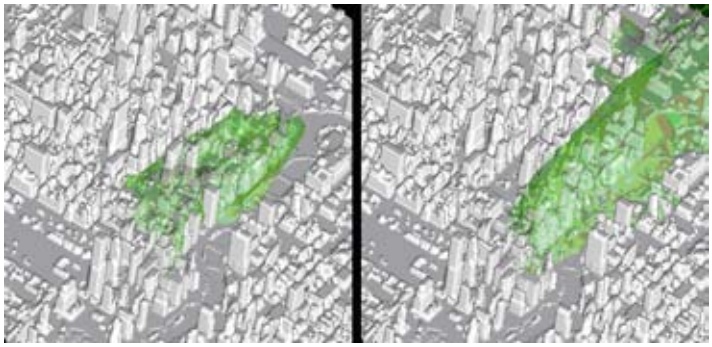
The fluid-dynamic dispersion code models the initial dynamics that are strongly affected by the precise release location, concentration, and type of agent, to determine the formation of a release cloud at a scale of 10–25 m. This information is then passed to the large-scale code, which models the evolution of the release over long periods of time. The large-scale code also provides atmospheric boundary conditions (e.g., wind speed and direction, thermal flux) for use in the small-scale code.

The Windy City

The Stanford group began with a model of downtown Chicago, a city that is already well characterized as the result of extensive modeling studies. They analyzed scalar transport and dispersion using their Chicago model and simulated a BWA release for two Chicago locations, in preparation for a grid refinement study to verify the sensitivity of the scalar concentration maps up to 12 minutes after the release.

Although the two release locations in the model were less than 200 m apart, the dispersion patterns are distinctly different *(see figure at right)*. In the simulation, high-speed wind channeling along the Chicago River entrained a contaminant plume and caused a fast release in the downstream city blocks. This effect was not observed farther from the river, where closely spaced tall buildings served to disrupt the flow.

The group was able to produce detailed maps of thermal heating (from sunlight) and wind speed and direction using the simulation code.



Simulations for downtown Chicago, 12 minutes after plume release, 30 m above the ground. The two locations are less than 200 m apart, but the plume on the right follows the channel of the Chicago River, while the plume on the left is farther inland.

Within the same computational infrastructure used for the Chicago simulations, the group is developing a model for fluids that do not have one constant value for viscosity, with the intent of representing rodlike and particulate BWAs. The group is modeling the effects of long elastic chains (such as polymers or proteins) in fluids, drawing on a large body of existing literature and computational resources. Their model is now fully functional, and it produces valid results for flow conditions that are more laminar than turbulent. Future work will test the limits of the range of turbulence and shear conditions for which the model is valid. The group will also incorporate nonhomogeneous concentration effects into the model.

Real-World Data from Oklahoma City

More recent simulations *(see figures, page 2)* focus on downtown Oklahoma City, the site of the July 2003 Joint Urban Atmospheric Dispersion Study (http://ju2003.pnl.gov). This study, cosponsored by the U.S. Department of Energy, Department of Homeland Security, and the Department of Defense's Defense Threat Reduction Agency (DTRA), featured ten releases of nontoxic sulfur hexafluoride gas and three types of nontoxic perfluorocarbon tracer gases in and around Oklahoma City buildings. This was the largest-ever U.S. urban atmospheric study, involving 150 scientists, engineers, and student assistants, 200 wind measurement stations, and 200 sampling stations.

continued on page 4

Dispersion of BWAs in Attack Zones

continued from page 3

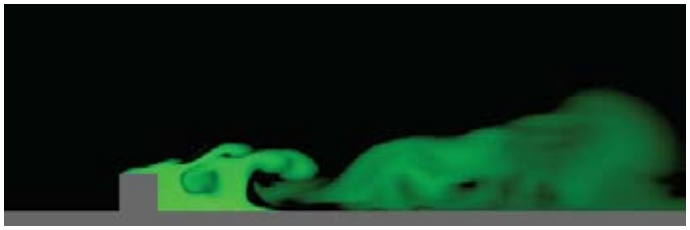
The Stanford group's 20-minute numerical simulations (*box, below*) showed that the direction and intensity of the wind have a profound effect on the flow characteristic in the region of the release. The calculations tracked the spread of a simulated black carbon tracer, under conditions replicating those for the real-world study. The simulated tracer was released at the same location for both simulations, under early-morning and late-afternoon conditions, with the wind shifting to the opposite direction from one simulation to the next. The simulations demonstrated the influence of the tracer plume on visibility and surface solar radiation.

Wind field data from the large-scale model was used to initialize the high-resolution computational fluid dynamics model.

The group continues to validate their computational tools using the Oklahoma City data. They intend to demonstrate the applicability of both the large-scale atmospheric code and the high-fidelity small-scale tool as applied to this problem, and to develop the capability to transfer information between the two codes to accurately predict both the detailed initial release and the long-term behavior of the agent release.

Studying the Wake

In a second area of this project, the research group has performed a detailed study of the dispersion effects downstream of an elongated obstacle, such as a building. This area of work will support the small-scale, high-resolution calculations that predict flows around and over objects of arbitrary shape (e.g., buildings).



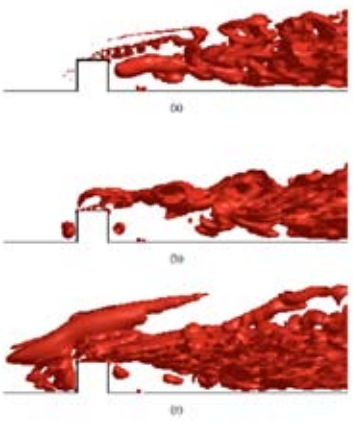
Two-dimensional simulation of turbulent flow in the wake of a building.

In this case, the high-fidelity code is used with highly refined grids, and the results are compared to existing detailed experimental measurements. The numerical simulation agrees exceptionally well with the mean flow measurements, the turbulent fluctuations, and the transported scalar statistics.

Additional simulations using low-fidelity Reynolds-averaged models illustrate the limited predictive capabilities of these schemes. The predictions for scalar and recirculation bubble concentrations, vary significantly, depending on the type of model used.

At present, the Stanford group is completing an investigation of the detailed dispersion downstream of the obstacle to identify the importance of large-scale three-dimensional effects *(see figure below)*.

In addition to the simulations, the Stanford team is developing a new computation flow code that will be the first to conserve a combination of properties, including potential enstrophy, vorticity, energy, and mass, when arbitrary boundaries are treated. This capability facilitates model-building by specifying which aspects of a system change and which remain constant.✯



3D turbulent flow simulations. Top: inflow fluctuations ignored. Middle: random inflow fluctuations imposed. Bottom: force with most unstable modes.

Oklahoma City Simulations

The Stanford team ran two simulations for virtual black carbon tracer plumes emitted from the same downtown Oklahoma City location. One simulation replicated the conditions for July 16, 2003 at 07:00 LST and the other for July 25, 2003 at 17:00 LST. The wind blew in opposite directions on these two days. (LST, local sidereal time, denotes the position of the sun in the sky rather than the local time zone.)

The simulations were done on four size scales: global (4 degrees latitude × 5 degrees longitude resolution), U.S. (about 50 km resolution), Oklahoma (120 m S–N × 120 m W–E × 20 m vertical resolution), and Oklahoma City (12 m S–N × 12m W–E × 20 m vertical resolution).