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1. INTRODUCTION

Operational systems predict the consequences of atmospheric releases of hazardous materials for real-time emergency response, pre-event planning, and post-incident assessment. Such systems provide federal, state, and local agencies, emergency planners and responders, public health officials, military personnel, and other users with critical information on which to base life-and-death decisions on safe zones for siting of incident command posts, sheltering-in-place or evacuation advisories, the need for protective equipment, and the utilization of hospital and health care resources.

A range of operational modeling capabilities is required to support different types of release events, distance scales, and response times. Fast-response deployable models are used to perform hazard assessments and initial response functions, and can serve as a backup when connections to a reach-back center are not available. Higher-fidelity three-dimensional dispersion models, coupled to real-time observational data and numerical weather prediction model output, are used for real-time response and support expert quality-assured predictions and refined assessments. Computational fluid dynamics models, which explicitly resolve urban structures, are used for high fidelity applications including vulnerability analyses and planning studies.

This paper will briefly discuss the types and capabilities of models used or under development for emergency response systems, customer products, supporting data, and a few representative examples of operational systems. Some selected research priorities are summarized in the final sections.

2. EMERGENCY RESPONSE MODELS

Models of atmospheric transport and dispersion must incorporate knowledge of:

- the physical properties of the airborne material
- the release mechanism (geometry, time-varying release rate, dynamic processes)
- complex meteorological conditions (including spatial and temporal variations) and
- the characteristics of the terrain and structures surrounding the release location.

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2.1 Regional-Scale Dispersion Models

Dispersion models simulate mean wind advection, turbulent diffusion, wet and dry deposition, gravitational settling, degradation and production processes (e.g. radiological decay chains, chemical reactions, biological viability).

Gaussian models (plume and puff) have undergone extensive development. Gaussian plume model are attractive for their relative simplicity of mathematical formulation (analytic expressions), limited input parameter requirements, and computational speed. Such models can be reasonably reliable in situations involving simple flows, such as unidirectional steady-state flow over relatively flat terrain, and have been used with some success in rural settings. They are also often used to determine long-term average concentrations for regulatory applications.

While most analytic models in common use assume constant wind and turbulent diffusivity values, resulting in a Gaussian concentration distribution, some models incorporate an analytical solution to the advection-diffusion equation that accounts for vertical variations in the mean wind and diffusivity. This results in more realistic non-Gaussian vertical concentration distributions. Gaussian puff models can incorporate temporal, horizontal, and vertical variations in meteorological conditions. Such models can be used over a larger range of distances and scales.

Lagrangian models (puff and particle) provide more detailed resolution of boundary-layer processes and dispersion. The advent of efficient numerical modeling techniques and improved computational performance have made these models accessible to the general user community. Lagrangian puff dispersion algorithms represent concentration distributions as overlapping Gaussian distributions. Lagrangian particle models use Monte Carlo methods to simulate the dispersion of fluid marker particles.

2.2 Source Models

Initiation of a dispersion simulation requires the specification of the material type, quantity, release duration, and various physical/chemical properties (e.g., particle size distribution, molecular weight). Source models provide the (time-varying) spatial distribution of source material (e.g., point, line, volume) and the total source mass (or activity) emission rate. For aerosol sources, the mass or

activity distribution is needed as a function of particle size.

Dynamic source models are needed to simulate buoyancy- or momentum-driven plume rise from continuous sources such as fires or stack emissions, cloud rise from quasi-instantaneous explosive sources, and some types of weaponized releases. Specialized source models are provided by the Nuclear Regulatory Commission for radiological releases based on knowledge of the operating conditions at nuclear power plants. The CAMEO/ALOHA system (see below) has extensive source and material databases for toxic industrial chemical (TIC) releases.

For initial response to real-world events when minimal information is available, pre-defined source terms are needed which provide the user with reasonable defaults (including best-case, most likely, and worst-case scenarios) to initiate an atmospheric dispersion simulation. These pre-defined source terms should represent plausible airborne release scenarios, which can be selected based on observable conditions (e.g., sprayer or tank size, explosive damage, etc.)

2.3 Meteorological models

Gaussian plume models typically use only a single constant wind velocity and stability class to parameterize turbulence diffusion. Such models are therefore valid only over distance and time scales for which this representation is adequate.

Diagnostic meteorological models derive mean wind, turbulence, and other variables at specified times from observational data and land-surface characteristics via a combination of interpolation, extrapolation, and similarity-theory parameterizations. Such models are commonly used for emergency response applications, due to their capabilities for ingesting real-time observational data and their computational speed. Diagnostic models incorporate terrain and atmospheric stability effects via a variational adjustment process, which enforces mass-conservation. Land-surface characteristics and surface heat and momentum fluxes can be used to diagnose horizontally-averaged properties of the mean wind and turbulence.

Many emergency response systems acquire numerical weather prediction (NWP) model output (providers include the National Weather Service, the Fleet Numerical Meteorological and Oceanographic Center, and the Air Force Weather Agency) and/or run in-house versions of these models. NWP models forecast the time evolution of the flow field by solving the nonhydrostatic, compressible form of the dynamical equations. The models incorporate relevant physical processes such as explicit moist physics, cumulus convection, and radiation, as well as parameterizations for subgrid-scale mixing (Figure 1).

Most current emergency response modeling systems drive dispersion models with weather forecast model output, rather than directly integrating dispersion processes into NWP models. This allows relatively rapid hazard predictions to be made for multiple scenarios based on the same meteorology.

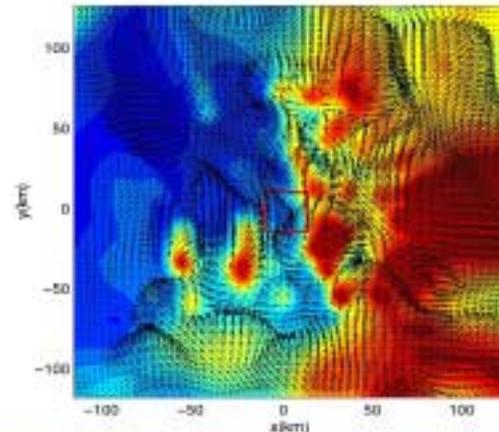


Figure 1. Example of NWP model output of winds from a simulation of the Salt Lake City basin (colors indicate terrain elevations).

2.4 Urban Models

The urban environment poses unique challenges for emergency response modeling. Detailed examination of flow in urban areas reveal the development of separation and stagnation zones around buildings, turbulent wakes and vortices, interacting wake regions from neighboring structures, and street canyon channeling.

A variety of models are being developed for simulating the complex behavior of flow and dispersion in the urban environment. Empirical urban models are derived from wind tunnel and field experiment data. Canopy parameterizations simulate the area-averaged effects of metropolitan areas, while computational fluid dynamics (CFD) models explicitly resolve the effects of individual buildings.

Rotach (1997) proposed a simple diagnostic parameterization, which incorporates the overall reduction of the mean velocity and the increased turbulence in the urban roughness sublayer. Hanna and Britter (2002) have developed parameterizations of the spread of pollutants within the urban canopy as a function of urban morphology parameters and observed meteorological data.

Urban canopy parameterizations have been developed for numerical weather prediction models, which incorporate the effects of drag, turbulent production, anthropogenic and rooftop heating, and radiation balance terms. Such models have been shown to improve the representation of urban flow

fields. However, canopy models cannot capture features caused by individual obstacles.

An example of an empirical modeling approach which explicitly incorporates building effects near the release site is provided by the Urban Dispersion Model (UDM). The UDM is an empirical Lagrangian puff model (Griffiths, 2001), which models interactions between puffs and obstacles explicitly, when the puff is of roughly comparable size to or smaller than the obstacle, using a simple procedure. In the urban-array region, where groups of obstacles are too close together to be considered individually, the dispersion is Gaussian (when averaged over time) with the bulk characteristics of the surface obstacles determining the rates of dispersion.

CFD models provide the highest fidelity transport and diffusion simulations (Figure 2). Such models solve the full 3-dimensional Navier-Stokes fluid dynamics equations together with appropriate physics submodels, for turbulence, radiation, surface heat budgets and other processes affecting the airflow. The resulting meteorological fields are used to drive solutions to the conservation-of-species equation using either steady-state conditions based on the Reynolds-Averaged Navier-Stokes (RANS) approach or via a coupled system using the time-dependent large-eddy simulation (LES) approach.

While CFD models are computationally expensive compared to Gaussian or Lagrangian models, the cost is repaid by the generation of significantly more detailed model data. CFD models are able to capture transient phenomena, such as plume arrival and departure times and peak concentrations. Accurate knowledge of peak concentrations is critical for determining the impacts of many chemical releases, for which the health effects depend on instantaneous or short-term peak exposures rather than the time-integrated dose.

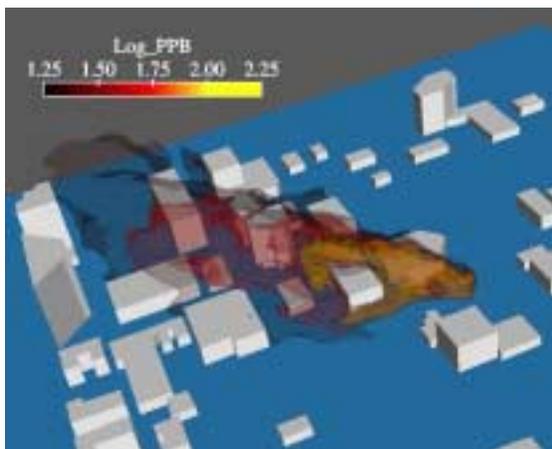


Figure 2. Example of a CFD model simulation of contaminant concentrations for building-scale urban applications.

2.5 Indoor Models

At any given time, the majority of the population may be indoors. Since indoor and outdoor concentrations can differ significantly, quantitative predictions of the indoor exposures resulting from outdoor releases are critical in determining whether occupants are safer evacuating or sheltering in place. Building infiltration models (Chan et al., 2004) are being developed for both residential and commercial buildings, by coupling outdoor plume models with building air exchange rates. For residential buildings without special provisions such as safe rooms, a simple well-mixed box model in which the indoor concentration is assumed to be spatially uniform provides an adequate representation. For larger houses and commercial buildings, multi-box models will be needed, as well as detailed knowledge of the air circulation and HVAC systems.

Multi-zone models predict steady-state airflows and the dynamic transport of pollutants indoors by representing the building as a collection of well-mixed zones (Feustel, 1990). Such models have been used to predict airflow and gas transport in multi-story, low- and high-rise residences, small office buildings controlled experimental test houses and single-family houses (see Sextro, 1999, and references cited therein). CFD models are under development for the simulation of airflow in large indoor spaces (e.g. auditoriums).

Specialized systems are being developed for interior infrastructure protection (e.g., airports, subways) against chemical/biological (CB) incidents. The PROTECT WMATA subway crisis management system includes facility hardening, detection, emergency management information systems, transport modeling (using a subway piston model coupled to atmospheric plume models), engineering countermeasures, decontamination, and emergency response (Policastro et al., 2003). This system is operational in a multi-station/tunnel system in the Washington D.C. subway system.

2.6 System and Model Evaluation

Emergency response modeling systems must be extensively validated using analytic benchmark cases (evaluation of numerical models with known, exact mathematical solutions), tracer field experiments (evaluation under real-world conditions), and operational use (testing of modeling system usability, efficiency, consistency, and robustness). Two key new data sets are being provided by the DOE's VTMX and URBAN 2000 Salt Lake City tracer experiment and the recently completed Joint Urban 2003 field study in Oklahoma City, supported by DTRA and DOE/DHS.

3. CUSTOMER PRODUCTS

Dispersion models predict quantities such as the time-integrated or time-averaged air concentrations,

peak concentrations, and deposition. These quantities must be converted into products useful to emergency responders (Figure 3), including maps of plume hazard areas, affected populations, health effect risk levels, protective action guidelines, and geographic data (maps, terrain, aerial photography). Other potential value-added information include wind observations (barbs) and/or model wind field plots.

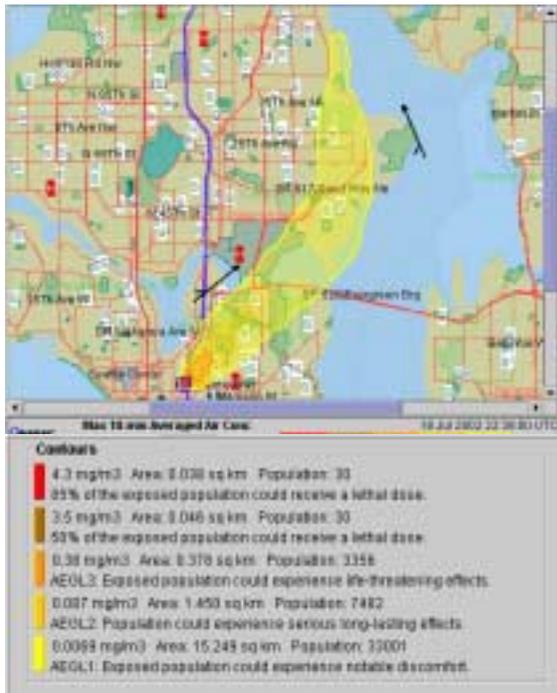


Figure 3. Example of customer value-added products, including plume, geographic data, health risk level, and affected population.

Most emergency response systems provide deterministic best estimates, sometimes generated with conservative modeling assumptions. Uncertainty quantification would enable decision makers to understand the likelihood of an event, to evaluate the potential need for additional real-time data acquisition and updated simulations, and to form contingency plans.

Uncertainty estimation for simulations of a complex, time-dependent system is a new and ambitious endeavor, which will require the exploration of a variety of methods. A full uncertainty analysis of a release event would take into account the uncertainties in all input parameters (e.g., the meteorological fields and source attributes), incorporate the sensitivity of the model outcomes to those parameters, and produce quantitative uncertainty ranges on output results of interest. Methods must also be developed for interpreting and presenting uncertainty estimate and guidance to users and responders.

Monte Carlo analysis builds a probability distribution for predictions from a suite of model runs, generated from a randomly sampled set of input variables. Statistical goodness-of-fit tests can then be performed to determine the best model predictions using available measurements. Response surface methodology (RSM) also builds uncertainties from a suite of runs, but utilizes classical experimental design theory to generate the inputs for the event simulations. Given the natural atmospheric stochasticity and the discontinuous aspect of complex terrain in many locations, bifurcation analysis may be necessary.

Sensitivity analysis decouples input uncertainty from model processes algorithms to provide an understanding of the sensitivities of model outcomes to the input parameters. Computed sensitivities can be re-coupled with input uncertainties to quantify prediction uncertainty.

4. SUPPORTING DATA AND TOOLS

Emergency response systems require access to a variety of meteorological data. National or global multi-purpose operational systems maintain robust, redundant automated real-time meteorological data acquisition systems, which provide real-time access to observational data and/or a variety of numerical weather prediction model output (global, mesoscale, local, and urban).

Operational systems also require extensive global databases of geographical, land-use, source term, dose response, population, and critical facility information. For urban modeling, building databases and processing tools need to be developed to support efficient grid generation.

5. OPERATIONAL CAPABILITIES

A number of operational emergency response systems exist to serve a variety of sponsors and customers. A few representative examples of nationwide capabilities are outlined briefly below. A more complete set of capabilities is provided in publications from the Office of the Federal Coordinator for Meteorological Services and Supporting Research (OFCM, 2002) and the National Research Council (NRC, 2003).

5.1 DOE/DHS

The National Atmospheric Release Advisory Center (NARAC) is a Department of Energy (DOE) and Department of Homeland Security (DHS) asset (see <http://narac.llnl.gov>). NARAC includes deployable Gaussian plume models for rapid-response and hazard assessment (HOTSPOT, EPICode), the core operational regional-scale models ADAPT (diagnostic data assimilation model), LODI (Lagrangian particle dispersion), and an in-house urbanized version of COAMPS (the Naval Research

Laboratory's numerical weather prediction model). The system also supports specialized models (e.g., nuclear blast and fallout) and a computational fluid dynamics model for building-to-urban scale simulations. NARAC's modeling capabilities (Nasstrom et al., 2000; Sugiyama et al., 2002) are supported by a real-time meteorological data acquisition system and extensive global databases of geographical, land-use/land-cover, source terms, dose response, and population information. Users request, view, and distribute NARAC predictions through the *NARAC iClient* and the newly developed *NARAC Web* software.

On-duty or on-call operational and technical staff are available 24x7 at Lawrence Livermore National Laboratory (LLNL). NARAC currently supports on the order of 5-10 alerts and emergencies, 100 interactive exercises, and 2000 automated responses each year. It is expanding its user base to support a wide variety of local, state, and federal agencies. NARAC currently is working with over 80 *iClient* users and over 300 Web users in 13 states. Under the Department of Homeland Security (DHS) Local Integration of NARAC with Cities (LINC) program, pilot projects are underway in Seattle, New York City, Albuquerque, Fort Worth, and Cincinnati to integrate NARAC capabilities with local emergency management agencies and responders. As part of this program in 2003, NARAC supported a major national exercise (TOPOFF2 in Seattle) and the real-world Staten Island barge fire in New York City.

NARAC directly supports the DOE/DHS regional and national Nuclear Incident Response Teams (NIRT), and the Federal Radiological Monitoring and Assessment Center (FRMAC). As part of this effort, NARAC is integrated with operational capabilities provided by other DOE laboratories, including Sandia National Laboratories, the Remote Sensing Laboratory, and Los Alamos National Laboratory.

5.2 DTRA/DoD

The Hazard Prediction and Assessment System (HPAC) was developed by the Defense Threat Reduction Agency (DTRA) to predict the effects of hazardous material releases and collateral effects on military and civilian populations. HPAC is a stand-alone PC based system designed to support the warfighter in battlefield situations. HPAC integrates source term models, weather data, terrain and land-use data, with material transport algorithms. The core HPAC model is the Second-order Closure Integrated Puff Model (SCIPUFF), which provides predictions of both the average concentration as well as the statistical variance resulting from random fluctuations in the flow field. An urban version of HPAC is scheduled for release in the near future, which contains both empirical and simplified (drag representation) CFD models.

Other DoD models include the U.S. Navy's VLSTRACK model, which provide hazard predictions for chemical and biological (CB) agents and a wide

variety of CB munitions. The Joint Effects Model (JEM) is currently under development to provide a unified Department of Defense model.

5.3 NOAA/EPA

The CAMEO/ALOHA system, developed jointly by the NOAA Ocean Service's Office of Response and Restoration and the Environmental Protection Agency (EPA), is a widely-used first responders' toxic industrial chemical emergency response modeling capability (see <http://response.restoration.noaa.gov>). The system provides an extensive chemical property database and source term models for a variety of chemical releases (broken pipelines, leaking tanks, evaporating pools, etc.), coupled to a Gaussian plume model.

The NOAA Air Resources Laboratory (ARL) and the National Weather Service (NWS) provide simulations of the transport and dispersion of pollutants using the hybrid Eulerian and Lagrangian model, HYSPLIT, coupled to NWP model output, such as the 12-km NWS ETA model. HYSPLIT is run in both automated and on-demand modes. The NOAA ARL READY web site provides access to NWP model data and HYSPLIT simulations (see <http://www.arl.noaa.gov/ready>).

6. DATA-MODEL INTEGRATION

An emerging aspect of emergency response is the importance of methods for incorporating measurement data into predictions and analyses. Data-fusion products provide situation awareness analyses by interpretation of available data. Data assimilation directly incorporates data into models.

6.1. Meteorological data assimilation

The accuracy of predictions of the consequences of NBC release events can be dramatically improved by incorporating higher resolution, more representative meteorology from observational data obtained from local observational networks (mesonets), radar-derived precipitation, and satellite analyses of winds, temperatures, and clouds. The development of variational or related methods for analyzing remote sensing data from lidars, wind profilers, radar, and/or sodar provides more realistic detailed 3-D estimates of the urban wind field, turbulence, and mixing layer depth—the critical parameters in determining atmospheric transport of hazardous materials. Numerical weather prediction models typically incorporate either 3-D or 4-D variational data assimilation algorithms to incorporate observations.

6.2 Event reconstruction

Effective mitigation or response to an unexpected or terrorist release requires rapid estimation of unknown source terms based on the available data, as well as accurate predictions of the future dispersion of the released material. In real-

world events, the source term is often poorly defined and for a clandestine terrorist attack may be completely unknown. The first indication of a release may be provided by sensor measurements, observations, and/or casualties. Event (or source) reconstruction tools are therefore needed which:

- Produce *quantitative* estimates of principal source-term parameters, including the location, quantity, and release time (time-varying release rate)
- Provide continuous *dynamic* interpretation of sensor data and improvement of both source estimates and consequence predictions of the transport of CB agents, as additional observations become available
- Incorporate *disparate* types of observational data (sensor data, casualties, etc.)
- Take into account the error intrinsic to *both* measurements and model representations of flow and dispersion processes
- Estimate the *uncertainty* and the *distribution* of possible source parameter configurations consistent with both data and models
- Guide sensor siting and deployment for improved characterization of CB agent releases and reduction in measurement uncertainty

A variety of approaches are being pursued to treat the event reconstruction problem including heuristic methods (backward trajectories, ensemble simulations) and Bayesian-inference stochastic sampling algorithms (indoor and outdoor applications) and non-linear optimization.

The development and operational use of event reconstruction tools is now becoming feasible due to the convergence of numerical modeling approaches, remote and deployable sensor technologies, high performance computing (ASCI-level platforms), and operational deployment of detector networks. These technologies are at the forefront of a revolutionary new paradigm for treating dynamic complex problems, which involve inextricable linkage and mutual optimization of sensor data and models (the use of data to steer models and of models to guide data collection.)

7. CONCLUSION

Operational systems simulate agent transport and provide quantitative estimates of the resulting health risks to the exposed population. A broad range of validated atmospheric flow and dispersion models are needed to cover a broad range of spatial and temporal scales and source types and to provide the appropriate level of detail, fidelity, and performance required for pre-event scenario planning, emergency response, and post-event assessments.

In order to meet the challenges of future threats, an expanded set of transport-and-fate capabilities are needed. The importance of both urban modeling and data-model integration has been discussed above. An improved understanding of boundary layer physics

for stable, nocturnal, transitional, and coastal conditions is also needed. Accuracy can be improved by enhancements to physical process models, such as precipitation scavenging, resuspension, multi-phase chemical kinetics, explosive releases, and fire models. Sensor data networks and real-time data feeds are needed to supply new meteorological and material detection measurements. The development of a standardized set of customer products and conventions is increasingly important as the use and range of customers of emergency response systems expands.

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