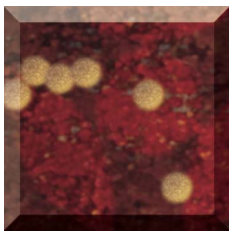

Modeling the Transport and Dispersion of Airborne Contaminants: A Review of Techniques and Approaches

James F. Garten, Charles E. Schemm, and Arthur R. Croucher

Recent events have significantly increased interest in modeling the time evolution of airborne contaminants. This capability can be used to plan and evaluate the effectiveness of sensor systems that would warn of something harmful in the air, aid real-time decision making regarding regions to quarantine or evacuate during an actual event, and analyze what really happened after an event. This article reviews the abilities and limitations of such predictive models through a discussion of a coupled model approach used at APL. The Regional Atmospheric Modeling System (RAMS) is employed to predict meteorological data (winds, temperature, etc.), since even in the best operational scenarios, the available meteorological information is often inadequate. The RAMS predictions are used to drive an atmospheric transport and dispersion model that predicts the time evolution of a cloud of contaminants.

INTRODUCTION

Intelligent and effective preparations for and responses to biochemical agent attacks, dirty bomb explosions, nuclear accidents, etc., require the ability to model the transport (motion) and dispersion (spreading) of airborne contaminants. The time evolution of a contaminant "cloud" depends on the four-dimensional (space plus time) wind magnitude, direction, and associated turbulence levels, as well as the four-dimensional temperature and humidity. As shown conceptually in Fig. 1, these variables could cause high concentrations of a hazardous agent to persist near the surface for an extended period of time, while concentration levels could decrease rapidly in others because the cloud spreads much more rapidly vertically and/or horizontally. Predicting a cloud's evolution, and specifically the cumulative hazard to particular regions on the surface, is largely an exercise in understanding the meteorological (MET) conditions.

There has been longstanding interest in having one or more sophisticated, integrated numerical models to calculate comprehensive predictions of contaminant concentration levels. Such predictions can provide estimates for the net exposure risk (i.e., the cumulative dose) at certain locations in the aftermath of an attack or accident. These, in turn, are crucial insights for real-time decision making. APL has been concerned with evaluating the performance of such models and, in particular, studying the effects of MET conditions that vary over space and time on predicted contaminant

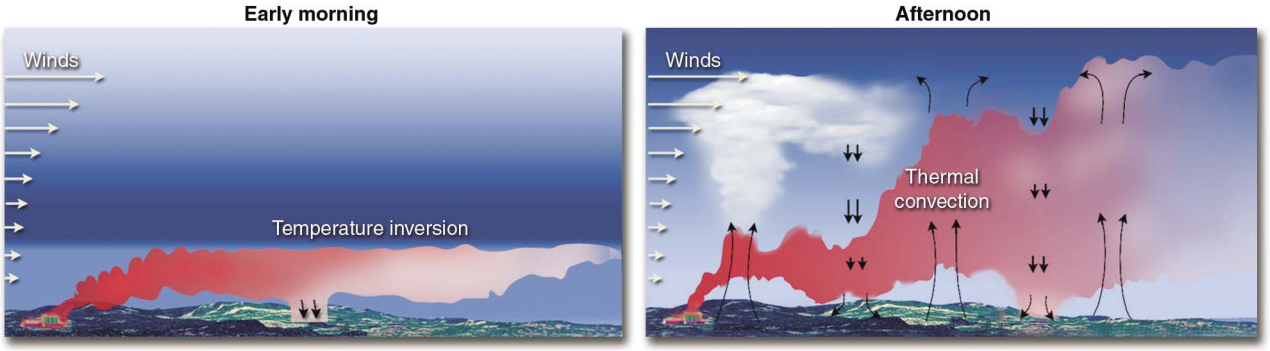

Figure 1. Conceptual illustrations of contaminant cloud evolution under two qualitatively different environmental scenarios.

concentrations. This article summarizes the abilities of some of these models, discusses the effects of MET conditions on cloud evolution, and describes the potential applications for proven numerical predictive tools.

END-TO-END MODELING APPROACH

Consider the possible methods for computing the time evolution of a cloud concentration field. The most precise approach would require the velocity field and other relevant MET variables (temperature, humidity, etc.), as well as the cloud concentration, to be known at some initialization time for an appropriate spatial resolution. A model would then time-step the three-dimensional solution forward in time, calculating new velocity, MET, and cloud concentration fields from the current ones. Because of the disparity in scales involved (scales of hundreds of kilometers or more may be required for the velocity evolution, while the cloud concentration may vary on scales of fractions of a kilometer) and potentially complex terrain and other details, such a high-resolution model is simply not feasible for many cases of interest. On the other hand, it might be well suited for regional- and national-scale pollution studies.

One means toward practicality is to use a coupled model approach in which two distinct models are run sequentially, with the output of the first used as input to the second. The first model is typically a computational fluid dynamics (CFD) code that forecasts wind velocities and other MET variables of interest over a spatial domain large enough to encompass the contaminant cloud during the time period of interest (see additional discussion in the "Meteorological Inputs" section). With this step completed, it can be assumed that the velocity and MET variables are "known" for the times and over the spatial regions of significance to a potentially much smaller-scale contaminant cloud evolution. The second model then starts from an initial cloud concentration field and predicts the time evolution of that field as it responds to the known external MET conditions. Results are interpolated as needed from the spatial and temporal resolution of the first large-scale model to those of the second small-scale dispersion model. APL's implementation of such a coupled model approach to transport and dispersion modeling is shown schematically in Fig. 2.

Approximations to the cloud concentration field can make calculations much more rapid, and hence of greater practical use. With the velocity and MET environment known, it is possible to represent the three-dimensional cloud concentration field, without any specific spatial grid, via a workable number of parameters. The time evolutions of these representative quantities are then modeled within the known environment in lieu of using the actual (gridded) concentration field.

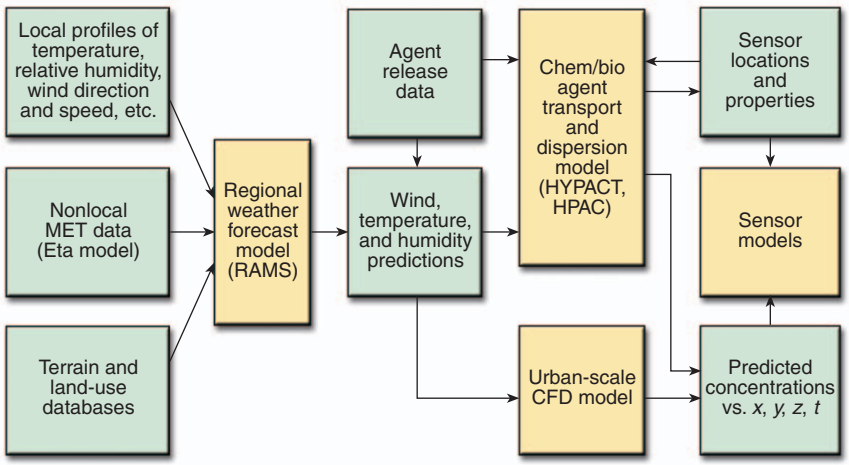

Figure 2. Conceptual diagram of an APL-developed end-to-end model that uses (1) meteorological (MET) data and predictions and (2) a transport and dispersion model to predict contaminant cloud concentration levels. Note the option to use the HPAC (Hazard Prediction and Assessment Capability), HYPACT (Hybrid Particle and Concentration Transport), or urban-scale CFD (Computational Fluid Dynamics) model for the transport and dispersion model. The diagram also illustrates one of the intended uses for such predictions: input into sensor models. ("Eta" is NOAA's National Center for Environmental Prediction model; RAMS = Regional Atmospheric Modeling System.)

The major types of cloud transport and dispersion models, and their primary advantages and disadvantages, are summarized in the next section. The particular CFD code that APL uses to provide MET input is discussed in the "Meteorological Inputs" section.

TRANSPORT AND DISPERSION MODELS

Gaussian Plume Models

Gaussian plume models[1,2] are predicated on the supposition that a cloud's actual concentration field can be approximated through the use of Gaussian shape functions of the form

$$F_G(\eta, \sigma \quad \exp\left\{-\frac{\eta^2}{\sigma^2}\right\}, \tag{1}$$

where η is the independent variable and σ is a width parameter.

In the simplest case, we assume that one of the principal axes of the cloud is in the vertical direction and uses eight parameters to approximate the cloud concentration field: the total mass of the cloud M, center of mass of the cloud (x_m, y_m, z_m), relative orientation of the cloud with respect to specified horizontal x-y axes represented by the angle θ, and three Gaussian-width parameters ξ_1, ξ_2, and ξ_3. The analytical equation for the concentration field for such a cloud is

$$C(x, y, z, t) = \frac{M}{\xi_1 \xi_2 \xi_3 \pi \sqrt{\pi}} F_G(x', \xi_1) F_G(y', \xi_2) F_G(z', \xi_3), \tag{2}$$

where $x' \equiv (x - x_m)\cos\theta + (y - y_m)\sin\theta$ and $y' \equiv (y - y_m)\cos\theta - (x - x_m)\sin\theta$. (Visualize an infinite series of inset footballs, with the surface of each football representing one concentration value, a value that decreases exponentially with the square of the distance from the center location.) The problem of modeling the time evolution of the cloud concentration is now reduced to modeling the time evolution of the eight quantities; even the total mass could be allowed to change in time because of the potential for chemical reactions, response to solar heating, etc. The known MET environment is used to predict the center-of-mass motions and the rates of spreading of the cloud (through the cloud widths).

Some Gaussian plume models take more sophisticated approaches. In particular, the Hazard Prediction and Assessment Capability (HPAC)[3] model used at APL[4] assumes that a cloud is a superposition of many Gaussian "puffs," each being described by its own set of eight parameters that are allowed to evolve in time.[5] In principle, this allows for more complicated initial cloud shapes and for puffs to split or recombine as time advances.

In addition to the implicit requirement that clouds be horizontally oriented, the most serious shortcoming of the Gaussian plume model approach is the inability to predict how quickly real clouds move and redistribute themselves vertically under particular MET conditions. In some instances, the presence of an inversion and/or low turbulence conditions may cause a cloud to hug the surface for an extended period of time, while in other instances ground heating and turbulence may cause a cloud to move and spread upward much more dramatically. This shortcoming mostly affects the predicted cloud concentrations near the ground because as the cloud center of mass moves upwards and/or the cloud spreads vertically higher, the predicted concentrations near the ground drop accordingly (potentially by orders of magnitude or more).

Lagrangian Transport Models

Another approach to express a cloud's concentration field with a reduced number of parameters is to represent the cloud by a large number of individual particles moving within the known MET environment.[2,6–8] At each time step, the location of each individual particle changes as given by $\vec{x}_i(t + \Delta t) = \vec{x}_i(t) + \vec{u}_i(\vec{x}_i, t)\Delta t$ for particles $i = 1, 2, 3, ..., N_p$, where N_p is the total number of particles. The velocity field in this equation ($\vec{u}_i$) includes both the "known" mean wind velocity and random components estimated from turbulence theory, using the mean MET variables as drivers. The number of particles needed to represent the cloud faithfully will vary with the complexity of the flow and the cloud, which may both increase significantly for longer simulations.

Some Lagrangian particle models augment the vertical component of this equation with additional effects. In particular, the Hybrid Particle and Concentration Transport (HYPACT)[9] model, also used at APL,[10] includes buoyancy and stratification effects. The inclusion of stratification makes this model arguably more physical than Gaussian plume models like HPAC. No assumptions are made regarding how quickly the cloud particles move upward beyond using the known velocity field and the natural spreading due to the turbulence. Furthermore, particles can move upward or downward as they are wont, whereas Gaussian plumes typically only move upward or remain stationary in the vertical.

Eulerian Transport Models

The primary disadvantage of Lagrangian models is the large number of particles that must be tracked to obtain representative concentrations at times and distances far removed from the release point. A more viable approach is to numerically solve a scalar transport and dispersion equation for the concentration of each chemical and biological agent of interest:

$$\frac{\partial C}{\partial t} = \vec{u} \cdot \vec{\nabla} C + \vec{\nabla} \cdot \left(K_C \vec{\nabla} C \right) + S_C \,, \qquad (3)$$

where $\vec{u}$ and K_C are the mean wind velocity and nonlinear eddy-viscosity coefficient, respectively, from the known velocity and MET fields, and S_C is a source/sink term meant to represent processes such as deposition, chemical reaction, etc. This type of equation is referred to as a "Eulerian" solver.

HYPACT includes a Eulerian solver option in addition to the Lagrangian solver discussed previously. The only requirement is that the initial contaminant cloud be large enough, and the grid spacing small enough, so that it can be effectively represented as a concentration field. When the grid spacing cannot be made small enough to describe a cloud's initial concentration field accurately, a Lagrangian calculation must be used to predict the evolution of individual particles, at least until the cloud has spread over a sufficient number of grid cells for a smooth concentration field to be determined. (Converting the particle position data to a cloud concentration field poses its own set of problems.) If results are desired for later times, then a Eulerian calculation can be initialized from this intermediate concentration field. HYPACT includes the option of running both Lagrangian and Eulerian solvers in sequence, hence its designation as a "hybrid" code.

Models for More Complex Situations

The models summarized above are used mostly to predict cloud evolution in the "free atmosphere," i.e., outside the influence of complex geometries such as buildings, streets, and trees. It is, however, important to predict the transport and dispersion of contaminants around and within buildings, within rooms, and under a plethora of other specialized geometrical/situational constraints. References 11–15 discuss approaches to predicting contaminant concentrations in such complicated geometries (see also the article by Scorpio et al., this issue).

METEOROLOGICAL INPUTS

General Discussion

No matter how good the design and implementation of a numerical transport and dispersion model, the quality of its predictions for cloud concentration levels is limited severely by the accuracy of the input MET information. The wind direction and speed determine where the cloud moves and how fast, and both may vary significantly with the height above the surface, causing different horizontal slices of the cloud to move in different directions and/or at different rates. Atmospheric turbulence levels control the rate at which the cloud spreads, and variable wind shear may cause this dispersion to be nonuniform (for example, the rate of spread of an initially circular cloud might be greater in one direction than another). Turbulence levels may also depend on the height above the surface, and all of these quantities may evolve over the lifetime of the cloud.

The vertical profiles of temperature and humidity must also be known, at least qualitatively, as these variables determine the vertical stratification and, in particular, the locations of inversion layers that affect the vertical migration and spreading of contaminant clouds. In a "mixed layer"[1,2,7] of the atmosphere, turbulence in the vertical velocity is sustained because convective and shear-driven instabilities outweigh buoyant effects and dissipation. Typically, a mixed layer begins at the surface but may be anywhere from centimeters to kilometers high; elevated mixed layers can also exist in regions that begin and end above the surface.

Turbulence is nearly always present in the atmosphere and spreads a contaminant cloud in the horizontal directions. However, within a mixed layer, turbulence in the vertical velocity typically spreads, or mixes, a contaminant cloud toward a uniform vertical distribution (within the vertical extent of the mixed layer), and this can occur much more quickly than the cloud spreads in the horizontal direction. The constituents/contaminants within a mixed layer do not penetrate into the region above the mixed layer to any significant degree (as illustrated in Fig. 1). Of course, if a cloud begins *above* the height of the mixed layer (e.g., from an aerial spray), then it will not penetrate into the region *below* the height of the mixed layer.

The height of the mixed layer can evolve over time and is derived from a threshold on the ratio between the horizontal wind components[1,2,7] and the vertical gradients of the virtual potential temperature, i.e., $\theta = (1000/p)^{R_d/C_p}$, where p is pressure in millibars, $R_d = 287$ J K^{-1} kg^{-1} is the dry gas constant, and $C_p \approx 7R_d/2$ is the specific heat at constant pressure.

These MET variables all affect the key quantity of interest in contaminant dispersion studies: the concentration levels of the cloud near the surface. Often, predicted concentration values are used to estimate the net exposure, or dose, inflicted on particular locations. Incorrect specifications of the MET data will cause significant errors in the predicted concentration levels, and these, in turn, will lead to inaccurate dose estimations, perhaps by several orders of magnitude or more. Clearly, this would be unacceptable for some applications, although false negatives (severe underestimation of surface dose) are typically tolerated less than false positives (severe overestimation of surface dose).

MET Considerations and Specifications

Many practical issues are involved in the use of real-time cloud concentration level predictions. For one, the needed MET data must be readily available and in a form ready to be ingested by the transport and dispersion model. HPAC includes some options[3] to

simplify this requirement. One option is that the HPAC user may simply specify a single wind speed and direction for all places and times, and the software will use climatological databases to "look up" other MET data, given the location and time of the cloud source. While this approach should yield a commonsense warning for regions at risk from the cloud, there could be significant errors in the surface concentration estimates, and hence the dose estimates, due to possibly significant departures from the climatological averages.

Alternatively, the HPAC user may also specify a horizontally uniform mixed-layer height as well as turbulence level estimates, which should, if accurate, improve the quality of the surface concentration and dose estimates. Figure 3 shows two sample HPAC results for a cloud released 30 ft above the surface, with and without an inversion, starting at 1000 ft. Without the inversion, the mixed layer is effectively infinitely high; therefore, the cloud spreads more in the vertical direction and surface concentration levels are reduced more quickly. This results in the smaller 2-h cumulative dose estimate shown in the figure.

HPAC's most comprehensive option is to ingest MET fields in toto; however, this option is not yet as effective as it could be (as of HPAC Version 4.3), largely because the models internal to HPAC (e.g., the terrain model) are not necessarily consistent with the gridded MET fields, which introduces errors into the transport and dispersion model part of HPAC. The Defense Threat Reduction Agency, which manages HPAC development, plans to address these issues in future versions.

Whether using HPAC or some other transport and dispersion model, a robust method is needed to specify the three-dimensional MET fields, ideally as functions of time. APL uses the Regional Atmospheric Modeling System (RAMS)[16] for predictive estimates as a surrogate for actual MET fields (Fig. 2). RAMS uses modified Navier-Stokes fluid flow equations, turbulence models, and many atmospheric/surface interaction models to evolve the MET fields in time on a user-specified spatial grid. Any coupled MET-prediction/transport-dispersion model will have difficulties similar to the HPAC problems mentioned above (inconsistent terrain models, etc.). One advantage of the alternative HYPACT model is that it was deliberately designed to directly and transparently ingest RAMS MET predictions. Unfortunately, this is simultaneously one of the disadvantages of HYPACT; at present, it can *only* be run from RAMS output data.

Figure 4 shows two sample HPAC results for identical clouds released in a MET environment predicted by RAMS. In Fig. 4a, the MET environment was assumed to be constant in time, while in Fig. 4b it was assumed to evolve in time as predicted by RAMS and fed into HPAC. The differences apparent in these cumulative surface doses again illustrate the need for accurate MET information.

Initialization values for the RAMS MET fields can come from gridded large-scale mean MET profiles, local MET profiles, or blends of both. However, obtaining initialization values for the RAMS surface states (e.g., soil moisture and temperature, sea surface temperature) can be nontrivial.[17] To ease this difficulty somewhat, many users run RAMS in "continuous forecast" mode, that is, RAMS simulations are initialized at so-called synoptic times (0000, 0600, 1200, and 1800 UTC) and run for 24-h forecast periods. At each synoptic time (or possibly more often if local measurements are recorded), the RAMS predictions can be "nudged" toward known

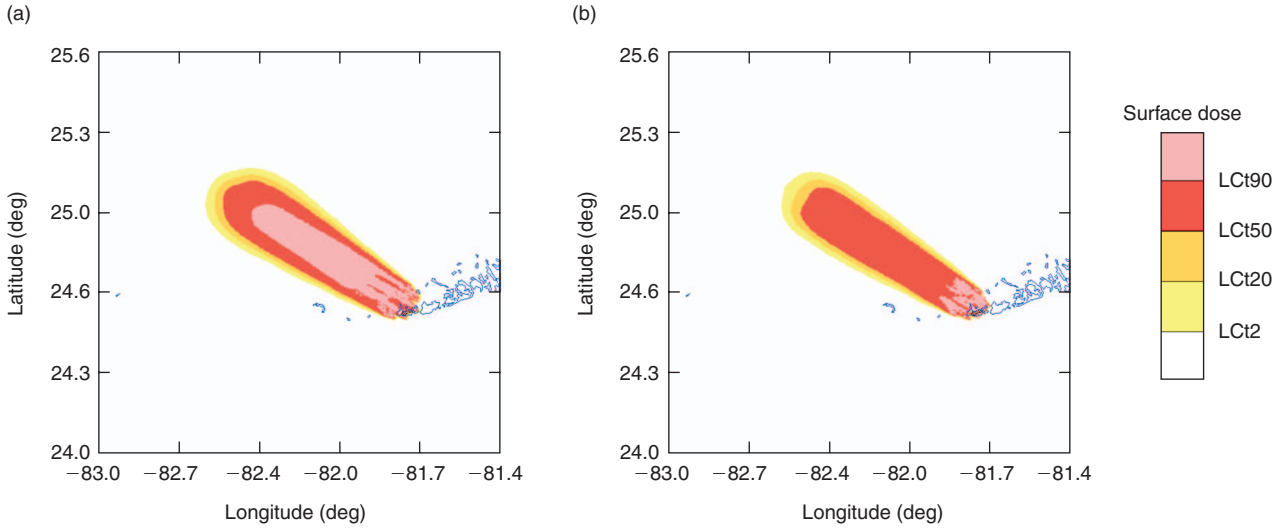

Figure 3. Two-hour cumulative surface dose levels of anthrax as predicted by the HPAC model from a point of release 30 ft above the surface: (a) with a mixed-layer height specified at 1000 ft, and (b) for a stable, standard atmosphere. The dose levels are estimated relative to expected fatality levels (e.g., the LCt50 contour, or lethality contour 50%, indicates that an average of 50% of the population exposed to that dose would not survive).

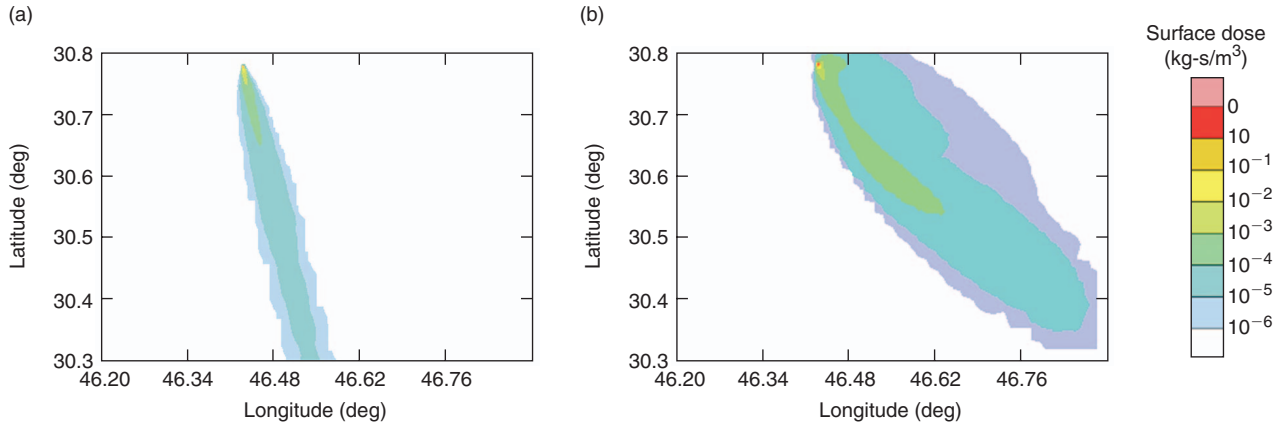

Figure 4. Four-hour cumulative surface dose levels of vapor GB (a toxic chemical) as predicted by HPAC for a surface point release using RAMS MET predictions (a) fixed in time and (b) updated over time.

or assumed large-scale values. This method ensures that a current forecast is always available and reasonably accurate.

MODEL VALIDATION

To be confident in using transport and dispersion model predictions, it is necessary to test (validate) the model under controlled situations. However, a thorough validation experiment can be fairly difficult to conduct. (RAMS has been tested against data for a wide range of conditions, and so we consider it to be validated for its intended purposes.) As can be inferred from the previous section, the details of the actual MET environment in which the experiment takes place must be understood to a reasonable level. Unfortunately, most experiments that might have been used for validation studies recorded little beyond the local average wind speed and direction. Even if sufficient MET data are recorded, the actual cloud concentration levels must be recorded at enough spatial and temporal locations to make comparisons to the predictions meaningful. With a few important exceptions (e.g., Ref. 18), most experiments have only recorded cloud concentration levels at one spatial location, or at most in one horizontal plane (at a fixed height).

Another approach to model validation is to compare the model predictions to known theoretical predictions for simplified MET conditions. Regrettably, comparisons can be somewhat circular because the models are based on particular physical relationships, equations, and algorithms that may also form the bases for the theoretical predictions. Still, such comparisons are important as they verify the ability of the model to produce expected results for special, simplified situations.

With these issues in mind, intermodel comparisons can clearly be tricky. Two different models may yield different predictions, not so much because one is "better" than the other but because they are based on different physical assumptions and/or they use the input MET data differently. That being said, it is worth illustrating important differences observed between sample HPAC and HYPACT predictions.[10] Figure 5 shows a horizontal slice of cloud concentration values 2 m above the surface as predicted by HYPACT and HPAC for identical initial conditions. The distributions are clearly different; most notably, HPAC predicts a much more symmetric shape, and also predicts that the cloud will spread out much more quickly in the horizontal directions. These differences could be due to differences in the underlying models or to the problems mentioned earlier with MET initializations. An actual two-dimensional lidar measurement of two clouds indicates that real clouds are also elongated in the direction of the mean wind (Fig. 6). This suggests that HYPACT may provide a more realistic prediction for this particular example, though the effects of the MET initialization on HPAC predictions are uncertain.

MODEL APPLICATIONS

Reliable, predictive tools for the transport and dispersion of contaminants in the atmosphere have many applications. Faster models such as HPAC can be used in real time to aid decisions regarding evacuation, quarantine, and allocation of responding resources. After an event, models such as HYPACT can be used to revise real-time estimates to more accurately predict surface dose exposure levels in different regions.

An effective transport and dispersion model can also be used to generate synthetic data. Such data could be employed as a general planning aid for field tests and, more importantly, to model the response of particular point and standoff sensors. All practical sensors have some functional shortcomings or at least trade-offs with respect to their capabilities. Synthetic data with modeled instrument responses provide a relatively inexpensive means to evaluate sensor and system

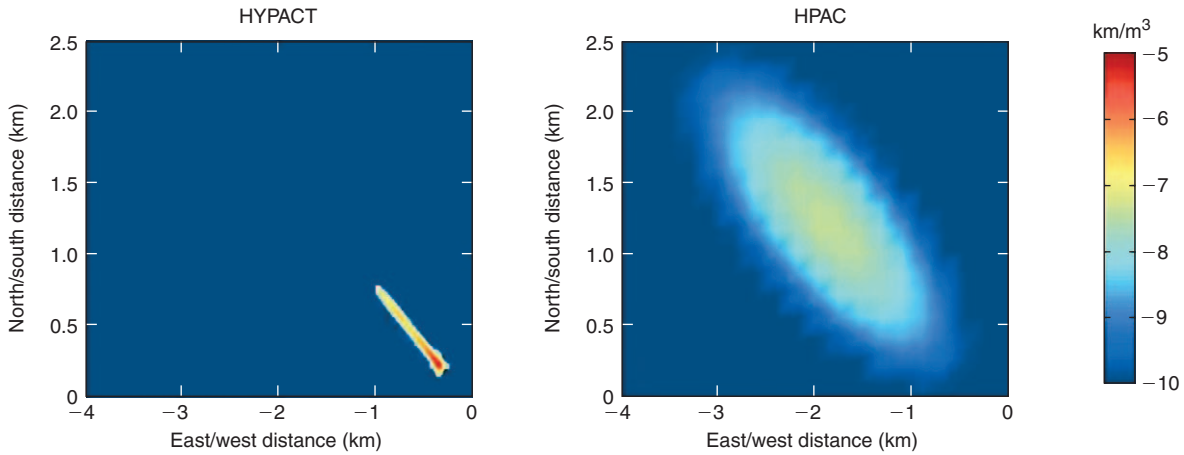

Figure 5. Near-surface cloud concentration values 2 m above the surface as predicted by HYPACT and HPAC, using identical RAMS-provided MET predictions for input, 20 min after a point release.

performance when compared to the expense and technical difficulties of actual experiments. Another use for synthetic data sets is to simulate the response of a suite of sensors. Imagine an attempt to protect a certain area or region—be it a semi-permanent military base of operations, a permanent military base, or a city—from biochemical agent releases. It would be useful to know how many sensors would be required to give adequate warning that a contaminant cloud was approaching the protected area. The overall effectiveness of various sensor layout schemes (how many of each type of sensor, where to place them, etc.) could be evaluated using synthetic data so long as one has adequate confidence in the representativeness of the data. Developmental work to accomplish these goals is ongoing.[19]

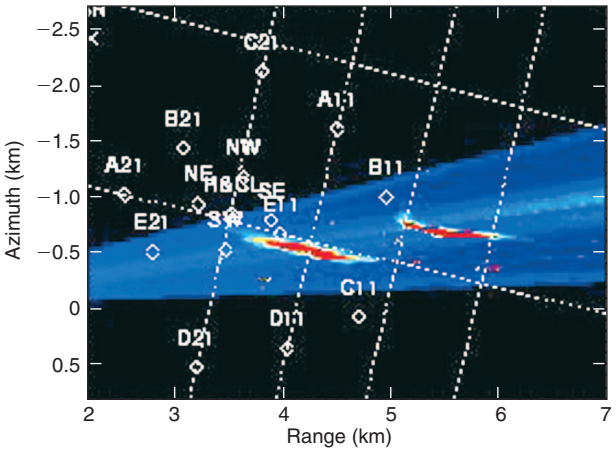

Figure 6. An actual lidar scan measured 20 min after the point release of a simulant. The dark blue region, where the response was due only to background atmospheric particulates, shows the lidar's aggregate field of view from a 10 second, 60 degree scan. Other colors correspond to larger responses than could be due to background particulates and indicate the presence of two clouds within the field of view. Further discrimination tests would be required to determine if these clouds contained harmful particulates.

CONCLUSIONS

Today, there is significant interest in developing defensive infrastructures to guard, protect, and warn against airborne contagions and contaminants. Capabilities to model the transport and dispersion of such particulates play a crucial role in these development efforts because they can be used not only to aid real-time decisions but also to provide synthetic data for planning, testing, and evaluation. This article has used the discussion of a coupled model approach toward these ends to review the abilities and limitations of different modeling techniques and approaches. Understanding these limitations and being able to explain them to the people who would make the real-time decisions are clearly key goals in planning real-time response strategies.

On a subtler note, evaluating whether synthetic model predictions are sufficiently representative of the way particulates would move and disperse in the real world will be crucial to developing confidence in sensor system layout designs. Because of the expense of real-world experiments, such designs will be developed according to how they respond to synthetic data. It could be tragic, indeed, if a sensor system performed very well in response to synthetic data but not very well if at all to an actual event.

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