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Improved Atmospheric Transport for Risk Assessment

D. Cooper*, and J. Kao

Abstract

This is the final report of a two-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). To effectively respond to airborne CBW attacks in urban settings, we must understand the vector of the threat, *i.e.*, where is the effluent going and when will it get there. These answers are needed both in real time (who should be evacuated?) and afterwards (where should the cleanup be focused?). Certainly, advanced multiscale models are essential to this task. No model has value, however, until it is normalized and validated by measured data. Our experience in atmospheric transport has demonstrated that the quality of model estimations is tightly coupled to the fidelity of the data and the effectiveness of its assimilation. We have started to quantify the improvement of accuracy of atmospheric transport and dispersion models that follows from enhanced remote sensing of meteorological parameters. The proper use of remote sensing data requires sophisticated assimilation techniques into advanced models, so the whole project emphasizes the synergy of the newest techniques for remote sensing observation, data analysis, data assimilation, and dynamical modeling. Our work quantified the value of various levels of data for improving effluent tracking and prediction, and allows tradeoffs between the cost of data acquisition and its impact on accuracy.

Background and Research Objectives

Various DOE and national atmospheric programs, including the DOE/NN transport and fate thrust, are developing sophisticated models. The ability to track chemical and biological warfare (CBW) releases will be limited by the available data. Simple model initialization with single point observations of meteorological data has been shown to be of limited value. The data possibilities range from conventional meteorological stations to enhanced remote sensing platforms. However, the paradigm of data assimilation and integration has never been evaluated in terms of benefit versus utility. Several questions need to be resolved:

- How much data is needed to adequately normalize and validate a three-dimensional (3-D) model?

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- What are the advantages of remote sensing data systems compared to conventional platforms?
- How many measurement units are required for a given urban area?

To get answers, we need to make data analysis, model integration, data assimilation, and field deployment to work collectively. Our work represents a trade-off study of the quantity and cost of data against model accuracy in predicting the transport and fate of a unique event such as an accidental release of toxic gases or a chemical or biological agent release in an urban environment.

Importance to LANL's Science and Technology Base and National R&D Needs

Los Alamos National Laboratory (LANL) has developed atmospheric modeling tools and application procedures for a series of practical problems that require the attributes of multiscale rapid response and real-time prediction in complex-terrain meteorological and emissions scenarios. Our perspective gained from successfully addressing these problems has promise in meeting the problems of CBW transport. Existing mesoscale and small-scale models available at LANL certainly provide a framework for interpreting atmospheric conditions in terms of the radiative, hydrodynamic, thermodynamic and photochemical processes that govern the atmospheric structure. The LANL Higher Order Turbulence Model for Atmospheric Circulation (HOTMAC) has been used for modeling boundary layer 3-D dispersion over more than a decade. It has a two-way nested-grid capability and a physically based turbulence parameterization. Another in-house model is RAMS (Regional Atmospheric Modeling System). It is a nonhydrostatic, compressible model also with two-way nested-grid capability.

In collaboration with the National Center for Atmospheric Research (NCAR), LANL has been developing a new hydrodynamic model (HIGRAD) to simulate high-gradient flows such as those that lidar can resolve. As this tool has become available, it has shown considerable utility in characterizing convective transport between the earth's surface and the lower atmosphere. HIGRAD would be an excellent tool to estimate the transport and mixing of pollutants and trace materials in the unstable boundary layer, a domain in which traditional diffusion models have been notoriously poor.

In contrast to many existing "static" data assimilation techniques, we use a "dynamical" data assimilation method. This technique is carefully designed to make

maximum use of spatially distributed measurements and is suitable for spatial scales of 10 to 100 kilometers. The idea was initiated during Desert Storm Operation. When the United Nations troops were under the threat of being attacked by Iraqi chemical weapons, LANL was contacted by the U.S. military to design an in-situ forecast (or "now cast") capability for wind circulation and associated dispersion with lidar measurements, so that a warning of approaching chemical plumes could be issued in time. The technical challenge posed by this highly practical application drove us to continue the development of the technique since the Gulf war.

There are two phases involved in this data assimilation approach. The first phase is to use the adjoint method to recover the full 3-D wind, temperature, and humidity fields from the corresponding lidar measurements. The adjoint method basically employs a comprehensive 3-D model to determine the state of dynamic and thermodynamic fields that generated the time sequence of observations that lidar made. In doing so, we first make an initial guess for the unobserved state and do pure model prediction for the time period in which lidar observations were made. A cost function is subsequently defined, which measures the difference between the model predictions and the lidar observations. We then construct a set of adjoint equations to determine the sensitivity of the cost function to the initial guess errors. So the initial guess can be adjusted iteratively until the minimum errors are reached. The final guess can now be called the recovered state that led to the observations.

The second phase is a straightforward prediction using the recovered state, which can now be called the initial condition, for an extended period of time in which new observations by lidar will be repeatedly incorporated into the model. As time goes on, the recurrence of phases 1 and 2 formulates an ultimate data assimilation procedure and the initial guesses at later times can be more accurately made. Furthermore, the sensitivities of the adjoint equations to the errors of source locations and strengths can be determined in a way similar to the initial conditions described above.

The dynamical data assimilation technique improves our ability to track plumes forward from their release and backward from their detection. The technique provides several benefits including:

- tracking and predicting airborne CBW threats,
- dynamical assimilation of meteorological measurements into models, and
- integration of high-resolution modeling with enhanced remote-sensing data.

Scientific Approach and Accomplishments

The complexity of transport, diffusion, and chemistry in predicting and tracking effluents from a CBW release requires that model and field measurements cover scales extending from releasing spots to area-wide effluent dispersion within a single dynamically and thermodynamically consistent framework. Limited temporal and spatial resolutions in modeling and measurements can lead to ambiguous determination of relations between sources and receptors. Models with high temporal and spatial resolutions are essential to resolve the transient phases in diurnal cycle and terrain complexity, such that thermally induced near-surface flow and photochemically induced species transformation can be accurately depicted. Unfortunately, high-resolution meteorological data from either conventional or remote sensing measurements for a targeted site are not consistently available. Therefore, data utility becomes an important issue in the CBW program. In practical terms we must decide how much data to buy and, because measurements can be costly, we want to buy just enough data to do the job.

In order to reach our research goal, data assimilation plays an essential role. Data assimilation is defined as the determination of the best estimate of the state of the atmosphere, given all the available information about the atmosphere along with a dynamical, predictive model that encompasses the governing atmospheric processes. A Newtonian relaxation method of data assimilation has been successfully incorporated into the LANL models. We use a more sophisticated data assimilation scheme in our research that not only "massages" data into a model for better predictions, but also helps to formulate an inverse modeling procedure for deducing source locations and strengths from a time/space sampling history.

Two logical steps are required to test our assimilation scheme. An experimental demonstration of the value of the full suite of meteorology data is certainly a requisite. However, before initiating such a potentially expensive demonstration, it is prudent to perform preliminary work on the experiment design and utilization of currently available data sets. Our particular attempt here is to

- quantify the "benefit function": *gain versus density and cost of conventional meteorological data*, and
- design a definitive field test in conjunction with the full suite of remote sensing techniques that the CBW program may eventually require.

The existing data sets include:

- El Paso, TX, 1994 and 1996 (terrain, urban, multiple profiles, lidar winds—LANL and others)
- Brush Creek, CO, 1984 (terrain, tracers, multiple profiles, Doppler lidar— LANL and collaborators)
- Rocky Flats, CO, 1992 (terrain, tracers, multiple profiles, lidar— LANL and others)
- METROMEX, D. C. area, 1988 (NOAA)
- SCAQS, Los Angeles Basin, 1986 (terrain, urban, tracers, multiple profiles— multi-agency).

Naively, there is a 5:1 rule for data assimilation. For example, if we are modeling a 5 km x 5 km grid, we would require a measurement every square kilometer. Anything sparser might lead to aliasing problems by misrepresenting the circulation pattern. To overcome this problem and use sparser data, a nested-grid version of our model is used. Our measurements are mapped to the coarser grid in which the finer grid for the domain of interest is embedded. Through the two-way interaction of the finer and coarser grids, a successful data assimilation is still obtainable.

Development Challenges for Follow-On Work

Assimilation of Single Doppler Wind Components

Since Doppler wind measurements only provide the line-of-sight (LOS) wind speeds, the true wind speed and direction are derived assuming horizontal homogeneity within the coverage of the laser beams at an altitude. The assumption of homogeneity may not hold well for boundary layer circulation. Under such a circumstance, we may have to work with the LOS winds for a reconstructed 3-D wind field that the model can utilize in order to proceed with the adjoint scheme described above. The Kalman Filter Method can be used for assimilating the single component LOS winds. This method is generally used to provide an optimal estimate of a physical system that minimizes the analysis error variance in a model being assimilated with available data. Unlike the adjoint method, the Kalman filter does sequential estimation, which continuously blends data and model forecast as data come in. Thus, it provides the optimal 3-D gridded wind data at any time step given previous observations. Moreover, the Kalman filter can also produce a forecast of both the model state and its error covariance (information about the accuracy of the analysis), if the adjoint method is not desirable in situations where data density is not

sufficient.

Inclusion of Chemistry in Models

As Differential Absorption Lidar effluent detection technology matures with time, there is a need to incorporate chemistry information into the modeling system for CBW problems since released gas-phase and particulate pollutants are valuable trace materials for detecting and tracking purposes. Distributions of chemical materials can only be determined by a coupling of gas photochemistry with aerosol microphysics within a comprehensive dynamical framework. In order to interpret measurements, predict the effectiveness of remediation strategies, and parameterize the complex and nonlinear interactions between releasing spots and area-wide scales, comprehensive and yet fast 3-D simulations of chemistry remain to be implemented. In our approach, an optimized, coupled integration of the photochemical and aerosol systems will be tuned for the project. The first major component, the Chemistry Aerosol Tracer (CAT) routine, has been demonstrated at LANL for its ability to perform complex, stiff, chemical/aerosol integrations within the LANL Global Circulation Model (GCM). CAT adopts the fastest available numerical scheme to solve the stiff chemistry and aerosol microphysics systems efficiently enough for inclusion in massive 3-D environmental grids.

Turbulence within Canopies and Rough Elements

This topic is dedicated to the understanding of the nature and formation of intermittent gusts in canopy and urban complex transport and how they interact with the surface. Recent observational studies have illustrated that the turbulent transport within and above canopies can be characterized as organized and coherent eddies rather than random and chaotic. These organized eddy structures account for more than 60% of the fluxes of momentum, heat, and water vapor. However, the mechanisms responsible for the formation and evolution of the intermittent eddies have not yet been resolved. We postulate that these eddies are closely related to high-frequency wake turbulence generated by interaction between air flow and canopy obstacle elements. The existence of the obstacles, in turn, helps to organize the wake turbulence. Since wake turbulence has a smaller time scale than boundary layer turbulence, its interaction with shear turbulence and mean flows leads to intermittent transport. Our integrated capability should be a convincing tool for the improved understanding of the processes described above.