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OFCM

OFFICE OF THE FEDERAL COORDINATOR FOR
METEOROLOGICAL SERVICES AND SUPPORTING RESEARCH

Federal Research and Development Needs and Priorities for Atmospheric Transport and Diffusion Modeling

JOINT ACTION GROUP FOR ATMOSPHERIC
TRANSPORT AND DIFFUSION MODELING
(RESEARCH AND DEVELOPMENT PLAN)

FCM-R23-2004
Washington, DC
September 2004

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Front Cover Graphic: On Friday, February 21, 2003, a fuel barge that was unloading fuel at a storage facility on Staten Island exploded. The barge was unloading 4 million gallons of unleaded gasoline. Smoke and flames climbed hundreds of feet into the air. A plume of smoke originating from the fire was carried over lower Manhattan and was captured in this photograph by Gregory Bull (AP Photo)

FEDERAL COMMITTEE FOR
METEOROLOGICAL SERVICES AND SUPPORTING RESEARCH

WORKING GROUP FOR
ENVIRONMENTAL SUPPORT TO HOMELAND SECURITY

JOINT ACTION GROUP FOR ATMOSPHERIC TRANSPORT AND DIFFUSION
MODELING (RESEARCH AND DEVELOPMENT PLAN) (JAG/ATD(R&DP))

Federal Research and Development Needs and Priorities for Atmospheric Transport and Diffusion Modeling

FCM-R23-2004

September 2004

Office of the Federal Coordinator
for Meteorological Services and
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FOREWORD

In August 2002, the Office of the Federal Coordinator for Meteorological Services and Supporting Research (OFCM) published the comprehensive report, *Atmospheric Modeling of Releases from Weapons of Mass Destruction: Response by Federal Agencies in Support of Homeland Security*. This publication, prepared by the OFCM's Joint Action Group for the Selection and Evaluation of Atmospheric Transport and Diffusion Models (JAG/SEATD), provided a comprehensive summary of Federal capability to provide atmospheric transport and diffusion (ATD) modeling support and has become a valuable resource in support of the homeland security/defense missions.

The JAG/SEATD report also made a number of recommendations for future work, regarding ATD modeling support, which was endorsed by both the Interdepartmental Committee for Meteorological Services and Supporting Research (ICMSSR) and the Federal Committee for Meteorological Services and Supporting Research (FCMSSR). Among the recommendations was the need to address the research and development required to advance the state-of-the science of ATD modeling in support of critical homeland security/homeland defense activities.

In October 2003, the OFCM established the Joint Action Group for Atmospheric Transport and Diffusion Modeling (Research and Development Plan) (JAG/ATD(R&DP)) to address this recommendation head on. Each agency that participated in the JAG/ATD(R&DP) shared the common goal to: Identify the most pressing research needs facing the Federal ATD modeling community as it strives to support the homeland security mission and to recommend a strategy that will eventually satisfy those needs.

This report, *Federal Research Needs and Priorities for Atmospheric Transport and Diffusion Modeling,* represents a commitment by each of the responsible Federal agencies in the OFCM Federal coordinating infrastructure to work in a collaborative and synergistic way to address this critical homeland security issue, and the report's recommendations are the result of careful deliberation by the members and are based on their collective skills, experiences, and vision.

The next step is for the participating agencies to work together in a collaborative and cooperative manner to incorporate these recommendations into agency plans and programs in order to improve Federal ATD modeling capabilities. The completion of this task in a timely and coordinated manner is vitally important to the Nation. Close coordination with the academic and private organizations will also be required, and the user community must be involved in the process from start to finish.

I wish to extend my deepest appreciation to the JAG members, alternates, technical advisors, and subject-matter experts who brought unprecedented knowledge and experience to the table and who demonstrated outstanding teamwork in developing this report. I am also deeply grateful for the outstanding leadership of the JAG cochairs, Dr. Walter Bach and Ms. Nancy Suski. The quality and comprehensiveness of the report reflects highly on the insight, professionalism, and dedication of all the participants and the report provides a solid foundation for future R&D efforts, regarding environmental support to homeland security.

Samuel P. Williamson
Federal Coordinator for Meteorological Services
and Supporting Research

September 23, 2004

MEMORANDUM FOR: Mr. Samuel P. Williamson
Federal Coordinator for Meteorology

FROM: Cochairpersons

SUBJECT: Federal Atmospheric Transport and Diffusion Modeling
Research and Development Plan

The Joint Action Group for Atmospheric Transport and Diffusion Modeling (Research and Development Plan) (JAG/ATD (R&DP)) has completed the tasks assigned in the JAG/ATD (R&DP) Terms of Reference. We are pleased to provide the subject report, titled: *Federal Research and Development Needs and Priorities for Atmospheric Transport and Diffusion Modeling*.

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EXECUTIVE SUMMARY

Atmospheric transport and diffusion (ATD) modeling is a challenging and dynamic field of research, and the Federal agencies have played a critical role in applying advances in the field to satisfy pressing national needs. Federal resources have proven to be vitally important to these efforts because ATD models typically must describe atmospheric processes in the most changeable and complex part of the atmosphere. For homeland security applications, the end-user's need for timely and accurate ATD information in the urban environment is one of the most pressing national needs.

In October 2001, the Office of the Federal Coordinator for Meteorological Services and Supporting Research (OFCM) established the interagency Working Group for Environmental Support to Homeland Security (WG/ESHS) at the request of the Federal Committee for Meteorological Services and Supporting Research (FCMSSR). In January 2002, the WG/ESHS formed the Joint Action Group for the Selection and Evaluation of Atmospheric Transport and Diffusion Models (JAG/SEATD) to study the nonproprietary atmospheric transport and diffusion (ATD) modeling systems in use by federally funded operations centers. In August 2002, the JAG/SEATD's definitive report was published, and its recommendations were endorsed by FCMSSR.

Among the recommendations was the need to further study the research and development (R&D) requirements related to ATD modeling. In October 2003, the Joint Action Group for Atmospheric Transport and Diffusion Modeling (Research and Development Plan) (JAG/ATD(R&DP)) was formed under the WG/ESHS and charged to:

- Develop a methodology for characterizing and prioritizing the research and technical needs, and for linking those needs to stated operational requirements.
- Consult with subject-matter experts as required (based on the needs of the JAG members).
- Identify the tools required for transitioning successful research results into operations through interagency cooperative efforts like observational and modeling test beds, field and urban studies/experiments, and a common model evaluation methodology.
- Develop a comprehensive plan that documents the research and technical needs of the ATD modeling and operational communities. The plan should prioritize the most pressing R&D needs and provide a roadmap to address those needs within the OFCM coordinating infrastructure. Expanded feedback on the plan was solicited during the 8th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling on July 14, 2004, and the OFCM Urban Meteorology Forum, *Challenges in Urban Meteorology: A Forum for Users and Providers,* on September 21-23, 2004, which included participation from the academic, public, and private sectors.

This report is the culmination of the JAG/ATD(R&DP)'s efforts. The report describes the research and development needs, based on user-community needs, and recommends a number of strategies to address those needs in order to provide a reliable capability to use atmospheric transport and diffusion as an instrument of local and national emergency response or planning. The principal topics addressed by the report include:

- A discussion of user needs for *consequence assessment systems* (a general name for typical applications in which ATD models are employed, including but not limited to emergency response/recovery and preparedness planning applications).
- Interpretation of the ATD modeling capabilities required to support what users need from their consequence assessment systems.
- Analysis of the gaps between the required capabilities and current Federal ATD modeling capabilities (requirements pull), plus opportunities for new and emerging science and technology to fulfill user needs better in the future (technology push).
- Strategies to fill the gaps and provide improved capability through an interrelated set of coordinated R&D activities implemented by Federal agencies with ATD modeling programs or related research, development, or technology transition programs.
- Prioritized recommendations for implementing the R&D strategies.

User's Needs

The emergency preparedness and response environment includes a number of activities during which consequence assessment of an airborne hazard is relevant. Planning activities start in anticipation of a specific incident to help everyone prepare to respond. Response activity begins when an incident occurs. Response activity then transitions into recovery activity. Incidents that involve the release of an airborne hazardous material can range from a relatively straightforward situation that that can be handled by local responders to a complex situation that involves elements of all three activities described and requires resources from many different organizations; i.e., incidents of national significance.

Users recognize that ATD models of the consequence assessment system are imprecise. They desire—and create—ways to work with the limitations of the information. Models give little or no expressions of probability and uncertainty, so they are insufficient to help many users make sound decisions. This fact imposes two complementary demands on model development. First, we must provide a reasonable measure of the uncertainty in a prediction or its probability distribution, and then secondly, we must communicate the implications of quantifying the uncertainty in ways the users can apply**.**

Research Needs

Advances in current ATD modeling are likely to come from improvements in meteorological model predictions and from measurements at the scales of interest. The former are closely related to better representations of atmospheric boundary layer (ABL) processes by improved parameterizations, initial conditions, boundary conditions, and representations in complex, especially urban, environments. As existing modeling and observing capabilities are improved, the realization that the ATD process is partly stochastic, rather than entirely deterministic, will enable uncertainties in the modeling process to be quantified. The modeler must then learn with the user how to communicate this uncertainty information to the user in ways that are relevant to the user's decisions.

Models and data must come together and complement one another. Techniques to localize and/or quantify source characteristics by fusing information from concentration sensors, ATD models, and other measurements are lacking or untested. To meet user requirements for timely modeling predictions, faster methods are needed to determine the quality of observed data, merge the acceptable data into modeling frameworks, and estimate concentrations rapidly across several scales of motion. Finally, to ensure the quality of the model estimates and provide the benchmark for improvements, the skill of the prediction and its robustness need to be assessed on a continuing basis.

To advance the state-of-the-science in ATD modeling, we must meet these R&D needs:

- Bridge the gap from mesoscale to microscale/urban scale.
- Improve characterizations of surface boundary conditions in model parameterizations and in input data sets (initial conditions and boundary conditions). In particular, better methods are needed to obtain, maintain, and apply land cover data for urban and surrounding environments.
- Test and refine the physical basis for sub-grid-scale parameterizations.
- Characterize dispersion in complex environments.
- Develop methods and technologies for improving ensemble construction and interpretation.
- Develop and test techniques to better estimate wet and dry deposition and chemical interactions.
- Improve tracer materials and measurement technology.
- Improve boundary layer atmospheric measurement capability.
- Improve and evaluate data acceptance and assimilation techniques for both initial conditions and boundary conditions.
- Develop physics-based evaluation metrics that recognize the fundamentally different sources for variations in observed and model-predicted values of downwind hazard concentration.

A tabular summary of these needs and priorities follows.

Table ES-1. Summary Table of R&D Needs with Prioritization Factors

R&D Need	Time Sensitivity	Short-Term Gain	Overall Level of Effort	Lead Time	Ultimate Gain Potential
Bridge the modeling gap	near term	average	moderate	average	exceptional
Characterization of surface conditions & input data sets	near term	average	high	average	exceptional
Test and refine physical basis for sub-grid-scale parameterizations	longer term	average	moderate	average	exceptional
Characterize dispersion in complex environments	immediate	average	high	average	high
Improve ensemble construction and interpretation	immediate	minimal	high	short	exceptional
Techniques to better estimate wet and dry deposition	near term	average	moderate	average	high
Physical and high-resolution computational models	near term	average	moderate	average	exceptional
Improve tracer materials and measurement technology	immediate	high	moderate	short	exceptional
Improve boundary-layer measurement technology	immediate	high	high	short	exceptional
Improve and evaluate sensor-fusion techniques	immediate	high	moderate	moderate	high
Data QA/QC for model fit and data assimilation	immediate	average	moderate	moderate	high
Develop physics-based model evaluation methods	near term	high	low	average	exceptional

Research and Development Strategies

The JAG identified two capstone goals for the R&D plan: *quantifying uncertainty* and *interpreting the implications of this uncertainty to users*. The JAG then identified six program elements needed to support the capstone goals. To achieve the goals, it is essential that the elements of the strategy be sustained, evaluated, and allowed to evolve as the knowledge base grows and the capabilities for ATD modeling improve.

Capture and Use Existing Data Sets. This element focuses on assembling the available (open access) data sets from the many years of ATD experiments and model testing into a modern data format. The data are in various forms and available on many types of storage media. Both the data and the expertise of the participating scientists are at risk of being lost. These rich data files are the only source of concentration data which can currently be used to quantify uncertainty in ATD models.

Model Evaluation Standards. Procedures for evaluating the performance of ATD modeling systems are not standardized across the Federal agencies or ATD model user communities. Further, the existing procedures may not fully deal with the complexities introduced by comparing calculations and observations having different inherent space and time averaging. Without common reference standards, model development and implementation tends to remain "stovepiped" within the developing agency, while other development efforts are discounted or go unused.

Bridge the Modeling Gap. Top-down modeling (large to small scale) and bottom-up modeling (small to larger scales) do not merge across scales from 50 meters to 5 kilometers in realistic environments. This fact points to a fundamental lack of knowledge of how to model the processes at these scales. In all models, there is an element of turbulence carried in the smallest scales and the unresolved processes. Although there is perpetual optimism that higher-resolution models will give better results, current operational experience does not substantiate the optimism.

Improved Measurement Capabilities. Measurements are fundamental to advancing the realism of a science-based description or prediction. In ATD modeling, improving the capability to measure concentrations of tracers and atmospheric variables (e.g., wind velocity, turbulence, temperature) *at the scales of ATD model use* is essential to R&D leading to better ATD models. Quantifying the uncertainty in model variables requires in situ and/or remote measurements at the modeled scales. Most applications of ATD models are at much finer scales than are the available data, especially in populated areas. To develop better parameterizations, measurements are needed to understand processes not resolved within models. Measurements are also needed to help bridge the model gap. Tracer measurement capabilities are needed to provide data for quantifying the uncertainty in ATD model predictions.

Local/Regional Siting of Instrumentation. Each locality has a unique morphology. Many localities want to provide a network of instruments, within budget limitations, that will reasonably represent wind and turbulence fields needed for ATD concentration fields in emergency conditions. No one plan fits all these sites. Strategies are needed to make reliable recommendations through a combination of modeling exercises, optimization processes, and experience in other areas.

ATD Test Beds. Most ATD model studies come in defined field campaigns operated to maximize the probability of success. Within this context, benign, simple, and non-taxing weather conditions were preferred although terrain conditions may have been complex. Controlled tracer releases are sampled and atmospheric measurements are made as densely as capabilities and resources permit. As accidental releases and terrorist incidents are not scheduled, little is known about performance of ATD models under daily conditions. Recently, fledgling infrastructures for routine ATD forecasting based on model and local information, such as NOAA's DCNet, have developed in several urban areas. The JAG proposes a strategy of establishing test beds in appropriate areas across the country to address and test ATD models, model needs, and model capabilities on a continuing basis. By operating and performing evaluations continuously, by testing new ideas and instruments, and by interacting regularly with users, an ATD test bed becomes a crucible in which ATD modeling is made robust and refined from an art into a demonstrated and verified operational capability. The initial number of test bed installations should be limited so that operational procedures can be developed and refined without squandering scarce resources. Once the prototyping lessons have been learned, the set of installations could expand to cover more locations of priority interest, with each additional location chosen to represent different challenges from those already in place or being installed.

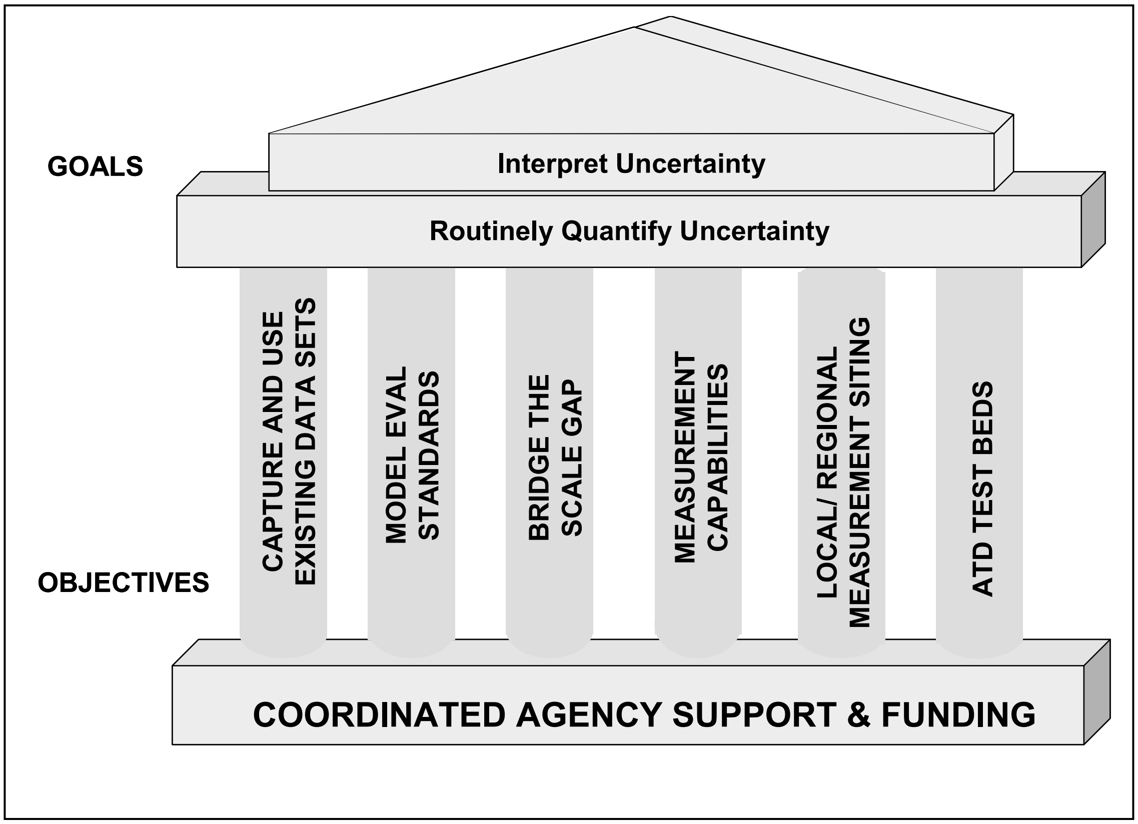

Figure ES-1. Six R&D objectives need to be achieved to support the ultimate goals of quantifying uncertainty and communicating its implications to users.

Recommendations

The recommendations are intended to support and guide Federal agency efforts to prioritize and obtain the necessary resources for their most pressing research needs. Additionally, they were developed to encourage multiagency collaboration and cooperation on shared objectives while helping to facilitate the participation from the academic and private sectors and the coordination of Federal activities with state, regional, and local governmental agencies.

The R&D elements will require a robust, coordinated effort by the multiple Federal agencies engaged in research, development, or application of ATD modeling systems. No one agency holds all the capabilities needed to affect the recommended course of action. Shared responsibilities, shared vision, and shared resources are essential to success. Without the resource base and sustained direction that a well-coordinated Federal effort can provide, the R&D needs cannot be met within time horizons consistent with national policy priorities.

Implementing recommendations are provided for the following seven areas:

- Quantify model uncertainties and interpret their implications to users.
- Capture and use existing data sets.
- Implement ATD test beds.
- Develop standards for evaluating modeling system performance.
- Improve the spatial and temporal scale interactions between meteorological and ATD models.
- Improve measurement technologies.
- Design and conduct special studies and experiments.

Implementing the recommendations will require a sustained effort over more than a decade. Some of the implementing actions will produce returns in the near term—within the next 2 years. Other actions will provide some benefits at intervals along the way, even though the most significant benefits may require a decade or more to be realized. Many of the limitations in capability identified in the report, however, are systemic, resulting from a lack of coordinated effort across agencies and agency programs, but they can be successfully overcome with the commitment and coordination of resources and facilities, particularly the agency teams of individuals dedicated to advancing the operational state-of-the-science of ATD modeling.

1.0 INTRODUCTION

The fundamental reason for modeling atmospheric transport and diffusion (ATD) is to predict the concentration in the atmosphere of hazardous material released from a source or sources (one or more points of release) as the material moves from the source to other locations. The predictions from an ATD model of concentration as a function of space (location) and time, plus other information, can be used for a variety of purposes. Hypothetical releases at particular points and under different conditions (the planning scenarios) can be used by *planners* to identify potential zones of hazardous threats and prepare effective responses to these scenarios. In an actual release situation, the threat may require emergency *responders* to take immediate action to protect health and safety of those in the zones of hazardous threats or to provide aid to those injured or exposed. Model predictions of where concentrations did (and did not) reach levels of concern are also important during the *recovery* phase, which may extend long after the immediate emergency. For less immediate dangers, such as those from *continuing release* of air pollutants with potential long-term effects, the planning, response, and recovery activities may weave into one another. Response activities, in particular, will periodically rise and fall as concentration levels of the hazardous material rise and fall over time.

At the most basic level, an ATD model predicts how motions in the atmosphere—wind and turbulence fields—transport and diffuse the material of interest after its release. Perfect prediction of the smallest motions in the atmosphere is not possible. Inherent constraints arise from limited information about the source, the atmosphere, and the time available to generate a prediction. The information needed about the source and the state of the atmosphere is always limited. Furthermore, some of the motions involved must be described stochastically or as nonlinear dynamic processes. Consequently, getting useful results from an ATD model is always a compromise between timeliness and completeness in portraying how the atmosphere acts on the released material. This tradeoff between timeliness (or resources for the modeling activity) and completeness is starkest for emergency response to an actual incident. No matter how much better the ATD modeling results could be in an hour or two, by then they are likely to be too late to help the first responders. Even the planner cannot wait forever or invest unlimited resources in a single model run. If planning for the one situation that does occur is to be appropriate, many scenarios must be considered and evaluated. Timeliness (and to a lesser extent, resource constraints) are less of an issue for long-term recovery, but the completeness standard often rises very high in that context of use.

Another practical demand on many real-world applications for ATD models stems from the consequences that variations in the prediction of hazard zones can have on large numbers of people. In urban areas, planners and responders are often faced with difficult triage decisions: who most needs help and needs it most quickly? When the complex morphology of urban areas is added to the prediction task—the irregular land-water interfaces of coastal bays and inlets, mountain-valley structures, or just the height and spacing variations of the modern urban built environment—the demands on the ATD model to identify the hazard zones accurately become extreme. *ATD models typically* *must describe atmospheric processes in the most changeable and complex part of the atmosphere.*

The events of September 11, 2001, dramatically sensitized the American public to the magnitude and range of potential terrorist actions aimed at civilian populations. The Nation is now far more aware of the potential threats from airborne technological hazards, such as releases of chemical, biological, radiological, and nuclear (CBRN) materials, not only from a deliberate action with hostile intent but also from industrial and transportation accidents. There is also an increased (and appropriate) expectation that all levels of government will improve their capabilities to share information, coordinate responses, and collaborate on preparations to better protect the public. Thus, there is a new sense of urgency associated with the research needs identified in this report.

1.1 Purpose

Given the objectives of ATD modeling and the constraints and current concerns as sketched above, there is value in a systematic approach to determining the most effective ways to lessen the constraints while making ATD modeling systems more useful for their intended applications, particularly applications of most pressing concern. This report presents a research and development (R&D) plan for providing the ATD modeling capabilities needed to meet established needs of the user communities, with special emphasis on enabling the National strategy for responding to domestic CBRN incidents. Although the report emphasizes homeland security and homeland defense applications, many of the capability improvements identified here will benefit other applications as well, such as air quality monitoring or emergency preparedness planning and response for accidental releases of hazardous materials.

The report includes:

- A discussion of user needs for consequence assessment systems (a general name for typical applications in which ATD models are employed, including but not limited to emergency response/recovery and preparedness planning applications);
- Extraction of ATD modeling capabilities required to support the users needs;
- Analysis and prioritization of the gaps between the required capabilities and current Federal ATD modeling capabilities (requirements pull), plus opportunities for new and emerging science and technology to fulfill user needs better in the future (technology push);
- A strategy to fill the gaps and provide improved capability through an interrelated set of coordinated R&D activities implemented by Federal agencies with ATD modeling programs or related research, development, or technology transition programs; and
- Recommendations for next steps in implementing the R&D strategy.

The R&D plan and recommendations presented here are intended to support and guide Federal agency efforts to fund their most pressing research needs and to encourage multiagency collaboration and cooperation on shared objectives. The plan will help to facilitate participation from entities in other sectors (academia and industry) and coordinate Federal activities with local, regional, and state governmental entities.

1.2 ATD Models in a Consequence Assessment System

For all the applications of ATD models mentioned above (and discussed more fully in chapter 2), users actually work with a complete consequence modeling system (or the functional equivalent of such a system, composed of several pieces). Figure 1 shows how an ATD modeling system fits within a complete consequence assessment system. The functions typically considered as part of the ATD modeling system are represented by the bold black boxes. The other functions are in lighter boxes.

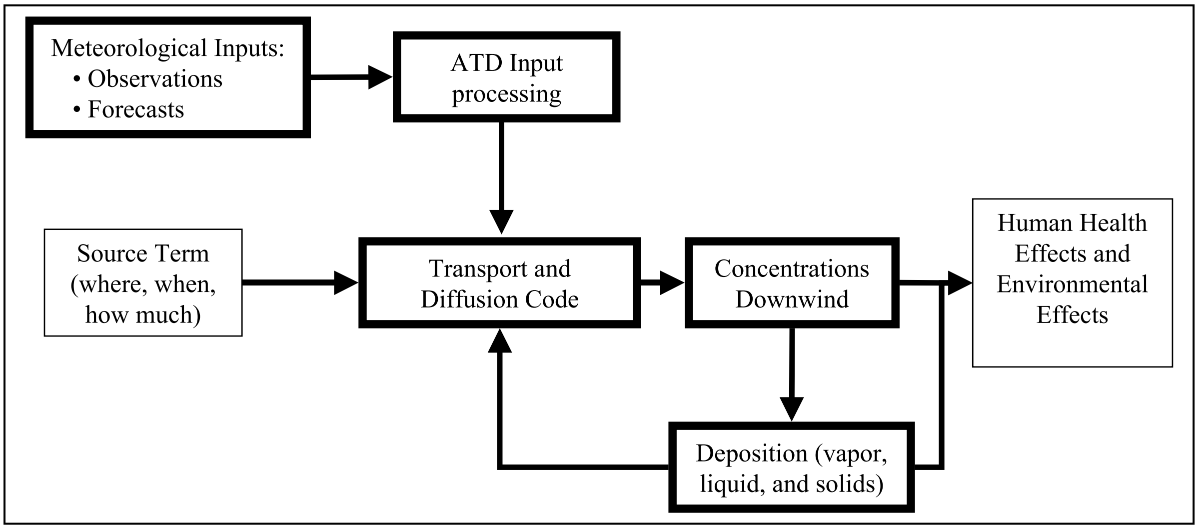

FIGURE 1. The functional components of a complete consequence assessment system, with its embedded ATD modeling system shown by bold lines.

The purpose of a consequence assessment system is to assess the consequences of specific hazards on people and the environment. To do this, the functional components must work together, passing information from one component to the next as shown by the arrows in figure 1.

- The **source term** component includes information about the identity and physical state of the hazard or hazards for which consequences are being assessed, the release mechanism(s) involved, and the mass of hazard released per unit time. For CBRN weapons, the release mechanism is the agent delivery system. For an industrial accident, it could be a leaking transfer line or burning truck trailer.
- **Meteorological inputs**, in simple terms, describe the local weather conditions at the time a source term release occurs and forecasts for these conditions through the time the substance is airborne. At a minimum, ATD models require inputs on wind speed and direction and a measure of turbulent activity, with the implicit assumption that these conditions do not change. A more complete meteorological

specification may include clouds, precipitation, temperature, pressure, humidity, surface heat and momentum fluxes, and more complex turbulence parameters.

- **ATD input processing** involves processing the available meteorological forecast information and observational data to prepare it for use in the modeling done by the transport and diffusion code. Input processing might, for example, include a diagnostic model in which available wind observations are used to estimate three-dimensional wind fields that reflect the impact of local terrain and conserve mass. It may also involve *data quality acceptance and quality control* (data QA/QC), such as applying criteria for whether additional observational data are accepted into the model run after initialization. ATD input processing may be used when meteorological observations are ingested into a localized wind field forecast. It may also be used to generate a nowcast (forecast for the next 1 to 6 hours) using the forecast fields from a prognostic meteorological model as a first guess and refining them by assimilating observational data that were not available at initialization. Sometimes these input processing functions are not considered part of the ATD modeling. For reasons that will emerge in chapter 3, this report includes them as a component within the ATD modeling system.
- **The transport and diffusion code** is the software engine that computes advection (transport solely by the mass motion of the atmosphere) and diffusion. The code describes, in sets of computation instructions to a digital computer, the combined effects of time-averaged transport (which has traditionally been viewed as a deterministic process) and diffusion. The principle mechanism of diffusion is turbulence, which has traditionally been represented as a stochastic process. A deterministic process is governed by and predictable in terms of definitive laws, such as dynamic equations. A stochastic process evolves in time according to probabilistic equations; that is, the behavior of the system is determined be one or more time-dependent random variables.
- **Deposition** refers to the way in which the ATD modeling system represents processes that remove the hazardous material of interest from the air carrying it and deposit it on the Earth’s surface (land or water). Substances released into the atmosphere will continue to reside there, continually diluted by mixing processes, until they are removed by reactions with other components of the atmosphere or are deposited to the surface. In some instances, deposited materials have the potential for subsequent resuspension by wind or volatilization.
- **Concentrations downwind** refers to the model’s prediction of how much of the hazard of interest (what concentration) will be in the air at particular locations and times after the release.
- **Human health and environmental effects** are the consequences of ultimate interest to most users of a consequence assessment system. From the prediction of concentrations downwind and other information, potential impacts on human health and safety and on the environment are estimated.

In conformance with the terms of reference under which this R&D plan was prepared, the functional requirements for characterizing the source term or the human health and environmental effects components of a complete consequence assessment system will not be analyzed. R&D needs are not defined for the capabilities needed in those components, nor does the R&D plan include activities to address capabilities needed in those areas. However, these components are considered from the perspective of being, respectively, an essential input to and output of the ATD modeling system. As such, they do influence the capabilities required within the ATD modeling components and the R&D to provide those capabilities.

The analysis in chapter 3 will return to figure 1 to analyze in detail the capabilities needed for each component of an ATD modeling system. For the moment, however, the principal message of figure 1 is that, for the purposes of this R&D plan, *an ATD modeling system is always a tool for the larger purpose of a consequence assessment application*. Differences in the specific objectives of that application will often mean that the ATD modeling system must be tailored to *fit the tool to its task*.

1.3 Scope and Context of the R&D Planning Activity

The activity leading up to this ATD R&D plan began shortly after the terrorist attacks on the World Trade Center and the Pentagon on September 11, 2001. In December 2001, under the direction of the Federal Committee for Meteorological Services and Supporting Research (FCMSSR), the Federal Coordinator for Meteorology established the Joint Action Group for the Selection and Evaluation of Atmospheric Transport and Diffusion Models (JAG/SEATD). The task of the JAG/SEATD was to evaluate the ATD modeling systems available to address threats to homeland security. The group's final report, published in August 2002, included a list of candidate research needs and concluded that the current ATD modeling systems available for Federal agency and military use should be refined and prioritized to reflect operational needs (OFCM 2002). The FCMSSR concurred with this recommendation, as documented in Action Item 2002-2.1 of the Record of Actions from the FCMSSR meeting of October 12, 2002. The Federal Coordinator for Meteorology then initiated a phased effort to address the recommendation.

For the first phase, the Federal Coordinator established the Joint Action Group for Atmospheric Transport and Diffusion Modeling (Research and Development Plan), or JAG/ATD(R&DP), and charged it to perform the following tasks:

- Review the proceedings from the Office of the Federal Coordinator for Meteorology (OFCM) special session at the George Mason University (GMU) Transport and Dispersion Modeling Conference (OFCM 2003) and identify any additional research needs that resulted from the conference.
- Review the results of the Joint Urban 2003 experiment at Oklahoma City (DTRA/DOE 2003).
- Identify any scenarios that are not addressed satisfactorily by the modeling systems documented in the JAG/SEATD report.

- Develop a methodology for characterizing and prioritizing the research and technical needs and for linking those needs to stated operational requirements.
- Consult with subject-matter experts as required (based on the needs of the JAG members).
- Identify the tools required for transitioning successful research results into operations through interagency cooperative efforts like observational and modeling testbeds, field and urban studies/experiments, and a common model evaluation methodology.
- Develop a comprehensive plan that documents the research and technical needs of the ATD modeling and operational communities. The plan should prioritize the most pressing R&D needs and provide a roadmap to address those needs within the OFCM coordinating infrastructure.

This R&D plan is the response of the JAG/ATD(R&DP), hereafter referred to as “the JAG,” to the above terms of reference. Expanded feedback on the plan was solicited during the 8th Annual GMU Conference on Atmospheric Transport and Dispersion Modeling on July 14, 2004, and the OFCM Urban Meteorology Forum on September 21-23, 2004, which included participation from the academic, public, and private sectors.

Research areas that were considered within the scope of phase 1 included but were not limited to meteorological inputs and input data processing, directly measured dispersion inputs, and transport and diffusion calculations. Research needs associated with but not limited to source characterization, common default source terms, chemical mixtures, chronic health effects, and common frameworks for the display of results in geographic information systems (GISs) will be included in a later phase.

To understand existing Federal operational modeling capabilities, the JAG has relied heavily upon the earlier JAG/SEATD study (OFCM 2002). The JAG/SEATD explored these capabilities in considerable detail but with limitations imposed by incomplete understanding of each modeling system. The JAG/SEATD determined that, of the 29 distinct ATD modeling systems it studied, many emphasized processes and factors that were peculiar to a specific application. Some of these systems provided a commendable representation of atmospheric dispersion processes. Many were integrated into consequence assessment systems with extensive source characterization and health effects for specific substances. These capabilities reflected investments by the Federal agencies that developed the ATD modeling systems over a significant period.

The current JAG studied the R&D needs listed in the JAG/SEATD report, as well as the report’s recommendations. It also reviewed the proceedings from the OFCM special session of the 7th Annual GMU Transport and Dispersion Modeling Conference (OFCM 2003) and the National Research Council report, *Tracking and Predicting Atmospheric Dispersion of Hazardous Material Releases, Implications for Homeland Security* (NRC 2003). From the review of these documents, the JAG developed a preliminary list of research needs.

Next, the JAG conducted teleconferences and several panel sessions dedicated to specific topics, to facilitate as much participation as possible by Federal agency representatives and subject-matter experts in drafting early versions of the R&D Plan. Subject-matter experts were invited to assist in reviewing and revising the list of candidate R&D needs. The JAG also reviewed the Joint Urban 2003 field experiment (DTRA/DOE 2003) and discussed a framework for transitioning successful research results into operations through interagency cooperative efforts. Among the cooperative efforts considered were test beds for observing systems and modeling, field studies and experiments including ones conducted in urban areas, and a common model evaluation methodology.

The JAG considered whether there were incident scenarios of recognized importance for which all of the current ATD modeling systems were totally unsuited. The conclusion was that all of the identified scenarios can be at least minimally addressed by one or more modeling systems. The JAG also discussed the challenges from releases of CBRN material due to high-altitude intercepts of ballistic missiles. In consideration of these realities, the R&D plan proposed in this report makes thorough and imaginative use of all available tools to address the dispersion issues confronting the Nation. Overall, the R&D plan reinforces the need for expanded theoretical and physical modeling studies, for dedicated field studies conducted in the circumstances of intended application, and for close coupling of all such activities with the development of improved models. These elements of an overall strategy accept and build upon the standard approach of continuing exploration of contributing processes. They acknowledge the powerful needs of current times and the urgency with which new and refined products are desired. They recognize that rapid transfer of the findings to the user community is necessary. To accelerate this transfer to operations, an essential element of the proposed strategy is to deviate from the usual approach to meteorological research and couple the user community more closely with the R&D program for ATD modeling.

The JAG prepared a draft R&D plan in time for review within the OFCM coordinating infrastructure prior to the 8th Annual GMU Transport and Dispersion Modeling Conference in July 2004. The main elements of the plan, including the recommendations for next steps in implementing it, were presented at that forum during a special OFCM session. This session enabled representatives from the public, private, and academic sectors to comment on them. Their comments were used to revise the report as appropriate.

The R&D strategy and recommendations in this report were presented at the OFCM Urban Meteorology Forum in September 2004 to solicit feedback from non-Federal organizations. This forum provided an opportunity for commercial interests and academic institutions to consider how their resources complement or supplement the approach to research and advanced development described in this document.

The report will be submitted to FCMSSR, through the Federal Coordinator and the Interdepartmental Committee for Meteorological Services and Supporting Research, for its endorsement of the report's recommendations. After the FCMSSR review, the responsible agencies within the Federal meteorological community will coordinate an approach for implementing the recommendations.

1.4 Structure

The report consists of six chapters and five appendices. Chapter 1 provides an introductory view of the purpose of ATD modeling systems and introduces the plan's scope, context, and general argument structure. Chapter 2 describes the operational needs of users of ATD modeling systems from their perspective, with particular attention to the similarities and differences in operational context and consequence assessment requirements of the major segments of the user community.

Chapter 3 interprets the operational user needs into required capabilities of ATD modeling systems and the inputs to those systems. Chapter 3 also begins the analytical task of comparing these requirements with existing capabilities, to identify gaps between what current systems can now do and what users need them to do. Chapter 4 goes further into this assessment of capabilities against requirements. It focuses on three broad areas:

- Improvements to both ATD models and the meteorological models that typically provide input data for them;
- Improvements to measurement technologies, to provide both the data needed to improve results with current modeling capabilities and the data required to take full advantage of the proposed modeling improvements; and
- Improvements required at the interfaces between data and models—areas that require a joint analysis and will involve accommodation and innovation from both sides.

Chapter 5 presents the set of interlocking program elements that the JAG adopted as the best approach for addressing the R&D needs identified and prioritized in chapters 3 and 4. The exposition of each program element covers the capabilities to be achieved through it, the rationale for this element as the best approach to meet user needs, and the relationships among the elements as components of an overall R&D Plan.

Chapter 6 contains the JAG's recommendations for actions to implement the plan in Chapter 5. Most of the recommendations include specific implementation actions to be taken if the basic recommendation is endorsed by FCMSSR.

The appendices include supporting details for the main lines of argument in chapters 3 through 5. Appendix A provides a historical perspective on the current state of meteorological and ATD modeling capabilities. It includes brief summaries of a set of past ATD field studies, which the JAG considers to be prime candidates for capturing existing data for new R&D objectives (section 5.3). Appendix B is a summary of current ATD modeling capabilities and R&D programs. It supports the analysis of gaps and opportunities in chapters 3 and 4. Appendix C is a more technical treatment of some of the key considerations underlying the general argument of chapter 3 and section 4.1 on the necessity to incorporate more probabilistic methods, representations, and output information in ATD modeling systems. Appendix D is a glossary of acronyms used in the report. Appendix E lists the JAG participants.

Reference information for the technical literature and other source citations in the body of the report (chapters 1 though 6) is listed after chapter 6 and before Appendix A. Each of appendices A through C contains its own reference list.

2.0 USER NEEDS

The consequence assessment systems introduced in chapter 1 can serve a variety of applications. While the scope of this document is primarily focused on the emergency preparedness and response needs of the homeland security community, consequence assessments are important in other applications as well. All of these applications utilize the fundamental building blocks of figure 1 and face the challenge of properly employing ATD modeling systems in complex environments, such as urban and coastal areas.

This chapter explores the range of user activities and their specific needs within the area of emergency preparedness and response, while identifying common needs that extend across these diverse application areas. These needs are the principal drivers that determine what the ATD modeling system must provide within any specific application's consequence assessment system. This statement foreshadows a major theme of this report: early and continuing involvement of the user community is essential in the development and product improvement process.

The JAG invited users from local, state, and Federal agencies to discuss their current use of ATD modeling systems, shortfalls in their ability to perform consequence assessment, and how their needs and requirements could be better met. These representatives included firefighters, state emergency managers, and Federal emergency responders and managers. Their perceptions of current capabilities and needs are the basis for most of this chapter.

2.1 The Emergency Preparedness and Response Environment

The emergency preparedness and response environment includes a number of activities during which consequence assessment of an airborne hazard is relevant. Planning activities start in anticipation of a specific incident to help everyone prepare to respond. Response activity begins when an incident occurs. Response activity then transitions into recovery activity. Incidents that involve the release of an airborne hazardous material (HAZMAT) can range from a relatively straightforward situation that can be handled by local responders to a complex situation that involves elements of all three activities (response, planning, and recovery) and requires resources from many different organizations.

The same personnel may be (and often are) involved in planning, response, and recovery activities. These personnel include:

- The local, state, and Federal emergency responders—law enforcement officers, firefighters and HAZMAT technicians, emergency medical personnel, and on-scene commanders;
- Government officials and emergency managers, many of whom will have important decision-making roles; and
- Federal agency decision makers, executing their operational missions.

For domestic incidents of national significance, the roles and responsibilities of the Federal agencies are defined in the National Response Plan and its associated annexes (DHS 2003). The incident management process is described in the National Incident Management System. Requests for Federal assistance and information flow up through the local jurisdiction's (e.g., city or county) emergency operations center to the state level, and then to the Department of Homeland Security (DHS). In domestic incidents of national significance, such as terrorist incidents and other high-visibility, multi-jurisdictional events, DHS may designate a Federal officer to serve as the local DHS representative and provide senior leadership, strategic guidance, and Federal operations integration (DHS 2004).

Release Event
What was released?
When?
Where?
How Much?

Observations
Direct
Sensor
Casualty

Risks
How many?
For how long?

Consequence management
How to minimize and/or manage impact?

FIGURE 2. Questions of concern to users of ATD modeling predictions for emergency preparedness and response.

For an incident involving the atmospheric release of a hazardous material, these users all need answers to the questions shown in figure 2. These fundamental questions remain relevant whether the hazardous release incident is small in scale and handled entirely by local response personnel or becomes an incident of national significance, spanning multiple jurisdictions and requiring Federal response support.[1] Current capabilities to answer these questions vary among Federal, state, and local response agencies. Locales that have industrial or manufacturing facilities, containing substantial amounts of hazardous materials, may be better prepared in terms of personal protection equipment, sensors, and stand-alone modeling capability than those without such hazards. Military and other Federal installations that store or handle hazardous material may have capability to respond to CBRN releases. The military may also provide support services to civilian agencies as an integral element of its homeland defense mission.

Four common themes recurred in the comments from most of the users who spoke with this JAG:

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[1] The 2002 annual report of the National Atmospheric Release Advisory Center (NARAC 2002) states, "Effective preparation for and response to the release of toxic materials hinge on accurate predictions of the dispersion, ultimate fate, and consequences of the chemical or biological agent. Of particular interest is the threat to civilian populations within major urban areas, which are likely targets for potential attacks."

- The safety of people is the first priority.
- All emergencies are local, and most are short-lived.
- The end user of the ATD results needs actionable information.
- Inconsistent data products and distribution protocols can cause confusion and inefficiencies in the emergency response.

Not surprisingly, one of the first and most important needs expressed by emergency responders is the need for effective communication and early indication of where the contaminant is going. Equally important is gaining an understanding of where it is likely ***not*** to go. A communications link between the HAZMAT or other emergency personnel and personnel with ATD expertise is often preferred to having the modeling capability "onboard" or at the scene. A "reach-back" capability is desirable because responders are busy dealing with public safety issues including medical response, potential evacuation, and incident characterization. They do not have the resources to run models and interpret results.

Emergency responders requested more useful and uniform products and a standard protocol for distribution and display of hazard predictions to the response community. They emphasized the need for established procedures to rapidly disseminate hazard area predictions to all levels of the response team. The use of GIS-based displays with overlays of near real-time hazard information could be especially important for large-scale incidents, involving multiple response agencies and potentially affecting large segments of the local and/or regional population.

The products need to be easily displayed and uniform in content. While users wanted a reach-back capability when needed (for example in a major incident), they also want an on-scene capability for making rapid decisions during smaller scale incidents. Above all, emergency responders asked for the capability to deliver the information needed into the hands of those working to save lives.

The user panel expressed the following key needs.

- Improvements are needed in the national capability for consequence assessments for preparedness and response applications:
    - Capability for modeling more than one substance at a time;
    - Realistic planning scenarios that can be built quickly and simply, to include a variety of hazards and local weather scenarios;
    - Scenarios that include common industrial chemicals, especially ones that could be weaponized;
    - Planning scenarios for CBRN agents, utilizing local building terrain and weather profiles;
    - Improved infiltration models; and
    - Capability for modeling flammability and explosivity.

- Information must be displayed in the emergency manager's display system (which may or may not be GIS-based) in accordance with the organization's standard operating procedures.
- A standardized set of products should be tailored to the needs of the particular end user:
  - Multiple product sets for multiple users;
  - Regular updates;
  - Realistic predictions which depict forecast uncertainty; and
  - Timely products—the key to saving lives.
- Training and coordination among Federal, state, and local responders are critical to efficient communications during an event.
- Users must be brought into the development process early and often.

2.2 User Needs in Other Applications of ATD Modeling Systems

2.2.1 Military Applications

The primary military requirements for ATD modeling *in theater* are for force protection and civilian population protection. CBRN materials are expected in modern military encounters on the battlefield. In data-denied areas, the military needs improved capabilities to sense weather and hazard parameters within an operational area. Accurate guidance on the use of hazard protection equipment (protective garments, masks, etc.) to defend against chemical or biological agents is critical for conducting military operations.

The key questions of importance to emergency preparedness and response (figure 2) are still the questions that military users need to answer, but the form and content of a useful answer may be different. For CBRN incidents, military applications involve planning and response phases similar to those for civil emergency preparedness. However, the resultant actions may differ and will be driven by military needs.

Meeting the needs specific to military applications will require:

- Improving current capabilities of weather-parameter and hazard-sensing systems that can be remotely deployed and monitored;
- ATD planning for installation protection and for joint and coalition operations, covering both deliberate releases (hostile actions) and accidental releases (e.g., destruction of enemy munitions containing CBRN and accidents during the removal or storage of CBRN-containing materiel); and
- Enhancing the capability to acquire and process the weather and hazard-sensor data; including assimilating the data into meteorological and ATD models.

2.2.2 Air Quality Monitoring Applications

The 11th Prospectus Development Team of the U.S. Weather Research Program observed in its July 2003 final report that there are at least three groupings of users of air quality information: the public, decision makers, and researchers (Dabberdt et al. 2004). The public is the largest user group, and the broadcast media provide the means of disseminating air quality information from its official source to the public. Decision makers that use air quality forecasts include Federal agencies, civil authorities (e.g., state and local departments of health), emergency response organizations, and the private sector (power, transportation, health care, and others). Among the Federal agencies that use these forecasts are the U.S. Environmental Protection Agency (EPA), the U.S. Forest Service in the Department of Agriculture, and the National Park Service in the Department of the Interior. Both public and private sector organizations use air quality forecasts to authorize and plan operations such as prescribed burns or pollutant-emitting operations at power plants and chemical manufacturing plants. Researchers who use air quality forecasts include air quality and environmental scientists, regulatory scientific advisors, and atmospheric scientists conducting field measurement studies.

The key questions of importance to emergency response also apply to air quality users; however, the form and content of a useful answer may be different. There is likely to be more emphasis on the capability for planning, and some of the decision elements involved, such as regulatory considerations, differ because the reasons for interest in air quality only partially overlap with the objectives of emergency response. Forensic applications in air quality are similar to those used in emergency response when ATD models are used to backtrack from observed concentrations to a release point. This application of ATD modeling may be necessary when the actual amounts and chemical makeup of the source material are unknown, as in an accidental release. Other uses of ATD models in air quality assessment are distinct from the way these models are used in a consequence assessment system.

For air quality forecasting, three-dimensional meteorological and chemical observations and advanced data assimilation methods are essential. In addition, meeting ATD modeling needs specific to air quality applications will require:

- Improved physical understanding of the atmospheric boundary layer (ABL);
- Better land-surface models;
- Better representation of winds and turbulence across varied spatial and temporal scales;
- Better understanding of clouds and cloud processes that affect chemical fate and transport; and
- Improved capabilities for estimating uncertainty and predictability and for evaluating models.

Information about other pollutants, including particulate matter, is important when considering the long-term health impacts on the population. For example, the air quality standards for fine particles are calculated using an annual average because national ambient air quality standards are set for pollutants that the public is generally exposed to for long periods of time. A shorter-term average standard would be more helpful when assessing the impact from short-term events or peak concentrations in long-term events. In the case of a fire or some other large source of particulates, the general practice is to move people away from the most intense concentrations of smoke. In responses to events that last on the order of days to a year (e.g., a landfill fire), however, managers need guidelines to decide how much short-term exposure a population can tolerate at any given time.

2.3 ATD Information Required for Hazard Response Decisions

The preceding sections showed that, across a range of applications for ATD modeling systems, the basic questions are the same. The user needs to know what the hazard is, when and where it is a threat to people (or other consequences), and the seriousness of the potential health and safety impacts to people and the potential environmental impacts.

For both health and environmental issues, the consequences can range from acute effects of short-term exposure to more slowly developing consequences of long-term exposure to levels too low to produce acute effects. For acute effects, spikes in the concentration of an airborne hazard are typically of interest. Therefore, the ATD model prediction needs to provide information on the spatial variability in hazard concentration on a time scale consistent with the time required to produce an acute effect. To assess effects from longer-term exposure to lower concentrations of a hazard, the time-averaged concentration of the hazard is needed. Many potential airborne hazards, including most CBRN agents, can potentially have acute and long-term effects, so both kinds of information are often relevant to the user.

Flammable materials are another class of potentially hazardous materials. When mixed with air in the right concentration range (i.e., between lower and upper concentration limits for the particular material), the material can explode if a source of ignition is present. If other combustible materials are within or near the explosion volume, the explosion can set off a rapidly growing fire. Users of a consequence assessment system for this class of hazards want to know when and where the concentration could be within the explosivity limits. This requirement is much like that for acute exposures—spikes in the airborne concentration at a time and place can be enough to reach the lower limit of explosivity.

For all of these consequences, the bottom line for the ATD modeling system is that ***the users want to know about the concentration of the hazard as a function of space and time***. In many instances, the user will want to know about both the peaks in the concentration at small time and space scales and the time-averaged concentration at spatial scales relevant to the consequence of interest. ATD predictions of concentration as a function of space and time must meet accuracy objectives for all places and conditions of concern, especially coastal urban areas. Physical processes to which ATD models are sensitive must be adequately treated, including land-sea breezes, urban heating effects, and urban effects on local winds. In densely populated regions of concern, small changes in the predicted hazard area can have substantial impacts on user decisions.

2.4 Constraints and Tradeoffs in ATD Modeling to Meet User Needs

Planning, response, and recovery activities have different constraints on timeliness for receiving a relevant prediction and on the comprehensiveness and completeness required for a prediction to be useful. The optimal tradeoff among these constraints will be different for different activities, different applications, and even specific characteristics of an incident (e.g., the hazard released and its consequences of interest, the amount released, the location of release, and the areas potentially affected).

As emphasized above, timeliness is the most important constraint for the responder but not the only one. One of the most important needs that emergency responders expressed to the JAG is for early indication and effective communication of the plume direction. Equally important is gaining an understanding of where the plume is likely ***not*** to go.

Most responders desire a comprehensive *reach-back* capability, which allows the local ATD modeler (or the on-scene user) to access technical support in getting predictions from the ATD modeling system that reflect the specific characteristics of the incident at hand. A single, direct line of contact from the incident command post to the supporting expertise is needed, rather than a complicated system that requires an expert to operate at the front lines. Most responders prefer an ATD modeling tool that is simplified for the response environment. They are too busy dealing with the immediate threats to health and safety to run complex models or to analyze results that do not tie directly to the decisions confronting them.

Specific emphasis on meteorological studies for planning purposes should be given to coastal zones, complex terrain, and urban environments where local heterogeneities have significant impact on dispersion. Users were especially aware of the special challenges raised by urban environment*s*. In urban areas, the presence of buildings and other structures affects not only the flow fields but also the structure and intensity of atmospheric turbulence. The R&D and test and evaluation communities need to seek user input on these urban challenges, the practical approaches users have found to dealing with them, and the kinds of information that would be of most benefit. Accurate databases on the built environment are required to model these surface-atmosphere interactions at scales relevant to ATD in urban environments.

Standard dispersion methodologies are based on descriptions of processes developed in the absence of buildings and urban street canyons. The influence of such urban complexity is known to be major, but relatively little is known concerning the best way to capture the consequences of site-specific surface features in the descriptions of turbulence used in dispersion calculations. In addition, building infiltration and exfiltration should be represented.

2.5 "If I Can't Have Certainty, Tell Me How Bad It Could Be, and Where"

Emergency responders do not want ATD model predictions couched in terms of mathematical measures of uncertainty or highly technical statements about probability. They do not know how to use such information. These measures of uncertainty bear no immediate and clear relationship to the decisions for which the users want information on hazard concentration as a function of space and time. This point was made most strongly by the first responders among the users who met with the JAG. While some decision makers may understand how to use uncertainty estimates, this fact also generally applies to planners and recovery operators as well.

The fundamental issue for the model developer can be expressed simply: Users want certainty in the information they get, so they can act quickly and decisively. The nature of the modeling situation (to be discussed in section 3.1), however, means that no ATD modeling system can provide predictions with certainty, at least not for situations of interest to real-world users.

Because users understand that there are limits to ATD modeling capabilities, they apply their intuitive estimate of uncertainty in order to err on the side of safety. A better option than relying on an intuitive safety margin is for users to have information on uncertainty interpreted into a form they know how to use. Rather than mathematical measures of uncertainty or probability, users asked for answers to these kinds of questions:

- What is the [reasonable] worst case to prepare for, and where could it occur?
- What areas are safely out of danger?
- Where could thresholds of interest (e.g., concentrations with lethal or other acute effects, longer-term exposure thresholds, explosive concentrations) be exceeded and when?

Many users are aware of the uncertainties in source characterization, in other model inputs such as fine-scale winds and land cover, and in modeling simplifications made to get results within time constraints. In many cases, users are dealing with the same types of uncertainty in their decisions. Knowing how users understand and work with these uncertainties can help developers find ***useful*** ways to present prediction uncertainties and probabilities to the user.

Reducing the uncertainty in ATD model predictions is an obvious goal for model developers. At the same time, model developers, users of model predictions, and all who assess progress in improving consequence assessment capabilities must understand that there will always be uncertainties in modeling complex, dynamic systems. The task for the modeling system researcher-developer is first to identify the sources of uncertainty in a given modeling system and provide reasonable measures of the uncertainty in a given set of predictions from the system. The second task—which may be the harder of the two because we know less about it—is to ***find ways to communicate to the user the implications of these uncertainties for that user's decisions.*** It is not enough to provide measures of uncertainty that are defensible within the model developer's world. Developers and representative users from the range of applications to be served will have to work together to determine how to make this essential information useful. The next task is to provide users with tools that meet their needs, which must be accomplished as part of development. The transition of R&D products into working tools must begin while the tools are still under development and before they are declared operational.

3.0 MODEL CAPABILITIES REQUIRED TO MEET USER NEEDS

Chapter 2 showed how the needs of those who use consequence assessment systems lead to the requirement that an ATD modeling system within the larger consequence assessment system predict accurately and usefully the concentration of the airborne hazard (or hazards) as a function of space and time. The predictions must be relevant to the actual conditions at the time of an incident. Users typically need to know who is not endangered, as well as who may be in danger. They want to know which locations are likely to be within a hazard area, which locations are safely outside the hazard zone, and the quality of these estimates.

Users know that ATD modeling systems do not produce perfect predictions. They desire—and find—ways to work with the limitations of the information, but the modeler's measures and expressions of probability and uncertainty are insufficient to help many users, particularly emergency responders and managers, make sound decisions. This user need imposes two complementary demands on the model developer. The first demand is to provide a reasonable measure of the uncertainty in a prediction or its probabilistic distribution. The second is to communicate the implications of this uncertainty measure or probabilistic distribution in ways the user can apply.

This chapter interprets all of the above user needs into requirements on ATD modeling systems, in terms relevant to assessing the further R&D that should be done. Section 3.1 describes how the temporal and spatial scales for which models have been designed limit their applicability to other scales, either to get input for the model or to apply its results in the real world. Section 3.2 returns to the major functional components of a consequence assessment system, as introduced in chapter 1, to examine how the requirements on the ATD modeling system flow down to requirements on each of its components. It describes current capabilities in each component, compares them with what is required, and identifies both challenges and opportunities in meeting the requirements. Section 3.3 examines, from the standpoint of actions available to the research, development, and test/evaluation communities, ways to

Uncertainty in ATD Model Predictions

The total model uncertainty is measured by the variance between the predicted and the observed quantity over a large number of events that have similar properties (an ensemble). In a recent discussion of the mathematical basis for understanding model uncertainty (Rao 2004), the components of the total model uncertainty are divided into:

(a) Internal factors such as the numerical approximations to the governing equations, modeling errors, and the treatment of dynamical processes;

(b) External factors such as data used to execute and evaluate the model, model parameterizations, and the initial and boundary conditions; and

(c) The stochastic component or inherent uncertainty, due to the natural variability of the atmosphere.

The model developer can minimize the first two components of uncertainty by addressing the several factors contributing to each. The third component cannot be eliminated and is only quantifiable in a statistical sense. Furthermore, we can expect inherent uncertainty to vary as a function of averaging time, location, and the ensemble parameters.

For the analysis of R&D needs, the essential relationship between measurements (observations) and identifying, quantifying, and minimizing model uncertainty must be embraced. The inherent uncertainty cannot be estimated without measurements. Progress toward reducing the first two components of uncertainty also depends on having appropriate observations and on continually improving the techniques used to obtain them.

undertake the task of improving the transition of modeling capability into useful tools for users. In effect, it analyzes capabilities, gaps, and opportunities at the output interface from the ATD modeling system to the consequence assessment system.

The exposition in this chapter draws on two prior reviews of ATD modeling capabilities, each of which included recommendations on R&D needed to address deficiencies. The National Research Council (NRC 2003) reviewed current capabilities in dispersion modeling, identified deficiencies and research needs, and recommended actions to provide more accurate information. The 11th Prospectus Development Team of the U.S. Weather Research Program addressed meteorological research necessary to improve air quality forecasting (Dabberdt et al. 2004). The JAG performed its own survey of current capabilities, which are summarized in Appendix B.

3.1 Consequences of Model Scale

Atmospheric processes are classified by the horizontal dimension and time periods of typically observed phenomena. Choosing an appropriate ATD model requires knowledge of the physical processes that should be treated for the intended application. It also requires an appreciation of the uncertainties associated with the tradeoffs made by the developer in constructing a model of the physical processes that are dominant or relevant at a particular scale.

For purposes of ATD modeling, there are three major scales of interest:

1. ***Macroscale*** applies to processes having spatial dimensions of 2,000 km or greater and influencing temporal variations of 3 days or longer.
2. ***Mesoscale*** applies to processes having spatial dimensions of 2 km to 2,000 km and influencing temporal variations of 1 hour to 3 days.
3. ***Microscale*** applies to processes having spatial dimensions of 2 km or less and influencing temporal variations of 1 hour or less.

These three are further subdivided by decades of distances, from larger to smaller, indicated by α (alpha), β (beta), and γ (gamma), as shown in figure 3.

As the scale becomes smaller, the effects of some processes become increasingly more difficult to treat explicitly or deterministically. Depending on the horizontal scale of interest, different atmospheric processes become significant. Turbulence—the gustiness superimposed on the mean wind—can be visualized as consisting of irregular swirls of motion called eddies. Eddies produce effects at the microscale. The small-scale phenomena associated with the microscale are so transient in nature that deterministic description and forecasting of individual eddies is virtually impossible.

The scales of atmospheric motions are interconnected and nearly continuous. Macroscale processes drive mesoscale and microscale processes as energy is transferred from larger to smaller scales. Conversely, small-scale processes can organize to develop larger-scale systems, such as convective storms. Many of the phenomena of interest for ATD occur in the troposphere—the portion of the atmosphere from ground level up to approximately 13 km. Most applications of ATD models are for incidents occurring in the atmospheric boundary layer (ABL)–the lowest few kilometers of the troposphere where people live. However, there are situations in which transport and diffusion in the upper atmosphere become critically important for ATD modeling.

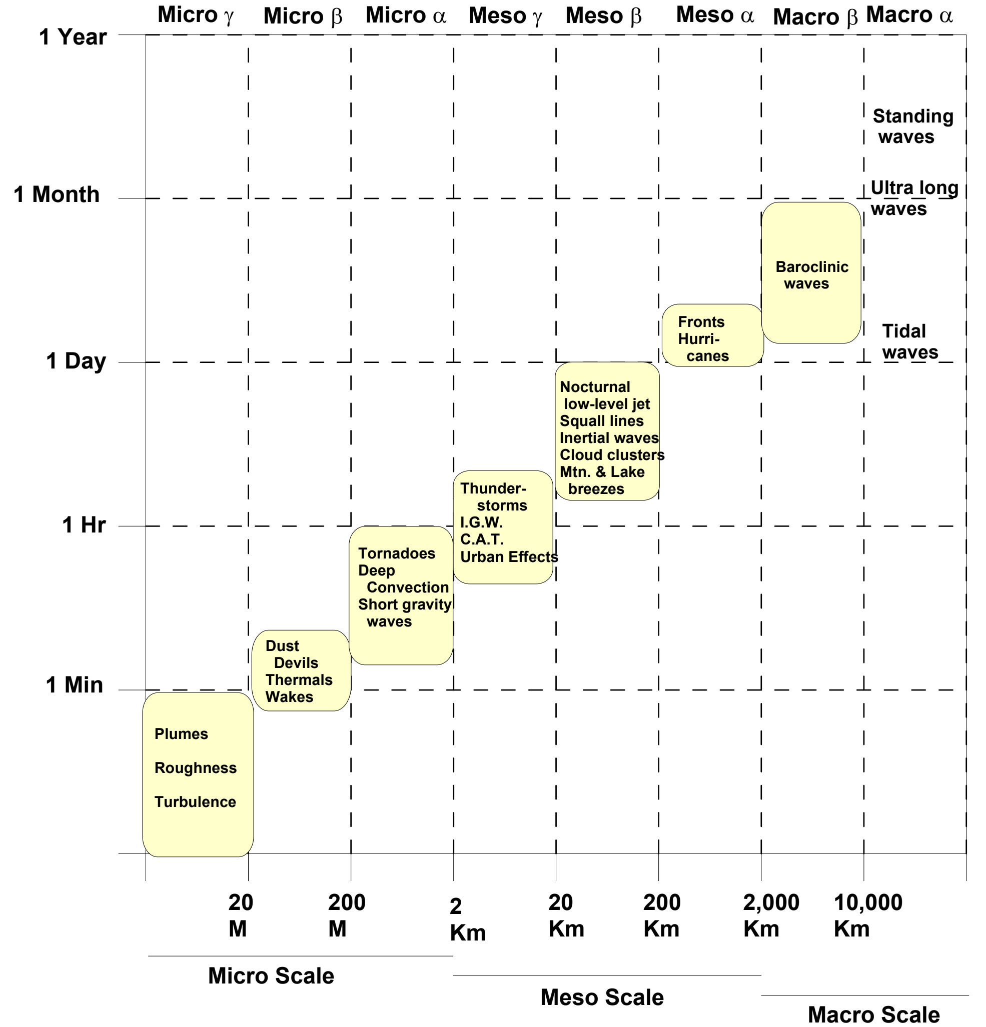

FIGURE 3. Scale definitions and different atmospheric processes with characteristic time and horizontal scales (adapted from Orlanski, 1975). C.A.T is Clear Air Turbulence and I.G.W. is Inertial Gravity Waves.

The horizontal and temporal dimensions of the incident to be modeled define the appropriate scale of the ATD model. The chosen ATD modeling approach should be appropriate for the circumstances, providing a comprehensive and concise description of effects at a particular scale of interest. ***Note:*** the horizontal grid increment is ***not*** the scale of the model. Full representation of the phenomena at the desired scale requires five or more grid increments. Appendix C contains a fuller discussion of ATD model construction and selection related to considerations of scale.

3.1.1 Consequences of Scale in Atmospheric Data

Atmospheric measurements may show scaling by their horizontal spacing or by the frequency of observations. Both the spatial and the temporal scale are important to understanding the relevance of observations and their applicability to models. Unlike the continuum of atmospheric motions, measurement scales show little continuity in space.

Table 1 lists common ground-based measurement systems used in the United States and some of their characteristics. The spatial scales they generally represent are also indicated. As the table indicates, the only systems that are truly available nationally are surface weather observations, the rawinsonde upper air system, aircraft data from the Aircraft Communications Addressing and Reporting System (ACARS), and the Doppler weather radar (WSR-88D) system. All of these systems are applicable to measurements of the meso-alpha and meso-beta scale processes. The specialty systems and tracer measurement capabilities are applicable to smaller scales but are available in a relatively few locations and for limited times.

TABLE 1. Spatial Scale and Observation Frequency of Common U.S. Meteorological Observing Systems

Spatial Scale	Observing System	Observation Frequency	Vertical Range	Spatial Separation	Spatial Range	Spatial Resolution
In Situ Measurements						
Meso-α	Rawinsonde	12 hourly	Surface to 30 km	400 km		
Meso-β	Weather observations	Hourly	2–10 m	60 km	Local	Local
Meso-β	Aircraft platform	10 to 1 Hz	Surface to 20 km	Variable	Continental scale over time	Platform dependent
Meso-γ	Tethered balloon	variable 10-30 min	1 km	Irregular	Local	N/A
Multiple	Tracer	1s to 30 min	Local	Irregular	None	Irregular
Micro-γ	Sonic anemometers	10 Hz	Tower height	Irregular	N/A	Tower spacing
Remote Measurements (Excluding Satellite-Based Systems)*						
Meso-β	WSR-88D weather radar	~100 Hz	100 m to > 15 km	200 km	250 km	1 km
Micro-α	Radio frequency sounders	15 min	100 m to >5 km	Irregular	Vertical only	Irregular
Micro-β	Acoustic sounders	10 to 30 s	20 m to 3 km	Irregular	Vertical only	Irregular
Micro-β	Doppler lidar	~500 Hz	~4 km, aerosol-dependent	Irregular	3 to 12 km	3 to 75 m range gate
Micro-β	Radio Acoustic Sounding System	~1 min	100 m to > 5 km	Irregular	Vertical only	Irregular

* Satellite-based observing systems are applicable to many of the scales listed but were not included among remote observing systems in this table.

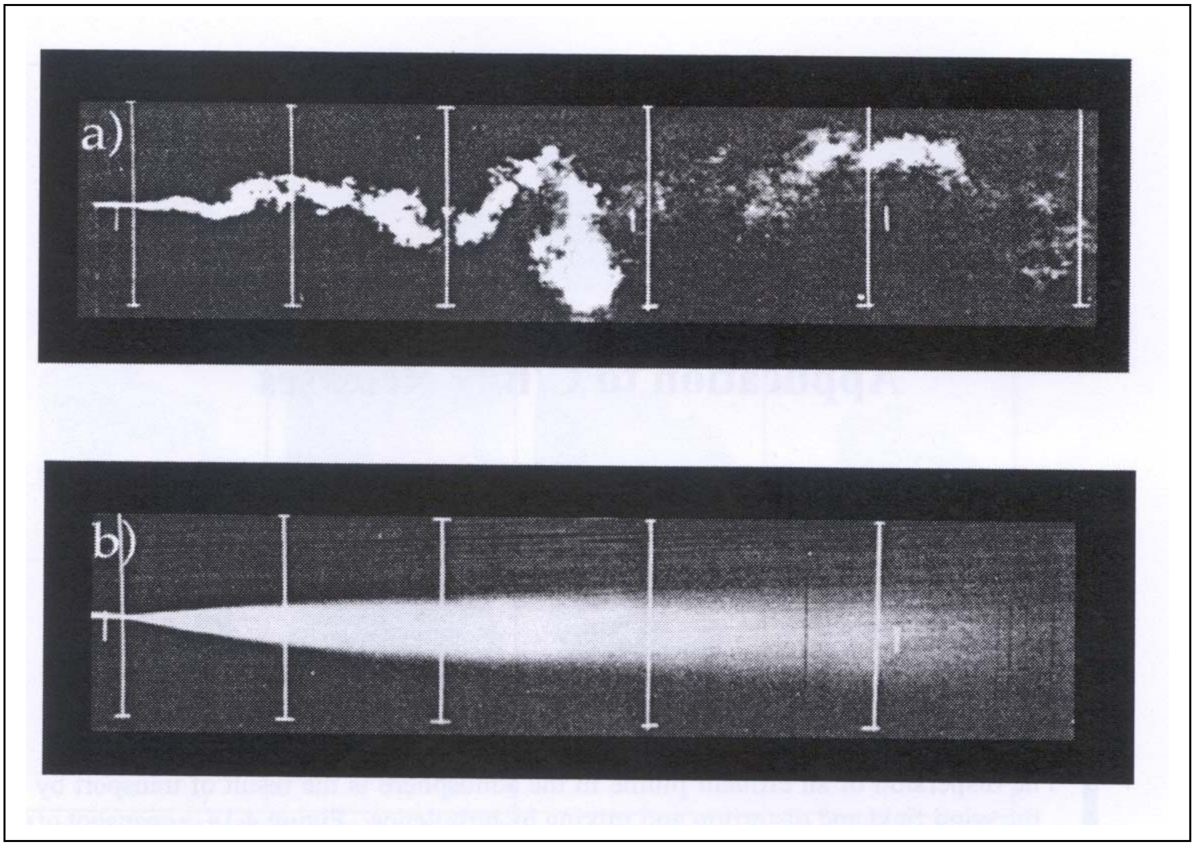

FIGURE 4. Concentration field of a simple flow (top) versus time-averaged distribution (bottom). Two images of the same release. In (a) we see a photograph of an instant during a point source release of smoke within a wind tunnel (view is taken looking down on the plume), where large and small swirls have distorted the plume into serpentine twists and turns. In (b) we see a time-average photographic exposure of the smoke release, where the time-average of the individual chaotic swirls are seen to have the "traditional" Gaussian plume shape used in ATD plume dispersion models. (Photographs are courtesy of U.S. EPA/NOAA Fluid Modeling Facility).

3.1.2 Consequences of Scale in Concentration Data

ATD models attempt to describe hazard zones by their boundaries and temporal extent. The meteorological portion of a model attempts to describe where material would go if the source was known, but the spatial and temporal distributions of the concentration are highly variable. As shown in figure 4, a single realization of a concentration field in a simple flow may bear little resemblance to a time-averaged distribution. At a given location, changes in concentration over time will depend on the sampling frequency of the sensor and its sensitivity. For high sampling rates, a sensitive sensor can detect a few intervals of large values and longer periods of low or no concentration. Depending on application, the time-averaged value may be more relevant or entirely inapplicable.

Short-term peaks in concentration, which are needed to assess acute effects or explosivity, are microscale phenomena. Many other characteristics that affect ATD predictions, such as concentration eddies in the vicinity of walls and urban canyons, are at the microscale. Meteorological models that are used to initialize ATD models are typically mesoscale models. Issues arise because of the scale differences between the meteorological model's process representations and grid spacing compared with the microscale representations needed by the ATD model.

For long-term health and environmental effects, time-averaged concentration is useful. Wind transport at local scales, however, has a large stochastic component that makes the time-averaged concentration a probability distribution with respect to space and time rather than a point value. To improve the information given to the user, the model researcher-developer needs to represent these stochastic processes realistically in the model and produce a probabilistic prediction that includes measures of the uncertainty in the point estimate (the probability distribution). Then effective ways need to be found to communicate to the user the implications of concentration as a probabilistic function of space and time.

Relevant to the components of an ATD modeling system, these scale issues affect many of the capability requirements and contribute to many of the capability gaps. Discussions of scale will recur repeatedly in section 3.2 and chapter 4, as the specific capabilities, gaps, and the R&D required to address the gaps are presented.

3.2 Requirements and Capabilities by System Component

The functional components of a consequence assessment system, which were introduced in chapter 1, are shown again in figure 5. Each component of the ATD modeling system (within the bold boxes) has its own requirements to become a functional part of the whole. These requirements can be compared with current capabilities in that functional component. Where the requirements are not fully met with existing ATD models (capability gaps), promising directions for further R&D can be identified on a component-by-component basis.

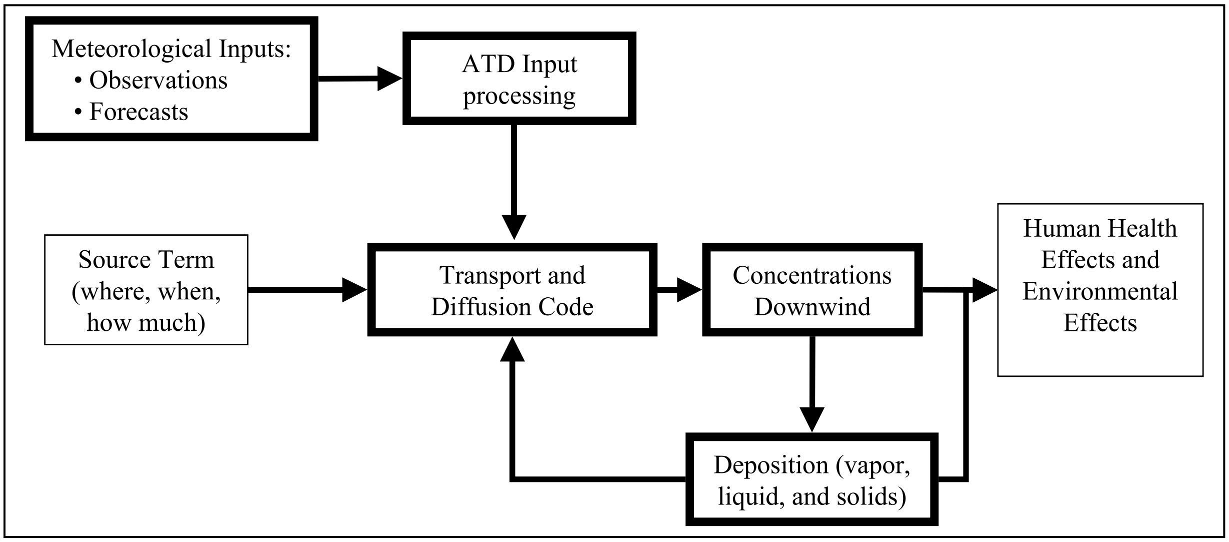

FIGURE 5. The functional components of a complete consequence assessment system. The embedded ATD modeling system is shown by bold lines.

3.2.1 Source Term

The source term component of a consequence assessment system includes information about the identity and physical state of the hazard, the release mechanism, and the mass of hazard released per unit time (emission rate). When ATD modeling is used in emergency situations, the characterization of the source term and the local transport and diffusion conditions are typically the largest sources of uncertainty. For users, the four questions listed in Figure 2 for the release event are source term questions essential to consequence assessment: What was released? When? Where? How Much? The mass of hazard released per unit time, or emission rate, is the key input derived from the source term that the ATD model needs to answer users' questions about where the hazard is going and in what concentration (concentration as a function of space and time).

To characterize near-field (less than 3 km) dispersion, it is critical to know the dilution and buoyancy of the source emissions in the immediate vicinity of the release. Uncertainties in the emission rate and initial dilution volume greatly increase the uncertainty in the near-field impact estimates.

As noted in section 1.2, this report does not address R&D needs for source term characterization. However, ATD modeling techniques can be coupled with concentration measurements made by sensors at some unknown distance from the exact location of the source term to back-calculate to a more precise estimate of the source location and emission rate. This approach, called ***sensor fusion***, can be defined for the purposes of this report as the combination and synthesis of information from networked sensors and predictive models to obtain more information about a chemical, biological, or radiological event than would be available from any individual sensor or diagnostic model alone. The networked sensors can include multiple sensor types, including in situ sensors and remote sensors, and other relevant sensors such as meteorological instrumentation. Section 4.4.1 explores sensor fusion techniques and their potential for reducing uncertainty in ATD model predictions downwind from the source location.

3.2.2 Meteorological Inputs

The meteorological inputs to an ATD modeling system may be data from observations, the output from a meteorological model, or a combination of observations and model output. At a minimum, ATD models require wind speed and direction and a simplified turbulence parameter as their meteorological inputs. A more complete specification of the meteorological parameters of interest may include input data on clouds, precipitation, temperature, pressure, humidity, surface heat and momentum fluxes, and a more complex characterization of turbulence. Mass structure and winds can also be measured directly, using a variety of in situ and remote-sensing systems and processing techniques.

In the absence of such detail, ATD models make assumptions to characterize meteorological conditions. Providing as much pertinent meteorological information as possible will improve ATD model predictions by decreasing the number of assumptions that must be made by the model. Before mesoscale meteorological model output was available, ATD modelers used surface and upper air meteorological observations from sites near the release location. In cases where the nearest available observations did not represent the meteorological conditions at the release site, the modeler would estimate the wind and turbulence conditions.

Mesoscale Models for Meteorological Inputs

While mesoscale meteorological models are executed at much finer grid resolutions than are macroscale (synoptic, global) meteorological models, they typically ingest boundary conditions from a macroscale model. With the sustained growth of computational resources, mesoscale meteorological models that provide acceptable descriptions of mesoscale atmospheric motions and turbulence were developed. These models have now been run operationally for over a decade, and the output from these models is used as input to the ATD model in cases where direct observations of local atmospheric conditions were not available and for the prediction of changes in conditions during transport and diffusion. The use of mesoscale meteorological model output has also allowed ATD model developers to account for additional atmospheric processes with self-consistent input. Although mesoscale meteorological models have proven capable of describing mesoscale atmospheric motions and accounting for atmospheric processes at the mesoscale, they have not yet been optimized for ATD models. Methods to refine these meteorological products before using them as input to the transport and diffusion code component are explored in section 3.2.3.

An advantage to using mesoscale meteorological model output (as opposed to macroscale models) to drive ATD calculations is the potential for improved resolution of localized wind patterns. Worldwide, many population centers are located near coastal regions with highly variable wind patterns. Thermally driven flows associated with land–sea interfaces and complex terrain, which are not resolvable by the coarser grid of macroscale models, can present significant challenges to the accuracy of ATD model predictions. Mesoscale models with horizontal grid lengths of about 12 km or less are capable of capturing some of the time evolution of such flows, potentially improving the accuracy of ATD computations for regions with these wind patterns.

For consequence assessment applications, modeling surface-layer fluxes, winds, and temperatures, even in a mesoscale meteorological model, is a challenge for many regions of interest. Surface fluxes are currently parameterized in numerical weather prediction (NWP) models using Monin-Obukhov similarity theory (Stull 1988). The atmospheric surface layer is defined as the inner region of the ABL, having approximately constant flux with height. It is generally on the order of 10 to 40 meters in depth for neutral to unstable conditions but can be considerably thinner in stable conditions. Because the atmospheric surface layer can be observed continuously using instrumented towers, there is a long history of studies measuring it under a variety of surface and atmospheric conditions. These observational studies have supported the development of detailed theoretical descriptions; however, as originally detailed, these theories are applicable to flat surfaces having uniform roughness, albedo, emissivity, moisture, and thermal conductivity. Real conditions, particularly in populated areas, often deviate significantly from these idealized conditions. So modeling the surface-layer fluxes, winds, and temperatures in real cases is difficult, even if the larger-scale winds (scales from tens to hundreds of kilometers) could be predicted exactly.

As an example of particular interest to many consequence assessment scenarios, surface irregularities (roughness elements) due to land use (trees, buildings, etc.) are a major challenge for modeling surface-layer properties. Especially in urban areas, large changes in surface conditions (parks, high rises, rivers, industrial zones, residential areas, etc.) can occur within distances of a kilometer or less. This variability affects the local state of the atmospheric surface layer. In major urban centers, tall buildings create “urban canyon” effects. The different types of surface irregularities found in urban areas are difficult to treat in a mesoscale model with a single practical theory for representing the surface layer. In fact, the flaws in current theory for modeling uniform surfaces may be small in comparison with uncertainties due to the effect of spatial surface irregularities found in major urban areas.

Another problem associated with high-resolution mesoscale modeling involves how information is passed from coarser to finer scales when models are nested (a smaller-scale model taking its initialization data and boundary conditions from a larger-scale model). For example, if there is an inconsistency in the nested models’ terrain or urban information databases, errors will propagate to all levels of a simulation. Some models currently in development have two-way feedback, which creates even more sensitivity to the initialization data.

Limitations in Using Model Fields for Meteorological Inputs

Although driving ATD calculations with mesoscale model predictions can, under favorable conditions (i.e., in other than complex environments), improve simulations of transport and diffusion due to localized wind flows, this approach is not without pitfalls. Slight misrepresentations of the temporal evolution (i.e., the timing) of local wind flows can severely degrade the accuracy of the predictions. Predicting the timing of meteorological events, whether synoptic (macroscale) or mesoscale in nature, is one of the greatest challenges in NWP. In these cases, ATD modelers should include phase errors as a contributory source of uncertainty and consider how best to quantify the uncertainty in the prediction stemming from this uncertainty in timing of key meteorologically driven events. Modelers must also have effective ways to communicate the impact of that uncertainty to users; for example, by showing plume development with and without the meteorologically driven event.

Forecast or diagnostic models at horizontal intervals greater than about 300 meters are incapable of explicitly representing ABL circulations, which are dominated by buoyancy and vertical wind shear. In daytime, buoyancy-driven circulations have lateral and vertical scales of the same order as the mixing height, which is typically one to two kilometers. These processes (which are turbulent from a larger view) mix the contents of the ABL. The nocturnal ABL is typically nonbuoyant, and stability resists vertical motion. It is poorly represented in current models because the lateral motion is typically weak, moving material without mixing. Intermittent turbulent events occur almost without local causes. This extremely complex and poorly understood environment is not modeled with skill.

The atmospheric surface layer occupies roughly the lowest tenth of the daytime mixed layer. Although the atmospheric surface layer is relatively well defined during the day it is less defined during the night. It is a zone of interaction, where heterogeneities in energy, momentum, and moisture dominate ATD processes. Eddy sizes in the atmospheric surface layer are proportional to the eddy's height above the surface. More than half of the energy fluctuations are unresolved. Since the ATD processes cannot be resolved, deterministic models do not apply. Predictions of concentration in this layer are the most important for consequence assessment because this is where human exposure occurs, but they are also the most difficult to make accurately.

The problem of accuracy applies even to relatively simple terrain. Hall and Basara (2004) found that operational mesoscale model predictions of wind speed and directions for the Oklahoma City airport had mean absolute errors in wind speed on the order of 2 ms^{-1} for forecast periods of 6 to 36 hours (figure 6). The mean absolute errors of wind direction were larger than 20 degrees. Other studies of model performance during different seasons and varied terrains found that wind speed errors are typically greater than 2 ms^{-1} and standard deviations in wind direction are greater than 50 degrees (Henmi 2003; Fast 2004). Although operational mesoscale models may have a small bias over many predictions, the predictions for appropriate wind speeds and direction for a given time and place can be expected to differ from concurrent observations.

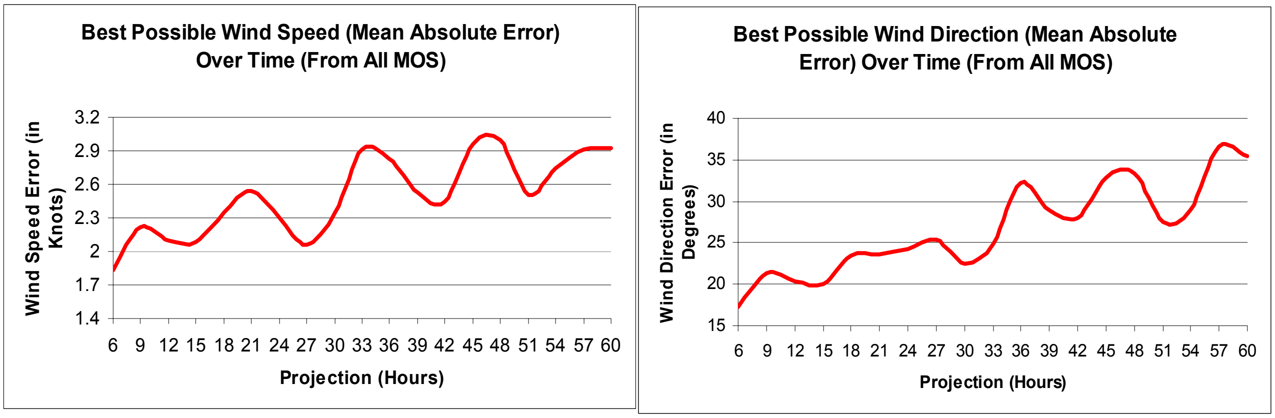

FIGURE 6. Mean absolute error in wind speed and wind direction, measured over a relatively simple terrain. Source: Hall and Basara 2004.

Clouds affect transport and diffusion of airborne materials in several ways. Diminished solar radiation from cloud cover reduces surface heating and convective mixing. Nocturnal cloud cover, even at high altitudes, reduces radiative cooling and influences the development and structure of the stable boundary layers. Insolation also can affect the chemical activity of various agents. Convection in clouds assists the mixing of air above and below the boundary layer: a process that contributes to the dilution of concentration levels at lower levels of the atmosphere. To reduce errors in the prediction of radiative fluxes, cloud information can be assimilated into a model rather than being represented by simple parameterizations. For example, remote-sensing methods can provide cloud mapping data, including inferred measurement of cloud height, for assimilation into mesoscale models.

Ensemble Forecasting of Meteorological Inputs

To provide some sense of the probabilistic variability of ATD outcomes, it is becoming more common to link ATD models to statistical information constructed from ensembles of mesoscale meteorological models. Means, variances, and correlations of meteorological parameters to be used in the ATD evaluations can be obtained by considering results from the multiple model realizations in an ensemble rather than relying on a single set of point-estimate input assumptions. Ensemble statistics can be obtained by including realizations in the ensemble either from differing models (a multi-model ensemble) or from multiple realizations of a particular model (a single-model ensemble). Multiple distinct realizations from one model can be obtained in various ways such as perturbing the initial conditions, varying the parameterization schemes, using combinations of these first two methods, or varying the grid resolution. Regardless of the ensemble building method, the objective is to characterize quantitatively the range of possible outcomes.

Significant research is still needed in this area. In particular, work is needed to determine the optimal number and types of ensemble members to produce a statistically significantly improved result. Advanced techniques for creating individual members of the ensemble are also of interest. Much development work is needed to link ensemble results from mesoscale meteorological prediction systems to corresponding ensemble systems of dispersion models and to evaluate the resulting probabilistic predictions. Most important, to make ensemble techniques useful to the user, research is needed on how to merge the probabilistic information in ensemble mesoscale meteorological solutions with ATD modeling systems to yield user-tailored probabilistic decision aids.

The WRF Modeling System

With support from multiple Federal agencies, the new Weather Research and Forecasting (WRF) mesoscale modeling system has been developed through an interagency collaboration of the atmospheric science research and operational communities. The National Oceanic and Atmospheric Administration’s National Weather Service (NOAA/NWS) is currently preparing WRF applications for operational implementation. The initial WRF system in the High Resolution Window domains will be run as an ensemble of six to eight model versions developed with two dynamical cores, multiple choices of physical parameterizations, and different anomalies in initial and boundary conditions. The number of ensemble members is expected to increase over time with planned increases of computational capacity. By the end of 2005, NOAA/NWS plans to implement WRF at 10–12 km resolution over all of North America. This North American WRF is expected to be replaced by an ensemble system as soon as computational resources allow. The WRF system is designed for applications with grids as fine as 1 km or smaller. Current computer capabilities allow WRF ensembles to be run at high resolution on regional or subregional domains that are smaller than the *national* weather forecasting requirements.

3.2.3 ATD Input Processing

Processing the input for an ATD model, for purposes of this report, includes refining meteorological inputs, whether from observational or model sources, to prepare them for use in the transport and diffusion code. Input processing techniques attempt to solve (or at least mitigate) several kinds of problems.

One set of problems addressed in input processing comes under the heading of *data representation*. Does a data value, whether an observation from an instrument or a model output value, truly represent the conditions that the model assumes it represents? For ATD modelers, data representation questions such as *Are these data representative?* typically mean *how well do the data meet the assumptions that this model makes regarding the data?*

The second type of input processing problem is *data* quality—how well does a measurement system capture the conditions it is intended to measure? The raw data in the direct signal output from a sensor can be in many forms. Most common signals are in the form of an electrical impulse, voltage, current, or resistance or a change in one of these properties. Quantifying the physical principle of the signals to a concentration, wind velocity, or pressure is the first step in ensuring data quality and is part of the sensor design. Data quality also depends on the sensitivity of the physical property it is intended to measure, changes in that property, and confounding environmental conditions. Calibration of the mean and variance of the measurement instrument to known references sets the precision of the measurement.

When each sensor is well calibrated and working properly, the measurement system as a whole may or may not be providing a realistic "observation" of the patch of reality it is intended to observe. At the level of accepting a set of data values from a measurement system, data quality acceptance/quality control (QA/QC) processes may identify outliers as potential instrument errors, interpolate for lost or missing data, or compensate for timing errors or irregularities. Furthermore, the exposure of the instrument and the heterogeneity of the instrument location must be factored into the assessment of acceptable data.

An ATD model generally assumes a correlation or coherence among the input data. In some instances, data incoherence arises from a data quality or data representation problem; in other instances, it results from incompatability of different input sources (observations and forecast models). When those data do not support the coherence assumption, the ATD model must provide rules for acceptance or rejection.

Development of guidelines for observation networks is one of the R&D needs that emerges from issues of data quality and data representation. In some ATD modeling systems, evaluating input data for either data representation or data quality is incorporated in the input processing operations. In other modeling systems, these characteristics must be examined independently. Data quality and data representation concerns are further magnified when the data are used to calculate derived quantities such as fluxes, scaling parameters, mixing height, wind shear, or thermal stability. The user of the input data needs to know the temporal or spatial averaging that has been used to produce the derived quantity.

Data assimilation is another concern in processing data for input to an ATD model. It overlaps with data representation and data quality but can also derive from other complications in the data–model interface. Weather forecast models are re-initialized at regular intervals using previous forecast fields and recent observations. In some instances, large differences between the forecast and the observation may occur. The initialization procedure is designed to weigh the forecast field and the observation within the context of expected variance in the values and the governing equations of motion. The new initialization may not include, or assimilate, the observation because doing so would violate other model constraints. This rejection of the observations by the model's rules for assimilating data may result from data representation problems (data that are not representative of scales that the model can represent), data quality problems, model errors (representations or parameterizations that deviate from the real processes being modeled), or a combination of these factors. The data quality and representation problems can be either in the data the model is now trying to assimilate or in data previously used for initialization or assimilation.

As this limited discussion illustrates, ATD input processing quickly becomes complex, consuming both time and resources (computational and human capital). While automated input processing is appealing, one approach does not fit all models or even all circumstances for the same model. As new instrumentation is developed, a major concern should be for internal consistency checks and usability (suitability) of the measurements in data input processing.

3.2.4 The Transport and Diffusion Code

The transport and diffusion code describes in algorithms the combined effects of time-averaged transport (which has traditionally been viewed as a deterministic process) and of atmospheric diffusion (which has traditionally been represented as a stochastic process). The entire set of computations is sometimes called the "ATD model," but that term is also sometimes used to mean the way in which transport and diffusion processes are represented when the set of instructions (the code) is run with an appropriate set of initialization data.

Federal agencies, the academic community, and others employ a large number of ATD modeling systems for a variety of purposes, including regulation, research and development, and emergency operations.[1] However, the JAG/SEATD report identified only a few basic types of operational ATD models, or transport and diffusion code approaches, in the modeling systems assessed by the JAG/SEATED (OFCM 2002, p. 1-

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[1] The JAG/SEATD reported that the FEMA Insurance and Mitigation Administration identified more than 140 ATD modeling systems in an internal report (OFCM 2002, p. 1-2).

4). These basic model types—box, plume, segmented plume-puff, Lagrangian particle, Eulerian grid, and computational fluid dynamics (CFD)—are defined and discussed in Appendix C. There are also only a few types of diffusion characterizations in use; the most common are empirical, statistical, similarity, eddy diffusivity, and second-order closure. The profusion of ATD modeling systems arises from the variations and combinations of these approaches combined with specializations made to handle unique problems, such as plume impaction on elevated terrain, concentration within the wakes of buildings, or heavy-gas effects.

Because of the stochastic component, all ATD modeling with a transport and diffusion code must be considered a forecast of possible outcomes. In addition, the sets of deterministic and probabilistic equations implemented in any given model provide only an approximation to the complex atmospheric conditions the model is meant to represent. Consequently, ATD modeling is always a compromise between getting a useful solution in an appropriate amount of time and realistically portraying the transport and diffusion of a released material within the atmosphere. These uncertainties introduced by the inherent probabilistic nature of the processes and by the compromises to make the model useful are in addition to the uncertainties in the input data.

Several techniques are used to apply ATD models to complex environments such as cities or coastal areas. The top-down approach uses multiple nests of finer-scale models within coarser grids to approximate the mean transport and turbulent flow at short temporal and spatial scales. This approach is useful when appropriate observation systems at the smaller scale are lacking. The bottom-up approach uses physical models—based on wind tunnels or flow channel experiments for example—or high-resolution computational models (discussed in section 4.2) to capture the larger-scale effects of the complex region being modeled and the fine-scale features of flows within the region. Physical models are used principally to build a knowledge base about a specific location and to provide appropriate data for improving the understanding of processes that are not measurable in the natural environment. Their advantage is that experimental conditions can be controlled; their disadvantage is that each experiment is only one possible realization of the stochastic variability. A middle ground, computational fluid dynamics (CFD) models, uses CFD codes adapted from the aerospace industry for examining turbulent atmospheric flows around single or multiple obstacles. In a sense, CFD models are numerical surrogates for wind tunnels or flow channels.

An emerging option for model refinement is to use remotely sensed data of actual conditions. Remote sensing can inform and update a model of the physical landscape on a recurring basis, allowing natural and manmade changes to be incorporated.

Finally, one of the principal user needs identified in Chapter 2 is seldom met at present. Most of the current operational ATD modeling systems for consequence assessment in civil emergency response applications are unable to provide information on the variability of hazard concentration on the shorter time scales needed to assess such consequences as acute effects of exposure or explosivity. A few modeling systems attempt to estimate the probability that such events could occur but are not specific as to when or where. Even CFD estimations cannot predict the exact stochastic pattern of dispersion. As a result, a forecast from even a very sophisticated ATD model has a large single-event uncertainty. At present, even ensemble-based ATD modeling systems predict only the ensemble-average dispersion pattern (the average over the multiple realizations in the ensemble) and the range of predicted ensemble variables, not the complete event-to-event variability. Because this variability can represent substantial uncertainties with respect to human health and safety risks, the ATD R&D community must do better at quantifying the uncertainty and communicating its implications effectively to those making emergency response decisions (or other decisions based on assessing consequences sensitive to this uncertainty).

3.2.5 Deposition (and Other Removal Mechanisms)

Substances released into the atmosphere will stay there, continually dispersed and diluted by mixing processes, until they are removed by reactions with other components of the atmosphere or are deposited on the Earth’s surface. Consideration of in-air reactions is essential in modeling the ATD of gaseous and biological agents. Nerve agents, for example, interact with atmospheric oxidants and with other constituents of the background air, gradually reducing the total amount of the hazard remaining in the air. Biological agents tend to be susceptible to ultraviolet radiation; hence, their active residence time in the air is largely controlled by their exposure to sunlight. Atmospheric reactions during transport can also be important for reactive liquids and solids.

Deposition Mechanisms

Precipitation is one of the most efficient mechanisms for removing pollutants and other substances from the air. The two precipitation-related processes of importance are *rainout* and *washout*.

Clouds serve as dynamic systems for processing air that passes through them, concentrating most pollutants in cloud droplets, which then coalesce and eventually fall to the surface (ground or water) as precipitation. This process of in-cloud scavenging is commonly referred to as “rainout.” For rainout to be an efficient removal mechanism, the hazardous material or pollutant must become directly entrained into a cloud. The scavenging efficiency depends on the chemical and physical properties of the pollutant in question, as well as on the dynamic characteristics of the cloud. Not all of the materials entrained in cloud circulations will be removed and deposited in precipitation on their first pass through a cloud. Sulfate particles, for example, are likely to pass through several clouds before being scavenged. For the gaseous and biological warfare agents of current concern, rainout appears likely to be important but has not been extensively studied.

Hazardous materials that are dispersing in the air near the surface will be scavenged by raindrops or other hydrometeors such as snowflakes, in addition to any rainout scavenging by clouds from which the precipitation derives. This process, called “washout,” is relatively inefficient for liquid or solid hazards unless the particles being scavenged are close to the size of the droplets scavenging them. Gaseous hazards, if they are soluble in water, can also be removed by falling hydrometeors, sometimes quite efficiently.

Dry deposition to the surface continues at all times, regardless of whether precipitation is occurring. Dry deposition is a far less efficient process than wet deposition but often removes similar amounts of material solely because the process is continuous, albeit slower.

The amount of deposition as a function of space and time is complex and difficult to predict in detail. For example, the factors of timing, amount, and location of precipitation are very important for wet deposition of dispersing materials. Prediction of clouds and precipitation mechanisms are a major focus of high-resolution mesoscale models. Although the best current models still have problems predicting the location and intensity of precipitation at scales of interest to potential users of the predictions, they do better when the driving forces are strong. Quantitative data on cloud-mixing processes and deposition are needed but are difficult to obtain.

Descriptions of deposition processes, particularly quantitative descriptions, need to be refined and tested. In future field studies and experiments on ATD, a component to measure deposition rates should be included wherever possible. This necessary work can build on the long history of relevant studies.

Resuspension

The arrow in Figure 5 from the Deposition box back to Transport and Diffusion Code represents the resuspension of hazardous material particles. For ATD modeling purposes, resuspended particles can be treated in the ATD model as a new release or emission to the atmosphere. In some instances, deposited materials will remain at the surface, with potential for subsequent resuspension into the air. Resuspension can be a major consideration for consequence assessment; radioactive particles in surface dust are a good example. In practice, resuspension of deposited materials will occur only when mechanical or volatility forces on the deposited material are sufficiently energetic. Such forces may be associated with vehicular traffic, foot traffic, or simply the wind.

Health and Environmental Consequences of Deposition

Atmospheric deposition provides the linkage between air concentrations of hazardous materials and surface environmental consequences. Although deposition constitutes a major *sink* for removing airborne hazardous materials, it is also a major *source* for studying and assessing environmental effects of hazards. Hazardous substances deposited from the air to the underlying surface are likely to enter into the biosphere. For example, if a nuclear or radiological material were deposited on the ground and inserted in an environmental pathway that led to human food sources, there would be human health consequences from this route of exposure.

3.2.6 Concentrations Downwind

Prediction of the concentration of a released hazardous substance as a function of space and time is the reason why consequence assessment systems incorporate an ATD modeling system. Once all the *appropriate* information about "concentrations downwind" has been delivered, the ATD modeling job is done; other components or players take that information as input for assessing the human health and safety consequences and environmental effects. A major theme of this report, however, is that deciding what information about concentrations is appropriate is not the sole province of either the ATD modeling community or the user community. Much work remains to be done by both communities to meet the user needs set forth in chapter 2.

3.3 Transitioning New Research and Development Capability to Operations

The term "operations" refers to the application of ATD prediction capability by a user to support that user's decision-making process. As discussed in chapter 2, consequence assessment tools are designed to support a range of operational planning, response, and recovery efforts. The ATD modeling system is likely to be only one component within a larger system for the overall consequence assessment. Transitioning ATD codes or systems from development to operations requires an understanding of the operational requirements, as well as how the ATD prediction capability will be used and how it will be integrated into the larger concept of operations.

Experience has proven that hazard assessment and decision information must get to the *right people* at the *right time*. The "right time" means that information must flow to the decision maker before it is too late for the mitigating action to be relevant. The "best" hazard analysis, if too late, is useless for response decisions, although it may still be relevant to forensic analysis during recovery activities. In addition to timeliness, the information must be operationally relevant.

For new ATD prediction capability to be successfully transitioned from R&D to operational use, the following areas must be addressed: usability; training; data connectivity; results communication; operational testing and evaluation, including production readiness; and documentation. Each area is discussed separately below, but there are major interrelationships among them that are critical to successful R&D. The successful program manager applies sound risk-management processes to invest in and coordinate activities in these areas. Keeping in mind that risks range from low probability of occurrence to high probability of occurrence and from small consequence to huge consequence, it is clear that the risk management plan must describe the risks to the program and prioritize them by degree of importance to the success of the program. The risk management plan should address all of the applicable risks, including acceptability; schedule; and technical, cost, and program risks.

The task of development is not complete until the new capability has been proven useful in operations. The work of the researcher must be guided by what users need and by what current capabilities cannot give them. To transition a new capability into operations in the time desired to meet national goals of preparedness, upfront and continuing interactions between users and researchers-developers must replace the leisurely, phased approach to research, followed by development, followed (perhaps) by operational deployment. No longer can the researcher or the developer walk away from the issues of transition as being someone else's problem.

3.3.1 Usability

Usability refers to the relationship between tools and their users. An effective tool allows the intended user to accomplish a given task in the best way possible. For ATD model codes that are either new or modified as a result of new research, the intended users should be clearly stated. As the level of user expertise with predictive modeling codes moves away from trained meteorologists and dispersion modelers, the need increases for more complex intelligence to be built into the modeling system to guide the user. For example, both novice users and advanced but infrequent users will probably need simple graphical user interfaces with standard defaults. More-expert users will want to use shortcuts and have more control over input parameters. Emergency response use will generally require a model that adapts to quickly changing conditions, provides clear guidance on input, and allows for unambiguous output. Regardless of user expertise, on-line help and error and range checking embedded in the modeling system software should be part of any operational system that will be used under stressful conditions.

In using dispersion models for planning or post-event analysis, the user friendliness of the modeling system is generally less critical. In nonemergencies, the more flexible time scale for providing an answer typically allows the user to analyze input and output more closely, get additional expertise or data, and explore a broader range of scenarios.

Without a clear understanding of the intended model use, the model user, and how information must flow to get relevant information to the right people at the right time, research-derived model enhancements will fail the usability requirement for transitioning to operations. Proper usability testing and implementation is critical for ATD models designed to define hazard areas where lives may be in danger. Usability testing should address a number of factors including fitness (how well the functionality fits the user need), ability to perform the intended task correctly, and how well the application fits the user expectations. Achieving this level of usability requires iterative interaction between users and developers, beginning well before a modeling product is ready for operational testing.

Prototyping can be an effective means to manage this and other technical risks. The user's inputs should be incorporated in the design of ATD modeling system improvements, and user feedback should be incorporated in subsequent prototype development cycles. In considering tradeoffs between capability and cost, a sensitivity analysis of new approaches or parameters should be part of the prototyping effort. The preferred software engineering methodology incorporates risk management techniques and engages users and other stakeholders throughout the software system life cycle. An example of such a methodology is the spiral model.[2]

3.3.2 Training

The model end user is rarely the model developer. Training of both the person who runs the model and the person responsible for making a decision using the model's output is critical for appropriate model use. Unfortunately, the decision makers often do not have the time and resources to be trained to use every tool intended to help them make a decision. Therefore, it is even more critical that the person running the model understand how to convey the implications for the decision maker of a forecast from the model (or from a set of models, depending on the user). As model forecasts become more sophisticated—for example, by incorporating reasonable and useful measures of uncertainty—the forecast itself must be presented in ways that are immediately meaningful to the decision maker. Model developers can no longer rely on the expertise of the person running the model to interpret this complex, sophisticated information and convey it concisely yet correctly to the decision maker. This means the developer (and behind the developer, the researcher) need to be "trained" on the user's decision-making environment just as much as those who run the model or make decisions using model output need training on the tool. In effect, the model must talk the decision maker's language. Therefore, those who create the modeling capability must also understand and "speak" that language.

Analogous to forecasting the weather with a meteorological model, any given ATD model has strengths and weaknesses, depending on the scenario and the environmental conditions known at that time. The forecaster needs to understand the model and the scenario details well enough to know how to adjust the forecast product. Unlike meteorological models that are run daily, thereby generating forecasts that can be evaluated every day, those who run ATD models are often intermittent users. They seldom have adequate data to evaluate the model or enough experience to make reasonable adjustments to the model output. Infrequent model use creates a unique set of problems, some of which can be addressed by usability in the model development. Others can be addressed through appropriate training. Training must address the entire range of users for whom the modeling system is intended to be an appropriate tool.

Although there are a variety of users, most operational objectives share a common requirement—generating consequence assessment information. At present there is no overall certification process for training personnel in ATD modeling. The most-effective training will cover more ground than just using a given model. It may, for example, include learning about the operational environment, exploring the basics of how air moves particles, understanding forward deployable technical solutions and expert reach-back services, and learning strategies for managing the risks of CBRN hazards. Workshops, formal courses, computer-based or on-line training, and tutorials are all mechanisms for providing training that should be considered when new ATD prediction

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[2] The spiral model was initially described by Barry Boehm in 1988. It is a "risk-driven determination of process and product; growing a system via risk-driven experimentation and elaboration; and lowering development cost by early elimination of nonviable alternatives and rework avoidance" (Boehm 2000).

capability is being transitioned into operations. In chapter 5, the advantages of test beds for ongoing and interactive training of both the users and the researcher-developers will be emphasized as the "hands on," experiential learning to complement these conventional approaches to user training.

3.3.3 Connectivity to Data Sources

Figure 5 identifies the major components of an ATD modeling system as meteorological inputs and input processing, transport and diffusion code, and deposition (fate of the dispersed material), with concentrations downwind as the output. The larger consequence assessment system includes source term characterization and effects on human health and safety and the environment from the dispersed material. All of these components may contribute data to the ATD model. The ability to connect to different data sources for inputs requires an information infrastructure to answer such questions as:

- Are the data available?
- Through what mechanisms are they available?
- What are the temporal and spatial scales for data retrieval?
- Are there standard formats?

Data connectivity also assumes an understanding of how the model will use the data input. An ideal operational system will have a seamless mechanism for both inquiry about access to potential data sources and utilization of the data received by the model.

3.3.4 Results Communication

Requirements for an operational ATD modeling system to communicate a forecast of hazard zones will depend on whether the forecast is for planning, response, or recovery (including post-event assessment). The situations with higher stress for users and less flexibility in timeliness of decisions require more emphasis on standardized, easy-to-interpret output. In emergency response, for example, standardized products for similar categories of threat (radiological, biological, chemical) will aid in the time-critical use of predictions. Planning and post-event assessment provide more opportunity for discussion and alternatives for presenting model output. Whether output is deterministic (a single best guess), probabilistic (probability distribution), or ensemble (combinations of different model outputs), communicating what the particular output conveys and its associated confidence or uncertainty should be considered integral and essential features of an operational system. In addition, an operational capability should provide interfaces for both the most widely available and the latest technologies for communicating output.

3.3.5 Evaluations of Modeling System Performance

This document uses "modeling system performance evaluation" to refer to a collection of engineering and scientific processes that enable modeling system developers to establish the degree of correctness of the software, how well the physical models and databases represent reality, and the fitness for use of an ATD modeling system. There are established guidelines and consensus approaches for evaluating ATD modeling system performance that must be incorporated in the overall processes of system development, evaluation, and transition to practice, especially when the ATD modeling system is integrated into a consequence system.

The manner in which a modeling system performance evaluation is conducted should depend on a number of factors, including the intended application, whether the modeling system will interface with a mission-critical system, and the amount and type of evaluation processes that were previously applied to the parts of the ATD modeling system. The processes in a modeling system performance evaluation include:

- **Science peer reviews**. During science peer reviews, the model's key constructs must be shown to be reasonable and defensible for the defined uses. A key part of the scientific peer review will include the comparison of modeled and observed evaluation objectives over a range of model inputs (e.g., maximum concentrations as a function of estimated plume rise, stability, or distance downwind).
- **Diagnostic and performance evaluations.** Diagnostic and performance evaluations are two types of statistical evaluations that are typically performed to assess different qualities of how well a model is performing. Both are needed to establish credibility within the client and scientific community. Diagnostic evaluations examine model capability to simulate individual processes that affect the results (e.g., droplet fall velocity using small-scale data sets, such as those from special field experiments, wind tunnels, or other laboratory equipment). Performance evaluations, particularly those conducted in circumstances of the intended application; enable one to decide how well the model simulates the average temporal and spatial patterns seen in the observations. Work is underway to develop a new generation of evaluation metrics that takes into account the statistical differences (in error distributions) between model predictions and observations.
- **Supportive analyses** (e.g., software verification, sensitivity, and uncertainty analyses). Software verification is the process of determining that a model implementation accurately represents the developer's conceptual description and specifications. These supportive analyses should be applied to ensure that the following four key tasks are completed:
    1. Modeling assumptions, limitations, and errors are adequately documented.
    2. The software development effort is well managed and controlled.
    3. Results produced by the modeling system are stable and predictable.
    4. The results of diagnostic and performance evaluations are well understood.

In summary, numerical comparison of model predictions with observed field data provides only a partial means for assessing model performance. Due to the limited supply of evaluation data sets, there are severe practical limits in assessing model performance. In this context, conclusions reached during the scientific peer reviews and the supportive analyses have increased significance in deciding whether a model can be applied in the circumstances defined by the model evaluation objectives. Therefore, setting up an evaluation program might include publishing peer-reviewed papers, hosting technical review boards, and having independent third-party reviewers.

3.3.6 Software Testing and Evaluation Including Production Readiness

When the ATD modeling system is integrated as a component system of the larger consequence assessment system, software testing must be conducted at all phases of the modeling system's life cycle, starting with unit-level testing and continuing through systems-integration testing. These activities provide confidence that the modeling system's *performance requirements* have been met and determine the degree to which the modeling system represents the real world *in the context of the intended use of the model.* The JAG/SEATD report reviewed the procedures currently in use by Federal agencies for testing and evaluating ATD modeling systems (OFCM 2002), and those procedures need not be reviewed again here.

Established test and evaluation procedures, including the model performance evaluation processes discussed in section 3.3.5 and their documentation, are essential parts of the process of transitioning from an R&D result to an operational tool. Implementation of new research results into new and existing ATD modeling systems should ensure that the following conditions are met:

1. New products of research should make a measurable improvement in and increase the value of the model results to the end user.
2. Software verification and validation procedures should be employed to ensure that new algorithms and techniques perform as intended. If the modeler and the researcher are not the same, then the model developer needs a mechanism to confirm that the new enhancement is being correctly implemented.
3. Usability testing has been completed, and the modeling system meets the needs of all its intended users. Operational test and evaluation should focus on the operational effectiveness of the system and its suitability for operational use.
4. Production readiness has been achieved by demonstrating reliable, sustained production. Production readiness also includes providing results within the required time constraints and providing backup against single points of failure in production, communication, and connectivity.
5. Comparisons with field data have produced no surprising discrepancies. To the extent model results are available, they should be compared with field data or historical data sets. While there will often be differences, the evaluation should be able to explain why the differences are acceptable.
6. Model-to-model comparisons are consistent for different modeling systems used in operations. If implemented correctly, new research will lead to model advances from the private, military, and public application sectors of the R&D community. Testing of multiple model implementations can provide valuable insight on potential problems.

3.3.7 Documentation

Public ATD models should have a range of documentation available:

- User documentation with point-and-click details for the intended user;
- Technical documentation so that other researchers or model developers can independently evaluate and test specific algorithms; and
- Quality assurance and testing documentation.

The code or modeling system should not be considered operational without these documentation components.

4.0 MODELING AND MEASUREMENT RESEARCH NEEDS

Chapter 3 examined ATD modeling system requirements (derived from user needs) and capabilities at the level of major functional components, such as the meteorological data inputs or the transport and diffusion code. This chapter identifies ATD modeling system capability gaps and R&D options to fill them by exploring modeling and measurement science and technology in greater technical depth. The objective is to identify the most promising scientific and technical opportunities to meet the ATD modeling needs.

ATD models require knowledge of the local wind and turbulence fields at the scales of interest of the population at risk. Because these scales vary by incident and potential consequences, the domains of interest are case dependent and not usually known *a priori*. Thus, the modeler's toolbox of capabilities and the skills to use them must cover a wide range. Nearby measurements are often not available, and conditions change rapidly, especially near the ground where people live and work and are most likely to encounter airborne hazardous materials.

Advances in current ATD modeling are likely to come from improvements in meteorological model predictions and from measurements at the scales of interest. The former are closely related to better representations of atmospheric boundary layer (ABL) processes by improved parameterizations, initial conditions, boundary conditions, and representations in complex environments. As existing modeling and observing capabilities are improved, incorporating the realization that ATD processes are partly stochastic rather than entirely deterministic will enable better quantification of the uncertainties in the modeling process. The modeler must then learn how to communicate this uncertainty information to end users in ways that are relevant to the users' decisions.

Models and data must come together and complement one another. Techniques to localize and/or quantify source characteristics by fusing information from concentration sensors, ATD models, and other measurements are lacking or untested. To meet user requirements for timely modeling predictions, faster methods are needed to determine the quality of observed data, merge the acceptable data into modeling frameworks, and estimate concentrations rapidly across several scales of motion. Finally, to ensure the quality of the model estimates and provide the benchmark for improvements, the skill of the prediction and its robustness need to be assessed on a continuing basis.

Section 4.1 explains the methodology applied by the JAG to prioritize the R&D requirements and opportunities presented here and in chapter 5. Section 4.2 focuses on modeling methods to address model deficiencies and unmet needs noted in Chapter 3. Section 4.3 does the same for measurement technology, including advanced sensor systems and methods for improving meteorological data inputs. Section 4.4 focuses on capability challenges related to the *interface* between data inputs and the ATD code. Understanding (and meeting) these interface challenges requires viewing them from both the data side and the modeling side (parameterization techniques, algorithm development, etc.).

4.1 R&D Prioritization Methodology

The JAG considered the following factors and associated questions when prioritizing R&D needs and opportunities.

- **Time sensitivity.** Is there a window of opportunity for achieving results? Does other R&D depend on this work (is it a prerequisite)? Is the user need that would be met a national priority of immediate concern, or is it a longer term improvement (longer term need)? The three values used for time sensitivity are *immediate*, *near term*, or *longer term*.
- **Short-term gains**. Can the R&D results be ready for transition to operations within 2 years of initiating the R&D effort? For the research needs discussed by the JAG, short term gains were rated as either *minimal, average,* or *high*.
- **Overall level of effort (LOE).** What are the total resources that the JAG members anticipate will be required relative to other R&D needs in this plan? Specific dollar amounts or ranges (i.e., quantitative cost estimates) were not considered. Instead, this factor includes the JAG's qualitative estimate of the relative scale of labor, infrastructure, and procurement costs. Within the research needs discussed by the JAG, the LOE was designated as either *low, moderate,* or *high*.
- **Lead time.** Is this a long-lead effort; i.e., an effort that must be planned and initiated a relatively long time before an initial operational capability can be realized, or could a coordinated effort started quickly reap benefits soon? Lead times were rated as either *short* (within 2 years), *average* (more than 2 years but less than 7), or *long* (up to 10 years).
- **Ultimate potential for gain.** What is the ultimate potential for gain relative to other research needs? Because all of the R&D needs selected by the JAG for this plan were considered above average in their ultimate benefits, the three ratings used were *above average*, *high*, or *exceptional*.

Table 2 illustrates how a hypothetical R&D need might be rated using the prioritization factors.

TABLE 2. Example of Prioritization Factor Ratings for a Hypothetical R&D Need

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
near term	minimal	moderate	long	exceptional

- This need is not an immediate national concern, but it should be addressed soon. The time sensitivity rating is therefore *near term*.
- This need is not expected to provide short-term gains because it has a long-lead time (between 7 and 10 years) before initial operating capability is likely to result. The JAG members therefore rated it *minimal* for short-term gains and *long* for lead time.

- Directed and applied research will be required to tackle this research problem, but it is not comparable to the largest efforts considered by the JAG. Therefore, its overall level of effort was rated as *moderate*.
- The ultimate potential for gain is great—among the highest of the efforts considered by the JAG. Therefore, its rating for ultimate potential gain is *exceptional.*

Given its exceptional potential for ultimate gain and the long lead required, the R&D to address this hypothetical need should be started as soon as possible. A carefully coordinated R&D plan should be developed to control cost, ensure that the potential gain is realized, and provide for ongoing evaluation of the requirement and the R&D direction over time.

As another example of the prioritization scheme, consider the kind of R&D effort that is sometimes referred to as "low-hanging fruit" because the benefits can be acquired relatively easily and quickly. An R&D effort of this kind might be rated as *high* for short-term gain, *low* for overall level of effort, and *short* for the lead time required. The "low-hanging fruit" metaphor is typically applied to something of value but not essential to have immediately or of the greatest ultimate importance. Its time sensitivity would therefore probably be *near term* or *longer term,* and its ultimate potential for gain might be *above average* or *high*.

4.2 Improving ATD Meteorological and Concentration Models

4.2.1 The Meteorological Model Components of ATD Modeling Systems

Predicting the concentration of airborne material at a given location and time after a release from a given source—the purpose of ATD modeling—cannot be isolated from predicting wind and turbulence, which is what a meteorological model does. The equations for conservation of mass (prediction of concentration given the source) of the airborne material are the same as for other scalar atmospheric variables, such as specific humidity and potential temperature. The sources and sinks (decay, chemical transformation, deposition) may vary by the material, but the movement of the material is controlled by the local wind and turbulence fields.

Because the process of estimating the wind and turbulence in the areas of interest to ATD is largely independent of the source term release event, the ATD modeling process is usually divided into a meteorological model and a concentration model. The former represents the wind and turbulence; the latter represents the relationship between source and concentration at a location given the meteorological conditions. When identifying the R&D needed to address capability gaps in ATD modeling, the capabilities of the meteorological modeling component of the system must be included.

For any given realization, an environmental prognostic model can depict only about two decades of distance scales. Therefore, as finer resolution is sought, the domain covered by a single realization must shrink. In four-dimensional atmospheric models, increasing the resolution by halving the grid sizes leads to at least an order of magnitude increase in computational burden. Distributed processing has helped reduce this burden but cannot eliminate it. Increased computational capabilities have enabled nested prognostic models to be run at lateral grid spacings of hundreds of meters. Model nesting, however, raises issues of its own, which are discussed below.

In the cascade of atmospheric energy toward smaller-scale motions, more information is required about issues at smaller scales. Instead of worrying about a few large processes, the modeler must contend with a multitude of small ones. Misrepresentation of actual processes with approximate expressions induces error and inhibits the quality of the model results. In Figure 7, moving from right to left represents the traditional top-down approach to modeling. The "bottom-up" processes of examining the flow from smaller scales, through physical modeling or simplified high-resolution numerical models (discussed in Appendix C) are represented in Figure 7 as progressing from left to right. In the range of scales from tens of meters to a few kilometers, the models do not adequately replicate atmospheric motions.

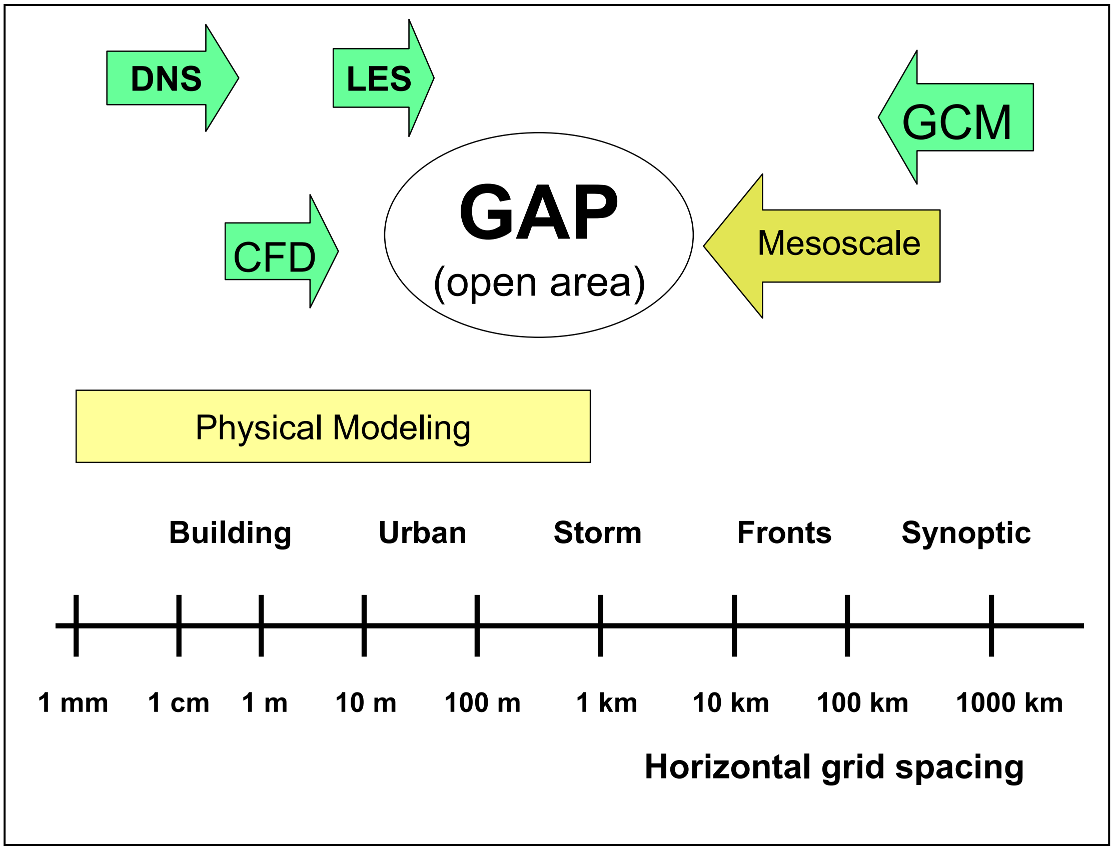

FIGURE 7. Transport and diffusion scales and model grid sizes. GCM = global climate models. Courtesy of T. T. Yamada.

4.2.2 R&D Needed to Improve ATD Modeling Components

This section identifies R&D requirements based on the preceding discussions of ATD modeling concepts and current capabilities. The rationale for each requirement follows the statement of the requirement. The rationale is followed by a prioritization assessment of the R&D to meet the requirement, using the prioritization factors and methodology introduced in section 4.1.

R&D Need: Bridge the gap from mesoscale to microscale/urban scale.

Deterministic modeling at grid scales that would allow representation of transport and diffusion phenomena characteristic of urban regions or subregions (100 m to 1 km) does not seem feasible in the near term. The accumulation of error limits the applicability of a top-down approach beginning with a mesoscale meteorological model nested in a synoptic model. The complexity of the near-surface environment requires finer and finer detail about surface features and their temporal changes. Although part of the problem may be addressed by more accurate approximations of sub-grid processes, it is difficult to develop estimation techniques that are sensitive to every nuance of a complex, poorly quantified feedback system like the urban atmosphere.

Top-down modeling is limited in its ability to represent ABL processes. An ABL process, such as three-dimensional, heterogeneous, anisotropic turbulence that scales with the boundary layer height Zi (about 1 to 2 km), cannot be represented with lateral grid scales of a few kilometers, regardless of the vertical grid spacing. In convective conditions, the lateral scales are about 1.5 times Zi. Consequently, there is a gap in capability between top-down modeling represented by mesoscale meteorological modeling, and bottom-up modeling represented by physical models and CFD models and LES. Unfortunately, the gap lies at the scales of phenomena that affect people. Considerable innovative thought is needed to bridge this modeling gap.

Useful improvements in nesting or initialization approaches include better forecasts of boundary layer height and the wind speed and direction profile as a function of grid size. The data from 915 MHz wind profilers, now available in many locations around the country, can provide the ground-truth data. These data are particularly useful for ATD modeling where ABL processes are often dominant. If the information requirements and ground truth are well defined, remote sensing could aid in providing input data to models and in model performance evaluation.

TABLE 3. Prioritization Factors for Bridging the Modeling Gap from Mesoscale to Microscale

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
near term	average	moderate	average	Exceptional

Bridging the modeling gap is a long-term objective that will not be easily met. Success in bridging the two decades of length scales that are still poorly measured (the gap area in figure 7) depends on meeting the other R&D needs for ATD modeling identified in this section. The initial efforts to quantify the uncertainty in existing meteorological models, fine-scale models, and physical models can be used to identify areas where more extensive research and model development are needed. Longer-term progress will depend on creative initiatives producing new, testable hypotheses about boundary-layer behavior and surface layer turbulence. This longer-term effort is essential to complete the modeling of the full spectrum of atmospheric processes at work in transport and diffusion.

R&D Need: Improve characterizations of surface boundary conditions in model parameterizations and in input data sets (initial and boundary conditions).

Accurate, well-resolved data on local surface conditions are critical to credible solutions of the equations describing ATD in the ABL. As noted in sections 3.2.2 and 4.2.3, key variables of interest are related to surface energy budgets and their spatial and temporal variations. Hence, information on surface type, surface cover and condition, surface temperature, surface moisture, and other characteristics is essential. In urban environments, the data must include accurate and up-to-date depictions of the buildings, as well as the often surprising amount of greenery and its effects on surface moisture and temperature. The three-dimensional distributions of surface characteristics and effects in urban environments are important because of the strongly three-dimensional nature of the wind, turbulence, and temperature fields in these areas. Remote sensing from aircraft and satellites will probably be the best solution (see section 4.3.2); however, ground-truth data and methods to test and correct the set of data intended as the initial conditions for ATD modeling will continue to be critical for improving accuracy and quantifying uncertainties (see section 3.2.3, ATD Input Processing). Further research is required to determine how accurate this description must be and the effects of scale on model performance. For CFD and laboratory (physical) models and perhaps for the next generation of high-resolution mesoscale models, the spatial resolution of the surface-boundary conditions will probably be on the order of a few meters.

Characterization of surface-boundary conditions will require collecting data over a wide range of known conditions in order to create a reliable ensemble of realizations for many possible circumstances. This effort must overcome a strong tendency in data collection experiments to look only locally in assessing surface energy characteristics and fluxes. Surface flux measurements are time-averaged values. As the averaging time increases, larger motion scales contribute to the measured fluxes. The height of the measurement above ground is important because of the upwind influences on the measurements. In stable boundary layers, near-ground stratification may separate the surface–air interactions from the processes used to measure them and from the sensors intended to measure them, (Mahrt, et al, 2001). Businger (1989) stated the issue clearly: "…for reliable flux measurements near the surface, we need to know the height of the convective boundary layer, the entrainment at the top of the boundary layer, and the mesoscale divergence and advection. We have hopes that, with remote sensing in the boundary layer, a significant portion of the required knowledge will be obtained."

TABLE 4. Prioritization Factors for Improving Characterization of Surface Conditions and Input Data Sets

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
near term	average	high	average	exceptional

Inclusion of local surface heterogeneity in initial conditions for ATD modeling will be a challenging objective. In the short to near term, capabilities exist to describe surface morphology at high resolution using airborne and space-based platforms. These capabilities are valuable for routinely identifying morphology changes over time. Translating these surface morphology data into representations of surface energy and momentum budgets at high resolution in day and night conditions is the more daunting challenge. Because many complex processes contribute to these budgets across a range of time scales, the large uncertainties in estimates will be hard to reduce. It will probably be necessary to continue the R&D effort over the long term with modest improvements in capability being achieved along the way.

Initial and lateral boundary conditions need to be more representative of the local environment. Progress will depend on the improved capability to characterize flows both laterally and vertically in the ABL through measurement at the scales of interest.

R&D Need: Test and refine the physical basis for sub-grid-scale parameterizations.

At each step in scale from the global to ABL modeling domains, approximations are made to account for physical processes that are too fine in scale to be resolved at the scale of the model. (Section 3.1 discusses the basics of model scales.) These approximations, called *sub-grid-scale parameterizations*, represent the unresolved processes using resolved grid values. They provide closure to the model (i.e., the model is closed when it has the same number of equations as independent variables). Because they are generalizations, sub-grid-scale parameterizations introduce sources of error. The cumulative effect is that the errors propagate (grow) as model output from one scale is passed as input to a model at a smaller scale. Well-designed models suppress the growth of accumulated errors, forcing them to dissipate; however, both theory and observation show that energy can transfer from small to larger scales. The consequences of such processes on a model realization are often suppressed or eliminated by the very techniques used to dissipate the errors from sub-grid-scale parameterization. Thus, two issues face the R&D community:

- How large are the errors from sub-grid-scale parameterization?
- How can these errors be reduced without interfering with accurate representation of real processes of energy transfer from one scale to another?

While the problems have been recognized, very few attempts have been made to resolve them. Recent basic research suggests that a bottom-up approach—representing the finer-scale processes at high resolution first and then generalizing to larger scales—allows the available data to be used effectively while improving the parameterizations that must be included for closure. Physical models provide a mechanism for measuring at very fine scales under controlled conditions so that the parameterizations can be suggested by data or physical insight and tested independently. The consequences of averaging small scales to accommodate larger grid sizes can then be evaluated. High-resolution computational models can be (and have been) similarly used to understand and improve parameterizations.

One suggested approach is to use grid-filtered equations rather than Reynolds stress models to assess the surface-layer energetics. The sub-filter-scale representations of these processes appear to have a wide range of stabilities (Sullivan et al. 2003).

A second approach uses the characteristic that atmospheric processes near the surface tend to scale with the height above ground level. One-dimensional closures connecting the first level or two of the model to the surface processes can be tested against observations, as Poulos and Burns (2003) have done. Their work showed significant scatter—suggesting unpredictability—in the Louis surface parameterization for stable boundary layers.

A third approach is to measure the atmosphere or concentrations at high resolution in all four dimensions. This will require instruments with greater capabilities than currently exist. As this cannot be done everywhere, selective experimentation will be required both routinely and in focused field campaigns. A common result of field programs, using new instrumentation, is the discovery of new phenomena and new insights into how the poorly resolved processes actually behave.

The problem of parameterizations for sub-grid or sub-filter scales was also recognized by the 11th Prospectus Development Team of the U.S. Weather Research Program in its final report on meteorological research needs for improved air quality forecasting (Dabberdt et al. 2004). Efforts undertaken as part of the U.S. Weather Research Program should be closely coordinated with R&D on meteorological models to support ATD modeling systems, since the atmospheric processes to be dealt with are the same in both areas of application.

TABLE 5. Prioritization factors for Testing and Refining the Physical Basis for Sub-Grid-scale Parameterizations

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
longer term	**average**	**moderate**	**average**	**exceptional**

Improvements in models and model components will largely depend on addressing the other R&D needs in this report. Models, both meteorological and ATD, will improve incrementally with a moderate level of effort as the recommended actions are taken to quantify uncertainty, capture existing data, establish ATD test beds, and improve measurement technologies. The potential for gain in improving decision aids for users is substantial, but it will be achieved incrementally as the state of the science is advanced through methodical R&D.

R&D Need. Characterize dispersion in complex environments.

The phrase "complex terrain" is often taken to mean mountainous or hill-valley terrain, but it can apply to any terrain that affects the wind and thermal structure of the atmosphere in ways that make concepts and predictive models based on homogeneous conditions no longer appropriate. Because the interactions of terrain features with atmospheric phenomena are really the point, a better term than "complex terrain" is "complex environment." For example, meteorologically speaking, coastal regions near large bodies of water are complex environments because the land–water interfaces often gives rise to land–sea breeze regimes. Similarly, dry regions adjacent to well-irrigated lands will generate localized wind fields. In mountainous areas, terrain steering, wind deflection, and irregular patterns of surface heating and vegetation will give rise to very complicated flow patterns. This is especially true at night when cold-air drainage into mountain valleys can produce significant jets of air moving above neighboring flatlands or basins at a time of day when the surface boundary-layer characteristics are particularly difficult to predict. In general, the common feature of all complex environments is the poorly understood impact of heterogeneous surface cover and surface energy budgets on local wind, turbulence, temperature, and moisture fields.

Urban areas are a particular focus of this report because CBRN events can be expected to occur primarily in urban settings. The enhanced roughness and changes in thermal characteristics of the urban landscape alter the meteorological fields over the city. At night, the thermal characteristics often lead to a heat island over the city, which can generate its own flow fields under light synoptic wind conditions. Around the central business district, where tall and large structures are usually clustered, one can expect to find flow deflections, flow channeling along street canyons, preferred sites for recirculating flows, and other organized flow patterns, such as wake vortices, strong vertical mixing, and greatly enhanced turbulence. To improve our understanding of complex urban environments, efforts are required to compile adequate building morphology data and to conduct useful field measurements to aid in validating and better parameterizing ATD modeling systems for urban environments. Thermal remote-sensing data can aid in documenting urban surface energy budgets by providing accurate observations of the thermal variation of urban landscapes at spatial resolutions from several meters to a kilometer.

Several urban ATD field studies have been conducted in the past 20 years, both in the United States and abroad. Despite their obvious importance, the number of these studies is small because of the expense and logistical problems in conducting field studies in actual urban areas. Our understanding of flow and dispersion in urban environments containing complex building clusters and street canyons is still inadequate. A major constraint has been the cost of making a sufficient number of in situ measurements at many locations over an extended period, especially measurements of the vertical profiles of key variables such as wind, turbulence, and temperature. Improvements in remote-sensing systems may lessen this constraint considerably while providing more representative data. Future urban studies should make extensive use of remote-sensing systems, such as radars, light detection and ranging (lidar), and sound detection and ranging (sodar), to provide both meteorological and tracer concentration data. Aircraft and satellite observations may become especially useful in understanding the processes controlling ATD over, around, and through cities. This understanding is crucial to improving predictive models. For an optimal fit between a remote-sensing system and an ATD model, both the model criteria and the phenomena to be observed must be thoroughly defined.

In a sense, the stable boundary layer (SBL) provides another type of complex environment. When an SBL is present, deep convective plumes do not exist to dilute hazardous materials released near the surface by mixing with higher-elevation air. Because of the SBL's strong surface stratification and weak or intermittent turbulence, the material remains concentrated near the surface for extended periods. SBLs occur almost nightly. Hazardous releases occurring at night (e.g., the fertilizer plant accident in Bhopal, India, in 1984) can expose large populations to concentrated doses of the hazard. Yet, SBL behavior is difficult to observe, generalize, and simulate because the weak, stratified turbulence of an SBL can be induced or maintained by a variety of processes, such as breaking gravity waves, Kelvin-Helmholtz instability, density current, or low-level jets (Banta et al. 2002). Recent high-quality field campaigns, such as CASES-99 and VTMX, have explored SBLs. Numerical studies at several scales, such as the GABLS LES study (Beare et al. unpublished) and the GABLs single-column model study (Cuxart et al. unpublished), have attempted to improve SBL parameterizations by defining intermodel variability and uncertainty due to numerical parameterizations.

SBLs are currently poorly parameterized in mesoscale models. The commonly used parameterizations (e.g., Louis 1979) frequently fail in two ways (Poulos and Burns 2003). First, the parameterizations often lead the model to predict too-rapid cooling of the surface, which suppresses turbulent mixing inappropriately. Second, they often maintain well-mixed layers that last too long and are too deep. In short, these parameterizations do not account for the intermittent sources of turbulent mixing mentioned above. Although the research community in boundary-layer meteorology is addressing the problem, substantial additional work is needed.

TABLE 6. Prioritization Factors for Characterizing Dispersion in Complex Environments

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	average	high	average	high

Initial efforts to quantify uncertainty in ATD modeling of complex environments will produce some near-term gains. Some efforts are already in progress, using existing tracer data from field experiments in cities and near missile ranges. One near-term activity should be to examine the existing archives of complex-terrain studies; however, field trials may not be sufficient to develop meaningful ensembles of realizations. Physical models of urban areas should be used to study uncertainty issues. Development of models for nocturnal transport and diffusion in cities can proceed from recent limited tests. For other environs, substantial R&D effort will be needed to understand and parameterize the nocturnal boundary layer in open, hilly, and mountainous terrain, as well as along coastlines. Significant advances in measurement technology may be needed to develop appropriate databases of meteorological and tracer data.

R&D Need. Develop methods and technologies for improving ensemble construction and interpretation.

Given the errors and uncertainties in initial or boundary conditions and in the model parts (e.g., numerical core, sub-grid-scale parameterizations), each run of a model produces a single realization in the ensemble of possible analyses (for a diagnostic model) or forecasts (for a prognostic model). As explained in section 3.2.2, an ensemble of possible realizations can be created by two basic approaches. The same model can be used to produce multiple realizations by perturbing initial conditions, using variable parameterization schemes, combining these two approaches, or using variable grid resolutions. A second approach is to use different models to produce the multiple realizations for the ensemble.

Sometimes the consensus (least different) realization in an ensemble is taken as the most likely solution. For weather forecasting, Fritsch et. al. (2000) found that the consensus realization gives better skill scores in large-scale flows than do other approaches to selecting the best weather forecast in an ensemble produced from multiple models. Although the consensus approach is now widely used and accepted for weather forecasting, its applicability to ATD modeling and the phenomena that become important at finer scales has not been established. In large-scale and strongly forced flows like hurricanes or severe storms, the ensemble approach gave better skill scores by various measures; however, the suitability of various ensemble approaches has not been established for weakly forced or ABL flows. The consensus technique has only rarely been used to examine ABL flows over the variety of surface morphology, diurnal conditions, and climatic regimes routinely encountered for ATD modeling. The JAG could find only one instance of the use of consensus selection in an advanced ATD model (HPAC) to estimate concentrations. Even for this one ATD model, there are limited comparisons of predictions using the consensus realization with observations. The scientific bounds and applicability of this technique within ATD modeling need careful experimental and theoretical study.

The complexity of near-surface flows and mixing suggests the variability may be large, and increased skill may be hard to demonstrate. Integration of local, near-surface measurements into larger-scale flow regimes has not been effective; the model and the observations often disagree about the distribution of mass (the pressure field) and momentum (wind and turbulence fields) because the scales of distributions contained in the model are much larger than the scales of the local observations. As local data become available at higher resolutions, the modeling approach of using large-scale forcing to drive local-scale models will have to bridge the scale gap. With sufficient local data, shorter-term, locally based predictions of wind and turbulence fields—and thus, predictions of concentration fields—will become feasible and reliable.

The top-down and bottom–up approaches to assessing data representation and assimilating data into models are important across the spectrum of motions. The top-down approach is driven by nesting of models to approach smaller scales. The bottom-up approach is driven by local measurements to analyze, diagnose, and predict present and future local conditions. At present, with a few exceptions, local data sources are too sparse. Remote measurement capabilities appear to be the best R&D pathway to meet this need to characterize the local wind fields for purposes of improved transport and diffusion prediction. Ensemble assimilation techniques must be developed for the local data utilization.

As noted in section 3.2.2, substantial R&D on ensemble methods is also needed on the following topics:

- The optimal number and types of ensemble methods to produce statistically significant improvements in results;
- Advanced techniques for creating the individual realizations in the ensemble;
- Development of techniques to link ensemble mesoscale meteorological prediction systems with ensemble ATD predictions and evaluate the overall uncertainty of the probabilistic results; and
- Communication of probabilistic information from ensemble techniques to users through user-tailored decision aids.

TABLE 7. Prioritization factors for Developing Methods and Technologies to Improve Ensemble Construction and Interpretation

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	minimal	high	short	exceptional

The ability to quantify the uncertainty in ATD predictions will provide invaluable guidance on where R&D resources (funding and talent) should be invested to optimize the return. Because of its tremendous potential for gain in improving the quality of ATD prediction products if used to guide other R&D investments, the need for improved ensemble construction and interpretation is immediate. The overall level of effort, however, will be substantial. Many aspects, such as characterizing the ABL or quantifying uncertainty in data-sparse environments, are likely to require an extended period of R&D. Nevertheless, even incremental improvements in our capability to quantify uncertainty will produce moderate to substantial product improvements for users of consequence assessment systems.

R&D Need. Develop and test techniques to better estimate wet and dry deposition and chemical interactions.

As explained in section 3.2.5, removal or transformation processes and resuspension of previously deposited material are important factors for predicting concentrations downwind and are critical for assessing related impacts on the terrestrial and aquatic environments. Improvements in the parameterizations of the model physics for these processes, together with better empirical coefficients, are needed to improve ATD model predictions.

Although both dry and wet deposition of airborne materials has been studied for decades, the airborne hazards of interest have generally been either radioactive products of nuclear testing or common air pollutants, such as sulfur, nitrogen, and mercury compounds. Removal or resuspension of other materials, especially small particles, is still difficult to predict. Wet deposition, whether by rainout or washout, is far more efficient than dry deposition, but it occurs only during periods of precipitation. Until more is known about these processes, especially as they occur in urban areas, improving modeling approaches to account for them will remain difficult. However, the importance is high because hazardous substances deposited in urban areas will find their way into run-off, wastewater, and aquatic ecosystems, with health and ecological effects that might be severe.

Focused studies of the both wet and dry deposition processes are needed. Additional process-level understanding is important for developing successful simulations. In the case of dry deposition, the necessary measurements and modeling will be particularly difficult in urban areas because of the heterogeneity and general complexity of the surface. For wet deposition, it is known that urban areas modify the precipitation regimes downwind, but it is not yet known whether this translates into more rapid scavenging of hazardous materials contained in the air. Carefully designed experimental programs will be required to address these questions. In addition to improving the representations of the contributing processes in models, accurate prediction of deposition, transformation, and resuspension effects requires the capability to merge real-time information (e.g., radar-derived values for rainfall rates and their spatial and temporal distributions) into the models. Prediction of exactly where precipitation will occur and at what rate requires characterization of many stochastic systems. At urban/local scales, predictions of where it will rain and at what rate are therefore likely to be best described in probabilistic terms.

TABLE 8. Prioritization Factors for Develop and Test Techniques to Better Estimate Wet and Dry Deposition

Time Sensitivity	**Short-Term Gain**	**Overall LOE**	**Lead Time**	**Ultimate Gain Potential**
near term	**average**	**moderate**	**Average**	**high**

Deposition from the atmosphere constitutes the linkage between atmospheric concentrations and ecological (and other environmental) effects. There is accordingly a long history of research on both wet and dry deposition of various substances, usually for periods of an hour or more. However, substantial uncertainty exists in current representations. Wet deposition models require significantly improved cloud and precipitation models for time, location, and intensity, with due allowance for the sometimes dominating role of processes that cannot yet be addressed deterministically. Dry deposition formulation will necessarily need to take similarly stochastic factors into account, in this case related to the heterogeneity of the surface. The contributing processes have been studied principally for contexts other than atmospheric turbulence and diffusion. The results will certainly depend on the substance being deposited.

This may be a difficult research effort, but the chances of success have improved with recent development of new measurement technologies. Use of remote-sensing methods (especially radar) and modern methods of chemical analysis could advance our understanding of wet deposition and its temporal and spatial characteristics. Likewise, new methods for measuring dry deposition rates are now ready for exploitation, particularly modifications of well-known and long-proven eddy correlation techniques.

4.2.3 Approaches for Model Improvement

Physical Model Simulations of Transport and Diffusion

Mathematical models of transport and diffusion must make substantial approximations for some of the fundamental fluid-dynamical processes involved, particularly those processes unresolved by the model. Numerical modeling can be supplemented and improved by using physical modeling (e.g., wind tunnels, water channels, or water tanks) to simulate the atmospheric conditions of interest. In these laboratory simulations, the primary variables can be controlled, and the time and expense are greatly reduced compared with full-scale field studies.

A physical model must duplicate certain nondimensional parameters if it is to provide a realistic simulation of ABL processes (EPA 1981; Snyder 1972). Unfortunately, not all of these dimensionless quantities can be matched simultaneously to their full-scale (atmospheric) values. Research has been conducted to provide advice on which quantities are most important for simulating ATD of neutral and positive buoyancy gases (EPA 1981) and of dense gases (Meroney 1986).

Laboratory experiments (wind tunnel, water channel, or water tank) have been used to investigate a number of ATD problems, including transport around individual buildings and industrial structures, through clusters of buildings, and in street canyons. Some of these have investigated the dependence of concentration fluctuations on the initial size of the source. Water channels have been used to investigate stable and neutral boundary layer transport around isolated hills. Water-tank experiments have been used to investigate convective diffusion and plume rise from explosions. Results from such laboratory simulations are the basis for many of the model parameterizations in current use for these situations.

Although laboratory simulations cannot fully replicate every characteristic of the full-scale condition of interest, they provide a cost-effective solution for exploratory research, confirmation of theoretical solutions, and construction of operational model parameterizations and estimation methods. Laboratory simulations are especially effective for investigating and characterizing the stochastic effects of ATD inherent in microscale flows around obstacles.

High-Resolution Modeling of Turbulent Flow

The fluid-modeling community has many years of experience in modeling turbulent flow regimes in a variety of circumstances. Special attention has been directed to turbulence near the interface of a fluid flowing past a fixed or movable surface, which is conceptually applicable to turbulence in atmospheric flows.

Direct Numerical Simulation (DNS). For air flows less turbulent than the atmosphere, DNS of carefully described, idealized atmospheric boundary flows can resolve turbulent eddies down to the molecular scale. Consequently, approximations are not required for very small eddies, but these conditions are applicable to only a limited number of ATD scenarios. Nevertheless, for turbulent flows near the ground, DNS has demonstrated important properties of surface-layer flows. The DNS approach can be used to help quantify processes and improve parameterizations for larger spatial scales.

Computational Fluid Dynamics (CFD). As noted in section 3.2.4, CFD codes, adapted from aerospace applications simulate mechanical turbulence in atmospheric flows around obstacles, particularly in urban settings. CFD grid spacings are several meters in the horizontal and vertical dimensions, so some representation of smaller scale processes is required. Inflow boundary conditions are often fixed in time, and larger scale motions are not usually included. In some cases, simple time variations can be imposed. In urban studies, CFD codes sometimes are embedded within prognostic mesoscale meteorological models, which provide time-varying boundary conditions for ATD simulations. In many cases, CFD codes do not account for the local sources or sinks of heat or their time variations.

The computationally intensive CFD approach can be used to study features of the complex wind fields in urban environments such as those found in the MUST, URBAN 2000, and Joint Urban 2003 field studies. An important feature of numerical simulations is that the external conditions can be controlled for many model runs, each of which has a slightly different initialization. The resulting ensemble of realizations can be used to obtain quantitative estimates of uncertainty in predicted concentration fields. Because CFD models have limited volume domains, their boundary conditions are often assumed rather than being calculated from larger scale simulations.

Large Eddy Simulation (LES). Historically, mesoscale meteorological models have employed horizontal mesh sizes that were much greater than the depth of the ABL. The entire turbulent energy spectrum of the ABL was therefore well below the resolution of mesoscale models, and turbulence parameterization methods were needed. By contrast, an LES has a horizontal grid of 10 to 50 m and can resolve the larger, more energetic, turbulent eddies in the ABL. However, even an LES is unable to resolve the finer scales of turbulence, so a sub-grid-scale parameterization is needed to account for energy exchange between the resolved grid and the unresolved grid. Recent field experiments (Sullivan et al. 2003) and modeling studies (Chow and Street 2002; Juneja and Brasseur 1999) have suggested several sub-grid-scale turbulence parameterizations that significantly improve the popular closures.

The LES has become a common tool for investigating ATD because the statistical properties of LES results show many similarities to those of atmospheric turbulence, especially for unstable and neutral stability conditions. However, because the physics of some processes in the stable ABL are not well understood, LES is still being refined for stable conditions.

Lagrangian particle models using resolved LES wind fields are often used to characterize ATD of material from various sources. Substantially different realizations of concentrations in plumes from point sources at the same or different locations within the volume are commonly calculated. The statistically similar behavior of plume characteristics (mean and variability) as a function of stability and release height has been demonstrated (Weil 2004). As with physical models or CFD, the ability to control conditions provides the opportunity to compile ensembles of realizations for uncertainty estimation.

Although the LES approach is commonly used, it is limited because the initial and boundary conditions are usually assumed rather than based on observational or modeled inputs. Since many LESs use cyclical boundary conditions, lateral motions typical of mesoscale phenomena cannot be included.

R&D Need: Continue the development and use of physical modeling capabilities and high-resolution computational models (DNS, LES, and CFD) to simulate transport and diffusion in boundary layer and complex flow regimes and to assess components of uncertainty of concentrations and meteorological factors

These modeling approaches are the foundation of small-scale modeling and attempts to link across the mesoscale–microscale modeling gap. They have many features that are in need of R&D efforts. The models provide a capability to specify the atmospheric state and develop ensembles of realizations. With concentration estimates, the approximate bounds to the inherent uncertainty of ensemble conditions can be assessed. We can gain significant insight and knowledge of the consequences of averaging concentrations, fluxes, and turbulence. Better parameterizations of scale-dependent processes can be developed. Quantified fields of concentrations, winds, and turbulence can be analyzed. These models will be used to test and evaluate consequences of high-resolution surface characterizations and boundary conditions. The models will be used to test new closure equations. Furthermore CFD- type modeling will continue to be used in complex geometries, so R&D on including energy budgets in the simulations is a crucial issue.

TABLE 9. Prioritization Factors for Development and Use of Physical and High-Resolution Computational Models

Time Sensitivity	**Short-Term Gain**	**Overall LOE**	**Lead Time**	**Ultimate Gain Potential**
near term	**Average**	**moderate**	**average**	**exceptional**

A significant effort in small-scale ATD modeling (physical and computational) already exists. Physical models can provide an “observational” database for assessment of ATD model performance in complex conditions. Appropriate fields from high-resolution computational models are available or are reasonably easily regenerated. Analyses of existing data sets, such as those derived from Joint Urban 2003, should begin immediately to assess uncertainty issues as a function of scale. Substantial progress should come rather quickly where data exist. The effort must be sustained, as other R&D efforts progress, to help confirm new approaches and close the modeling gap.

4.3 Improving Measurement Technologies

Measurement of atmospheric properties and processes at and below the scales of interest is essential to improvements in ATD modeling. The primary area of concern of ATD is near the ground—in the surface layers of the atmosphere—where the hazard comes in contact with the ecosystem and its effects are felt. Meteorologically, the surface layer is connected to the large-scale flows through the ABL and is the most variable portion of the atmosphere.

The ABL is unique in that it results from the interaction of the small-scale effects of surface properties with large-scale flow fields. Furthermore, the ABL responds to diurnal solar heating and radiational cooling processes, providing a three-dimensional turbulence structure whose height during the day is on the order of the boundary layer height and during the night is a sharply stratified two-dimensional turbulence with little vertical mixing. Measurement systems need to account for the wide variety of conditions and scaling lengths that arise even in open areas.

Within urban areas, measurements become more difficult to make and then to understand because of the scales of buildings and the variations in vegetation and surface conditions. The increase in degrees of freedom challenges assumptions about relationships between measured quantities and can invalidate modeling assumptions. As the information in Table 1 (chapter 3) suggests, the ABL and the surface layer are poorly and sparsely sampled for ATD uses, both for tracer material (for the evaluation of ATD model performance) and for characterizing the environment (wind, temperature, humidity, and turbulence).

The standard meteorological measurement methods for weather forecasting have not focused on observing the *entities* in atmospheric phenomena, such as eddies at different scales that cause the short-term fluctuations in airborne hazard concentration at a given point. Scanning lidar systems can now identify eddies and other fine-scale phenomena rather than simply measuring their effects on state variables at particular points and times. These technological advances in measurement open up entire new strategies for observing the atmospheric processes and phenomena that cause the variability in local air movements and, therefore, in hazard concentrations. These new observations will be able to feed the parameterizations in improved mesoscale models. They also may be able to provide the initial or boundary conditions for much more sophisticated and realistic representations of microscale phenomena in ATD codes.

To quantify the uncertainties in ATD predictions, measurements of the distribution for a meteorological input parameter are necessary--not just a point observation of the parameter. For example, it would be preferable to have an observation-based estimate of the standard deviation in the wind direction during an increment of time, rather than a single point value for the wind direction. Existing quality standards for meteorological observations used by NOAA/NWS, for example, aim for accurate point estimates and are not adequate for capturing this information about the temporal distribution of the parameter.

R&D Need: Improve tracer materials and measurement technology.

Field experiments are the preferred means for testing and improving transport and diffusion models. Controlled releases of inert gases or aerosols simulate the transport of active agents through the atmosphere. Measurements of concentrations of this tracer material over a given period at various locations provide “ground truth” for the concentration and its time history, defining the plume dimensions and the distribution of mass within the plume. Measurements of wind and turbulence properties and other atmospheric variables in the study area are taken at the same time.

Previous dispersion experiments are useful mainly for studying the gross behavior of the effluent plume, as they provide reasonably good spatial location of the plume's path and footprint. The experiments were well suited for evaluating concentration prediction models that produced results with time and space scales similar to those of the sampling network. Tracer technology, however, has not kept pace with turbulence measurement technology. Improvements in tracer technology—both the tracer material and its measurement—are essential for assessing progress in ATD modeling.

Tracer materials are an important part of field experiments. Their release characterizes the source terms of interest to ATD modeling. The measurement of tracer concentration as a function of distance and time from release defines the impact of ATD on a released material and thus the potential hazard zones. Selection of the tracer technique for an experiment can be a tedious task.

Tracers must be *inert*—minimizing the potential health or environmental hazards. Aerosol tracers need to replicate the aerosols of interest. The tracer aerosol should closely replicate the hazard aerosol in size distribution, dielectric properties (for remote sensing), and affinity for moisture (since aerosols swell at unsaturated humidities). For gas or aerosol tracers, low cost per unit mass is desirable. Detectability at highly diluted concentrations (10^{-9} dilution) is also highly desirable.

Instruments for detecting tracer concentration must have a *rapid sampling rat*e, as variations in concentration for intervals shorter than the instrument response cannot otherwise be measured directly. If the response rate is not adequate, coarser parameterizations of fluxes and surface deposition are required, intermittency of concentrations cannot be determined, and short-period events of high concentrations cannot be identified. Instruments also need a large dynamic range of measurement to capture high and low concentration events as they occur and with equal precision. The devices should provide the measurement for real-time analysis. Low cost per sensor is needed to allow for a large array of sensors. Concentration detection by remote-sensing techniques is highly desirable for future studies because point measurements can never provide sufficient coverage near the ground and aloft.

Few tracer system components—material or sensor—satisfy all these requirements. Trade-offs (except for safety) are usually required. At present, sulfur hexafluoride is the gaseous tracer of choice for urban and short-range studies, as in Joint Urban 2003, Urban 2000, and Pentagon Shield. Rapid-response sulfur hexafluoride detectors are expensive and not readily available. Consequently, the measurement campaigns for these studies were highly labor intensive and logistically limited. Some long-range studies have used perfluorocarbons (e.g., the ANATEX experiments), but long integration times (about 12 hours) were required to accrue enough material for analysis (Draxler 1991; Draxler et al. 1991).

Assessing and guiding future improvements in ATD modeling will depend on a concentrated effort to develop tracer materials and measurement technologies that meet these requirements. Adequate tracer studies must become routine so that ATD model performance can be regularly evaluated. Adequate studies are also needed to evaluate the sources of uncertainty in both measurements and modeling.

TABLE 10. Prioritization Factors for Improving Tracer Materials and Measurement Technology

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	High	moderate	short	exceptional

A concentrated effort to develop needed tracer technologies should begin immediately. It is impossible to routinely quantify uncertainty in ATD models in the field or in test beds without controlled tracer data. This effort is critical for the overall research objectives but may not be easily achieved because progress on development of fast-response sensors has been slow and remote-sensing capabilities will depend on the candidate tracer material. Having this capability is also essential to learning how best to communicate uncertainty to users.

R&D Need: Improve boundary-layer atmospheric measurement capability.

Atmospheric quantities other than hazard concentration, such as temperature, water vapor, and trace gases are also affected by atmospheric fluctuations. Short-term changes in wind speed and direction, which strongly affect the transport and diffusion of locally emitted contaminants, are of particular interest in the case of hazardous or toxic materials for which even short-term exposures to a threshold concentration may seriously affect human health and safety.

Fluctuations in wind speed, wind direction, and atmospheric temperature are probably among the easiest data to obtain. Appropriate instrumentation has been available for decades and has been continuously improved. With the recent decrease in cost of three-dimensional sonic anemometers (which offer the advantages of fast response, low threshold, and no moving parts), it is now possible to establish continuous, around-the-clock measurement programs for wind and temperature fluctuations at most locations of interest. The accuracy of these instruments remains reasonably good for sampling rates up to 20 Hz. Data can be collected easily using inexpensive small computers. Data transfer and centralized data collection and storage are probably the main remaining technical problems because of the amount of data that can be collected from even a modest-sized wind-sensor network in a relatively short time.

Even with an ability to collect large amounts of data, data collection at discrete points may cause problems of data quality and data representation (see section 3.2.3) because of the spatial and temporal variability of the wind and its fluctuations. In principle, this issue could be handled by an instrument array that is dense both horizontally and vertically. While this solution is not feasible for routine instrument networks, it is feasible for specialized networks and field studies. The correlation length is a measure of the consistency of observations taken at one location with those at another location using common averaging times (e.g., 1 minute instead of 15 minutes). Dense networks provide an opportunity to measure correlation length and assess the density of measurements needed to characterize a location and its surroundings (urban or rural). Joint Urban 2003 is a good example of a field experiment that employed a dense wind and turbulence network.

Remote-sensing techniques offer the potential for technology solutions to ABL measurement needs. The major advantage of a remote-sensing method is that a line or volume of the atmosphere can be sampled at a known, designed (often rapid) rate without the sensor needing to be in direct physical contact with the spatial points or volumes being sampled. Remote-sensing systems produce observations either by active or passive means. In an active system, the system transmits a signal and records the direct or indirect interaction of that signal with environmental conditions of interest. In a weather radar system, for example, the reflections of a transmitted radio wave from a scatterer are captured. Passive sensors typically rely on the thermal properties of the ground or the atmosphere, without an emitted signal. A typical passive observing system detects the infrared energy naturally radiated from the environmental condition of interest. Both active and passive approaches to remote sensing typically require additional extensive processing of the received signal to obtain the desired information about the environmental condition of interest.

Active systems such as radar, lidar, and sodar have been used to measure winds, temperature, and precipitation. Ground-based radar and sodar have been available to ATD modeling for many years to measure wind profiles, but they have not been networked for operational use. Implementation of clear-air radars, like the FAA Terminal Doppler Weather Radar system, provides wind fields at kilometer increments near major population centers. Efforts are underway to make similar use of the WSR-88D weather radar network. Recent availability of eye-safe Doppler lidar systems has permitted resolution of wind fields of urban and rural domains at resolutions measured in tens of meters. These systems generate volumetric data in tens of seconds. Improved and expanded lidar capabilities are being studied actively for both research and operational use. Airborne and satellite-based radar and lidar capabilities are becoming common. For directed-research programs, moisture and ozone are now commonly measured using remote-sensing systems on aircraft or satellites. The ATD R&D community must keep abreast of these developments as they relate to mesoscale through microscale applications.

Satellite-based or airborne passive remote sensors can provide land cover information across a range of temporal and spatial scales. Passive remote sensing is well suited to gathering current data on local surface radiances, which can be interpreted into information about surface conditions. Thermal remote-sensing techniques can help document the surface energy budget by providing accurate observations of thermal changes across the landscape at spatial resolutions from several meters to a kilometer. Multispectral and hyperspectral imaging in fine bands within the same view may become a means of quantifying subtle but significant differences in surface conditions. Research must continue on methods of translating the sensed radiation signal into information on surface properties on a timely, reliable, and comprehensive basis.

Remote-sensing systems that use sophisticated scanning techniques, such as push broom or framing techniques, have the potential to probe larger volumes of the atmosphere above a region than do local sensors; however, these systems have their limitations. Their view of the atmospheric volume can be degraded by precipitation or blocked by obstacles or clouds. They can be affected by unwanted reflections (clutter) or by scattering in the sensing medium. They may also have relatively coarse spatial resolution. Some systems (e.g., sodars) produce signals that can affect humans in the immediate area and, as a result, may be difficult to use in populated areas. Some remote-sensing systems, especially research-grade systems, are not well suited to autonomous operation. They require frequent or even continuous attention from skilled specialists. This requirement makes them expensive to operate.

Remote-sensing systems generally have a high sampling rate, which means that very large quantities of raw data can be acquired in a short time. This rapid data acquisition poses potential storage and transfer problems. Interpreting the data is often not straightforward and may require considerable expertise and experience. For example, correct interpretation of the data is often complicated by the noise of turbulence effects, which generally must be removed by time-averaging to reveal the mean patterns. Ground-truth data over the sensing volume are needed to ensure that the remotely measured variables and derived parameters agree with conventional data sources.

Finally, research is needed to improve the fundamental understanding of how models can incorporate a variety of remotely sensed data.

TABLE 11. Prioritization Factors for Improving Boundary-Layer Measurement Technology

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	**high**	**high**	**short**	**exceptional**

To realize short-term gains, further development of existing boundary-layer measurement capabilities should be accelerated and on-the-shelf improvements should be incorporated into existing measurement systems. New, low-cost instrumentation developments for measuring important boundary-layer variables and possibly fluxes, should be started by exploiting existing R&D mechanisms such as the Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs or agency-specific instrument development programs. New instrument development is often time consuming and expensive, so options to expedite the process should be explored through laboratories, academia, and industry. The measurement improvements will enable other R&D needs to be met.

4.4 Model–Data Interface Challenges

In the end-to-end functional analysis of ATD modeling systems provided in section 3.2, there are a number of capability gaps that occur at the interface where data come into the modeling system. Such capability gaps could be viewed as either an input data problem (too few data, questionable data, not the right data, etc.) or a modeling problem (model representations not powerful enough to predict from the data given, etc.). Innovative approaches to filling them often amount to some combination of advanced input processing, as defined in section 3.2.3, and model improvements. Two recurring themes in these interface challenges are determining the *impact of input data uncertainties* on the uncertainty in modeling system predictions and issues of data quality and data representation, as defined in section 3.2.3. The JAG identified R&D needs for three areas of these model–data interface challenges: sensor fusion, data representation and data assimilation, and model performance evaluation.

4.4.1 Source Characterization by Sensor Fusion

A comprehensive assessment of source characterization technology—either current capabilities or R&D needs to meet application requirements—is beyond the scope of this report and beyond the charge of the JAG. However, the use of sensor fusion, as defined in section 3.2.1, to back-calculate to the estimated source term location, emission rate, and release duration is within the scope of this report.

In certain hazard release scenarios, the first indication of a release will be alarms triggered by specific sensors at varying distances and directions from the exact location of release. The identification of the location and characteristics (emission rate, duration) of the source from these alarm data are often important objectives in response management. By combining data from networked sensors with predictive models, more can be learned about a release event than could be obtained from any individual sensor or predictive model alone. Sensor fusion modeling systems are being developed to backtrack from these initial sensor data to estimate the most probable source term location and emission characteristics.

The process of integrating sensor data with predictive models is intended to result in adjusted predictions that better describe the release event than would model calculations made without the sensor data. The predictive models produce calculations based on previously available information about the source term release. Several predictive models may be run separately to produce a single prediction, or they can be used to create an ensemble of predictions. Some predictive models can estimate aspects of the uncertainty in their description of the event. Although the mathematical problem may not allow a single, definitive solution, even the capability to narrow the possible range of locations or characteristics can be valuable to response decisions.

To explore the limits in characterizing the source term by coupling ATD modeling with monitoring data, Hanna, Chang, and Strimaitis (1990) analyzed data from the Project Prairie Grass diffusion experiment using Gaussian plume models. Two of the three models had been tuned to the release situation. The authors concluded that the source term emission rate could be estimated to no better than a factor of two, even with an advanced Gaussian plume model, a point source in ideal circumstances, and a near-surface release having a known release height and a constant emission rate. This limit on emission rate estimation may represent an ultimate uncertainty that cannot be reduced, but further investigation is warranted.

R&D Need: Improve and evaluate sensor fusion techniques.

The R&D areas for improving sensor fusion techniques include the following:

- Rapid interpretation of data streams from multiple sensors;
- Increased detection confidence with reduced system-level false alarms;
- Improved situational awareness for CBRN events;
- Estimates of the most probable source terms; and
- Refined model predictions of downwind hazards.

Sensor fusion methodologies with the potential to provide these improvements include inverse dispersion modeling, Bayesian statistical methods, adjoint methods, artificial intelligence, neural networks, fuzzy logic, and others. Sensor fusion techniques should be developed that can use data from a wide range of detector types, as well as other relevant non-sensor data, such as intelligence and medical information. Existing mathematical and statistical concepts should be evaluated and incorporated as appropriate, but new or more advanced concepts may be required because of the wide range of unknowns and uncertainties involved.

TABLE 12. Prioritization Factors for Improving and Evaluating Sensor Fusion Techniques

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	high	moderate	moderate	high

Sensor fusion has been targeted as a high priority for the Department of Defense (DoD) and the Defense Threat Reduction Agency. Research plans for various single or multiple approaches have been developed, and implementation of them has begun across a wide range of atmospheric scales. Candidate approaches can be evaluated in a relatively short time frame. Since the success of this R&D effort depends on the ATD modeling capabilities, sensor fusion capabilities should improve as ATD models improve. However, uncertainty due to the nonlinearity of ATD may limit capability improvements. Opportunities exist to understand this uncertainty and feed that understanding back into the ATD model improvement and sensor fusion capabilities. These synergies and dependencies across individual R&D needs are typical of what the JAG found in many areas for which quantifying ATD modeling uncertainties is a major objective.

4.4.2 Data Representation and Data Assimilation

Diverse sources of meteorological and agent-concentration data exist. The data are often taken at, or are representative of, varied time and space scales. Putting these data together in a coherent, physically realistic manner is the data assimilation process. As mentioned earlier, it may occur in one to four dimensions and cover a variety of scales. A key factor in data assimilation is how well the data fit the assumptions of the model: defined in section 3.2.3 as data representation. Prognostic models, for example, require initial conditions to describe the current state of the atmosphere in the volume being modeled and boundary conditions for that volume of atmosphere; namely, its inflow, outflow, and lower and upper sources or sinks of mass, energy, and momentum. The process of model initialization begins at global scales where radiosonde, satellite, aircraft, and other observational data sources are assimilated with previous forecasts for the new initial time to provide a comprehensive, updated, large-scale description of the atmosphere. As higher resolution grids are nested into subsets of the next larger scale, the initial and boundary conditions for the smaller grid must be provided to account for processes not represented at the larger scale.

At the larger scales, data assimilation approaches are undergoing intensive research and development. In the past two decades, physics-based assimilation of observations has replaced interpolation approaches. For example, in *nudging* techniques, a tendency term is added to the differential equation for each explicit variable in a full-physics mesoscale model such as MM5. The tendency term is proportional to the difference between the model predictions and observations; the observations are weighted in space and time, depending on the data type. Another approach comes from Sakaki's use of variational calculus, which opened the way to weighting observed data and constraints imposed by the equations of motion and conservation within the forecast model to produce three-dimensional initializations. This approach, called 3-D VAR, has become a de facto standard for major forecast centers. Attempts to incorporate temporal variability into the basic 3-D VAR approach, called 4-D VAR, lead to a complex set of equations that can only be solved approximately. Producing a 4-D VAR analysis is almost as time-consuming as the 72-hour forecast. Furthermore, it is closely coupled to the forecast model and its parameterizations.

More recently, ensemble techniques are being explored to improve the data representation fit of initial conditions. As noted previously, ensembles can be composed of several runs using the same model with different initial conditions, several runs using different models, or a set of runs with the same model but using different parameterizations. Another approach being explored for developing an ensemble is to use principles of Kalman filtering. These techniques appear to be independent of the forecast model. Generally speaking, most of these techniques have not been well tested with the finely nested grids needed for ATD predictions.

As grids are nested, typically in a ratio of 3:1, the meteorological data fields are usually interpolated to the finer grids without a physical constraint. Outside the ABL, this approach is reasonable. Inside the ABL, however, smaller scale processes that affect the turbulent state in the ABL are not represented. The usual assumption is that the finer-scale lower boundary conditions will develop (in the model state) after an initial adjustment period. Lateral boundary conditions are likewise interpolated and, at the inflow, driven by the larger scale forecast fields. Unfortunately, because there is a severe lack of observational data at nesting scales, these assumptions are not tested or directly verifiable. The overall forecast quality is a surrogate indicator of the validity of the assumptions. In traditional measures of performance, which use indicators such as bias and root-mean-square error, there appears to be a practical limit to improving forecasts (i.e., reducing forecast errors) by reducing grid size (Mass et al. 2002). This limitation can largely be explained by the fact that, as higher resolution is added to the forecast, the traditional forecast statistics become increasingly affected by slight errors in the location or timing of the mesoscale features. Research is needed to develop measures of performance for high-resolution mesoscale model forecasts that better quantify their value for use with ATD models.

Incorporating additional data on local winds and turbulence appears to have a positive effect on model performance at high resolution. As mentioned, the top-down approach of nesting appears to meet a practical limit near grid sizes of 5 km; however, the Army test ranges have had good results with operational modeling systems that use two-way grid interactions and an innermost domain resolution of about 1 km (Warner et al. 2004). For a wide range of weather conditions, models, and observational conditions, forecast models at that scale have large errors in wind-direction predictions—root mean square errors of about 40 to 60 degrees. Thus, inclusion of local observations in diagnostic and prognostic models of the wind field seems to be a reasonable and perhaps necessary approach to meeting user requirements for greater accuracy and useful information about predictive uncertainties.

Two other aspects of ATD modeling system performance place additional challenges on data assimilation R&D to improve the prediction of concentrations for the end users (emergency managers, operations officers, and researchers). First, for initial and intermediate response to hazard releases, data QA/QC for model fit (data representation) and data assimilation need to be automated (i.e., handled by software-embedded algorithms), without requiring expert “tweaking” by the model user. Second, the remote measurement technologies discussed in section 4.3.2 provide input data that require new capabilities on the part of the ATD model code to assimilate the data. Some software-embedded algorithms for data assimilation exist. However, as noted in section 3.2.3, assimilation of observations beyond $\boldsymbol{t_0}$ of a prognostic model is often restricted by the constraints necessary to perform the iterated computations. If the data to be assimilated diverge too far from the model’s predicted values for that space-time cell, the data are rejected.

One of the emerging remote-sensing technologies, Doppler lidar, offers promise for providing high-resolution local wind fields in a variety of conditions. Following developments in deriving wind fields from Doppler radar data, Lin, Chai, and Sun (2001) used 4-D VAR with Doppler lidar data to construct three-dimensional wind fields characteristic of the convective boundary layer. As noted above, pure 4-D VAR is computationally time-consuming. Warner et al. (2002) used less restrictive constraints to permit a rapid analysis of 3-D wind fields obtained from scanning Doppler lidars.

Coupled with backscattered energy from airborne aerosols, almost real-time estimates of aerosol plume position, and short-term estimates of future paths (nowcasts) are feasible. Newsom and Banta (2004) and Calhoun et al. (2004) have suggested other approaches to assimilate lidar data at high resolution. Parallel development of lidar technology and data processing techniques should help advance the knowledge of smaller scale motions in real boundary layers.

R&D Need: Improve and evaluate techniques for data QA/QC for model fit and data assimilation for both initial and boundary conditions.

Data assimilation issues are closely tied to the scales of motion of interest, the availability of data representing those scales, and the techniques (models) used to link the data to the current state of the atmosphere at that scale. At present, data assimilation practices using variational or ensemble techniques exist for mesoscale operational models. These models are nested in global models but use finer resolution terrain conditions from surface, satellite, and/or aircraft regional observations. As finer scales are needed, assimilation approaches must adapt as surface and near-surface data become more important—an issue closely linked to improving characterization of surface-boundary conditions as discussed in section 4.2.2. At finer scales, assimilation becomes more temporally sensitive (perishable) and acceptant of observations appropriate to the model scale. The assimilation must allow representation of finer-scale dynamical processes (a need closely linked to bridging the mesoscale to microscale/urban scale gap, as discussed in section 4.2.2). It must be able to accept data coming from emerging measurement technologies (closely linked to improving boundary-layer atmospheric measurement capabilities, as discussed in section 4.2.3. These improvements are particularly important for recognizing and incorporating into the model run the three-dimensional structure of the daytime and night-time boundary layers.

Data QA/QC issues increase as remotely sensed and higher density in situ data are incorporated into the analyses. As much as possible, these issues should be addressed by onboard processing at the sensor, but errors due to data transmission, omissions, and losses must be identified before the data are used. Because volumetric remote sensing provides large sets of data to control and check, tests and filters for rapid and automated data QA/QC must be developed. Automated capabilities are also needed to ensure data representation by assessing the applicability of the data for the intended use. Including error bounds with observation data is an essential step toward understanding and quantifying the sources of uncertainty in model predictions that stem from factors outside the model itself.

TABLE 13. Prioritization Factors for Improving and Evaluating techniques for Data QA/QC for Model Fit and Data Assimilation, for Both Initial and Boundary Conditions

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
immediate	average	moderate	moderate	high

Substantial development has occurred in data QA/QC and data assimilation at the macroscale and the larger mesoscale. Applications of 4D VAR and ensemble techniques for meso–β and smaller scales can be initiated without much difficulty for testing these techniques where appropriate measurements exist. Full implementation of assimilation techniques will become beneficial when data become more plentiful and regular in test beds or large networks (i.e., when instrumentation is developed and in operation). As model scales become smaller and approach the urban scale, data assessment issues will become more location-specific, adding challenges to automation of the process and requiring faster execution times. Results of this R&D will link with the design and implementation of urban regional monitoring networks.

4.4.3 Model Performance Evaluation Issues

Model performance evaluation basically comes down to comparing a model's predictions of concentration with the concentrations observed from field measurements. One can view the observed concentrations as a summation of three values: the ensemble average for the conditions present, the effects of measurement uncertainty, and the effects of unresolved processes (stochastic fluctuations). The modeled concentrations can be viewed as a summation of three values: the ensemble average for the conditions present, the effects of uncertainty in specifying the model inputs, and the effects of errors in model formulation (which may vary as conditions vary).

The concept of natural variability acknowledges that the details of the stochastic concentration field resulting from transport and diffusion are difficult to predict. In this context, the difference between the ensemble average and any one observed concentration value (realization) is ascribed to natural variability. The ensemble is the ideal infinite population of all possible realizations meeting the (fixed) characteristics associated with the ensemble. In practice, one will only have a small sample from this ensemble.

Measurement uncertainty in concentration values in most tracer experiments may be a small fraction of the measurement threshold. When this is true, the contribution of the measurement uncertainty to empirical determinations of the magnitude of natural variability can usually be deemed negligible.

One method for performing an evaluation of modeling skill is to average separately the observations and the modeling results over a series of non-overlapping limited ranges of fixed conditions, which are called "regimes." Averaging the observations provides an empirical estimate of what most of the current models are attempting to simulate; namely, the ensemble average. A comparison of the respective observed and modeled averages over a series of regimes provides an empirical estimate of the combined error associated with input uncertainty and formulation errors.

This method for evaluating model skill is not perfect. Some models provide estimates of the average concentration for a volume of air (grid averages), whereas the observations represent what is seen for some point in the volume of air. The variance in observed concentration values due to natural variability can be on the order of the magnitude of the regime averages. Hence, small sample sizes in the groups will lead to large uncertainties in the estimates of the ensemble averages. The variance in modeled concentration values due to input uncertainty can be quite large; small sample sizes in the groups will therefore lead to large uncertainties in the estimates of the deterministic error in each group. Finally, grouping data together for analysis requires large data sets, of which there are few.

R&D Need. Develop physics-based evaluation metrics that recognize the fundamentally different sources for variations in observed and model-predicted values of downwind hazard concentration.

The most important concept expressed in the discussion above of modeling performance evaluation is that the observations and the modeling results come from different statistical populations whose means are (for an unbiased model) the same. The variance seen in the modeled values results from differences between estimates of ensemble averages and differences resulting from modeling errors. The variance in the observations results from differences in ensemble averages, differences arising from sampling uncertainties, and an additional variance, which is not represented in deterministic modeling, caused by stochastic variations between individual realizations. Because of these differences in the populations for which variances are being estimated, a thorough reassessment is needed of how transport and diffusion models are evaluated. The currently accepted model evaluation methods directly compare the observed and modeled concentration values (in contrast to comparison of regime averages), an approach that assumes the observations and the model estimates have the same sources of variance. As explained above, this assumption is erroneous. Viewed in this context, comparisons of observed and modeled frequency distributions of concentration values for transport and diffusion models are questionable, unless the models are attempting to estimate not only the variations to be expected in the ensemble average as conditions vary but also the effects of unresolved stochastic fluctuations. Thus, asking whether a deterministic model can match observed extreme values amounts to requiring the model to succeed at a task it is fundamentally incapable of doing, except by compensating for input uncertainties and formulation errors. Until now, model evaluations have focused on evaluating a model for how it is used rather than on the basis of what the physics in the model is capable of estimating. For example, models are now often evaluated as a characterization of extreme values—a task for which few, if any, models incorporate the necessary physics.

Thus, the focus of model evaluation methods should be on assessing how well a model predicts those features of the concentration distribution (mean, variance, distribution) for which that model incorporates appropriate physics. While we cannot simulate exactly what is observed in time and space, we might (with suitable research) predict the average characteristics of the concentration distribution seen at each point (e.g., the mean, variance, and distribution). Of course, we only observe individual realizations, but if we properly predict the characteristics, the observed individual realizations will be within the predicted distribution of possible outcomes. If this approach to model evaluation is pursued, the evaluation methods can adapt to assess model performance as new model capabilities (e.g., probabilistic modeling) are developed.

TABLE 14. Prioritization Factors for Developing Physics-based Model Evaluation Methods

Time Sensitivity	Short-Term Gain	Overall LOE	Lead Time	Ultimate Gain Potential
near term	high	low	average	exceptional

Physics-based model evaluation methods must consider the internal, external, and stochastic components of model uncertainty. Models are evaluated unevenly, with different criteria applied by different developers. A reference standard or consensus-based methodology developed by an independent standards setting organization provides a standard by which developers and evaluators can uniformly evaluate modeling systems. This solution can be implemented rapidly by commissioning a standard-setting organization to develop and maintain (update) the standard. The sustaining activity by the organization will ensure the standard is maintained over time as experience is gained and innovation produces improvements.

4.5 Summary of R&D Needs

Table 15 is a compilation of the prioritization factors assigned to R&D needs in tables 3 through 14. Although this summary table brings all the R&D needs together, the assignments of prioritization factors need to be interpreted through the explanations given in the paragraphs following each of the component tables.

TABLE 15. Summary Table of R&D Needs with Prioritization Factors

R&D Need	Time Sensitivity	Short-Term Gain	Overall Level of Effort	Lead Time	Ultimate Gain Potential
Bridge the modeling gap	near term	average	moderate	average	exceptional
Characterization of surface conditions & input data sets	near term	average	high	average	exceptional
Test and refine physical basis for sub-grid-scale parameterizations	longer term	average	moderate	average	exceptional
Characterize dispersion in complex environments	immediate	average	high	average	high
Improve ensemble construction and interpretation	immediate	minimal	high	short	exceptional
Techniques to better estimate wet and dry deposition	near term	average	moderate	average	high
Physical and high-resolution computational models	near term	average	moderate	average	exceptional
Improve tracer materials and measurement technology	immediate	high	moderate	short	exceptional
Improve boundary-layer measurement technology	immediate	high	high	short	exceptional
Improve and evaluate sensor fusion techniques	immediate	high	moderate	moderate	high
Data QA/QC for model fit and data assimilation	immediate	average	moderate	moderate	high
Develop physics-based model evaluation methods	near term	high	low	average	exceptional

5.0 AN R&D STRATEGY TO MEET USER NEEDS

5.1 The Goals for ATD Modeling R&D

As the JAG considered user needs and the R&D to sustain continuous improvement of ATD modeling capability, a recurring theme was the necessity to quantify the uncertainty in ATD modeling predictions far more completely and accurately than is currently possible. Quantifying the uncertainty is essential for two reasons.

First, ATD models must routinely characterize both the deterministic and stochastic contributions to the modeled effects. The stochastic contributions may in many instances override the deterministic processes. As emphasized in chapter 2 and throughout this report, the ATD modeling community must do better at interpreting for the end users of its products the implications of the uncertainty in predictions for the ways in which the predictions will be used.

Second, effective progress in reducing the uncertainty (where possible) through continued R&D requires knowing how much there is and how much each factor contributes to the uncertainty in the product. As detailed throughout chapters 3 and 4, some sources of uncertainty in predictions can be reduced; others cannot (given the inherent nature of the processes involved or the limits of our science of them). Cost-effective progress in reducing uncertainty requires quantifying and distinguishing these various contributions to the uncertainty in the product.

The JAG identified two capstone goals for future R&D: *routinely quantifying uncertainty* and *interpreting the implications of this uncertainty to users*. Supporting these capstone goals are six objectives (figure 8). Some of the objectives, such as *multiple ATD test beds*, correspond roughly to a single program element in the R&D plan. Other objectives, such as *bridging the modeling gap*, will be achieved through contributions from several R&D program elements. Overall, the JAG expects that a sustained and concerted effort of a decade or more will be required to attain all the objectives to the degree envisioned in this report. However, throughout that duration, all of the program elements will produce useful interim results. To reach the capstone goals, the elements of the overall strategy must be sustained, evaluated, and allowed to evolve as the knowledge base grows and the capabilities for ATD modeling improve.

The synopsis below of each objective notes those program elements most directly related to obtaining the objective. Details of the program elements are discussed in sections 5.3 through 5.7; next steps toward achieving these specific objectives and the capstone goals are recommended in chapter 6.

Capture and Use Existing Data Sets. This objective identifies the need to assemble into a modern data format the available (open access) data sets from the many years of ATD experiments and model testing. These historical data are in various forms and storage media: punch card, paper, and electronic media. Oral histories from the participants will provide essential insights into the data quality, the understanding of objectives, and the

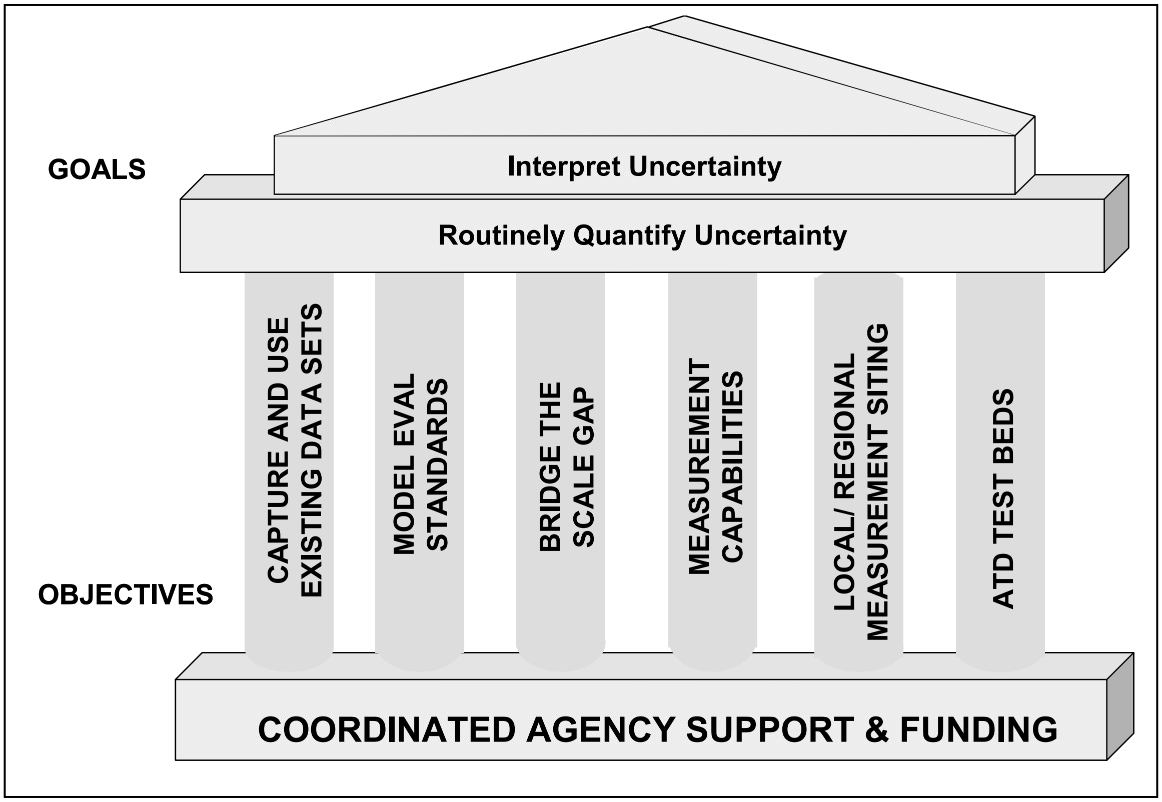

FIGURE 8. Six R&D objectives need to be achieved to support the ultimate goals of quantifying uncertainty and communicating its implications to users.

actual conduct of the field programs—all of which are in danger of being lost. These records of past ATD field experiments are the best extant source of concentration data currently available to quantify uncertainty in ATD models. The data from some of these experiments were not previously analyzed to the extent now technically feasible. The records from others are now worth studying for different objectives than before. Overall, they represent a resource that can quickly provide a useful base to begin assessing ATD model uncertainty. This objective can be achieved through the R&D program element described in section 5.3, Capture and Use Existing Data Sets.

Model Evaluation Standards. Procedures for evaluating the performance of ATD modeling systems are not standardized across the Federal agencies or ATD model user communities. Further, the existing procedures may not fully deal with the complexities introduced by comparing calculations and observations having different inherent space and time averaging. Without common reference standards, model development and implementation tend to remain “stovepiped” within the developing agency, while other development efforts are discounted or go unused. An all-agency effort to establish and maintain a current set of criteria for evaluating model performance by a recognized independent standard development organization (SDO) will alleviate this problem. This objective can be achieved through the R&D program element described in section 5.4, Foster Evaluation Standards for Modeling Systems and Components. Other program elements will help by contributing to the knowledge base needed to set standards and update them as needed.

Bridge the Modeling Gap. Top-down modeling (from larger to smaller scales) and bottom-up modeling (from smaller to larger scales) do not merge across scales from 50 m to 5 km in realistic environments. This points to a fundamental lack of knowledge of how to model the processes at these scales. In all models, there is an element of turbulence carried in the smallest scales and the unresolved processes. Although there is perpetual optimism that higher-resolution models will give better results, current operational experience does not substantiate this optimism.

The processes are primarily boundary-layer processes mixed with mesoscale phenomena and driven by the large synoptic flows. Specification of initial and boundary conditions for forecast models is difficult because of the complexity of the lower surface. Timing of flow features becomes more critical for ATD needs than for other forecast needs. Furthermore, smaller-scale features are typically lumped into sub-grid-scale processes and treated as a closure problem until some of the processes become effective in altering flows in significant ways. Feedback loops of small to large scale are poorly understood. In most ATD models, the crucial level of interest—within the first few meters above ground—is where the unresolved processes are dominant and mostly stochastic.

The objective of bridging the modeling gap can be met through the combined and coordinated efforts from several R&D program elements. The major contributing elements will be coordinated programs for improved measurement technologies (section 5.5), the multiple ATD test beds (section 5.6), and special studies and experiments (section 5.7). The additional analytical results obtained by capturing existing data sets (section 5.3) will provide early contributions toward this essential and difficult objective. Furthermore, the bottom-up approach of physical modeling and CFD and LES is critical to achieving his objective. Developments in theoretical constructs and understanding of basic processes within the gap will be keys to its closure.

Improved Measurement Capabilities. Measurements are fundamental to advancing the realism of a science-based description or prediction. In ATD modeling, improving the capability to measure concentrations of tracers and atmospheric variables (e.g., wind velocity, turbulence, temperature) *at the scales of ATD model use* is essential to all the identified R&D needs leading to better ATD models. Quantifying the uncertainty in model variables requires in situ and/or remote measurements at the modeled scales. Most applications of ATD models are at much finer scales than are the available atmospheric data, especially in populated areas. To develop better parameterizations, measurements are needed to understand processes not resolved within models.

Tracer measurement capabilities are needed to provide data for quantifying the uncertainty in ATD model predictions. They are also needed to build an experience base for users. Compared with meteorological model users, who routinely receive feedback on their forecasts, ATD model users rarely get real-time experience or feedback at present, except in emergency situations. Users need to build a base of experience with models and develop local knowledge through feedback from real experiences. There is no training ground like real (not "canned") hands-on experience.

Two of the R&D strategy elements will make major contributions to this objective of improved measurement capabilities: the coordination of programs for improved measurement technologies (section 5.5) and the multiple ATD test beds (section 5.6). Supporting contributions will come from further analysis of existing data sets (section 5.3), consensus evaluation standards (section 5.4), and special studies and experiments (section 5.7).

Local/Regional Siting of Instrumentation. Each locality has a unique morphology. Many localities want to provide a network of instruments, within budget limitations, that will reasonably represent wind and turbulence fields needed for ATD concentration fields in emergency conditions. No one plan fits all these sites. Strategies are needed to make reliable recommendations through a combination of modeling exercises, optimization processes, and experience in other areas. Major contributions to this objective can come from analyzing existing data sets (section 5.3) and the multiple ATD test beds (section 5.6). Parts of the coordinated programs for improved measurement technologies, particularly work on optimizing observational network design (section 5.5.2) will support this objective, as will aspects of the special studies and experiments (section 5.7).

ATD Test Beds. Recently, fledgling infrastructures for routine ATD forecasting based on model and local information, such as NOAA's DCNet, have developed in several urban areas. The JAG proposes a strategy of establishing test beds in appropriate areas across the country to address and test ATD models, model needs, and model capabilities on a continuing basis, just as weather forecasting operations and evaluations are conducted. By operating and performing evaluations continuously, by testing new ideas and instruments, and by interacting regularly with users, an ATD test bed becomes a crucible in which ATD modeling is made robust and refined from an art into a demonstrated and verified operational capability.

Most ATD model studies in the past were defined field campaigns operated to maximize the probability of success. Within this context, benign, simple, and nontaxing weather conditions were preferred, although terrain conditions may have been complex. Controlled tracer releases were sampled and atmospheric measurements were made as densely as capabilities and resources permit. As accidental releases and terrorist incidents are not scheduled, little is known from these past studies about the performance of ATD models across the spectrum of daily conditions. The proposed test bed infrastructure will provide this coverage, while building on the results from past studies.

The initial number of test bed installations should be limited so that operational procedures can be developed and refined without squandering scarce resources. Once the prototyping lessons have been learned, the set of installations could expand to cover more locations of priority interest, with each additional location chosen to represent different challenges from those already in place or being installed.

The ATD test bed objective amply illustrates the interdependence among the program elements and the synergy across major applications for ATD modeling. Activities that support air quality forecasting can also employ the test beds and contribute ideas to improve test bed capabilities. Experience developed in working with the test beds will aid in siting instruments to optimize their utility. Measurement innovations, in turn, will feed and stimulate modeling innovations. Models will have access to better parameterizations to close knowledge gaps. New approaches to ATD modeling will develop as test bed capabilities for experimentation and evaluation improve. Baselines for characterizing uncertainty will develop. Improvements in models by reducing uncertainty will be more readily quantified using the test beds, and the performance of different modeling systems or different configurations of one system will be more easily compared and objectively evaluated.

Multiple test beds are a major R&D program element, as well as a major objective. The extensive discussion in section 5.6 explains in greater detail why establishing and maintaining multiple test beds, with several in urban/city environments, is so important to the ultimate goals of quantifying uncertainty and interpreting its implications for users. In addition, the test bed objective will draw on other proposed program elements. Test beds need meteorological and tracer measurement capabilities to test siting strategies and to test and modify the instruments (section 5.5). Test beds should incorporate programs in which users and researchers work side by side in developing and using modeling systems and supporting tools (section 5.2). Standards are likely to evolve, based on test bed capabilities (section 5.4).

5.2 The R&D Aspects of Interpreting Uncertainty Implications for Users

This report addresses R&D needs, not training and outreach. However, some elements of training and outreach to users must be addressed because they impact the R&D process and outcomes. The most important of these elements concern the ability of users to understand how the limitations on model accuracy and precision—limits which the model researcher-developer quantifies in terms of the concept of uncertainty and the mathematics of probabilities—affect appropriate use of the model results. For example, users must have tools that incorporate probabilistic weather information with transport and diffusion applications and associated decision aids. As ensemble methodologies become more widely applied, traditional deterministic realizations will give way to statistical representations of plume evolution. It will be critical that the end user understand the difference between deterministic and probabilistic results and the subsequent effect on consequence management.

As emphasized in chapter 2, users do not understand, and do not care to learn about, mathematically expressed statements of "uncertainty." As important as those statements may be to the researcher-developer, they are difficult for most decision makers to understand and use constructively. They are even unlikely to be interpreted correctly by the person running the model in a real-life situation, unless that individual has an exceptional level of expertise and understanding.

In short, the ATD modeling system is not an operational tool for consequence assessment tasks until the end users know how to use it correctly. There is an experiential base on which to build, with both positive and negative cases from which to draw lessons.

The efforts to learn how best to make uncertainty information useful to the users of ATD modeling predictions must take into account the three time frames for model use identified in chapter 2: first response (first hour), intermediate response/recovery, and long-term planning/recovery. Research is needed on how to give each user category results that those users can work with effectively. From the discussion in chapter 2, here are just a few preliminary and general distinctions that are likely to be important:

- The most important information for the first responder is knowing what the hazard is and how to deal with it. Details of how the ATD modeler (whoever is running the model) got to the results and the mathematical uncertainties in the predictions are largely irrelevant. However, ways in which the uncertainties in the prediction could affect the response are important. These implications need to be communicated in terms relevant to immediate response decisions.
- In the recovery phase, accountability for each step from the beginning to the end of the modeling activity is necessary.
- Planners may want, and may be able to use in their larger planning, model predictions stated probabilistically.

ATD test beds, an essential ingredient in the R&D strategy (section 5.6), provide the infrastructure where users, developers, and researchers can interact. Users are there to be trained to use the new products and information in their activities. Planners can even use test beds as an integral and essential part of scenario building and what-if analyses (gaming) for preparedness planning. The developers and researchers get to see how users respond, what they need, and where they have difficulty with products in development. These types of activities validate the usefulness of the ATD modeling activity.

Independent, external consensus standards for evaluating modeling systems and tools (section 5.4) also play a major role in interpreting uncertainty for users. Such standards will:

- Build user confidence in products;
- Provide a science-based evaluation process for ATD products; and
- Provide a mediation/facilitation role in dialogue between developers and users on what is needed to do the job.

User training and the development of reach-back capability should be complementary activities. The effective integration of reach-back capability with tool dissemination to users is an intrinsic aspect of R&D, not just a post-R&D training issue. The National Atmospheric Release Advisory Center (NARAC) currently provides a national capability for training and reach-back in the context of incidents of national significance. Analogous training and reach-back support should be extended, perhaps through regional modeling centers, to incidents not at the nationally significant level, such as hazardous material spills. Reach-back capability for levels below incidents of national significance need ongoing coordination among existing infrastructure components, such as the NOAA/ NWS Weather Forecast Offices and regional ATD modeling centers.

5.3 Capture and Use Existing Data Sets

There are a number of existing high-quality ATD data sets from field research studies, which were conducted on terrain conditions ranging from very simple to very complex. The effects of hilly or mountainous terrain on winds and temperature have been studied for decades in the United States and abroad. Significant advances in understanding and predictive capability have evolved from this work. Many of the field studies sponsored by the U.S. Government used tracers, which makes the data potentially useful for testing and improving both meteorological models and ATD models.

Many of these data sets, which were initially used to develop or test parameterizations for ATD models, can yield additional, valuable results on concentration uncertainty. They are the only current source of data for this purpose. New analyses, using tools developed since the studies were first done, can glean useful insights from the high-quality data sets. For instance, data sets that were treated with deterministic models when the studies were done can be re-evaluated with improved representations of the physical processes, including probabilistic models that incorporate stochastic representations of aleatory uncertainties. Many of the issues now recognized as important for meeting user needs—such as short-term fluctuations in concentration and fuller quantification of uncertainties—were not major objectives at the time the studies were done. For example, in past experiments tracers were used to estimate time-averaged concentrations, not short-term fluctuations. In some instances, the data sets were not thoroughly analyzed initially because of agency-funding limitations. Appendix A includes a partial annotated list of the past studies known to the JAG members to have data sets with substantial untapped potential for further analysis.

One shortcoming of the data sets in their current condition is that they are housed in different laboratories and stored in different formats. The available data sets should be put into a format that allows the ATD research community to access and use them easily. For example, the Atmospheric Studies in Complex Terrain (ASCOT) program was sponsored by the Department of Energy (DOE) and conducted from the late 1970s to the early 1990s. The ASCOT data were stored at whichever DOE national laboratory was leading the field effort in that year. Data sets were collected at the Argonne, Lawrence Livermore, Los Alamos, and Pacific Northwest national laboratories, and probably elsewhere. Efforts are underway to collect and archive the ASCOT data sets.

It will be far more cost-effective to archive and re-analyze these data sets than to repeat the underlying field studies at great expense. (In fact, data capture, reanalysis, and preparation of the data in accessible format could be a good opportunity for graduate student research and/or employment.) The data capture activities should include transferring the experimental data and associated metadata into an electronic format that provides ease of access for analysts. For many of the studies listed in Appendix A, the effort should also include gleaning undocumented details and contextual information about the studies from the memories and expertise of the personnel who performed them.

Several of the longer range transport studies are already incorporated in NOAA's Data Archive and Tracer Experiments and Methodology (DATEM).[1] This archive may provide a framework for future archival activities.

For several of these valuable data sets, work is already underway to perform additional analyses. Several simulations of the Prairie Grass field experiments have been done using more recent modeling approaches (Irwin et al. 2003; Hanna et al. 1990; Irwin 1984). The Metropolitan Tracer Experiment (METREX) data (Draxler 1985) have been re-examined in some DCNet modeling efforts.

While some important cities and industrial facilities are located near mountains or in hilly terrain, much of the Nation's population and critical infrastructure are located near ocean coastlines or near large lakes. A modest number of field studies that collected both meteorological and tracer data within coastal zones have been conducted, usually for specific purposes such as testing and refining models of rocket effluent plumes. The data are often not as detailed as desired because it was difficult to make detailed measurements over large bodies of water, especially measurements aloft. Nevertheless, these data sets have value as a starting point for research on ATD in coastal urban environments.

Reanalysis of these data sets can provide insights for designing test bed experiments (section 5.6), optimizing observational network design (section 5.5.2), and for special studies (section 5.7). This would allow more rapid progress toward improving ATD modeling system products.

In terms of cost/benefit ratio, capitalizing on existing field data sets should be a top priority. With a modest level of effort, substantial short-term gains can be realized from these analyses in quantifying the uncertainty in existing ATD models and products. As discussed above, the strategy is time-sensitive with respect to providing input to the implementation of ATD test beds, planning for additional special studies, and capturing undocumented information about the past experiments while those who conducted them remain available.

5.4 Foster Evaluation Standards for Modeling Systems and Components

For this report, the term "performance evaluation" means ascertaining, as objectively as possible, how well a meteorological, ATD, or air quality modeling system is performing the tasks for which it was designed or used. The evaluation of model performance is essential to providing users with reliability measures and modelers with standard methods for assessing potential improvements. Various review groups have concluded that there is

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[1] For further information on DATEM, see the Internet homepage: http://www.arl.noaa.gov/datem/.

a need to develop a common process for development of "consensus-based" evaluation procedures and metrics (OFCM 2002, NRC 2003, Dabberdt et al. 2004). Models simulate only a portion of the natural variability, thus their operational tasks are limited by the assumptions made in the construction of the model and the physical processes that are characterized. Differences between what is predicted and what is observed result from a combination of errors in model formulation (which can lead to systematic biases), propagation of measurement and input uncertainties (which can be amplified due to nonlinear effects), and the fact that nature contains more variability than do the models.

The *Standard Guide for the Statistical Evaluation of Atmospheric Dispersion Model Performance,* ASTM D 6589 (2000), provides a framework for describing how observations and predictions differ. This standard employs the concept of ensembles, which in reality are imperfectly known. Ideally, one would compare the observed and predicted ensemble averages to objectively characterize any systematic bias in the model's predictions. This approach has had some success for evaluation of short-range dispersion models by sorting observations into pseudo-ensembles, but much work remains to be done.

Because uncertainties propagate forward in a prediction model, it is helpful to assess performance in a "front to back" sequence. For instance, the performance of the air quality/concentration model is dictated to a certain extent by any uncertainties in the characterization of the meteorology. The transport and diffusion of the emissions is based on the stated meteorological conditions. Often a portion of the emission specification (e.g., the dependence of surface spill evaporation on temperature and wind speed) is based on the representation of the meteorological conditions. Certain chemical processes are strongly influenced by the presence of and dynamics within clouds.

After reviewing the state of practice, the JAG concluded that standardized "physics-based" evaluation metrics are needed. Current skill scores and evaluation methods ignore the fact that the frequency distributions of the observations and predictions are inherently different; they have different sources of variation, as explained in ASTM D 6589 (2000). Thus, the JAG does not recommend attempting to catalogue and make use of current skill scores, as they have limited value, and then only if one realizes that seemingly correct predictions can be attained through a combination of offsetting errors. More sophisticated physics-based metrics would allow objective statistical tests to be made of whether differences in the results produced from various models should be deemed significant. From such statistical comparisons, measures of success can be developed.

Different user needs will likely require different ways of evaluating model performance. Nevertheless, evaluation of all ATD models will have many common points of concern. The Federal agencies should agree on meeting this need for common model performance methods and metrics through a group under the aegis of an SDO. (An example is ASTM International, Committee D22, which has already developed ASTM D 6589.)

This approach to standards development is consistent with, and perhaps required by, Public Law 104-113.[2] In addition, other considerations favor development of ATD model performance standards by a standing committee of technical experts from a variety of disciplines. The SDOs have proven systems for developing technical standards. If information is needed, they can hold technical symposia to address specific concerns. If experts from various disciplines are needed, an SDO has a vast resource of experts within its technical committees for consultation. SDOs routinely review existing standards for needed updates. A standing SDO committee can provide continuity in methods development under the standard. Perhaps most important, development of a standard by an SDO carries the cachet necessary for public acceptance.

With a view toward development of model evaluation methods, the JAG anticipates that the variety of user needs will provide fertile ground for development of a variety of performance metrics and methods tailored to specific user requirements. Furthermore, advances in modeling capabilities (e.g., models that provide a quantitative prediction of the distribution of possible individual outcomes) will place ever-increasing demands for development of new performance metrics tailored to specific user needs. In these dynamic conditions, a one-time definition of a set of performance metrics will not serve a useful purpose. A standing committee can provide continuity in standards development, acquire expertise over time, and leverage lessons learned to meet new demands over time.

Further work is also needed on performance standards for instruments to detect and measure hazardous airborne species, particularly hazardous gases. Although essential to consequence assessment systems for those hazards, this need is beyond the scope of this JAG's expertise and terms of reference. There are, however, other committees and working groups already established that can address these needs.

5.5 Coordinate Programs for Improved Measurement Technologies

Advances in all scientific endeavors come from the interaction of theory, model, and measurements. The measurement instruments to provide data for multiscale ATD modeling or for quantifying model uncertainties at the scales of interest to the users of ATD model predictions are scarce, and their use is far from routine. New and improved

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[2] On March 7, 1996, President Clinton signed into law *The National Technology Transfer and Advancement Act of 1995*. This law, codified as Public Law 104-113, serves to continue the policy changes initiated in the 1980s under Office of Management and Budget (OMB) Circular A-119, *Federal Participation in the Development and Use of Voluntary Standards,* which are effecting the transition of the Executive branch of the Federal Government from a developer of internal standards to a customer of external standards. Section 12 of Public Law 104-113, Standards Conformity, states that "… all Federal agencies and departments shall use technical standards (defined as 'performance-based or design-specific technical specifications and related management systems practices') that are developed and adopted by voluntary consensus standards bodies, using such technical standards as a means to carry out policy objectives or activities determined by the agencies and departments." Public Law 104-113 further states that "… Federal agencies and departments shall consult with voluntary, private sector, consensus standards bodies, and shall … participate with such bodies in the development of technical standards."

measurement techniques will add substantially to the development of theory and models appropriate for ATD user applications. Many parts of the modeling process need a variety of data types—for example, wind velocity, temperature, and flux data—so a variety of instrument types and capabilities are needed.

The instrument development process often requires a long lead time: typically a decade or more from prototype development to a fielded system. However, to overcome barriers and shortcomings in ATD modeling and its use within the time frame set by national priorities, this development lead time must be shortened. In both the near term and longer term, the focus should be on developing instruments that, once their capabilities are demonstrated, can be used routinely in the ATD test beds and in special studies of ATD modeling issues. In the near term, the emphasis should be on incorporating and extending existing technologies. Development of a nationwide system, akin to the WSR-88D NEXRAD system, remains a vision for the future.

The current trend toward compact, low-cost units closely networked into distributed systems is an appealing model for ATD instrumentation. An example is a distributed, compact phased-array Doppler radar system that is under development at the University of Massachusetts. Its key advantages are low cost, low maintenance, compact size, and connectivity. These features enable a network to be scaled to appropriate sizes and therefore widely applicable.

New instrument development should focus on the R&D problems identified earlier in this report (e.g., chapter 3 and section 4.3): initial conditions, boundary conditions, closing the modeling gap from microscale to mesoscale, and improving tracer capabilities. Both remote and in situ measurement technologies are likely to be used. The remote technologies may employ active sensors (e.g., radar or lidar) or passive sensing (e.g., radiometric techniques) from platforms on the ground or aloft (carried on aircraft or satellites). One can expect that new system developments will use concurrent advances in digital signal processing to extract data at a high rate and with sufficient resolution. These systems will provide on-board processing and communicate information to the appropriate users—modelers, data assimilators, or emergency responders.

5.5.1 Tracers

Improved tracer capabilities are essential to progress in ATD modeling. Without an effective tracer technology for routine measurement of controlled or otherwise known releases, evaluation of ATD model concentrations—their uncertainty, their time averages, their variance, their intermittency—cannot be achieved. The task of identifying a suitable tracer, as discussed in section 4.3.1, is interwoven with the tasks of developing in situ and remote-sensing capabilities. Tracer selection must consider the measurement capability, as well as the measurement and diffusion properties of the hazards the tracer will represent.

5.5.2 Meteorological Data

The meteorological data of principal interest are in the ABL—the least measured part of the ATD-modeled atmosphere. The ABL is essentially the connecting layer between the large scale flows above it and the land or water surface beneath it. It includes the fine-scale flows affected by surface conditions.

Some near-term gains can be achieved by extending the capabilities of cutting-edge technologies to improve temporal and spatial resolution of wind field measurements. In particular, the capabilities of WSR-88D (NEXRAD) radars to measure winds and retrieve temperature profiles in clear air need to be explored. Doppler LIDAR systems are resolving boundary-layer wind fields and aerosol features within the modeling scale gap. Measurements of boundary-layer height and wind profiles above 100 m are currently available with 915 MHz radar wind profilers at widely scattered locations. Their vertical resolution may be increased by using new techniques under development at NOAA's Environmental Technology Laboratory. However, the spatial variability of the wind profile is poorly captured by these systems. Adding mobility to eye-safe Doppler lidar measurements by placing them on aircraft, as suggested in a National Research Council report (NRC 2003), can expand the capability for area coverage, especially for emergency response to hazardous material ATD. Networking of smaller, more compact systems also promises greater capability.

Measurement of the temperature distributions horizontally and vertically at meso-gamma scales to microscales is important for understanding ABL processes, especially in transitional and stable conditions. The temperature (density) structure governs the buoyancy of the atmosphere. These conditions are particularly important for ATD near the ground because density currents can control local flows even in simple terrain, while momentum and kinetic energy from a low-altitude jet (30–100 m AGL) may also be driving near-surface processes. Horizontal thermal gradients define the urban heat island and drive mesoscale and microscale circulations by differential heating (sea breezes, mountain breezes), which affects local transport and diffusion.

The spatial variability of the temperature field would be a longer-term goal of a coordinated measurement program to support ATD modeling. Currently, most vertical temperature profile measurements are made in situ using balloons or kites to lift the sensors through the ABL. This process is labor-intensive and provides observations representative of only a small part of the atmosphere. Although current remote radiometric measurement techniques can produce local temperature profiles, they resolve the horizontal variability poorly, if at all. In most cases, the measurements using existing instrumentation have insufficient sampling rate and fidelity to compute heat flux profiles. High-resolution remote measurements of temperature profiles in the lowest 200 m of the atmosphere—comparable to in situ measurements on a meteorological tower—would provide major advantages for understanding processes at the surface and in near-surface layers. Raman scattering of selected electromagnetic frequencies is another promising remote-sensing technique still in early stages of development.

For the meteorological component of ATD modeling, atmospheric moisture needs to be measured with precision comparable to that of temperature measurements. Differential absorption lidar systems have been used to measure water vapor along lines of sight and within scan volumes. This technology needs further exploration and, if warranted, development for ATD and other ABL-sensing applications.

Measurement systems of the future need not be confined to the sensor technologies available today. Innovation in design and implementation of sensing systems must be actively encouraged and pursued. The atmosphere affects acoustic and electromagnetic propagation in ways that vary with the frequency of the wave phenomenon and the atmospheric conditions. Just as radar meteorology developed from the observation that clouds interfere with radar detection of aircraft, new sensing technologies for the future require critical thinking now about ways to acquire knowledge of atmospheric state variables from this “noise” in signals propagating through the atmosphere. From this perspective, a program for advancing measurement technology to support ATD modeling is highly dependent upon the sensor development community—in Federal laboratories, small business, industry, and academia—and is not confined to the meteorological community.

5.5.3 Implementation

Many Federal agencies and the National Science Foundation have existing programs to develop research instrumentation related to the atmospheric sciences. The DoD University Research Instrumentation Program provides for purchase of existing equipment or parts to make new sensor systems. Most agencies sponsor SBIR and STTR programs, which can provide substantial funding to move proof-of-concept and prototype systems toward commercial development. Coordinated efforts among the agencies are required to leverage their instrumentation opportunities to support ATD R&D.

5.6 Establish Multiple ATD Test Beds

For the purposes of this report, an ATD test bed is an infrastructure of atmospheric instruments including, as a minimum, an array of tower-mounted meteorological sensors capable of continuous observations. These observations should include not only measurements of the standard meteorological properties but also eddy fluxes of heat, moisture, and momentum. However, the JAG considers the type of test bed installation recommended in this report to be far more than a simple monitoring network. First, the test bed should provide a location and infrastructure to support the short-term deployment of other instrument systems, which could be ground-based, airborne, or satellite-based. Second an ATD test bed must have strategically located remote probing systems to yield wind speed and direction profiles, extending through the planetary boundary layer. Third, the test bed’s instrumentation should be tested and upgraded as developments dictate. Fourth, and most important, the observation data should be routinely scrutinized to improve the understanding of the wind, temperature, tracer, and turbulence fields (both horizontally and vertically) across and above the region encompassed by the test bed. Because of the importance that the JAG attaches to this element of the R&D strategy, a full discussion of several aspects of test bed implementation and operations are included below.

These basic requisites for an ATD test bed derive from the major reasons for implementing and sustaining a test bed infrastructure and operational capabilities. Section 5.6.1 presents the reasons related to meeting R&D needs detailed in chapter 4. Additional reasons for the test bed strategy, presented in section 5.6.2, relate to the critical work of transitioning existing and forthcoming ATD products into operations, as discussed in section 3.3.

While test beds are most often mentioned in connection with cities, an ATD test bed need not be limited to an urban environment. Section 5.6.3 presents the rationale for implementing a number (but not all) of the test beds in urban environments. Section 5.6.4 compiles requirements for effective implementation of multiple test beds, consistent with the strategy proposed here. Finally, section 5.6.5 notes some key management issues that must be addressed, if this strategy is to achieve its potential gains cost-effectively.

5.6.1 R&D to be Supported by ATD Test Beds

As a tool for R&D, test beds enable benchmarking of options for ATD modeling systems and components in specific applications and conditions (the ATD environment of the test bed location). The data from the test bed, whether by itself or supplemented by short-duration intensive studies, can be used to test and refine predictive models. Results from test beds can be used in validating ATD modeling systems and components and as input to decisions on selecting, refining, and extending the modeling system and products to improve their suitability for specific consequence assessment needs. The experimental data from test beds also provide feedback to fundamental research on ATD processes and conceptual model improvement.

As a permanently installed measurement system with supporting infrastructure and resources, a test bed can produce all-season, all-weather, 24-hour quantitative data on local environmental conditions. This capability is critical for broadening ATD modeling system performance evaluations beyond fair weather conditions and for establishing the historical base for ensemble forecasting. For R&D to improve ATD models, instrumentation is needed that can measure concentrations as a function of time and distance from release point (e.g., through use of tracers or surrogates), as well as measuring air transport and diffusion parameters.

Short-term deployments of additional instrument systems at a test bed, to supplement its fixed monitoring infrastructure, are useful both for testing new instrument systems and for advancing the understanding of ATD processes and factors at that location. Short-term deployments of remote-sensing systems, for example, can be used to update databases of surface-land interactions needed for microscale predictions even after the remote-sensing instruments are removed. Land cover, building location and spatial relationships, surface roughness, surface thermal variation, ultraviolet light intensity in open spaces, and urban canyon morphology, as well as other urban characteristics of importance to ATD models, can be derived from remotely sensed data and incorporated into the data infrastructure of the test bed.

After review and discussion, the JAG concluded that the best way to get the data needed to feed better stochastic models is to have test beds where measurements can be made over time, under the full range of meteorological conditions that can occur at a site of interest. Test beds are the best way to produce the measurements and parameterizations needed to characterize uncertainties. They can support R&D on quantifying uncertainty, such as ensemble techniques and Monte Carlo simulations, as well as R&D on probabilistic models (models that incorporate stochastic representations of the physical processes controlling transport and diffusion).

Because of the substantial level of effort and duration of investment needed to sustain not just one but multiple test beds, the benefits this strategy can provide relative to other field study approaches is worth consideration. Among the many merits of this strategy, the following are particularly significant:

- Test beds are necessary to support the long-term measurement of atmospheric processes in urban airsheds and the archiving of the measurement data with associated ATD modeling results.
- A well-instrumented, well-characterized test bed is an excellent tool for testing, evaluating, and incorporating measurement innovations in operational settings. An even better tool is to have multiple test beds, representing a range of complex environments (particularly urban environments), in which the strengths and limitations of various measurement innovations and approaches can be compared across environments.
- Test beds are excellent tools for research on data QA/QC and data assimilation techniques.
    - The permanence of test beds makes them uniquely well suited for R&D to improve the assimilation of surface-based, satellite-based, and airborne remote-sensing data into the mesoscale meteorological models that provide input to ATD modeling systems.
    - The strategy proposed here is consistent with test bed work by NASA and by NOAA on better methods of assimilating satellite data into regional meteorological models (for example, the WRF and Eta models), which are often used to feed ATD models.
- Test beds provide the infrastructure to encourage and support synergy and collaboration among developers working on different system components. (The DCNet installation provides a current example that should be encouraged and expanded.)
- Test beds provide the infrastructure and reproducibility needed to develop and test methodologies for optimizing observational network design in general and design for urban areas in particular. (Section 5.5.3 contains further discussion of optimizing observational networks.)

- A permanent test bed can be used to conduct experiments on "sources of opportunity," such as a benign but detectable emission from a point-source release. For urban environments, these opportunistic field studies can provide a cost-effective and pragmatic complement to planned experiments.

For all of these R&D functions, one needs an instrumented test bed with sufficient density of observations to provide ground truth for comparison with model predictions.

In addition to supporting R&D for ATD modeling, a test bed in an appropriate location can serve other R&D and operational objectives. Its monitoring infrastructure can improve local weather forecasts and nowcasts by characterizing the local variability of temperatures and precipitation. The monitoring network could be used, for example, to determine specific locations within the test bed region where freezing conditions are present, or whether an expected sea breeze front has propagated through the area. A test bed can also provide continuous support to air quality studies (essential nowadays in many urban areas) and provide assistance for emergency response when required.

Thus, the test bed capabilities proposed here can serve purposes other than increased understanding of ATD processes. This multiple use aspect may serve to increase the available funding through cost sharing and to add to the political support for the project. The multiple functions for an ATD test bed—particularly test beds located in densely populated areas—are important for sustaining the long-term (10 years or more) public and political support for the installation, without which the ATD modeling R&D cannot be fully achieved.

5.6.2 The Role of ATD Test Beds in Transitioning New Capability to Operations

Sections 2.6 and 3.3 make the argument that developers of ATD modeling systems must begin taking more responsibility for the successful transition of forecasts and related products into operations. The task of development is not complete until the new capability has been proven useful in operations. The JAG members agreed that test beds are probably the best approach for (1) bringing users into the development process early and (2) providing productive, ongoing interfaces between fundamental research, model development for application, and operational use of developed products. Particularly when located in densely populated regions, test beds provide the following benefits, which complement and support these R&D-relevant objectives:

- Test beds can accelerate user training in real environments.
- Test beds encourage sustained, repeated input and feedback from users.
- Test beds provide developers and governmental funding entities with a powerful tool for leveraging application support across diverse users and user communities.

As an example, test problems can be run at a test bed with users directly involved. The lessons learned from the exercises can be used by researcher-developers to refine the output the model must provide, if it is to meet those users' needs. The refined specifications for the output in turn define the modeling system's input data requirements. At the same time, all of the interactions with users help to educate them about the modeling system's output, including its measures of uncertainty and the implications of those measures for the users' decisions. Thus, the involvement of users in test bed exercises provides a training ground for emergency response personnel who can return to their response/preparedness roles and use the more sophisticated predictive results effectively when the improved products become operational.

5.6.3 Why Test Beds in Cities?

Stated simply, urban test beds are needed because that is where the need for properly performing consequence assessment systems (as defined in chapter 1) is greatest. In our larger urban areas, the population is at risk from increasing levels of hazardous aerosols and gases of many kinds, including urban pollutants that affect air quality. Many of these urban regions are also at risk from point- or line-source releases of CBRN hazards, unintended or deliberate. Test beds established in several cities will provide the data to improve the currently limited capability to forecast the ATD of airborne substances in urban areas, regardless of the substance in question.

As discussed in section 4.2.1, urban environments are complex with respect to factors affecting atmospheric transport. We need to develop and refine the capability to forecast the meteorological conditions of urban areas at the microscale relevant to reliable prediction of concentrations and exposure regimes downwind from source-term releases. The urgency of making progress in this area is intensified by the hard reality (discussed in chapters 3 and 4) that purely deterministic approaches fail to describe the range of possible outcomes necessary for emergency management decision making. This is especially true for environments characterized by deep street canyons, complex building morphology, and other land cover features that influence local wind conditions as much as, or more than, external meteorological conditions affect them. For the reasons discussed in section 4.2.4, coastal urban environments require special attention.

Locating a test bed in an urban area (or in a region of coverage that includes an urban area) also has the potential to leverage diverse interests into sustained support for the test bed. A test bed infrastructure, as well as the data and studies produced using the test bed, can support emergency preparedness planning. Using the test bed for disaster planning and response exercises conducted by municipal or regional authorities increases the developer–user interactions. As noted in the previous section, these interactions feed back into R&D efforts to develop products that are better suited to meet evolving user needs.

However, urban environments (or densely populated regions including suburban areas) are unlikely to provide coverage of all the environments of interest to all the consequence assessment communities described in chapter 2. Military operations, for example, or modeling of industrial accidents located away from population centers (such as transcontinental pipelines, nuclear power facilities, or military facilities) may be better served by an ATD test bed in a non-urban setting. (The special studies discussed in section 5.3 provide an option for covering some of these conditions.) The rationale for having a number of the ATD test beds in cities does not mean that all of them should be urban.

In summary, a number—and probably the majority—of the multiple test beds needed to implement this R&D strategy fully should be installed in high-priority urban regions. For a program of nationwide coverage sufficient for national interests, some of the test bed installations may not cover urban or even suburban regions. The siting decisions should reflect the objective of providing experimental coverage to test ATD modeling capabilities across the full range of environments in the Nation.

5.6.4 Requirements for Effective Test Bed Implementation

Test Bed Site Selection

The proposed ATD test bed strategy includes implementing multiple test beds. The number of installations must be adequate to represent the Nation's diverse environments, particularly urban environments in different meteorological regimes (air-land-water interactions and climatic patterns). For the strategy to be cost-effective, a limited set of ATD test bed sites must be carefully selected, representing the major climatic and meteorological regimes of the Nation.

The previous section explained the importance of siting a number of ATD test beds in urban areas or metropolitan regions. Another siting objective should be to locate several of the test beds in coastal or lakeshore urban locations. Previous studies near ocean coastlines and large lakes have been limited. Thus, an initial task in the test bed strategy will be to weigh these objectives, along with other factors such as the ability to leverage costs with other users, to determine the number and optimal locations for ATD test beds.

Baseline Capabilities of Each Testbed

As discussed above, the ATD infrastructure should aim to support R&D, the transition of products to operations, and local forecasting and air quality monitoring in urban areas. To accomplish these aims, each test bed installation needs the following capabilities:

- Operate and archive data continuously;
- Continually test and evaluate existing analysis techniques;
- Develop techniques for utilization of tracer sources of opportunity;
- Perform periodic, controlled tracer experiments in both simple and complex meteorological conditions; and
- Test and evaluate new measurement technologies and tracers.

Each test bed in the program must have adequate base instrumentation. There should be a baseline of instrumentation common to all the ATD test beds, to ensure that comparisons can be made across the different environments they cover. The lessons learned from one test bed installation should be used to optimize the installation of those that follow.

Involvement of User Communities

In line with the arguments for user involvement made in section 5.6.2, potential user communities for the test bed should be involved in installation planning from its early stages.

Long-Term Resource Commitment

Perhaps the most difficult requirement to fulfill—and one that must be addressed as part of the site selection process—is the provision of sufficient long-term funding to sustain implementation and operations over an extended period. For some of the R&D needs specified in chapter 4, a decade or more will be required to achieve the longer term results that the JAG has envisioned. The decision to proceed with a test bed program should be with full recognition of the commitment necessary to reap the potential return on investment. Periodic review and evaluation of R&D projects must be built into the test bed management approach to ensure that progress is being made and that the envisioned outcomes are still supportable.

Short-Term Gains

At the same time that many substantial results will come only from long-term efforts sustained over years, there will be valuable interim results and products from the test beds. One short-term gain will be the evaluation and comparison of alternative ATD modeling systems (and system component options deployed within one overall modeling system) under comparable conditions. Testing across multiple, comparably instrumented sites is essential for the ultimate goal of compiling a set of models fully evaluated for a defined set of scenarios. Appropriate selection of a model from this evaluated set can then be made for any of a wide range of applications important to users. The near-term results from evaluation of existing modeling capabilities will establish criteria for deciding what further R&D should be done for modeling and measurement systems and methods.

Partnering to Provide Sustained Support and Direction

Stable, long-term resource allocations from a single Federal agency or program are difficult to sustain over multiple years of budget appropriations and administration priorities without strong partnerships from within and outside the Federal sector. Partnering is also essential to ensure that users' needs at the local and regional levels continue to guide and inform each test bed's projects. The test bed program at the Federal level should provide mechanisms to involve state and local public entities as partners with Federal funding agencies, as well as engaging the academic R&D community. Public-private partnerships with mutually consistent long-term objectives should be encouraged.

Coordination across Test Bed Installations

The ATD test bed implementation program should require coordination across test bed installations to ensure that data are sharable and accessible. This coordination should include cross-installation activities and standards for data archiving, data access, and technical support to data users. There should also be coordination, where appropriate, with other atmospheric modeling efforts, including physical model facilities, modeling test beds for meteorological models, and air quality monitoring test beds for atmospheric chemistry and other air quality factors beyond transport and diffusion.

5.6.5 Test Bed Management Issues

This report does not recommend a particular management approach for ATD test beds. Implementing agencies and their partners will need to make decisions on a management structure based on a range of factors, many of which are beyond the scope of this report. However, there are some issues and concerns related to the program objectives presented in sections 5.6.1 through 5.6.4 that the selected management approach must be capable of handling.

For the proposed ATD test bed implementation strategy to be effective, long-term planning and continuity of direction are essential. The strategy also requires channels for communicating upcoming possibilities for collaboration and leveraging among interested parties on studies, test and evaluation programs, and operational training and exercises. One approach that is worth considering is to have a single executive director for a test bed installation (e.g., a test city), who would have a scientific/technical policy board for advice. However, the executive director would retain decision authority and responsibility for a coherent, productive, and sustainable program covering research, development, testing, and evaluation.

Program coordination and funding of test bed oversight functions by participating agencies could use any of several established mechanisms, such as competitive proposal solicitations. Existing contracting capabilities in the lead agency should be used as appropriate.

5.7 Plan and Conduct Special Studies and Experiments

In addition to a set of long-term test bed installations, special studies and experiments will be useful for particular purposes. These special studies would be field campaigns rather than sustained activities. A special study could be motivated by the requirement to address a specific, isolatable physical process, such as deposition or resuspension. It could be designed to explore transport and diffusion in a unique yet consequential environment, such as high-altitude droplet dispersion. Another rationale for a study could be to extend the utility of past field experiments (captured through the program element discussed in section 5.3) by relating historical data to current methodologies and instrument capabilities. A study could also be designed to extend recent test bed results to a broader range of conditions not covered by the set of operational test beds.

One example of an important physical process to be studied on a special basis is the resuspension of hazardous materials once they have deposited on surfaces through settling, precipitation scavenging, or sorption to local materials. Deposited aerosol particles may be resuspended by the direct action of the wind or by abrasion of the surface (by other particles, foot traffic, vehicles, surface treatment, and so on). Deposited chemical species that sorb to local particles may also be resuspended. Because resuspension depends on a suite of complex factors, including the particle and surface morphology, specific chemistry, and local fluid mechanical effects, resuspension models tend to be highly parameterized. In the absence of surface disturbance, resuspension rates decrease with time, hence resuspension is of greatest concern in the following cases:

- In the immediate short term after deposition;
- For highly toxic materials, where small resuspension rates could pose grave concern; or
- Where surfaces are likely to be disturbed, as during clean-up operations, normal urban operations, or large fluctuations in meteorological conditions such as a surface freeze followed by a quick thaw.

When winds shift, resuspension can lead to a secondary plume and deposition pattern. Studies are needed to explore and quantify the following issues: (1) What is the effect of changing meteorological conditions on resuspension, including wind gusts and temperature effects? (2) How can we best model urban and vehicular resuspension? (3) For disturbed conditions, on what time scale can surfaces be considered sufficiently clean? (4) When do sorbed chemical species resuspend, and are “dust flux” models sufficient to describe these effects? Resuspension can be studied in field experiments through secondary collections of the released species, after initial plume passage.

Special studies are also warranted for unique yet pertinent situations, such as high altitude releases, which have the potential to impact large populations. Field testing of a high altitude release would contribute to a better overall understanding of the risk and consequence associated with missile defense—an important national and homeland security topic. Previous studies of high altitude releases such as Cristal Mist (Diehl 1994; Kaman Sciences Corp. 1996) identified the importance of various high altitude processes, such as clear air turbulence, for predicting ATD and deposition. However, recent technological advances in remote-sensing and monitoring tools, notably lidar, could significantly improve upon earlier efforts. A carefully monitored and controlled meteorological study where stable droplets and/or particles are released at high altitude could be used to validate parameterizations of important processes associated with high altitude meteorology and dispersion. A possible field experiment would include the release of droplets/particles of different size (10 microns to 1 mm) and at different altitudes (above 1 km, above 10 km, above 20 km). The released droplets/particles could be carefully tracked and recorded as they settle and deposit over a large area. Depending on the altitude of release and droplet/particle size, the monitored area could be very large—potentially hundreds of square kilometers.

Repeating conditions of selected classic studies, but with new measurement technologies used alongside the old technologies, can increase the value of the old data sets by enabling cross-test comparability and longitudinal studies. Early field experiments were conducted within the then-available tracer and measurement technologies and with particular objectives. Results from these studies were used to develop, improve, or confirm ATD modeling assumptions and parameterizations. Recent significant advances in those capabilities offer the opportunity to revisit the classical field studies and evaluate and improve the parameterizations formulated in the classical arena. Reductions in uncertainty of models by the infusion of new technology can be quantified. Improved understanding of the earlier results may be possible. As an example, a large number of dispersion tests were conducted at Hanford, Washington, with zinc sulfide tracer particles, which have a high deposition rate. Comparative tests could enable data mining for the effects of deposition on the initial data and interpretation of field results (Doran and Horst 1985). In addition, certain meteorological parameters now understood to be crucial to transport and diffusion prediction, like surface heat flux and boundary-layer height, were not always documented in classic field studies. The results from the classic studies must be interpreted with estimates of these important parameters, introducing more variability and uncertainty than is necessary. If modern instrumentation and methods could be applied to the classic problems, a more complete set of measurements would result. This would provide a basis for improved characterization of transport and diffusion effects.

With respect to coverage of special situations, a permanent test bed facility cannot be established for every set of conditions of interest. The gaps can be filled in with one-time experiments that provide a basis for interpolating and/or extrapolating from test bed results and old data sets. Special studies and experiments can also focus on the roles of particular physical processes to improve process-specific parameterizations.

Test beds cannot cover all of the many challenges of ATD models. While urban domains are emphasized in this report, field campaigns in different circumstances will be needed to assess the multiscale properties of transport and diffusion. Some special studies may address terrain-driven and urban-driven flows, like the Department of Energy’s Vertical Transport and Mixing (VTMX) field study in 2000. Even after the initial study, the complex flows affecting lateral and vertical mixing in a stably stratified basin were not resolved. One conclusion of that study was the necessity for more temporally and spatially complete measurement of the sub-basin-scale motions near the ground and aloft.

One purpose of test beds is for routine, day-by-day investigations of ATD modeling capability and evaluation. On occasion, special one-of-a-kind studies will be needed to address particularly difficult modeling performance issues. Within the framework of a test bed, additional instrumentation may supplement the test bed’s usual instrumentation suite to conduct a major field campaign. Such studies would be based on specific science objectives.

Special studies can also be used outside the framework of the established test bed installations to address specific questions and issues. The greater understanding gained from a carefully designed special study could advance the theory and practice of atmospheric modeling. As an example, many individual field programs have examined components of the diurnal cycle for modeling mesoscale features. This field study produced a set of insightful science questions and issues, which are summarized in the following list, developed at the VTMX workshop in September 2002.

Issue 1. The performance of mesoscale numerical models in describing the wind, temperature, and turbulent structure of the valley atmosphere was mixed.

- Basic flow patterns and temperature fields were captured, but …
    - the timing of important events (e.g., flow reversals) was often off by one or more hours, and
    - details of the flows over certain segments of the valley were in error (e.g., jet structure, flow strength).
- The vertical temperature structure showed persistent biases, which are not yet understood.
- The agreement between modeled and observed turbulent heat fluxes and turbulent kinetic energy was unsatisfactory.

Issue 2. Aspects of radiational heating and cooling in valleys do not seem to be adequately accounted for in numerical models. For example, extreme cooling is observed in sinkholes.

- Can this behavior be explained and modeled?
- How relevant is this phenomenon to larger-scale valleys and basins?

Issue 3. Wavelike features and ascending or descending layers of air were common along the side walls and may be common elsewhere. Their significance for vertical transport and mixing is unclear.

- What is actually happening during these events?
- What causes them?
- Is there any hope that they can be modeled or predicted?
- Does it matter?

Issue 4. LES and DNS look promising, but can they deliver useful improvements in parameterizations for mesoscale models?

- How can we generalize from highly idealized modeling conditions to the real world?
- What insights into the basic physics of stable atmospheres can be gained?

This list does not exhaust all of the questions and issues that special studies could address, but it does reflect current questions, results, and issues that have arisen in the context of the VTMX program and other recent field studies.

6.0 RECOMMENDATIONS

The R&D elements presented in chapter 5 will require a robust, coordinated effort by the multiple Federal agencies engaged in research, development, or application of ATD modeling systems. No one agency holds all the capabilities needed to affect the recommended course of action. Shared responsibilities, shared vision, and shared resources are essential to success. Without the resource base and sustained direction that a well-coordinated Federal effort can provide, the R&D needs cannot be met within time horizons consistent with national policy priorities.

In this chapter, the JAG presents nine recommendations, covering implementation efforts in seven areas:

- Quantify model uncertainties and interpret their implications to users;
- Capture and use existing data sets;
- Implement ATD test beds,
- Develop standards for evaluating modeling system performance;
- Improve the spatial and temporal scale interactions between meteorological and ATD models;
- Improve measurement technologies; and
- Design and conduct special studies and experiments.

Implementing these recommendations will require sustaining the effort over more than a decade. Some of the actions can be accomplished and will produce returns in the near term: within the next 2 years. Other actions will provide interim benefits at intervals along the way, even though the most significant benefits may require a decade or longer for realization. A paragraph on timing considerations follows each recommendation below.

Many of the capability limitations identified in this report are systemic, resulting from a lack of coordinated effort across agency R&D programs aimed at understanding and modeling the fundamental drivers of ATD processes, such as boundary-layer processes. Coordinated efforts are also needed to develop capabilities to measure the spatial and temporal variability of the most changeable part of the atmosphere at the resolution required for ATD predictions. These limitations can be surmounted, but success will require commitment and coordination of resources and facilities. Particularly important are the human resources residing in dedicated teams with strong operational and science motivations.

6.1 Quantify Model Uncertainties and Interpret Their Implications to Users

The JAG views the two recommendations in this section as together forming the keystone for delivering vastly more useful ATD modeling products as operational tools for the user communities described in Chapter 2. The remaining recommendations define enabling science and technology to achieve the full potential of these keystone recommendations.

6.1.1 Improve ATD Modeling Systems to Routinely Quantify Uncertainties

As explained in chapter 2, most of what users need from the ATD modeling system embedded in their consequence assessment system comes down to predicting airborne concentrations of hazards as a function of space and time. To deal with the uncertainties in predicting these concentrations, the ATD model developer has a growing array of probabilistic techniques available. Yet, the users do not want mathematical expressions of uncertainty or probability; they want answers on which to base decisions and take action. The usual practice has been to give users point estimates of concentration, whether those estimates were derived from deterministic representations of the physical ATD processes or incorporated modeling of stochastic processes. However, the uncertainties in the data inputs to the ATD model, the approximate nature of the model constructs and parameterizations, and the stochastic nature of atmospheric turbulence all lead to uncertainties in individual realizations of a model. Quantifying these uncertainties is essential for two reasons. First, reducing the uncertainty through continued R&D requires knowing how much there is and how much each factor contributes to the uncertainty in the product. Second, the ATD modeling community must do better at interpreting the implications of the uncertainty in model predictions for the users of ATD modeling products.

Recommendation 1. ATD modeling systems should routinely quantify the uncertainties in their results. Implementation actions required for this recommendation include but are not limited to the following.

- Develop robust techniques to assess probabilities of occurrence of concentrations above significant threshold levels.
- Adapt (or develop) and verify measurement capabilities at or below the scales of interest for model predictions.
- Test, verify, and validate model improvements, including probabilistic methods of process representation, parameterization, and data acceptance/assimilation.
- Establish a shared data system with substantial sets of data to test and evaluate uncertainty quantification techniques.
- Develop techniques to quantify and reduce uncertainty in predictions through improved model–data interfaces, including but not limited to sensor fusion, data assimilation, and evaluation criteria.

- Develop analysis techniques that are applicable in nonlinear regimes to display important sources of uncertainty.
- Use the outcome from new techniques for estimating uncertainty to guide improvements in ATD models.
- Develop and implement processes for uncertainty displays in data-sparse environments.

Timing considerations for recommendation 1. Initial efforts to quantify uncertainty in current models, using existing databases, can begin immediately. At reasonable funding levels, 5 years will probably be required to conduct the necessary R&D on modeling methods and to improve measurement capabilities. Delays in starting or funding limitations will extend the time required. Some of the implementation actions listed for recommendation 1 will depend on progress in other actions in the list. For instance, techniques for estimating uncertainty that are applicable in nonlinear regimes will be needed before sources of uncertainty can be ranked in importance, as a guide to improving ATD models.

6.1.2 Effective Communication of Model Uncertainties to Users

To serve users better, the model development community must do two things differently. First, modeling systems must routinely quantify the various mathematical uncertainties in model results. Second, developers must find useful ways to communicate the practical import of these uncertainties to the users. For many of the applications discussed in chapter 2, users need to understand the impact on health and safety of concentration variability in space and time. For example, a model's predicted probability distribution for the concentration in an area of interest (hazard area) during a specified time interval might be represented as the probability that a meaningful health or safety threshold concentration will be exceeded. This way of presenting model results may be practical and useful for some types of users once they understand it. Other types of users may need or prefer a different representation of results.

Ongoing, sustained interaction between developers and users is the only way to determine which representations will work best for which users, while still adequately representing the uncertainty. For example, NASA has used product advisory boards, with members drawn from the state and local governments who are the customers (potential users) for remote-sensing data. The product advisory board participates throughout the product development process, commenting at critical milestones on the members' perceptions of the value of the emerging product.

Recommendation 2. The ATD modeling R&D community should work intensively and routinely with representative users to determine effective means of presenting information to users that incorporate the quantified uncertainties in model results. Implementation actions required for this recommendation include but are not limited to the following.

- Involve users in prototyping, testing, demonstration, and training sessions for probabilistic tools under development to determine which tools and representations are most useful and acceptable to specific user types and application contexts.
- Incorporate the feedback and advice from users on the utility of representations of probability and/or measures of uncertainty into the ATD model R&D process.
- As a requirement for the ATD test bed implementation proposed in recommendation 4, require planning and implementation with relevant user communities throughout the R&D programs conducted at a test bed facility.

Timing considerations for recommendation 2. Although current capabilities to quantify the uncertainties in ATD predictions are limited, *efforts to improve on current practices in interpreting uncertainty implications for users can and must start now*. Those in the ATD model R&D community who work with users in demonstration or training exercises should take every opportunity to seek "best practices" and innovative approaches that help users understand how to accommodate prediction uncertainties in their decision processes. The dialogue among model researcher-developers, modelers (those who run the models operationally), and users of the model predictions can start immediately.

6.2 Capture and Use Existing Data Sets

An abundance of data from previous field experiments exists in various forms and formats. The richness of these experimental data has not been fully exploited, particularly given advances in analytical techniques and new objectives of analysis since the experiments were conducted. These data sets constitute the nation's only current source of concentration data to quantify the uncertainty in ATD model predictions under actual atmospheric conditions. The studies were performed to achieve certain objectives, often related to air quality, such as estimating plume behavior in heterogeneous environments, transport and diffusion from elevated sources, or multi-state dispersion. They reflect a wide range of applications and learning conditions. However, few of these data sets have been analyzed using the probabilistic techniques now available.

These data and important unrecorded knowledge about the experiments from which they were collected are in danger of being lost to the R&D community with the aging of the experiments' designers and participants. Individual efforts to reanalyze these legacy data sets have occurred or are in progress. An immediate effort is needed to expand and coordinate the acquisition of the legacy data sets and supporting knowledge about the experiments, capture the data and supporting information in modern data files, and analyze the data using modern approaches and techniques. The OFCM, under FCMSSR instruction, could coordinate the multiagency effort needed. Appendix A describes a number of past experiments and demonstrations that this JAG views as important to capture and preserve. There may be others. Immediate action on these objectives is warranted because further work with these data sets using state-of-the-art and state-of-practice methods will aid in formulating initial estimates of the stochastic uncertainty in

ATD processes, designing ATD test beds, planning experiments for the test beds, and designing special studies and experiments.

A complementary objective to capturing and reanalyzing the legacy data sets is to increase their accessibility to the ATD modeling R&D community. For example, the OFCM could lead the effort to develop an XML standard for ATD-related data, taking into account any standards already developed or in progress for related types of data.

Recommendation 3. OFCM should convene an interagency effort to develop guidelines for acquisition, archiving, and access of data from previous field and laboratory ATD experiments. Implementation actions required for this recommendation include but are not limited to the following.

- Identify and communicate the reanalysis projects already completed or in progress.
- Prioritize the experiments and demonstrations from which data sets should be captured and preserved in accessible format.
- Adopt or adapt a data interchange standard as an archival format.

Timing considerations for recommendation 3. Data capture and archiving for the priority experiments can be completed in 3 years.

6.3 Implement ATD Test Beds

Multifunctional ATD test beds will support a variety of research, development, and product-transition activities required to fill existing gaps in meeting user needs. Among the activities enabled by ATD test beds are the following.

- Long-term measurement and archiving of measurement data on atmospheric processes and ATD modeling in urban airsheds;
- Accelerating iterative rounds of user input and feedback to implement recommendation 2;
- Accelerating user training in real environments (also essential to recommendation 2);
- Testing, evaluating, and incorporating measurement innovations;
- Developing techniques for using sources of opportunity (benign atmospheric releases, other than planned tracer studies, which can be detected and traced as they are dispersed downwind);
- Improving the assimilation of satellite-based and airborne remote-sensing data into the mesoscale meteorological models that provide input to ATD modeling systems;
- Fostering a coordinated approach to model–data interaction issues including but not limited to sensor fusion, data assimilation, and evaluation criteria;

- Providing all-season, all-weather, 24-hour quantitative data on local environmental conditions;
- Leveraging development efforts for users with diverse applications, such as weather nowcasts, air quality forecasts, public education and outreach, and transportation systems management; and
- Developing and testing methodologies for optimizing observational network design in general and network designs for urban areas in particular.

Because of the diversity of conditions across the United States and even among its major urban centers, the JAG assumes that multiple ATD test beds will be required. Urban locations are likely to predominate, but some nonurban settings will probably be appropriate as well. The sequencing and final number of test beds to be implemented and the appropriate types of locations for them should be initial tasks for an appropriately constituted body established by the stakeholder Federal agencies and referred to here as a joint (or multiagency) test bed authority. Coordination with parallel test bed development programs for atmospheric modeling goals (e.g., air quality and weather forecast modeling) is essential to ensure that the overall investment is cost-effective and efficient.

Recommendation 4. Participating Federal agencies, through the FCMSSR, should establish a multiagency test bed authority to oversee multiple test beds for urban and complex environments in locations selected on the basis of national and R&D priorities. This joint test bed authority should have authority to undertake the following actions:

- Assess the number of test beds required to meet research, development, and application transitioning needs for the Nation’s diverse environments. Implement those test beds consistent with these needs and overall resource constraints.
- Ensure that test bed implementation plans provide for adequate base instrumentation to achieve the intended research, development, and application objectives of the test bed.
- Incorporate user community feedback and advice on user training and technology transition activities at the test beds (supports recommendation 2).
- Coordinate solicitations for competitive proposals to use the test bed infrastructure funded through interagency memoranda of agreement or other mechanisms.
- Provide a point of contact for parties interested in using the test bed for experiments or projects supported by other means.
- Enter into and encourage partnerships with state and local entities, as well as public-private partnerships, for support and utilization of the test beds, in particular for technology transition and user training projects.
- Coordinate the ATD test bed implementation program with other atmospheric modeling test bed efforts.

- Establish and coordinate a program for sharing and archiving long-term measurement data across the ATD test beds, using the data interchange format or guidelines developed for recommendation 3.

Timing considerations for recommendation 4. Implementing and acquiring results from the ATD test beds are evolutionary efforts lasting for a decade and more. Embryonic test beds exist and could be brought up to the level of capability envisioned in this report. Plans for others are developing and must be actively nurtured.

6.4 Develop Standards for Evaluating Modeling System Performance

Accepted standards for evaluating modeling system performance are essential. This need can be met efficiently by the proven processes used by established voluntary standards development organizations such as ASTM International.

Recommendation 5. The OFCM should officially ask an existing standards development organization to establish and maintain a subcommittee to develop guidelines and standards for evaluating ATD modeling system performance. The Federal agencies involved in ATD research, development, or applications are encouraged to support this subcommittee.

Timing considerations for recommendation 5. A working group could be established within an existing consensus standards organization within 6 months. Release of an initial set of performance standards will require 2 to 3 years.

6.5 Improve the Spatial and Temporal Scale Interactions Between Meteorological and ATD Models

As described in section 4.2, there are gaps in model nesting or initialization capability that seriously affect the interactions between models at different spatial and temporal scales. The capability gaps in connecting top-down modeling from NWP-based meteorological models with bottom-up modeling approaches, such as physical modeling, CFD, or LES, are at the very spatial and temporal scales that have major impacts on consequence assessment applications, particularly applications for densely populated environments. One approach is to test and further refine the physical basis for sub-grid-scale parameterization in nested meteorological models. Other approaches to bridging this gap from the microscale or urban scale to mesoscale models should also be investigated.

Another area for improvement is characterization of surface boundary conditions at the three-dimensional spatial scales relevant to ATD modeling requirements in urban environments. Remote sensing from airborne or satellite assets will probably provide the data (see sections 6.6.1 and 6.6.3), but algorithms to test and correct the observation data set will be needed to attain the desired accuracy in model predictions.

Recommendation 6. The R&D communities in meteorological and ATD modeling should work together to conduct the research, development, and testing needed to address difficulties in interfacing models at different scales and to improve the capability of urban scale ATD modeling systems to handle fine-scale surface-atmosphere boundary conditions. Implementation actions include but are not limited to the following.

- Test and refine the physical basis for sub-grid-scale parameterizations. This will be the outcome of the bottom-up approach of using physical models and CFD and LES.
- Explore innovative approaches for bridging the gap from microscale (urban scale) ATD features and events to mesoscale meteorological models.
- Better characterize surface boundary conditions at urban scale, including methods for obtaining, maintaining, and using up-to-date land cover data.
- Address the issues in model initialization, nesting, and data assimilation. This will be the outcome of the top-down approach.

Timing considerations for recommendation 6. No specific timing considerations for this recommendation were identified. However, progress on bridging the gap from microscale ATD features and events to mesoscale meteorological model results used as initialization and boundary data in ATD modeling is essential to reducing the uncertainties in ATD predictions.

6.6 Improve Measurement Technology

6.6.1 Coordinated Measurements Technology Development Program

Measurements provide the ground truth for models and theory, as well as the data for model initialization and bounding. For progress in theory and modeling and for understanding the uncertainty in model variables, measurements of concentrations and atmospheric variables must be made at or below the scales of interest. Test beds will not realize their full potential with point sensors alone. Capabilities to remotely sense meteorological fields of wind, turbulence, and moisture fluxes rapidly and volumetrically should be actively pursued and quickly incorporated into test beds for evaluation and utilization. Technology to rapidly sense induced tracers in situ and remotely is essential for test beds and for special experiments. Some sensing systems must be mobile, rather than fixed at one location. In emergency response applications, airborne or ground-transportable systems are highly desirable for plume tracking throughout the depth of the boundary layer and not just at ground level.

Avenues already in place for instrumentation R&D can be leveraged for ATD instrumentation development. Many Federal agencies have small business innovative research (SBIR) and/or small business technology transfer (STTR) programs. These could be used as vehicles for a multiagency approach to enlisting the resources of the private sector and the university research community in innovative instrumentation technology R&D. The “bench scientists” in the Federal laboratories have creative ideas and capabilities to develop new instrumentation providing these measurement capabilities.

Recommendation 7. A coordinated Federal ATD R&D program should develop or improve evolutionary and revolutionary atmospheric sensors supporting ATD R&D and then transition the technology into tools for ATD model researchers, developers, and users. This coordinated program for measurement technology should tap the expertise from across the public (including Federal laboratories), private, and academic sectors. Implementation actions required for this recommendation include but are not limited to the following.

- Identify potential tracer materials and determine the most useful combinations of tracer material and detection techniques to improve ATD models and quantify uncertainty.
- Develop and test new atmospheric measurement technology, including those using remote-sensing techniques for volumetric measurements.
- Coordinate measurement technology development with modeling R&D (see Recommendations 1 and 6) to address major model–data interface issues, including but not limited to sensor fusion, data assimilation, and evaluation criteria.

Timing considerations for recommendation 7. Timing and priorities among the suggested implementation actions should reflect dependency relationships with other ATD R&D activities. For example, a reliable and cost-effective means for collecting large amounts of tracer data is essential for characterizing and quantifying the uncertainty in ATD predictions. Therefore, an early start, with high priority, should be given to selecting potential tracer materials. This selection should be completed within 2 years because it will dictate the direction of development for point and volumetric techniques for tracer measurement. Engineering development to lower cost and enhance mobility of sensor networks relative to existing systems could, if initiated soon, be completed within 5 years. Development and test of new, innovative systems for meteorological measurements will be an ongoing process, continuing over a decade and more.

6.6.2 Instrument Siting and Networking

Guidelines for siting sensors for meteorological variables or processes have generally been developed for open environments. In the complexities of urban, coastal, or terrain environments, these guidelines can rarely be met. The existing criteria are suitable for their intended purpose of observations to support regional weather forecasting. However, in urban environments, there are multiple purposes that meteorological sensor systems can serve. The CFD modeling community may want time-sequenced data near buildings, as well as away from buildings, to discern circulation patterns. To ensure that consistent and reliable measurements are made at ATD test beds, performance guidelines need to be established for siting instrumentation in complex environments that take these multiple purposes into account. Given the rapid advance in instrumentation technologies and the variability from site to site in terrain and local meteorological characteristics (e.g., diurnal wind patterns, air-land-water circulation and heat transfer patterns), traditional, deterministic design requirements for instrument siting are unlikely to work well for the intended purposes. Functional guidelines, in terms of desired performance from an instrumented site, are more appropriate.

Recommendation 8. The OFCM should establish a working group, representing the Federal agencies involved in ATD research, development, or applications, to establish performance guidelines for ATD and meteorological instrumentation systems in complex environments. Implementation actions for this recommendation include but are not limited to developing and testing procedures for designing local observation networks and siting instrumentation in diverse, complex environments.

Timing considerations for recommendation 8. A working group can be established through the OFCM in 3 months. Release of draft instrumentation performance guidelines will require about a year after that. Test of the guidelines will follow as required.

6.7 Design and Conduct Special Studies and Experiments

Many of the classic field transport and diffusion experiments upon which our modeling parameters are based date back to the 1950s to 1970s. Since then, significant advances have occurred in measurement technology, computational capabilities, and modeling algorithms. Among these advances are major reductions in the averaging times for meteorological or tracer sampling. Turbulence and its spatial variability are better characterized and captured in model representations. The importance of boundary-layer scaling has been demonstrated.

Special field studies, replicating several of the classical studies, should be conducted with modern measurement technology. Such studies will improve the data foundation for model parameterization, assess the improvements in understanding gained from advances in science, and demonstrate the merits of new measurement technologies. Another reason for special studies is to provide an adjunct to the fixed test beds, allowing other environmental settings to be studied and to extend model testing and verification and validation (V&V) to these settings. A key ingredient for such studies is the ability to measure tracer concentrations remotely in four dimensions at high space-time resolution and meaningful concentrations.

Like the design of the ATD test beds, design of special studies and experiments conducted at non–test bed sites should be informed by the results of the data capture and reanalysis efforts recommended in section 6.2 (see recommendation 4). These special studies will also prove more fruitful after some of the measurement technology improvements recommended in section 6.5 are available for use in them. Given these prerequisites and the high priority of proceeding with test bed implementation, special studies and experiments are intermediate-term to longer-term needs (3 to 7 years).

Recommendation 9. The Federal agencies involved in ATD research, development, or applications should establish a working group to design and oversee the conduct of a series of classical experiments. The design and selection of these experiments should reflect the information gained by capturing existing data (recommendation 3) and complement the infrastructure of ATD modeling system test beds (recommendation 4). Among experiments that the working group should consider are the following:

- Characterize fundamental uncertainty (due to atmospheric turbulence) through highly instrumented testing under simplified conditions (a "Daughter of Prairie Grass" study but incorporating new technology).
- A regional-scale study (covering about 5000 km^2) of the diurnal evolution of tracer transport and diffusion in the ABL in terrain-forced flows should be achieved within a decade. Such a study should use newly developed tracer technology to enable surface and airborne multidimensional remote sensing of concentration, even between urban structures. Surface and airborne networked Doppler lidar systems with overlapping coverage could be used to measure winds, turbulence, and stratified aerosol layers. The study should include low-altitude temperature and turbulence measurements for turbulence fluxes and a network of other measurement systems designed and deployed for the study location.

Timing considerations for recommendation 9. At least 3 years will be needed before new experiments can be defined and designed, depending on progress in reanalyzing old data sets (recommendation 3) and improving measurement technologies (recommendations 7 and 8).

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Appendices

APPENDIX A. HISTORICAL PERSPECTIVE

A.1 Historical Perspective—Meteorological and ATD Modeling

When creating a roadmap for the future, it helps to understand the path that brought us to our present position. The earliest comprehensive effort by a Federal agency to predict the transport and diffusion of airborne particles for public safety purposes began in the 1940s. As the nuclear age emerged, it became apparent that "radioactive fallout was an exceedingly complex issue, involving extremely long range transport through the air and affecting all aspects of the environment."[1]

ATD modeling is generally classified into two subgroups: emergency-response and air quality predictions. Emergency-response forecasting focuses on situations where chemical, biological, or nuclear materials are unexpectedly emitted into the atmosphere and where the source is unknown or poorly described. Air quality forecasting focuses on the U.S. Environmental Protection Agency's (EPA's) criteria pollutants, such as ozone, particulate matter, nitrogen dioxide, carbon monoxide, sulfur dioxide, and lead.

A.1.1 Emergency Response Modeling

In 1948, the U.S. Weather Bureau—the predecessor of today's National Weather Service (NWS) in the National Oceanic and Atmospheric Administration (NOAA), established the Special Projects Section. This office was the forerunner of the Air Resources Laboratory (ARL), now in NOAA's Office of Oceanic and Atmospheric Research. The Special Projects Section was at first funded solely by the Department Of Defense (DOD). Later, it was funded jointly by the DOD and the Atomic Energy Commission (AEC), which was the predecessor of the Nuclear Regulatory Commission (NRC) and portions of the Department of Energy (DOE). The Special Projects Section conducted research related to the U.S. nuclear weapons and atomic energy programs. After a few years, it also provided operational services in support of these programs.

Also in 1948, the U.S. Weather Bureau established and jointly funded with the AEC two research stations at Oak Ridge, Tennessee, and Idaho Falls, Idaho. The Oak Ridge research station was established to study the processes of atmospheric diffusion and understand the dispersion characteristics of the Oak Ridge area. Several other agencies subsequently contributed funds to develop these research facilities into what is now the Atmospheric Turbulence and Diffusion Division of NOAA/ARL.

The AEC and the DOD began joint tests of nuclear weapons in 1951, in the southwest Great Basin, a desert region northwest of Las Vegas, Nevada. A majority of the early tests in this weapons program were atmospheric tests. They showed that a good understanding of the atmospheric environment was necessary to characterize the transport and fallout of airborne radioactive products of the test events. In 1956 the AEC

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[1] Excerpted from a historical sketch of the Air Resources Laboratory, on the Internet at www.arl.noaa.gov/history.html.

implemented an Interagency Agreement with the U.S. Weather Bureau to establish a Weather Bureau research station in Las Vegas: the predecessor to the NOAA/ARL Special Operations and Research Division (SORD). The primary function of this research station was to support AEC/DOD test operations by taking local surface and upper air weather observations, preparing weather and trajectory/fallout forecasts, and providing expert meteorological advice to event scientists. These functions continue today, as NOAA/ARL SORD supports DOE's National Nuclear Security Administration (NNSA) at the Nevada Test Site (NTS). By the 1970s, the Field Research Division of ARL, as it is now known, had successfully participated in many experiments, which successfully pioneered the use of tracer technology and data analysis techniques.

In 1973, the DOE Office of Biological and Environmental Research tasked the Atmospheric Sciences Group at Lawrence Livermore National Laboratory (LLNL) to investigate the feasibility of developing an end-to-end, fully integrated system to provide reliable and timely assessment advisories to emergency managers at DOE nuclear facilities in the event of an accidental release of radioactive material to the atmosphere. To characterize the source of the release, this system was designed to rely heavily on downwind measurements and analysis of isotopes. In 1972 the AEC recognized the need for real-time estimates of transport and diffusion (Knox et al. 1981). To meet this need, LLNL developed the Atmosphere Release Advisory Capability (ARAC), which includes an advanced, three-dimensional modeling system of pollutant dispersion and the communications capability to disseminate predictions from this modeling system to local officials (Dickerson and Orphan 1976; Lange 1978; Sherman 1978). A facility to exploit the ARAC, now known as the National Atmospheric Release Advisory Center (NARAC), was officially established in 1979 with funds from a number of agencies, including the DOE. Since its inception, NARAC has responded to a number of accidents including radiological releases at the Three Mile Island nuclear power station in Pennsylvania (Dickerson, Knox, and Orphan 1979) and at the Chernobyl nuclear power station in the USSR in 1986. In 1984, NARAC responded to the atmospheric release of a chemical hazard, methyl isocyanide, at a fertilizer manufacturing plant in Bhopal, India.

Several of the DOE National Laboratories have conducted research in ATD modeling and related research areas. Sandia National Laboratory, for example, has a long of history of source term development for accidents at nuclear power plants. In 2002 the DOE Chemical and Biological National Security Program (CBNP) established the Local Integration of the NARAC with Cities (LINC) program. The CBNP, along with LINC, was transferred to the Department of Homeland Security (DHS) in 2003. The DHS used LINC during the TOPOFF2 exercise in 2003 to demonstrate a capability to provide local government agencies with advanced operational atmospheric plume predictions. NOAA developed a gas and chemical modeling system called CAMEO/ALOHA in 1992 to assist local fire departments in assessing the impacts of accidental releases of hazardous chemicals (NOAA and EPA 1992). ("CAMEO/ALOHA" stands for "Computer-Aided Management of Emergency Operations/Areal Locations of Hazardous Atmospheres.").

DOD was one of the first Federal agencies to fund the development, testing, and application of ATD models. Military interest in ATD modeling originated in the 1940s from a need to quantify the downwind hazards resulting from the use of chemical and biological munitions, including accidental releases of chemical agents at U.S. Army storage depots. With the advent of liquid-fueled rockets in the 1950s, military requirements for ATD modeling expanded to include accidental releases during the transportation, storage, and handling of toxic liquid propellants. Prior to the 1970s, most of the empirical data on ATD came from field studies conducted by DOD organizations such as the Deseret Test Center, Dugway Proving Ground, and Air Force Cambridge Research Laboratory. These field studies included the landmark Prairie Grass (Barad 1958; Haugen 1959) and Ocean Breeze/Dry Gulch (Haugen and Fuquay 1963) experiments. DOD continues to be one of the principal Federal sponsors of ATD field studies, with recent examples including the Mock Urban Setting Test (MUST) (Biltoft 2001) and Joint Urban 2003, which was conducted in collaboration with DHS. During the past 50 years, the Army, Navy, Air Force, and several DOD agencies have developed a series of ATD models to meet specific military requirements. Capabilities from the three major DOD ATD modeling systems are currently being combined into a single Joint Effects Model (JEM) for operational use by all services.

The mandate of the Defense Threat Reduction Agency (DTRA) is to safeguard America's interests from weapons of mass destruction (chemical, biological, radiological, nuclear, and high explosives) by controlling and reducing the threat and providing quality tools and services for the warfighter. DTRA was created in 1998 as the successor to the Defense Special Weapons Agency, which in turn succeeded the Defense Nuclear Agency (DNA) in 1996.[2] In 1996, DTRA developed the Hazard Prediction and Assessment Capability (HPAC) modeling system to calculate the effects of releases of biological, chemical, and nuclear agents. The HPAC modeling systems uses SCIPUFF, a Lagrangian puff model, to simulate transport and diffusion (Sykes et al. 1996).

A.1.2 Air Quality Modeling

In 1955, in response to a request from the Air Pollution Unit of the U.S. Public Health Service (a predecessor of part of the EPA), the U.S. Weather Bureau formed an air pollution unit under its Special Projects Section. It also detailed specialists to the Public Health Service to provide user-appropriate and scientifically credible air quality meteorological programs to support regulatory applications. Significant data collection and analysis efforts in the 1950s and 1960s led to a better understanding of air pollution episodes and the atmosphere's controlling effect on air pollution (Heidorn 1978; Holzworth 1962). During this period, the Weather Bureau issued regional advisories of air pollution potential over the eastern United States (Niemeyer 1960; Boettger 1961) and municipal air quality agencies began to predict pollution on the local urban scale (e.g., Thuillier and Sandberg 1971).

In 1965, President Johnson formed the Environmental Sciences Services Administration (ESSA) from two longstanding Department of Commerce agencies: the Coast and Geodetic Survey (established by President Jefferson in 1807) and the Weather Bureau (established by Congress in 1891). In 1970, President Nixon combined ESSA with seven

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[2] In 1948 DOD established the Armed forces Special Weapons Project. This effort led to formation of the Defense Atomic Support Agency in 1959, which became the DNA in 1971.

other earth science programs to establish NOAA. By then, NOAA/ARL had five Divisions: Idaho Falls; Las Vegas; Oak Ridge; Washington, D.C.; and Research Triangle Park, North Carolina.[3] Also in 1970, President Nixon established the EPA. As part of the Clean Air Act Amendments of 1970 and 1977, the EPA focused on setting air quality standards and controlling pollution at its sources. The NOAA group assigned to support the EPA, now known as the Atmospheric Sciences Modeling Division (ASMD) of NOAA/ARL, serves as the primary vehicle through which EPA supports research efforts in air pollution meteorology and atmospheric modeling. ASMD conducts research activities in-house and through contract and cooperative agreements for the National Exposure Research Laboratory and other EPA groups. ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control programs mandated by the Clean Air Act to the EPA offices of Air Quality Planning and Standards, Research and Development, and Air and Radiation. It also supports EPA regional offices and various State and local agencies.

During the 1970s and 1980s, air quality agencies prepared pollution predictions using objective statistical methods that required forecasts of atmospheric conditions as input (Aron and Aron 1978; Aron 1980; McCutchan and Schroeder 1973). In the 1980s, State Implementation Plans became a regulatory method to control air pollution at its sources by demonstrating how states would reduce emissions to meet the National Ambient Air Quality Standards. Numerical Eulerian grid models were used to develop State Implementation Plans by simulating historical air pollution episodes and demonstrating the effect of future emissions reductions. These models employed diagnostic wind field models to interpolate available meteorological observations to a three-dimensional grid (Collett and Oduyemi 1997). By the 1980s, the diagnostic models could be replaced with prognostic models (Chang et al. 1987). As prognostic real-time mesoscale meteorological models have matured, the air quality community has begun coupling them with air quality models, either keeping separate (offline) software for chemistry and meteorology (Vaughan et al. 2002; Hogrefe et al. 2001; Jakobs et al. 2001; McHenry et al. 2001) or using an integrated (online) approach (Grell et al. 2000).

Air chemistry models describe the fate and transport of atmospheric chemical constituents in both the gas and the aerosol phases. They now track about 100 chemical species, interacting through mechanisms involving hundreds of chemical reactions. Because of the important role that aerosols play in radiative transfer, weather, and health impacts, most air quality models now include detailed descriptions of aerosol dynamics and calculate size-resolved aerosol composition, radiances, and photolysis rates interactively with the cloud and aerosol fields. With today's computational power and efficiencies, air chemistry models can simulate pollution distributions in urban air sheds with spatial resolution of a few kilometers or they can cover the globe with horizontal grid spacing of less than 100 kilometers. These models are able to provide quantitative information on the distributions of many of the atmosphere's key trace gases and aerosols. Air chemistry models have become an essential element in atmospheric

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[3] The ARL Cincinnati Office was moved to Research Triangle Park, North Carolina in 1969 specifically to provide support to the EPA.

chemistry studies. They also provide science-based input for decision makers locally, nationally, and globally.

Although meteorological and chemical processes are strongly coupled, until recently the chemical processes in air quality modeling systems were usually treated off line from the meteorological model, as in EPA's Community Multiscale Air Quality modeling system, whose output provided the transport function (Byun and Ching 1999). This type of system is usually termed a chemical transport model (CTM). In the newer online approach there is no CTM; the chemical processes are represented within the meteorological model. The online approach has a number of potential advantages for air quality forecasting, such as better characterization of the time-resolved dispersion of air pollutants.

Within the context of mesoscale meteorological modeling, the Weather Research and Forecasting (WRF) model is being developed cooperatively by many government laboratories and universities led primarily by the NOAA, the National Center for Atmospheric Research (NCAR), DOD, and the Federal Aviation Administration. The WRF model is well suited to become the cornerstone for a next-generation air quality prediction system.[4] This model, currently under development, is nonhydrostatic, with several dynamic cores as well as many choices for physical parameterizations to represent processes that cannot be resolved by the model. This flexibility allows the model to be applied on many scales. A first version of an online WRF-based air quality prediction system for ozone prediction already exists (http://box.mmm.ucar.edu/wrf/WG11); the chemical modules are based on the online MM5/chemistry model (Grell et al. 2000). The official future release of this model (planned for 2005) will include many additional chemical modules from other air quality prediction systems and a choice of offline coupling.

A.2 Field Studies

This section lists and summarizes ATD field studies that could prove useful for supporting future ATD research initiatives. The list is not exhaustive; it represents those studies that the JAG members considered to be of greatest potential value for ongoing R&D efforts, as discussed in chapters 5 and 6.

A.2.1 Point Source Dispersion Experiments

Dispersion of Near-Surface Releases

1. **Round Hill** was conducted in 1954/55 and 1957 using sulfur dioxide tracer (Cramer, Record, and Vaughan 1958). Ten-minute samples were measured for sulfur dioxide along three arcs (50, 100, and 200 m) downwind of a point source release. The release height for the 29 experiments in 1954/55 was 30 cm; the release height for the 10

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[4] Background information on the WRF model and the latest applications and development news can be found on the Internet at http://wrf-model.org/.

experiments in 1957 was 50 cm. Receptor height was 2 m. Site roughness was greater than 10 cm. A unique feature of the 1957 experiments was that sampling was conducted for the first 0.5 min and 3-min of the 10-minute sampling periods.

2. **Project Prairie Grass** was conducted in 1956 with sulfur dioxide tracer (Barad 1958; Haugen 1959). It included 68 ten-minute samples taken at 1.5 m intervals along five arcs (50, 100, 200, 400, and 800 m) downwind from a point source release of sulfur dioxide 46 cm above ground. The 20-minute releases were conducted during July and August of 1956, with an equal number of cases run during the daytime and nighttime. Sampling was done during the 10-minute period in the middle of the 20-minute release. Site roughness was 0.6 to 0.9 cm.

3. **Green Glow** was conducted in 1959 with zinc sulfide tracer (Fuquay, Simpson, and Hinds 1964; Nickola 1977). Thirty-minute samples of zinc sulfide were taken along six arcs (200, 800, 1600, 3200, 12,800, and 25,600 m) downwind from a point source release 2.5 m above ground. Receptor height was 1.5 m. Site roughness was 3 cm.

4. **Hanford-30** was conducted in 1960–1961 with zinc sulfide (Fuquay, Simpson and Hinds 1964; Nickola 1977). Zinc sulfide samples were collected at 20 to 75 minutes along five arcs (200, 800, 1600, 3200, 12,800 m) downwind from a point source release 2.5 m above ground. Receptor height was 1.5 m. Site roughness was 3 cm.

5. **Dry Gulch** ws conducted in 1961–1962 with zinc sulfide (Haugen and Fuquay 1963). Thirty-minute samples of zinc sulfide were collected along five arcs (853, 1500, 2301, 4715, and 5665 m) downwind of a point source release 2 to 3 m above ground. Receptor height was 1.5 m. The terrain was sloping mesa cut by deep ravines; vegetation was mainly grasses with occasional brush and trees.

6. **Ocean Breeze** was conducted in 1961–1962 with zinc sulfide (Haugen and Fuquay 1963). Thirty-minute samples of zinc sulfide were collected along three arcs (1200, 2400 and 4800 m) downwind of a point source release 2 to 3 m above ground. Receptor height was 1.5 m. The terrain was rolling sand dunes covered with dense palmetto and brushwood.

7. **Hanford-67** was conducted in 1963–1973 with zinc sulfide, fluorescein, rhodamine B, and krypton-85 tracers (Nickola 1977). Ten-minute and 30-minute samples of zinc sulfide, fluorescein (uranine), rhodamine B, and krypton 85 were collected along eight arcs (from 200 to 12800 m) downwind of a point source release, mostly at 2 m with several at 1 m. Receptor height was 1.5 m. Site roughness was 3 cm. There were 23 experiments, most using dual tracers, including 14 with releases at both 2 and 26 m.

8. **Mountain Iron** was conducted in 1967 with zinc sulfide tracer (Hinds and Nickola 1967; Hinds 1968). Several 5 minute, but mostly 30 minute samples of zinc sulfide tracer were collected along arcs ranging from 260 m to 11.4 km from a 2 m point source release. The experiment site was rugged rolling terrain near the central California coast.

9. **Hanford-83** was conducted in 1983 with sulfur hexafluoride tracer (Doran and Horst 1985). Thirty-minute samples were collected for zinc sulfide and sulfur hexafluoride, which were jointly released from a point source 2 m above ground. Six experiments were run, with sampling at 1.5 m above ground and along five arcs ranging from 100 to 3200 m downwind. Site roughness was 3 cm. These experiments were conducted at the same site as the Green Glow, Hanford-30, and Hanford-67 experiments and had the objective of better characterizing the deposition properties of zinc sulfide.

10. **MADONA** was conducted in 1992 with sulfur hexafluoride and propylene gas tracers (Cionco et al. 1999). The multination Meteorology and Diffusion over Non-Uniform Areas (MADONA) field study was conducted at Porton Down, Salisbury, Wiltshire, United Kingdom. MADONA combined high-resolution meteorological data collection with diffusion experiments using smoke, sulfur hexafluoride, and propylene gas during unstable, neutral, and stable atmospheric conditions. The objective was to obtain terrain-influenced meteorological fields, dispersion, and concentration fluctuation measurements using specialized sensors and tracer generators. Thirty-one days of meteorological data were collected during the period September 7 through October 7, 1992. Twenty-seven diffusion experiments were conducted from September 14–23, 1992. Puffs and plumes of smoke and sulfur hexafluoride were released simultaneously for most of the experiments. This well-documented database is suitable for the evaluation and validation of short-range wind field and ATD models. The database was originally placed on CD-ROM in a structured way by the Chemical and Biological Defence Establishment, Porton Down. This database is now available from the Riso National Laboratory, Denmark, at <http://www/risoe.dk/vea-madona/ndescribtion.htm>.

Dispersion of Elevated Releases–Rural, Simple Terrain

1. **Hanford-67** was conducted in 1963-1973 with zinc sulfide, fluorescein, rhodamine B, and krypton-85 tracers (Nickola 1977). Ten-minute and 30-minute samples of zinc sulfide, fluorescein, rhodamine B, and krypton-85 were collected along eight arcs (from 200 to 12,800 m) downwind from a point source release. Receptor height was 1.5 m. Site roughness was 3 cm. There were 46 releases at 26 m and 20 releases at 56 m. There also were releases at 111 m, but no meteorological data are available for these cases.

2. **Cabauw** was conducted in 1977–1978 using sulfur hexafluoride tracer (Nieuwstadt and van Duuren 1979). In a series of 15 experiments, sulfur hexafluoride tracer was released at either 800 m or 200 m, with sampling at 1.5 m above ground along a single arc that ranged downwind from 3 to 5 km (depending on wind direction). Sampling was for two consecutive 30 minute periods. Site roughness varied from 10 to 20 cm, depending on wind direction.

3. **Kincaid** was conducted in 1980–1981 using sulfur hexafluoride tracer (Bowne et al. 1983). The sulfur hexafluoride tracer experiments conducted at Kincaid involved a release from a 183 m stack with a buoyant plume rise on the order of 200 m. There were 171 experiments conducted during April, May, and August of 1980 and May

and June of 1981. Measurements were made of near-surface hourly concentrations and hourly meteorology. There were twelve roughly defined receptor arcs ranging from 0.5 to 50 km from the release.

4. **Teruel** was conducted in 1985 with sulfur hexafluoride tracer (Sivertsen and Irwin 1987, 1996). Ten experiments were conducted in which sulfur hexafluoride was released from the 343 m stack of the 1200 MW Teruel coal-fired electric power plant. Two consecutive 15-minute samples were collected 1.5 m above ground along three arcs at approximately 10, 24, and 48 km from the stack. The plant is located 600 m above sea level on the southern side of the Ebro valley, midway between Madrid and Barcelona. Site roughness was estimated to be about 30 cm. A key objective of these experiments was to characterize the decrease in the transport speed (and thus the increase in the transport time) as the plume flowed toward the coast and into the strong sea breeze.

Dispersion of Elevated Releases–Rural, Complex Terrain

1. **Cinder Cone Butte** was conducted in 1980 using sulfur hexafluoride tracer (Snyder et al. 1985). During the autumn of 1980, 18 nighttime or early morning 8-hour tracer experiments were conducted at the 100-meter high hill at Cinder Cone Butte, which is near Boise, Idaho. The main tracer was sulfur hexafluoride; Freon 1381 was also used in ten experiments. Sampling was conducted with a network of approximately 100 samplers located on the slopes of the hill.

2. **Hogback Ridge** was conducted in 1982 using sulfur hexafluoride tracer and Freon 1381 (Snyder et al. 1985). In October 1982, 11 nighttime or early morning 8-hour tracer experiments were conducted along an approximately 1.5-km section of the 90 m high Hogback Ridge near Farmington, New Mexico. A network of 110 samplers located on the slopes of the ridge collected samples of sulfur hexafluoride and Freon 1381.

3. **Tracy Power Plant** was conducted in 1984 using sulfur hexafluoride tracer (Snyder et al. 1985). A feasibility study was conducted in November 1983, with a full-scale study in August 1984, at the Tracy Power Plant, which is located about 27 km east of Reno, Nevada. The site is located in the Truckee River Valley, with mountains surrounding the power plant on all sides. Peaks as high as 460 m above the stack base afforded opportunities for plume impaction in many directions. The power plant was maintained in warm standby condition as sulfur hexafluoride was injected in the base of the 91.4 m smokestack. The feasibility study consisted of 10 experiments during November 7–19, 1983, for a total of 90 hours of sampling at a network of 53 samplers. The full-scale study consisted of 14 experiments during August 8–27, 1984, for a total of 128 hours of data collection at a network of 110 samplers, mainly during late evening or early morning hours.

4. **ASCOT Studies**. Beginning with an exploratory field study in The Geysers geothermal region north of San Francisco, California, in 1979, the DOE funded a multi-year multi-organization study of ATD in complex terrain. The work included

both multiple tracers (sulfur hexafluoride, several perfluorocarbons, and other materials) and detailed micrometeorological measurements using both point and remote-sensing instruments. From 1979 to 1982, this work centered on valleys and basins astride the California coastal range. The emphasis then shifted for several years to a complex of simple individual valleys in the oil shale region north of Grand Junction, Colorado. Interest then shifted to the Front Range of the Rocky Mountains, near the DOE's Rocky Flats facility northwest of Denver. A field study was also performed in the ridge valley terrain of eastern Tennessee, which is typical of many areas near the Appalachian Mountains. Funding for ASCOT ended in the early 1990s.

5. **Model Validation Study.** Because of tightened limits on human exposures to the products of both normal and abnormal rocket launches at the Cape Canaveral Air Station and Vandenberg Air Force Base ranges, the Rocket Exhaust Effluent Dispersion Model, which was used to predict concentrations from launches, was leading to too many weather-induced launch delays. In hopes of reducing the number of expensive launch delays while still protecting public health, the Air Force funded a series of transport and diffusion studies at the two sites in 1995 and 1996. To simulate the elevated releases expected from a rocket, a blimp was used to release sulfur hexafluoride tracer. Near-ground releases were also used. An extensive network of time-integrating samplers and a small network of mobile fast-response samplers mounted in vans were used to measure ground-level concentrations. Fast-response analyzers were also mounted in two Global Positioning System (GPS)–equipped light airplanes to measure concentrations aloft. Both launch ranges have extensive meteorological systems in place. These were supplemented by point and remote-sensing instrument systems. Three 3-week seasonally spaced studies were performed at Cape Canaveral Air Station; one study was conducted at Vandenberg Air Force Base. Although the Cape Canaveral area is flat, the site is considered complex terrain because of the land–water contrasts and the wide range of land types. Vandenberg is in the midst of quite complex terrain. Both sites are subject to land–sea circulations.

Point Source Releases in Urban Terrain

1. **St. Louis** was conducted from 1963 to 1965 using sulfur dioxide tracer (McElroy and Pooler 1968). From the spring of 1963 to the spring of 1965, 26 daytime and 16 evening experiments were conducted involving 1-hour releases of zinc sulfide from two site locations (Forest Park and a rooftop release from the Knights of Columbus Building). Sampling (total dose) was conducted typically along three arcs that ranged from 1 to 7 km from the release site, with a few cases having an arc at 15 km. The initial lateral dispersion was estimated at 50 to 60 m (length of a typical city block, 160 m, divided by 4.3), with larger values when the wind was diagonally across the block. The initial vertical dispersion was estimated at 20 to 30 m. The authors concluded that dispersion from low-level sources in urban areas for downwind distances of less than 800 m is conjectural.

2. **Copenhagen** was conducted in 1978–1979 using sulfur hexafluoride tracer (Gryning and Lyck 1984, 2002). This series of ten tracer experiments in the Copenhagen area was carried out under neutral and unstable atmospheric conditions. The sulfur

hexafluoride tracer was released without buoyancy from a tower at a height of 115 m and sampled at 2–3 m above ground level on up to three crosswind arcs at 2–6 km from the point of release. Three consecutive 20-minute averaged tracer concentrations were measured, allowing for a total sampling time of 1 hour. The site was mainly residential, having a roughness length of 0.6 m. The meteorological measurements performed during the experiments included standard measurements at multiple heights on the tower of tracer release, as well as three-dimensional wind velocity fluctuations at the height of release.

3. **METREX**. During all of 1983, fluorocarbon tracer was released at several locations around the Washington, D.C., beltway as part of the Metropolitan Experiment (Draxler 1985). The scale of this experiment, which was larger in both space and time than most urban studies, was intended to test dispersion models over the long term. Some supplementary meteorological data were collected in addition to the usual information from the sites around and within the Washington, D.C., metropolitan area.

4. **Indianapolis** was conducted in 1985 using sulfur hexafluoride. (Murray and Bowne 1988). Sulfur hexafluoride was released from an 84 m stack with buoyant plume rise. There were 170 experiments conducted during September and October of 1985, with measurements of near-surface hourly concentrations and hourly meteorology. Measurements were taken along twelve roughly defined arcs ranging from 0.2 to 12 km from the release.

5. **Lillestrom** was conducted in the town of Lillestrom (near Oslo), Norway, in 1987 using sulfur hexafluoride tracer (Haugsbakk and Tonnesen 1989). The experiments took place in a flat residential area with buildings and trees ranging from 6 to 10 m in height. The surface roughness was about 0.5 m. Sulfur hexafluoride was released from a mast 36 m above the ground. Near-surface samples were collected along three arcs for two sequential 15-minute periods. The crosswind tracer concentration profiles were well determined for all trials, enabling a relatively accurate estimate of crosswind-integrated concentration. The temperature during the tracer experiments was low (approximately -20° C), and the ground was snow-covered.

6. **Kit Fox** was conducted during late August and early September 1995. A "billboard" (flat plate) obstacle array was set up in the desert at Frenchman Flats at the Nevada Test Site. Local roughness was enhanced with a much larger array of much smaller obstacles. Carbon dioxide was used as the somewhat dense gaseous tracer, and an array of instruments provided horizontal and vertical meteorological measurements. The test is well documented and would make a good addition to a national archive.

7. **URBAN/VTMX** was conducted in 2000 with sulfur hexafluoride tracer (documentation at <http://urban.llnl.gov/experiment.html> and <http://www.pnl.gov/vtmx/>). The URBAN 2000 experiment, which was conducted during October 2–25, 2000, consisted of six intensive observation periods with nighttime releases of sulfur hexafluoride in downtown Salt Lake City, Utah. During this same period, the Vertical Transport and Mixing (VTMX) meteorological field

measurement program took take place in the Salt Lake Valley. VTMX was designed to study the processes contributing to vertical transport and mixing of momentum, heat, and water vapor in the lowest few thousand feet of the atmosphere. The Salt Lake Valley was chosen as the study site because the surrounding mountains often contribute to the development of cold pools (i.e., conditions in which colder air is trapped in the valley while warmer air is found at higher elevations). Vertical transport and mixing processes in these conditions can be particularly difficult to describe. Flows over the mountains and out of the canyons, as well as winds generated by the temperature contrasts between the Great Salt Lake and the valley floor, may generate wind shear and atmospheric waves. These phenomena can in turn modify the vertical structure of the atmosphere.

8. The **Mock Urban Settings Test (MUST)** was conducted during September 10–27, 2001, at the Dugway Proving Ground in Utah using propylene as the tracer (Biltoft 2001; Biltoft, Yee, and Jones 2002). A mock building array was created by placing shipping containers in a 10 x 12 regular aligned grid. Each shipping container was 12.2 m wide, 2.42 m deep, and 2.54 m high. They were aligned with the long face perpendicular to the prevailing nighttime drainage winds and daytime upslope winds. The plan area density of the array was 13 percent and the height-to-width ratio was 0.2, the latter indicative of the isolated roughness flow regime. Tracer gas puffs or plumes were released from positions within or immediately upwind of the MUST array. Tracer dispersion through the array was measured using fast-response photoionization detectors. A 32 m tower and several 6 m towers within the MUST array provided vertical sampling, while four sampling lines of photoionization detectors provided lateral dispersion information. Sixty-eight usable trial events, consisting of 63 continuous releases and 5 sets of puff releases, were completed during MUST, providing 16 hours of continuous release data and 4.75 hours of puff data for analysis.

9. **BUBBLE** was conducted in 2002 using sulfur hexafluoride tracer (Gryning et al. 2003). Between June 15 and July 12, 2002, a series of four experiments were conducted in Basel, Switzerland. Sulfur hexafluoride was released approximately 1.5 m above the rooftops with rooftop sampling at 12 locations distributed close to the release and extending out to about 1.6 km. The mean building height in the area was 15.1 meters, and the mean plan area density was 48 percent. Each experiment provided six 30-minute samples, starting at approximately 1400 LST. The aim was to perform the tracer experiments under Clara Wind conditions, a thermally-driven wind system that develops over Basel in the afternoon on cloud-free summer days and is characterized by persistent winds from the northwest.

10. The **Joint Urban 2003** Field Experiment was conducted in Oklahoma City, Oklahoma, during July 2003 (Halvorson et. al. 2004; <http://ju2003.pnl.gov/study.html>). Its focus was characterizing the flow of sulfur hexafluoride tracer gas in an urban environment. More than 150 government, university, and private sector participants supported high-resolution atmospheric measurements and other instrumentation during the experiment. The field program consisted of six daytime and four nighttime intensive observation periods, each lasting approximately eight

hours and typically including four puff releases and three 30-minute releases. The Joint Urban 2003 database (approximately 3 terabytes) is maintained by Dugway Proving Ground.

A.2.2 Possible Urban Testbeds

1. NOAA/ARL implemented a dispersion measurement testbed, **DCNet**, in the Washington, D.C., area to provide the best possible basis for dispersion computations needed for both planning and possible response.

2. The Brookhaven National Laboratory's Environmental Measurements Laboratory initiated the **Urban Atmospheric Observatory** in 2003 to establish a dense array of meteorological instrumentation, remote-sensing and satellite products, and model output, as well as radiation detection (gamma spectrometer) and aerosol measurements in a small area in the heart of downtown Manhattan in New York City.

A.2.3 Long Range Transport Studies

1. The **Atlantic Coast Unique Regional Atmospheric Tracer Experiment (ACURATE-82/83)**, which was conducted in 1982 and 1983, consisted of measuring the krypton-85 air concentrations from emissions of the Savannah River Plant in South Carolina (Heffter, Schubert, and Meade 1984). For 19 months from March 9, 1982, to September 30, 1983, 12- and 24-hour average air concentrations were collected at five locations along the United States east coast at distances of 300 to 1000 km from the plant (Fayetteville, North Carolina, to Murray Hill, New Jersey). Measurements were made of hourly krypton-85 emissions from the plant (in curies) and of air concentrations (in picocuries per cubic meter). Ambient background concentration at each measurement station was subtracted from measured concentrations. Background varied by latitude, increasing to the north due to the prevalence of nuclear fuel reprocessing in the northern latitudes.

2. The **Across North America Tracer Experiment of 1987 (ANATEX-87)** consisted of 66 perfluorocarbon tracer releases (33 each from two different locations) every 2.5 days from January 5 to March 26, 1987 (Draxler and Heffter 1989). Air samples were collected for 24-hour periods continuing over 3 months (January 5 to March 29) at 75 sites covering most of the eastern United States and southeastern Canada. Perfluorotrimethylcyclohexane was released from the site at Glasgow, Montana. Perfluorodimethylcyclohexane and perfluoromonomethylcyclohexane were released from the site at St. Cloud, Minnesota. Release units are recorded in grams; air concentrations were recorded in picograms per cubic meter. The two tracers released from the St. Cloud site were released at the same time and therefore do not provide any meteorologically independent data.

3. The **Cross Appalachian Tracer Experiment (CAPTEX-83)** was conducted during September and October of 1983 (Ferber et al. 1986). It consisted of six 3-hour releases of perfluorocarbon tracer, four from Dayton, Ohio, and two from Sudbury, Ontario, Canada. Samples were collected at 84 sites 300 to 800 km from the source as

3- and 6-hour averages for about 48 hours after each release. One additional short (30 minutes) tracer release from Dayton was not evident in the sampling data.

4. The **Idaho National Engineering Laboratory releases in 1974 (INEL74)** consisted of about two months of krypton-85 releases, from February 27 to May 5, 1974, with continuous 12-hour sampling from February 27 to May 4, 1974, at 11 locations in a line about 1500 km downwind (Oklahoma City, Oklahoma, to Minneapolis, Minnesota). The same ambient background concentration (13.7 pCi/m^3) was subtracted from all stations (Ferber et al. 1977, Draxler 1982).

5. The **Oklahoma City 1980 experiment (OKC80)** was a single release of two different perfluorocarbon tracers on July 8, 1980, over a 3-hour period (Ferber et al. 1981). From July 8 to July 11, 1980, 3-hour samples were collected at 10 sites 100 km downwind and at 35 sites 600 km downwind from the Oklahoma City release point.

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APPENDIX B. FEDERAL CAPABILITIES AND RESEARCH AND DEVELOPMENT PROGRAMS

The dispersion modeling and consequence assessment capabilities of Federal departments and agencies are described below. Programs and activities of the Departments of Commerce, Defense, Energy, and Homeland Security are covered, as are programs in the National Aeronautics and Space Administration (NASA) and the U.S. Environmental Protection Agency (EPA). The information on programs presented here was current as of September 2004. Program details are subject to change.

B.1 U.S. Department of Commerce, National Oceanic and Atmospheric Administration

Within the context of atmospheric dispersion modeling, the National Oceanic and Atmospheric Administration (NOAA) is the principal supporting agency for atmospheric forecasts. NOAA provides meteorological and other products tailored for response applications. In partnership with the EPA, NOAA provides the dominant first-responders' dispersion model capability, the CAMEO/ALOHA modeling system, which is now in use by 10,000 to 20,000 emergency responders nationwide. NOAA provides dispersion forecasts based on the Nation's operational domestic mesoscale weather data and prediction models, both routinely (four times daily for selected sites) and on an around-the-clock on-demand basis. Through its 122 Weather Forecast Offices, NOAA provides weather and dispersion forecasts nationwide. Through its Realtime Environmental Applications and Display System (READY), it provides the dispersion forecasting capability that is a central element of the emergency systems of a large number of States and other emergency response organizations.

NOAA provides forecasts of dispersion for international applications through its role as one of seven international sources recognized by the World Meteorological Organization. The other Regional Specialized Meteorology Centers for dispersion are located in Canada, Australia, Russia, England, France, and China. The NOAA modeling system is used by Australia and China.

NOAA is a principal sponsor of the Weather Research and Forecasting (WRF) model. The WRF model is being developed as a collaborative effort among the Mesoscale and Microscale Meteorology Division of the National Center for Atmospheric Research (NCAR), the Environmental Modeling Center of the NOAA National Centers for Environmental Prediction (NCEP), the Forecast Research Division of the NOAA Forecast Systems Laboratory, the Air Force Weather Agency (AFWA) in the Department of Defense (DOD), the Federal Aviation Administration, the Center for the Analysis and Prediction of Storms at the University of Oklahoma, and other university-based scientists.

B.2 U.S. Department of Defense

B.2.1 U.S. Northern Command

The mission of the DOD is to provide the military forces needed to deter war and to protect the security of the United States. Within the DOD, the U.S. Northern Command (NORTHCOM) is the lead activity for homeland defense.

NORTHCOM plans, organizes, and executes homeland defense and civil support missions. Specifically, it will conduct operations to deter, prevent, and defeat threats and aggression aimed at the United States, its territories, and interests within its assigned area of responsibility. As directed by the President or Secretary of Defense, NORTHCOM provides military assistance to civil authorities, including consequence management operations.

Under NORTHCOM is the Joint Task Force for Civil Support (JTF-CS). The mission of JTF-CS is to provide command and control for DOD forces deployed in support of the Department of Homeland Security, Federal Emergency Management Agency (DHS/FEMA) to save lives, prevent injury, and provide temporary critical life support. DHS/FEMA is responsible for managing the consequences of a chemical, biological, radiological, nuclear or high-yield explosive (CBRNE) incident in the United States or its territories and possessions. As part of DOD's overall effort in support of the Terrorism Incident Annex added to the Federal Response Plan in 1997, JTF-CS is prepared to respond to requests for assistance from the lead Federal agency (LFA) following a CBRNE incident. When approved by the Secretary of Defense, JTF-CS supports the LFA in charge of consequence management—most likely DHS/FEMA.

B.2.2. Defense Threat Reduction Agency

The Defense Threat Reduction Agency (DTRA) safeguards America's interests from CBRNE used as weapons of mass destruction (WMD) by controlling and reducing the threat and providing quality tools and reach-back services for the warfighter and first responders in the event of a terrorist attack or hazardous material release. In an incident, DTRA will be asked by the LFA to participate in all National Special Security Events.

DTRA Operational and Analytical Support

DTRA provides operational and analytical support to the DOD and other organizations for critical WMD defense and response to related catastrophic events. Dispersion modeling and consequence assessment capabilities are an important element of this support. DTRA provides scientific and physics-based software tools that are easily deployed on a laptop personal computer. As part of its suite of consequence analysis tools, DTRA supports the user with on-demand meteorological data servers that provide real-time and forecasted four-dimensional weather, terrain, and land-use data from NOAA, U.S. Air Force and Navy, DTRA, Air Force Combat Climatology Center, and NCAR. DTRA supplies the research and development, training, and technical support needed for automated software systems to accurately predict the effects of hazardous material releases into the atmosphere and their impact on civilian and military populations. The agency also supports emergency response for matters involving WMD events through the use of deployable Consequence Management Advisory Teams (CMATs), a 24-hour, 7-day-per week (24/7) continuous operations center, and technical reach-back support. Technical reach-back support, through the 24/7 Operations Center, provides DTRA assistance to user's with immediate CBRNE response and consequence management needs. DTRA's active development program is bringing new software tools to the user, providing decision support information consistent with operational concepts integrated vertically across all echelons in a Common Operating Picture environment. All these tools are available in a web-based, collaborative, net-meeting-type, geographical information system (GIS) environment for the use of operators, warfighters, and first responders. DTRA has a proven record of transitioning research and development software tools for operational use.

DTRA Research and Development Programs By Topic Area

Hazard Prediction and Assessment. DTRA's Hazard Prediction and Assessment Capability (HPAC) program relies on various types of weather products to support transport and diffusion calculations and corresponding hazard predictions. Currently, DTRA provides three types of weather analyses in real time to its HPAC users: historical weather, observations, and forecasts. In addition to providing the HPAC user community with 24/7 operational meteorological data, the DTRA meteorology program is engaged in basic and applied atmospheric R&D to further improve its hazard assessment tools.

Numeric Weather Prediction (NWP). DTRA provides NWP data to its customers from various models with grid resolutions from as coarse as 80 km to as fine as 1 km. For applications such as collateral effects from large nuclear strikes, coarse global-scale data suffice to characterize the fallout pattern over regional areas. At the other extreme, a chemical attack on a city or in a populated open area requires knowledge of the wind flow at resolutions corresponding to the local terrain: typically on the order of a few kilometers. Therefore, DTRA conducts basic research to improve NWP capabilities in general with particular emphasis on advances that can improve high-resolution modeling.

Current research efforts funded by DTRA include expanding the capacity of mesoscale models to incorporate remotely sensed datasets such as radar and satellite-derived wind fields, the creation of high-resolution local analyses, and the potential use of emerging urban observational networks. Other projects are focused on improving land use parameterizations to provide better specifications of the urban canopy. Since DTRA makes use of data from numerous NWP modeling systems, research also is being conducted to determine biases associated with these systems and the appropriate measures of NWP forecast accuracy of these models at differing model resolutions.

Weather Uncertainty. Meteorological predictions are inherently uncertain due to the stochastic nature of the atmosphere. Therefore, forecasts of meteorological quantities are incomplete if not accompanied by estimates of forecast precision. An accurate characterization of NWP forecast uncertainty is imperative when applied to atmospheric transport, dispersion, and associated downwind hazard assessment. Due to the probabilistic framework of the HPAC toolset, DTRA is particularly interested in capturing the variability in predicted values of meteorological variables for inclusion in transport and diffusion calculations.

Current research efforts designed at improving uncertainty estimates are focused primarily on the application of ensemble methodologies. In particular, DTRA-sponsored studies are currently investigating such issues as the minimum number of ensemble members needed to construct a statistically significant ensemble, real-time ensembling of DTRA's operational NWP data sets, ensemble generation at the mesoscale, and the validation of ensemble members through real-time model performance statistics. Also, DTRA is sponsoring a university study directed toward improving the existing empirical uncertainty model within HPAC.

Data Manipulation and Dissemination. Several developmental efforts to improve the dissemination of data to DTRA customers are ongoing, including the development of new architecture and software for the Meteorological Data Servers system. Once complete, these systems will provide state-of-the-art ingest, data manipulation, and server capabilities for DTRA's user community. DTRA is also actively involved in the development of advanced methods to reduce meteorological data transfer times. This research is directed toward intelligent methods of "thinning" large high-resolution NWP data sets to reduce overall size and improve delivery to end users.

B.2.3 U.S. Army

The Army has the responsibility to provide fundamental knowledge of the atmospheric boundary layer (ABL) over land to all U.S. armed services. Army programs concerned with ATD include the Atmospheric Sciences R&D program within the Army Research Laboratory, the Chemical Stockpile Emergency Preparedness Program (CSEPP), and the Army Research, Development, Test, and Evaluation (RDT&E) Meteorology Program.

Atmospheric Sciences R&D program. This program within the Army Research Laboratory is located at the Army Research Office (Research Triangle Park, North Carolina) and the Battlefield Environment Division (Adelphi, Maryland, and White Sands Missile Range, New Mexico). The program is broadly based to address the wide spectrum of physical conditions of the ABL and its influences on Army operations and systems. The program is divided into three general research areas: Atmospheric Sensing, Atmospheric Modeling, and Atmospheric Effects.

- *Atmospheric Sensing.* ATD-related concerns in this area include rapid detection, identification, and quantification of chemical and biological agents, both gases and aerosols, and in situ characterization and volumetric remote sensing of the state of the environment.
- *Atmospheric Modeling.* Within this area, the ARL focuses on understanding and modeling the diurnal dynamics of the ABL and on assimilation and fusion of volumetric measurement of atmospheric state variables at high resolution in

complex and urban domains. The effort results in the fusion of data with appropriate models to provide a real-time picture of the present state of the ABL and its likely development over short time periods, especially as they apply to ATD nowcasting. While working to reduce the uncertainty in data-fused model results, the Army Research Laboratory recognizes the need to communicate that uncertainty together with best estimates of expected ATD conditions in user-friendly products to decision makers at all echelons.

- *Atmospheric Effects.* End users of ATD modeling systems are often most interested in quantifying the effects of the atmosphere and assessing its impacts on their systems, operations, and personnel. ATD-related concerns are to provide those parameters at the spatial and temporal scales needed to determine relevant effects such as visibility effects of aerosols and dosage effects on personnel. The research results are incorporated into the weather modeling and support functions of the integrated meteorological system deployed to support training and field operations.

Chemical Stockpile Emergency Preparedness Program. The U.S. Army serves as DOD Executive Agent for the chemical weapons stockpile. Chemical weapons are stockpiled at eight locations: Aberdeen, Maryland; Lexington, Kentucky; Anniston, Alabama; Newport, Indiana; Pine Bluff, Arkansas; Pueblo, Colorado; Tooele, Utah; and Umatilla, Oregon. As a signatory to several international treaties, the United States has agreed to destroy its stockpile of chemical weapons. The Congress mandated in Public Law 99-145 that the Army provide *maximum protection* to the workers, general population, and the environment during the storage and destruction of these chemical weapons.

CSEPP focuses on the protection of the general population in the unlikely event of an accident involving the chemical stockpile. At the national level, the program is jointly managed by the U.S. Army Chemical Materials Agency and FEMA. The Program Office is at Aberdeen Proving Ground, Maryland. CSEPP provides funding and technical assistance to ten states and 41 counties in the vicinity of the chemical stockpile. (Newport is located approximately six miles from the Illinois border and Umatilla is located approximately three miles from the Washington border).

The D2-Puff model serves as the primary chemical hazard prediction tool in support of the US Army stockpile and non-stockpile programs. (The non-stockpile program handles demilitarization of chemical weapons or agents not included in the stockpile as defined by treaty and law, such as items uncovered from old ordnance disposal sites.) This segmented plume model is used daily in the planning for and potential response to accidents involving the chemical weapons stockpile. The primary stockpile chemical agents include the nerve agents sarin (designated GB in Army applications) and VX and the blister agent mustard (designated H in Army applications). The primary non-stockpile chemical agents include mustard, phosgene, and lewisite. The primary accidents of concern include spills, explosions, fires, and stack releases.

The D2-Puff model incorporates several sources of real-time meteorological data, both on-post and off-post. Meteorological towers have been built specifically to support the modeling system on the depots as well as in several nearby communities. In addition, the modeling system captures data from nearby NOAA National Weather Service (NWS) and university sites, as well as NOAA/NWS forecasts available via the Internet. With these data, the model continually generates wind fields and hypothetical chemical plume projections to support ongoing chemical weapons storage and demilitarization operations. The model typically updates every 15 minutes to account for temporal and spatial variability in the wind field due to the surrounding complex terrain.

The modeling system connects Army depot operations centers with State and county emergency managers to allow rapid transmission of emergency management information. This information includes an automated communication system, a GIS, a model to support shelter-in-place strategies, and report summaries.

The Army RDT&E Meteorology Program. The Army RDT&E Meteorology Program at Dugway Proving Ground, Utah, is responsible for providing operational meteorological support to U.S. Army RDT&E activities. The program is a user of ATD models, not a developer. However, as the principal DOD test center for chemical and biological defense systems, Dugway Proving Ground has a long history of ATD model R&D. It continues to provide technical assistance to other DOD agencies in ATD model R&D, including conducting field dispersion tests or experiments. Operational meteorological support of field tests involving releases of simulants of chemical and biological agents also requires that Dugway Proving Ground use ATD models in essentially the same ways that they are or could be used for homeland security applications.

The Army RDT&E Program also sponsors applied R&D on mesoscale meteorological modeling. These efforts benefit ATD modeling because the accuracy of the gridded mesoscale model output used as inputs to ATD models is at least as important to the validity of CBRNE hazard assessments as the accuracy of the ATD models themselves.

B.2.4 U.S. Air Force

Air Force Weather resources are organized into a three-tiered structure to conduct worldwide operations and support homeland defense. The Air Force Weather Agency (AFWA) is the strategic-level center. It provides meteorological satellite processing, weather models (mesoscale NWP, cloud analysis/forecast, snow depth, surface temperature, and land-surface models), strategic-level weather products, and specialized support to Special Operations Forces and the intelligence community. The second tier consists of the Operational Weather Squadrons (OWSs), each of which supports a specific geographic area of responsibility. Each OWS provides forecasts, warnings, and advisories to a large number of Air Force and Army active duty, Reserve, and National Guard locations, which support numerous U.S. sites. The level of support is second only to NOAA/NWS. The OWSs provide homeland security support to NORTHCOM when tasked. The third tier consists of Combat Weather Teams, which provide mission-tailored support to local base and tactical units of the Air Force, Army, Special Operations Forces, and other specialized military units. The Combat Weather Teams also provide the observations from their locations, which are disseminated to AFWA and, in most cases, also to the World Meteorological Organization for worldwide use.

B.2.5 U.S. Navy

The Navy's capability to provide operational support for homeland security is based on its expertise in conducting a Rapid Environmental Assessment and providing real-time environmental support, based on that assessment, for naval forces. The Navy's strengths in characterizing the environment through observations and modeling, together with its distributed facilities and effective network for communications and data exchange, are substantial contributions to the national requirement for the best meteorological and oceanographic support to the mission of homeland security. The Navy operates two primary Meteorology and Oceanography (METOC) production (modeling) centers, three regional METOC centers, and numerous facilities and detachments throughout the United States that work closely with NOAA operation centers. The Navy's METOC community also owns seven military survey ships equipped with the latest oceanographic digital data collection systems to survey critical areas worldwide.

B.3 U.S. Department of Energy

B.3.1 Nuclear Incident Response Teams

The Department of Energy (DOE) and the DHS are jointly responsible for the Nuclear Incident Response Team (NIRT) assets that would be used in response to a domestic nuclear release incident. A February 28, 2003, memorandum of agreement (MOA) between the two departments established a framework for DHS to use various DOE assets. The MOA delineates functions and responsibilities for the control, utilization, and exercise of, and the standards for, NIRT assets. NIRT assets, with the exception of the Radiological Assistance Program, which may continue to self-deploy under circumstances where self-deployment is currently authorized, will deploy at the direction of DHS for domestic events in connection with an actual or threatened terrorist attack, major disaster, or other emergency in the United States. NIRT assets include the:

- Accident Response Group;
- RAP;
- Aerial Measuring System (AMS);
- National Atmospheric Release Advisory Center (NARAC);
- Federal Radiological Monitoring and Assessment Center (FRMAC);
- Radiation Emergency Assistance Center/Training Site; and
- Nuclear Emergency Support Team.

B.3.2 National Atmospheric Release Advisory Center

NARAC, which is located at Lawrence Livermore National Laboratory (LLNL), provides atmospheric plume modeling tools and services for chemical, biological, radiological, and nuclear (CBRN) airborne hazards—both gases and particles. These capabilities employ real-time access to worldwide meteorological observations and forecasts via redundant communications links to resources of NOAA, the U.S. Navy, and the U.S. Air Force. NARAC can simulate downwind effects from a variety of scenarios, including fires, radiation dispersal device explosions, hazardous material (HAZMAT) spills, sprayers, nuclear power plant accidents, and nuclear detonations. A database of potential sources is maintained for input to NARAC models. The NARAC software tools include stand-alone local plume modeling tools for end user's computers, and Internet web-based software to provide reach-back access to advanced modeling tools and expert analysis from the national center at LLNL. Initial automated, advanced three-dimensional predictions of plume exposure limits and protective action guidelines for emergency responders and managers are available in 5 to10 minutes. On-duty or on-call NARAC staff can follow up these initial products with more detailed analyses developed immediately, 24/7. NARAC continues to refine calculations using on-scene information, including measurements, until all airborne releases have stopped and the hazardous threats are mapped and the impacts are assessed. Model predictions include the three-dimensional and time-varying effects of weather, land use, and terrain. NARAC provides a simple GIS for display of plume predictions with affected population counts and detailed maps. It can also export plume predictions to other standard GIS systems.

NARAC supports the NIRT, the regional RAP teams, AMS, FRMAC, the DHS under the DOE–DHS MOA, and 40 DOE and DOD online sites. NARAC's operational support to 5 cities and 53 State and Federal organizations across the country has been successfully demonstrated under DHS and DOE oversight.

B.4 U.S. Department of Homeland Security

The capabilities of the DHS Emergency Preparedness and Response (DHS/EP&R) Directorate include an agency-wide GIS Service Center, which has evolved since 1994 from the Mapping Analysis Center (MAC). The MAC had originally supported the FEMA Emergency Support Team and the Response and Recovery Directorate. At the GIS Service Center, the results of the various modeling software packages are incorporated with remote-sensing data and imported into multiplatform GIS software for subsequent analysis. Experts in the scientific and modeling community determine the parameters used to operate these highly complex and complicated programs. DHS/EP&R maintains Internet and Government intranet sites, as well as a continuity of operations site with a capability almost identical to the GIS Service Center. DHS/EP&R is in the process of installing secure classified communications.

B.5 National Aeronautics and Space Administration

As an R&D agency, NASA has invested in three areas applicable to ATD: sensor technology, platform technology, and modeling and computing.

Tropospheric chemistry is considered to be the next frontier of atmospheric chemistry, and understanding and predicting the global influence of natural and human-induced effects on tropospheric chemistry will be the next challenge for atmospheric research over the foreseeable future. NASA's interest in trace gas species in the troposphere has driven investment in a number of active sensing techniques, e.g., differential absorption lidar. Experimental airborne prototypes are being developed and tested in various suborbital missions for tropospheric profiling of chemical species and may be adapted or used in homeland security applications.

NASA is also investing in autonomous suborbital platforms that simultaneously enable in situ planetary exploration and improve the targeting capability of Earth observational systems. Investments in airspace improvements that provide unmanned aerial vehicles (UAVs) with access to the National Airspace System and with in-vehicle technology for safe robotic flight in populated areas can directly enable in situ observations of hazardous airborne material without endangering pilots.

For many years, NASA has invested significantly in the development of data assimilation systems (DASs), especially global systems for medium-range weather forecasting and for climate, and in the study and understanding of forecast and modeling uncertainties. This data assimilation work now extends to the development of land-surface DASs and their integration into atmospheric simulation systems, to the development of an ocean DAS, and to collaboration with the National Weather Service to build a mesoscale atmospheric DAS. NASA's data assimilation work is also being applied to the study of the Earth's carbon cycle and to the study of global precipitation and of the Earth's hydrologic cycle.

While much of NASA's work with data assimilation and with forecast and modeling uncertainty has been applied to spatial and temporal scales much larger than those relevant to ATD modeling, a great deal of the technology that has been developed and many of the lessons that have been learned can be transferred directly to smaller scales. The real challenge is to build a program where people from a varied range of disciplines can talk to each other.

NASA has had extensive experience in using observation system experiments (OSEs) to evaluate the impact of various observations on global-scale atmospheric predictions and in using observation system simulation experiments (OSSEs) that first simulate the atmospheric observations and then predict the impact that these simulated observations would have on atmospheric predictions. These same OSE and OSSE techniques can be used to determine the impact that on-site data will have on ATD simulations and thereby help build ATD sensor networks.

NASA has invested heavily in multi-model ensemble techniques to better understand model and observation uncertainty. Ensemble Kalman filters have been used to estimate model spread and to thereby significantly reduce the number of ensemble members necessary, compared with those needed in a straightforward Monte Carlo approach. The agency has also carried out research on the use of the breeding vector to generate optimal forecast ensembles. All of these ensemble techniques can be fully adapted to the art of data assimilation for ATD modeling.

B.6 U.S. Environmental Protection Agency

As explained in appendix A, section A.1.2, the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory (ARL), NOAA, serves as the primary vehicle by which EPA funds its research efforts in air pollution meteorology and atmospheric modeling. ASMD conducts research activities in-house and through contract and cooperative agreements for the National Exposure Research Laboratory and other EPA groups. ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, especially the Office of Air Quality Planning and Standards. ASMD has identified five major research themes, summarized below, to guide its future research program development and resource planning efforts.

B.6.1 New Directions to Criteria Pollutants and Air Toxics Modeling

This research theme addresses the original and still primary area of research for which ASMD was created. The main research product is state-of-the-science modeling tools for assessment and mitigation of criteria pollutants and air toxics. Following the “one atmosphere” concept, the main tool for computer simulation of a multitude of air quality issues is currently the Community Model for Air Quality (CMAQ) system. While the CMAQ is adaptable to various meteorological models, ASMD has used only the Pennsylvania State University–NCAR Mesoscale Model (MM5). Future efforts will involve a gradual transition to the WRF model, which will be the next-generation mesoscale model for both research (replacing MM5) and operational forecasting (replacing the Eta and Rapid Update Cycle models). ASMD is becoming increasingly involved, especially in the chemistry component. WRF-Chem will be an "on-line" meteorology-chemistry model, representing a major step forward in the state of the science.

Current research includes upgrades to the meteorology–chemistry interface program, upgrade linkages to the WRF model, initial testing of WRF-Chem, and installing the PX-land surface planetary boundary layer (PBL) model into WRF-Chem. Upgrades are being made to the emissions processors to include wildfire, fugitive dust, and sea salt emissions. New gas-phase chemical mechanisms, readers, and solvers are being installed into CMAQ and tested. Research is being conducted to improve the condensed chemistry for long-term simulations. Updates are being made to the cloud dynamic processes and aqueous chemistry. A new version of CMAQ is scheduled for release in June 2004.

Improvements are being made to the CMAQ photolysis rates and radiative transfer model, including the addition of feedbacks between aerosols and radiation. A sectional model for treatment of aerosols is being added to CMAQ. The CMAQ plume-in-grid model is being extended to include aerosol chemistry. The CMAQ code is being optimized to reduce execution speed with testing on various platforms and compilers. Research is underway to include simulation of mercury chemistry and fate in CMAQ.

The plume dispersion model AERMOD is being updated to include dry and wet deposition. Fluid and wind tunnel simulations are being conducted to investigate sub-grid-scale phenomena, dispersion within convective boundary layers, and urban canyons. Computational fluid dynamics (CFD) modeling is being conducted in support of wind tunnel simulations of flow and dispersion around the World Trade Center site as part of the post-September 11, 2001, risk assessment for the New York City area. Research is being conducted to characterize sub-grid concentration distributions, including large eddy simulation with air chemistry and the probability distribution function of emissions.

B.6.2 Air Quality and Global Climate Change

From the air quality perspective, global climate change may make it more difficult in the future for the United States to achieve its air quality standards or goals at the regional and local level. Conversely, air pollution emanating from the United States, including methane, carbon dioxide, particles, and other constituents, may be exacerbating the rate of climate change. Climate change impacts act on long time scales (decades to centuries) and thus are difficult to detect. ASMD has established three research areas that address simulations of global air quality and the attendant effects of climate change: (1) assessment of intercontinental transport, (2) assessment of global climate change on regional/urban air quality, and (3) assessment of regional air quality on global climate change.

One current research activity involves MM5 regional climate modeling simulations based on downscaled global climate model results for current and future years. Another activity is investigating emissions processing for current and future climate change conditions.

B.6.3 Air Quality Forecasting

A national real-time air quality forecast model will equip State and local air quality agencies with a tool for making accurate, multi-day predictions of air quality. The public can use these forecasts to reduce individual exposure to harmful levels of ozone and particulate matter during elevated pollutant episodes. The real-time modeling results can also be used for aiding decision makers in issuing air pollution advisories, for regulating controlled burns, and for helping the public to visualize air quality patterns. The goal of this emerging research program is to design, develop, and test models for real-time forecasting of airborne material. The goal of this research is to construct an operational national air quality forecasting system for ozone and particulate matter. This research theme supports EPA’s mission “to protect public health and welfare” and NOAA’s mission “to forecast changes in atmospheric conditions.”

Current research under this theme includes: (1) evaluation of summer ozone and fine particle simulation results for 2002 and 2003 for the northeastern United States, (2) collaboration and assistance to NOAA/NCEP in installing improvements and efficiencies in the operational modeling system for air quality forecasts, and (3) improved aerosol and radiation process treatment in the WRF-Chem air quality model to allow for meteorological and chemical feedbacks.

B.6.4 Multimedia Modeling

Many of the most difficult challenges facing the EPA span environmental media. Specific multimedia issues of concern include mercury, pesticides, hazardous waste, and excess nutrients. Effectively addressing these issues requires an improved understanding of cross-media processes. This research area will address the interaction of the atmosphere with adjoining media critical to nitrogen/nutrient cycling, acid deposition, and ozone formation and destruction, as well as the behavior of mercury and other toxic pollutants in the environment. Research activities include development of a multimedia nitrogen deposition model.

B.6.5 Data Management and Analysis Research

Many of the environmental issues currently being addressed will require simulations that demand significantly more computational resources and more complex model configurations than present activities require. As the scope of models increases and the models become more sophisticated, the amount of data they consume and generate will also increase. One area of ongoing research is to develop and test methods to address these data management issues.

A second area of ongoing research is to develop and test methods for data analysis and visualization. The growing volumes of data collected and generated will increasingly strain our ability to analyze the data. Much data analysis still relies on a human being looking at the data or at summaries of the data. This approach will become increasingly impractical as data volumes increase.

The ability of our modeling systems to replicate meteorological and chemical processes can only be determined through rigorous model evaluation. A third area of research is to develop and test improved methods for summarizing and characterizing model performance.

Research being conducted within this theme includes development and testing of model evaluation metrics that assess the ability of regional-scale modeling of ozone and aerosols to replicate seasonal spatial and temporal trends. A comparison is planned to assess the performance of several regional-scale mercury models. Quality assurance analysis tools are being developed for assessment of MM5 meteorology and the emissions processed for use in CMAQ.

APPENDIX C. ATMOSPHERIC TRANSPORT AND DIFFUSION MODELING CONSIDERATIONS

C.1 Hierarchy Theory

Most environmental models implicitly employ hierarchy theory in their construct, which in turn employs the concept of scale. Hierarchy theory is an extension of systems theory that attempts to analyze the effects of scale on the organization of complex systems. Simon (1973) was one of the first to argue for hierarchical systems in which each level communicates a small set of information or quantity of material to the next heigher (slower and coarser) level, and each level is formed from the interactions among a set of variables that share similar speeds (and geometries). O'Neill (1988) expanded this idea by shifting attention from the small-scale view to a multiscale view that recognized that processes could develop mutually re-enforcing relationships. Hierarchy theory has been used to separate the large and slow processes from the small and fast processes. Many have argued that environmental phenomena tend to have characteristic spatial and temporal scales (Simon and Ando 1961; Delcourt, Delcourt, and Webb 1983; Urban, O'Neill, and Shugart 1987). This hypothesis is supported empirically by the fact that many physical and ecological phenomena arrange themselves approximately along the 45° line as depicted in figure C-1.

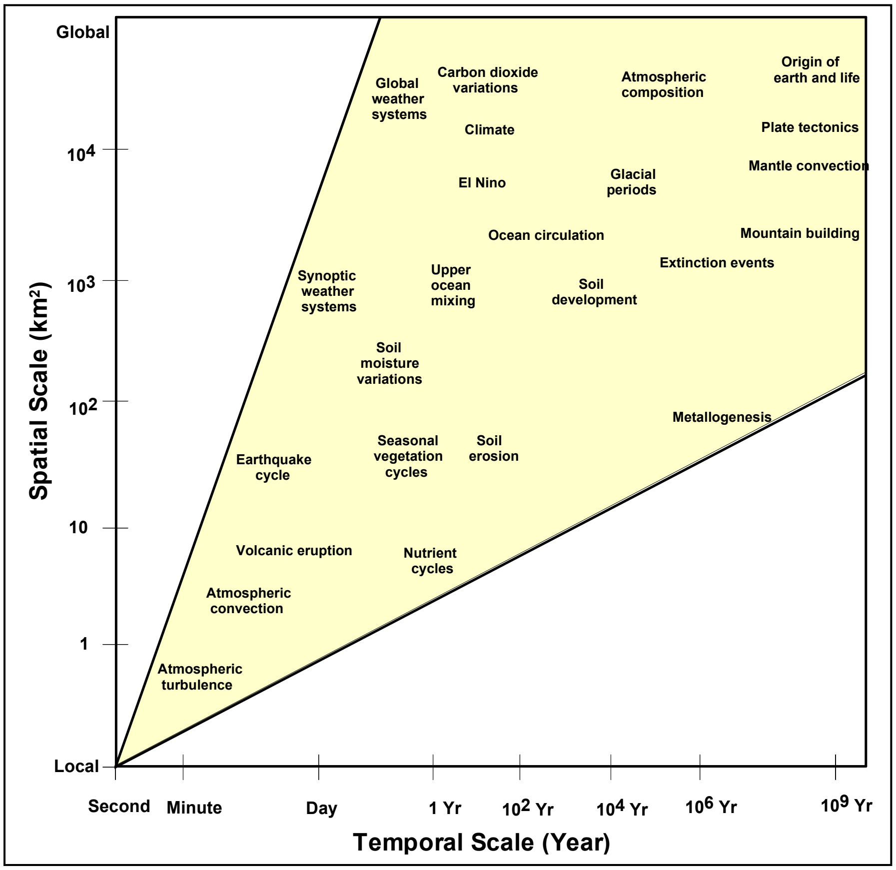

FIGURE C-1. Depiction of various physical and ecological phenomena. Adapted from NASA Advisory Council 1988.

C.2 Scale

Depending on the horizontal scale of interest, different atmospheric processes take on greater or less significance. For the atmospheric processes shown in figure 2, the horizontal scale of motion seems to be the better quantity to use for classification (Orlanski 1975). These scales are all interconnected. Large-scale atmospheric processes (e.g., climatic and daily synoptic weather systems) drive smaller scale processes as energy is transferred from large to small scales. Conversely, small-scale processes can organize to develop large-scale systems: for example, convective storms developing from smaller disturbances. Many of the cases of interest in ATD occur in the troposphere, the portion of the atmosphere up to 15 km above the ground. However, there are cases when transport and diffusion within the upper atmosphere are important (e.g., protecting air

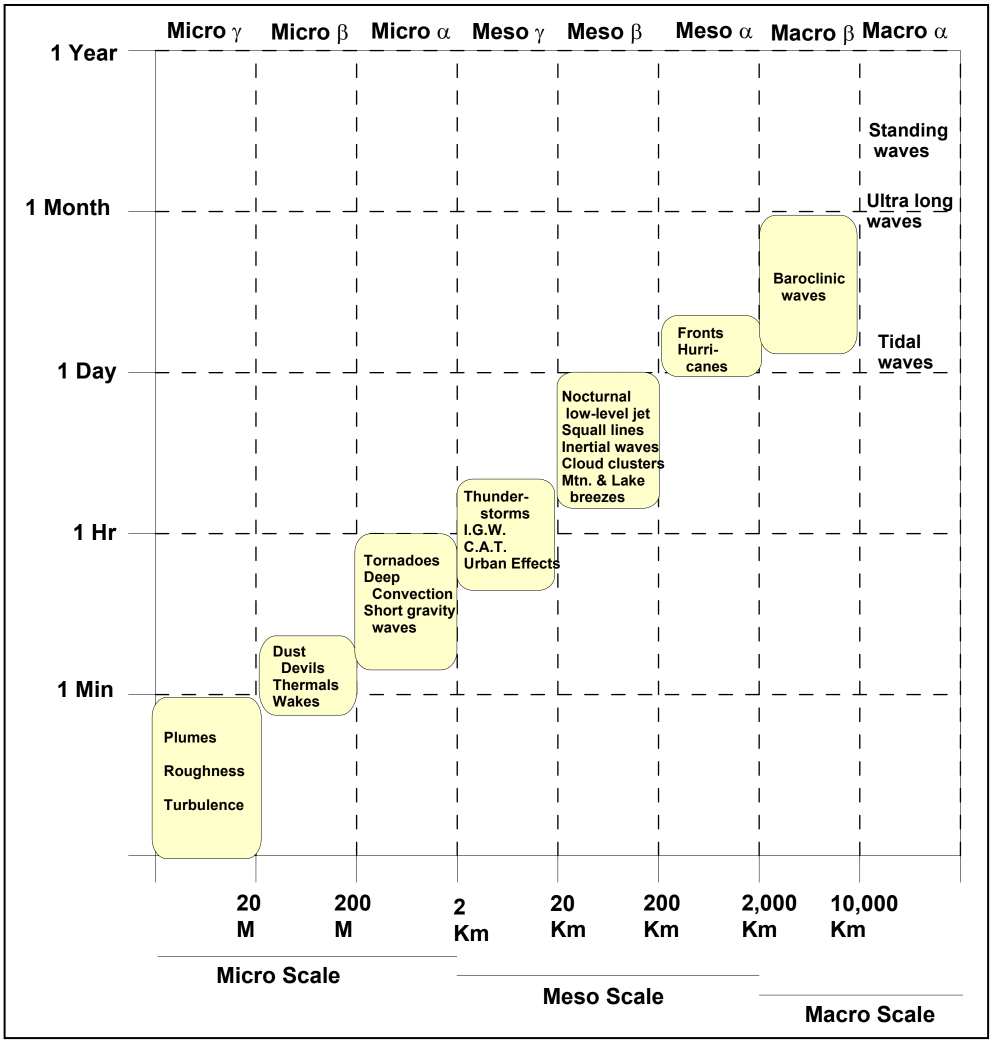

FIGURE 2. Scale definitions and different atmospheric processes with characteristic time and horizontal scales (adapted from Orlanski 1975). C.A.T is Clear Air Turbulence, and I.G.W. is Inertial Gravity Waves.

traffic from volcanic ash, tracking the path of materials from major explosions, or tracking the dispersion of materials originally constrained within the lower atmosphere but which slowly leak into the layers of air aloft).

The atmospheric boundary layer (ABL) is defined for the purposes of this discussion as the lower part of the atmosphere, which is directly influenced by the presence of the earth's surface during the diurnal cycle. This includes the diurnal evolution of solar heating and radiative cooling and the transitions between those states. For ATD, the three-dimensionality of the ABL is crucial to understanding the physics of its variability and, most important, for modeling the variability. With the exception of convective clouds, fronts, or terrain uplift, the troposphere above the ABL exhibits quasi-horizontal flow; vertical motions are slow and gradual. Within the ABL, the earth's surface, through heating and cooling the air and friction over various roughness elements coupled with sources and sinks of moisture, produces three-dimensional turbulence and intermittent processes, which seldom reach truly steady-state conditions. An integral aspect of this diurnal variation is that some of the material originally constrained in the lower atmosphere "leaks" into the layers of air above it. This leakage is accelerated by the action of deep convection, whether or not accompanied by clouds.

The upslope and downslope winds resulting from differential heating and cooling would not be explicitly treated in a model of ATD at the continental scale, but they would be of great concern if the scale were reduced to a local region. Mexico City is an example of a location where proper characterization of the interaction of local and mesoscale airflow circulation patterns is fundamental for proper characterization of transport and diffusion. Mexico City is located in a basin and is surrounded on most sides by hills and mountains. Observations and mesoscale analyses provide evidence that the local circulations are highly complex. A conceptual diagram depicting some of these processes is shown in figure C-3. Mexico City is not unique. Many major cities are located in valleys along major rivers, where upslope and downslope flows are common, or along shorelines of lakes and oceans, where land-sea breezes are common.

The choice of horizontal scale plays an important role in the formulation and selection of an atmospheric model. According to hierarchy theory, describing effects at some scale (the scale of interest) requires at least three levels (scales) for both comprehensiveness and conciseness: (1) the next smaller scale, which provides information up to the scale of interest, (2) the scale of interest, which constrains processes at the next lower scale and provides information up to the next larger scale, and (3) the next larger scale, which constrains processes at the scale of interest. At each scale, a decision must be made as to which physical processes will be represented and how explicitly each selected process will be treated. For instance, at a fine scale the potential evapotranspiration depends on physical parameters such as temperature, vapor pressure deficit, wind speed, surface roughness, precipitation, and soil moisture status, as well as biological parameters such as stomatal conductance (Monteith 1965). At subcontinental scales, Thornthwaite and Mather (1955) show that the potential evapotranspiration can be predicted adequately using a monthly mean temperature and precipitation and latitude (to determine length of day). The nature of the process has not changed with scale, but the relative contribution of explanatory variables has.

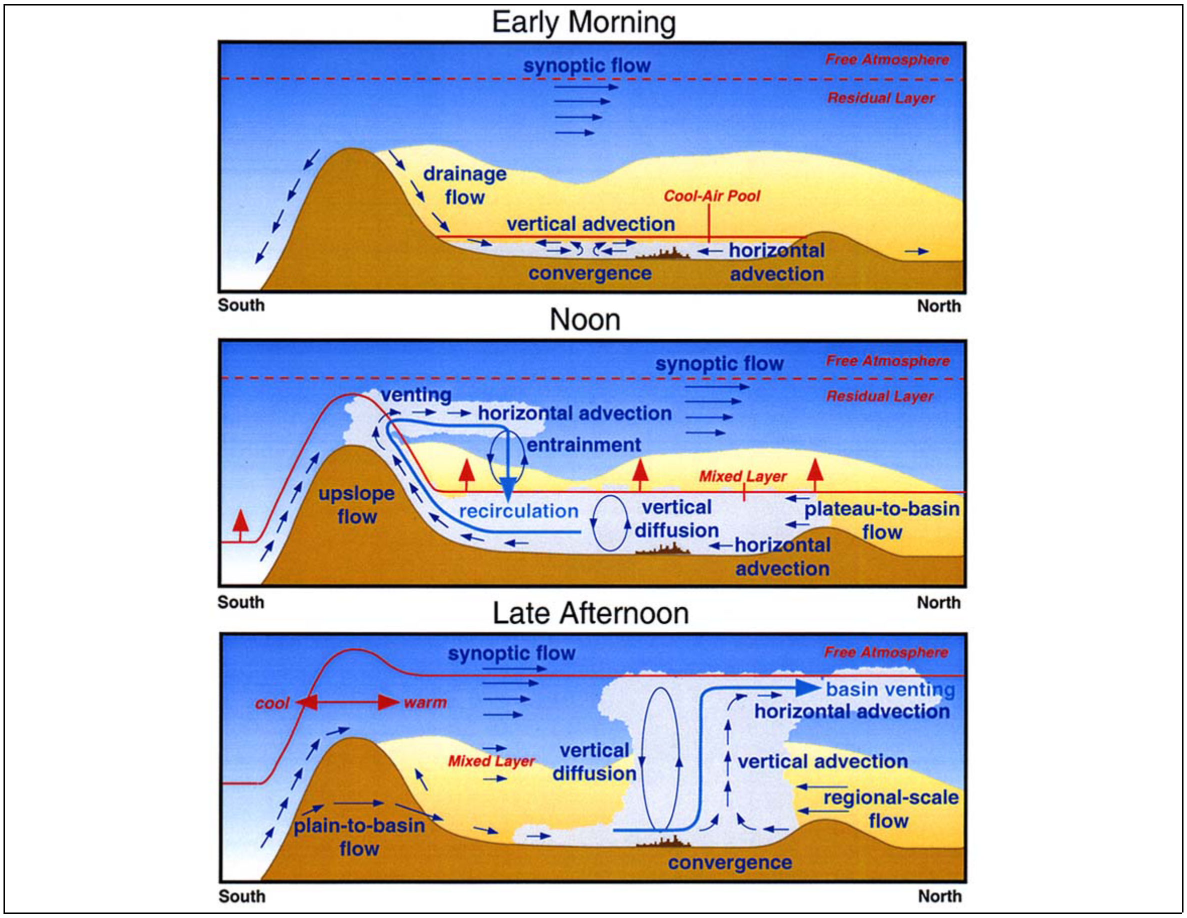

FIGURE C-3. Conceptual diagram depicting some of the meteorological processes associated with pollutant transport within the Mexico City Basin. (Contributed by Jerome Fast of Pacific Northwest National Laboratory, operated by Battelle Memorial Institute for the U.S. Department of Energy. http://www.pnl.gov/atmos_sciences/as_meso5.html.)

Aggregating a large number of processes or decomposing a complex system into a smaller number of levels is similar to approximating the solution of differential equations using a truncated Taylor series. The magnitude of the truncation errors depends on the nature of the processes (e.g., nonlinear interactions, feedbacks, and time delays), spatial heterogeneity, and the uncertainties of available model input and model parameterizations. Because of the feedbacks and interactions, it seems difficult to build a model that spans more than two orders of magnitude ("Carl Walters Rule of Thumb," personal communication from Dr. Gerry Peterson).

C.3 Predictability

A composite of the spectrum of horizontal kinetic energy in the troposphere is shown in figure C-4. In its average state, the atmosphere has a large amount of energy in long wavelengths and decreasing energy as scales become smaller. The energy spectrum (energy per unit wave number interval) decreases as wave number increases (wavelength decreases). The energy spectrum shown in figure C-4 encompasses six decades. As illustrated in figure C-2, the time scales of the motions compress and expand with spatial scale, so that in general, small-scale actions affect short time periods.

Numerical weather prediction models have been successful over the years because the kinetic energy spectrum decreases toward the smallest scale processes and the atmosphere is essentially a weakly stratified fluid, exhibiting quasi-horizontal flow. As computational facilities exploded in capacity and capability, operational weather models have successfully transitioned from the larger scale synoptic flows with horizontal grid sizes of ~200 km to more detailed mesoscale models with horizontal grid sizes of ~20 km or less and representation of terrain influences, oceanic interactions, vertical motions, and larger scale cloud systems. Research and operational models at Army test ranges go to smaller grid lengths (~ 1 km) and include more and more processes of cloud physics, radiative transfer, and land surface interaction and texture. As the grid size is decreased, time steps are decreased, and more details of the small scale processes must be accounted for within the model. From a simple theoretical construct, Lorenz (1969) estimates the spatial scales for loss of predictability as a result of small errors in a uniformly turbulent two-dimensional atmosphere. His results, shown in figure C-5, indicate that the predictability is lost after an hour or so for motions on scales below 40 km.

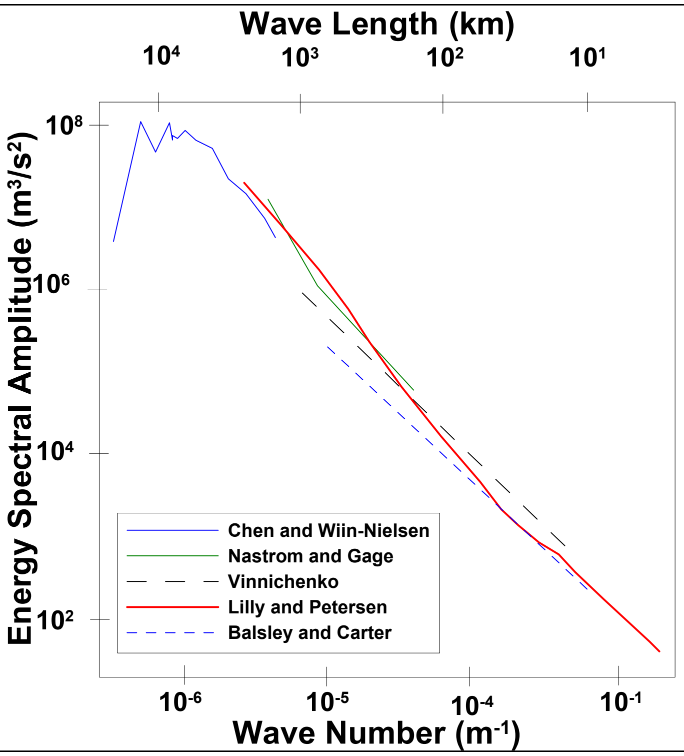

FIGURE C-4. Composite spectra of two-dimensional energy obtained from various sources. Adapted from Lilly 1985.

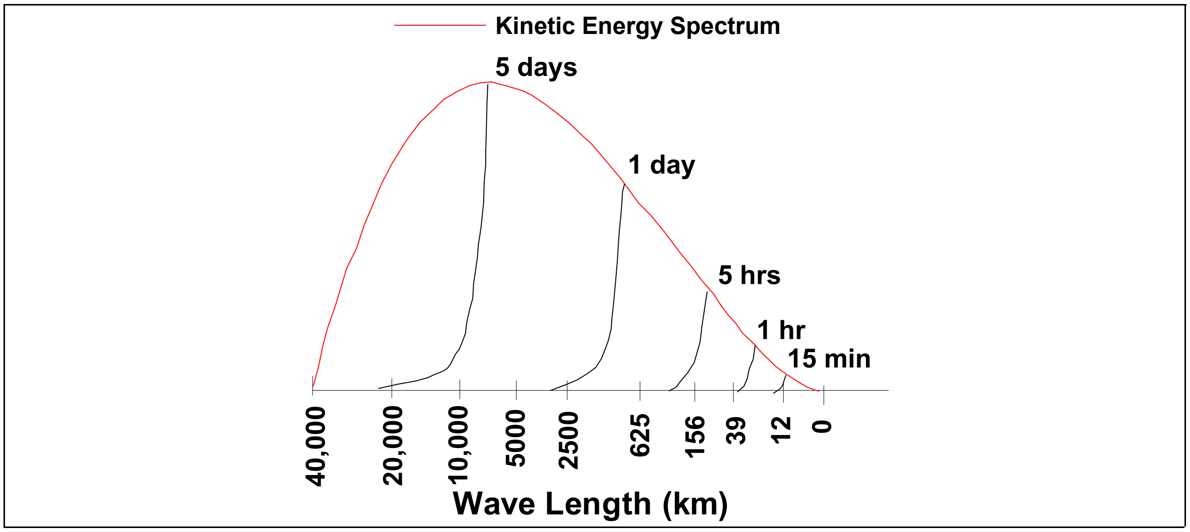

FIGURE C- 5. Results of a closure model calculation of the rate of loss of predictability of two-dimensional flow where the kinetic energy spectrum is given by the upper (red) curve. The short (black) parabolic areas show the left edge of the unpredicted spectrum as it proceeds to larger scales. Adapted from Lilly 1985 and Lorenz 1969.

Observations by Van der Hoven (1957) suggest that the spectrum of the intensity of horizontal wind fluctuations near the ground often shows a separation of scales, as in figure C-6. Large-scale motions of transient weather systems (highs and lows, fronts and storms) are at the left of the figure. A secondary peak representing diurnal processes occurs at about 12 hours. Processes of the order of an hour or so show little intensity compared with these longer processes or those with shorter periods (10 minutes, 1 minute). Although there is some scientific debate about the persistent presence of this "mesoscale gap," the data suggest that mesoscale models may be more effective in representing the larger scale processes than those at smaller scales.

The energetics of ABL turbulence scales are relatively small compared to larger scale flows. This means that these flows have less structure and change more rapidly than do larger scale flows. The memory time of the flow is short and the correlation times and lengths of ABL motions are small. To maintain predictability, high-resolution models may need to be refreshed more often with changing local conditions—insolation, winds, and surface moisture—at the scales of interest. Historically, these processes have been approximated by parameterizations using forecast values of larger scale flows. Where complex terrain is a dominant factor, this conventional thinking remains to be well tested and can be best considered a first approximation to be used with caution until better understanding develops. In anticipation of the discussion to follow, it should be emphasized that dispersion over cities can display the characteristics of severe terrain complexity.

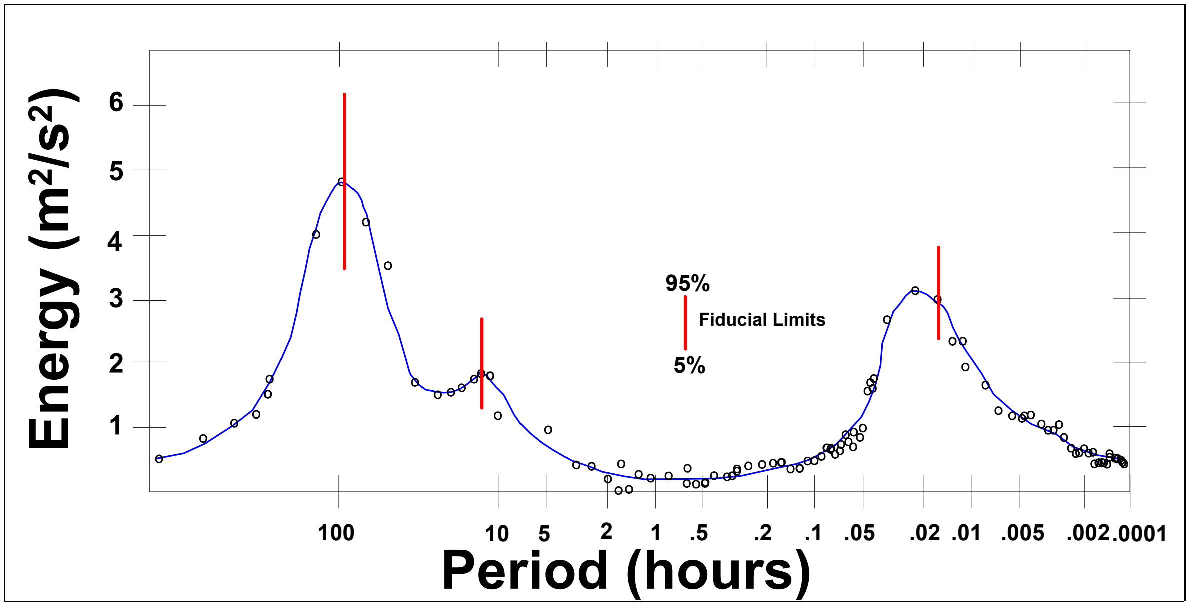

FIGURE C-6. Horizontal wind-speed energy spectrum at Brookhaven National Laboratory at about 100 m height. Data analyzed were collected during the period from June 1955 through February 1956. The statistical significance of the major peaks and gaps of the spectrum is shown by the 5% and 95% confidence (fiducial) limits. Adapted from Van der Hoven 1957.

As the scale of atmospheric motion becomes smaller, the effects of some processes become increasingly more difficult to treat explicitly or deterministically. Turbulence, the gustiness superimposed on the mean wind, can be visualized as consisting of irregular swirls of motion called eddies. Usually turbulence consists of many different size eddies superimposed on each other with different relative strengths. Compared with the other scales of meteorological motions, turbulence is on the small end of scale, as shown in figures C-1 and C-2. Phenomena such as turbulence with a spatial scale smaller than about 3 km and a time scale shorter than about 1 hour are classified as microscale. The small-scale phenomena associated with the microscale are so transient in nature that the deterministic description and forecasting of each individual eddy is virtually impossible (Stull 1988).

Physical models—such as wind tunnels, flow channels, and convection tanks—have been used successfully to investigate stochastic effects embedded within local-scale flows. These physical models have the distinct advantage of controlling boundary and initial conditions, high-resolution measurements, and repeatability. Such control permits a large ensemble of realizations and the potential for measuring inherent uncertainty. Figure C-7 illustrates how physical modeling results can be used to investigate the effect of temporal or spatial averaging. Vortex shedding from the corners of the building is apparent in the instantaneous pictures for both cases, but there is an obvious difference in the structure of the plumes. The tall building has a thin sinuous plume with much meandering, which is similar in some respects to the classical von Karman vortex street in the wake of a two-dimensional cylinder. This structure is not as pronounced in the wake of the wide building, which appears to have a more random internal structure (Lee et al. 1988).

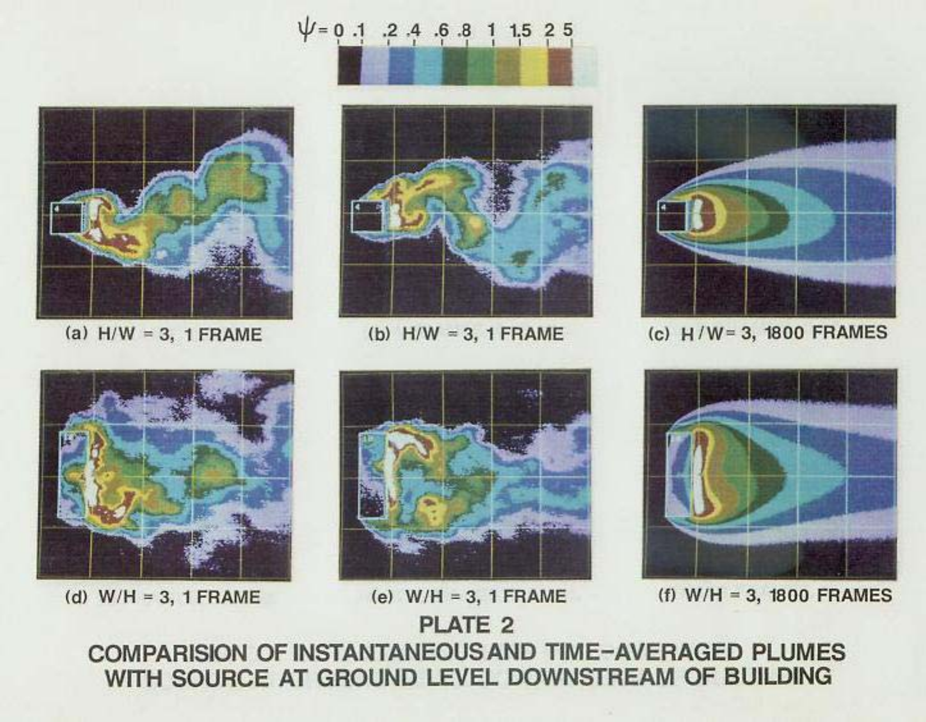

FIGURE C-7. A video image analysis of smoke concentration in wind tunnel flow fields (Lee et al. 1988). The smoke source is centered on the lee side of the building at the surface. The plate illustrates the very large differences between instantaneous and time-averaged plumes for a tall building, H = 30 cm, and a wide building, H = W = 30 cm, where W is the cross-stream width of the building. Photographs were collected at 30 frames per second. The relation between the digitized smoke intensity and the vertically nondimensional integrated concentration, ψ, of the smoke particles was obtained from calibration experiments in which the smoke was replaced by a mixture of ethane and air.

Most operational ATD models predict the ensemble mean transport and diffusion for the conditions specified. However, atmospheric releases are individual realizations from imperfectly defined ensembles. As illustrated in figure C-7, the within-ensemble variance of certain processes can be quite large. For instance, the first-order approximation of the lateral concentration profile of a plume is the often-assumed Gaussian shape. Inspection of tracer plumes reveals fluctuations superimposed on this Gaussian shape of the order of a factor of two. These fluctuations are not addressed or characterized in most operational transport and diffusion models (ASTM 2000). The approximation thus inherently constrains the predictability one can anticipate from such a model.

At the microscale, the direction of transport cannot be treated deterministically (Irwin and Smith 1984; Weil, Sykes, and Venkatram 1992), which precludes the possibility of simulating the concentration time series as would be seen at some fixed receptor location. In the simplest of circumstances, the microscale transport direction of a plume can be defined to about 25 percent of the overall width of the plume, which typically is on the order of 20 degrees in width. As the winds become light and variable, the uncertainty in the transport direction increases. At the microscale, the transport direction is best viewed as a stochastic variable having a large variance.

Only rarely is the centerline of a plume a straight line. In reality, because the initial plume dimensions are small in comparison with the length scale of the turbulence, the plume of dispersing material waves back and forth in a serpentine fashion in both the vertical and horizontal dimensions, as shown in figure C-7. The resultant plume meander contributes to the time-integrated plume spread but complicates determination of the time history of concentration values at some fixed point relative to the release point. The plume meandering causes the plume to be present at a given point only intermittently. A frequently cited model used for characterizing the process just described is the Gifford (1959) fluctuating plume dispersion model.

Further inspection of the crosswind profile of the instantaneous plume reveals that the vertical and lateral concentration profiles are not smooth bell-shaped curves but are “grassy-looking profiles, with many local deviations (greater and less) from the envisioned smooth bell-shaped profile.” Various models have been proposed to characterize the combined effects of random concentration fluctuations within a plume that in turn is randomly varying (meandering). Wilson, Robins, and Fackrell (1982) note that the variance of the concentration fluctuations is seen to be strongly dependent on height above the surface, which “…can pose difficulties in hazard assessment because variations in receptor height of only a few meters cause significant changes in the predicted variance and thus the probability of observing a specified concentration.”

C.4 Model Selection and Application

Part of the problem of model selection is knowing the horizontal scale of the various transport and diffusion processes of concern. Another part of the model selection problem is understanding which transformations and removal processes are of concern. Figure C-8, which depicts some of the major atmospheric processes typically addressed in transport and diffusion models, illustrates that not all processes are of interest at all scales. (Note that figure C-8 is not intended to provide guidance on when a process *must be* addressed.) For example, whether a model provides a means of characterizing buoyant plume rise is of no concern, even in the near field, unless the emissions are buoyant. Modeling systems that estimate the impacts of inert species typically focus on short transport distances where little dilution has occurred and concentration values are at their highest levels. Such models focus on characterization of diffusion, local flows, building effects, and initial source effects (e.g., buoyancy and explosive dispersal). Modeling systems that estimate impacts of chemical and radioactive species that form during transport are less concerned with microscale effects and are more concerned with mesoscale and macroscale processes. These models must address the consequences of variations in time and space of meteorological conditions that affect transport and diffusion.

Transport and diffusion models are typically employed for two circumstances: (1) for the assessment of near-field impacts from one or more releases (e.g., involving transport distances of 5 km or less), and (2) for the assessment of long-range impacts from a radioactive or very toxic release (e.g., involving transport distances of 30 km or more). In the first instance, where the plume dimensions are small in comparison to the dominant

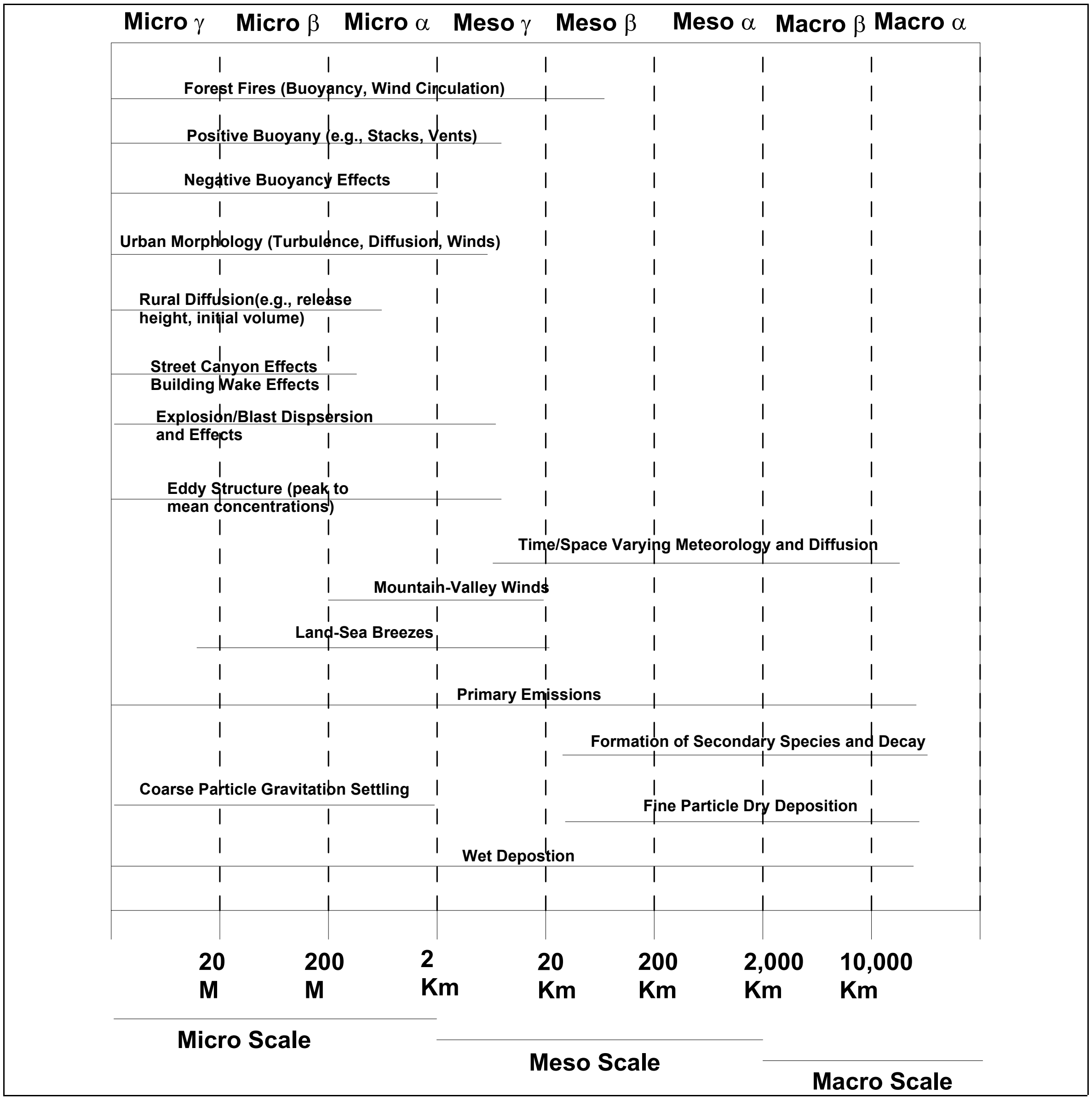

FIGURE C-8. Depiction of varying horizontal scale transport and diffusion processes likely to be of most concern.

turbulent eddy sizes, it will not be possible to simulate the actual transport explicitly. Turbulence and counter-gradient flows will make the near-field transport a highly stochastic process. For near-field impact assessment, the transport times are sufficiently short that the chemical/radioactive species being modeled can usually be treated as inert. In the second instance, the transport will still be uncertain but can be treated with more confidence. Counter-gradient flows are sufficiently short-lived that they can be neglected for longer-range transport problems. Whether the chemical or radioactive species can be treated as inert will depend on the species. As shown in Figure 8, many of the processes of interest for near-field impact assessment become of less importance for problems involving longer transport distances.

Most transport and diffusion models characterize emissions as coming from one of three source types: point, volume, or area. For any given application, the user must select the source type characterization that best represents those qualities of the release deemed to be most relevant to the questions being posed. Inevitably tradeoffs and compromises will be needed. Consider the situation depicted in figure C-9. This photograph of a point-source emission was taken in early morning, when there was significant buoyant rise and stable atmospheric conditions. The rising gases are stabilizing at different heights where there are significant differences in the direction of the transport winds. Do we simulate this as one plume or two plumes with different plume rises?

FIGURE C-9. Photo taken by Walt Lyons from his office window, which looks due south toward Denver, on a late spring day. (The year is uncertain but may have been 1997.) Contributed by Walter Lyons, President of FMA Research, Inc., Yucca Ridge Field Station, 46050 Weld County Road 13, Ft. Collins CO 80524.

For each source and source type, decisions have to be made as to the rate of release, the temperature of the gases (if hotter or colder than ambient temperature), and the initial dilution volume at the release—all of which may vary in time. For instance, the initial dilution and rate of release of emissions are critical if concentration values are desired close in to the release point, but the initial dilution is of less concern at distances much beyond 10 km downwind of the release. The successful application of a model is thus one of knowing what questions are being posed, what capabilities are present in the models, and what the tradeoff consequences are as one tailors the application of the model to a particular situation. We can envision a model as a tool that can be used in a variety of ways. To apply a tool successfully takes wisdom (i.e., experiential knowledge as well as academic knowledge). A hammer, a stone chisel, and a suitable block of marble in the hands of an experienced sculptor can create a statue, but in the hands of one who is not a sculptor (or an apprentice who is just learning the trade), just a pile of smaller stones.

Tennekes (1990) challenged the atmospheric modeling and measurement communities with three requirements:

- No observation is complete without an appropriately sampled estimate of the variance of the properties observed.
- No forecast is complete without a preceding estimate of forecast skill.
- No model calculation is complete without a calculation of its variance.

Taking all of the above aspects under consideration, one can conclude that the appropriate choice of an ATD model depends on five selection parameters:

- A definition (or redefinition) of the information to be gained or the decision to be made;
- The selection of the scale of interest;
- A knowledge of the physical processes that likely should be treated for the intended purpose;
- An appreciation of the uncertainty associated with the tradeoffs made in the model's construction; and
- The limits of predictability associated with any modeling system for the scale of interest.

C.5 General Model Types

Models of environmental processes are approximate representations of reality. Each model involves a set of tradeoffs, taking into account objectives such as whether it will be used to aid understanding, to estimate changes that might occur, or to determine where areas might be affected if a release were to occur. There are six general model types: plume, segmented plume and puff, Lagrangian particle, box, Eulerian grid, and computational fluid dynamics (CFD).

1. A **plume model** assumes that conditions are horizontally homogeneous (everywhere the same) and steady state as shown in figure C-10(B). As shown in figure C-10(A), plume models attempt to capture some essence of what is seen, but they make no claim to depict reality. Plume models are useful for quick estimates near a release, so long as the wind direction is relatively steady, the wind speed is greater than 1 to 3 m/s, and the distances downwind from the release are on the order of 20 km or less.

2. A **segmented plume and puff model** divides the emissions into a series of overlapping volumes (or puffs) so that one no longer need assume horizontal homogeneous conditions or require conditions to be steady state, as shown by the example in figure C-11. Developing the time- and space-varying meteorological conditions is resource intensive. These conditions include detailed terrain and land use data, meteorological observations from many locations within the domain, and a capability to model the local flows and circulations (either by dynamic or empirical models). Puff models have been used to study mesoscale transport and diffusion of species whose chemical or radioactive transformations can be represented using time-dependent decay approximations.

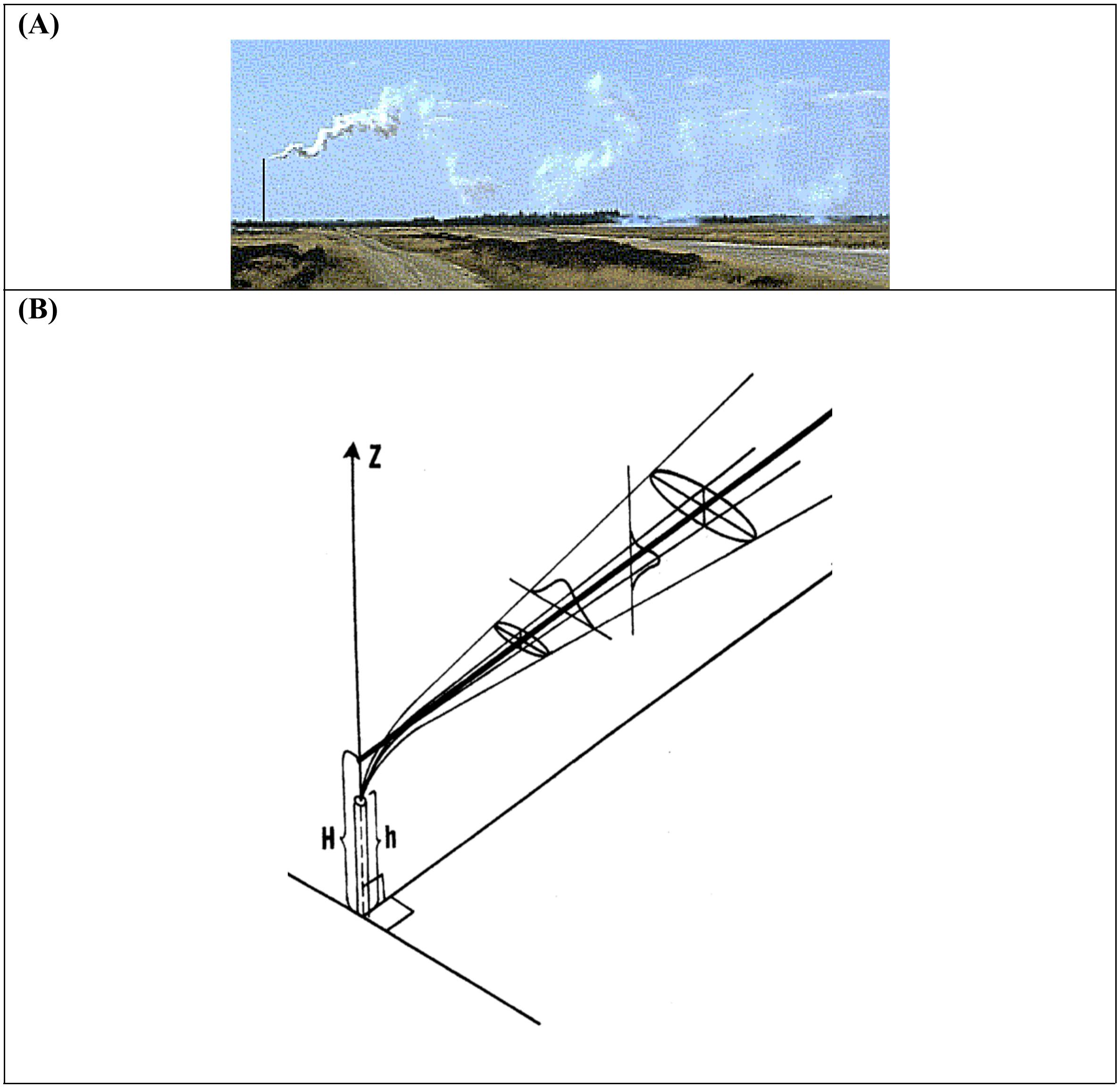

FIGURE C-10. (A) Diffusion of smoke from a tall stack during a sunny afternoon. (B) Idealization that would be used in a Gaussian plume model to characterize the diffusion from such a tall stack.

3. A **Lagrangian particle model** divides the emissions into thousands of tiny masses or particles that are individually tracked as they are stochastically transported downwind, as shown by the example in figure C-12. Each particle is “moved” at each time step by pseudo-velocities that take into account the three basic components of transport and diffusion: (1) the transport due to the mean wind, (2) the turbulent diffusion caused by the (seemingly) random fluctuations of wind components (both horizontal and vertical), and (3) the molecular diffusion (if not negligible). As shown by Hanna (1979), it is a plausible assumption to describe both Eulerian and Lagrangian wind vector fluctuations by a simple Markov velocity process (autocorrelation process of the first order). Particle models can be used to investigate

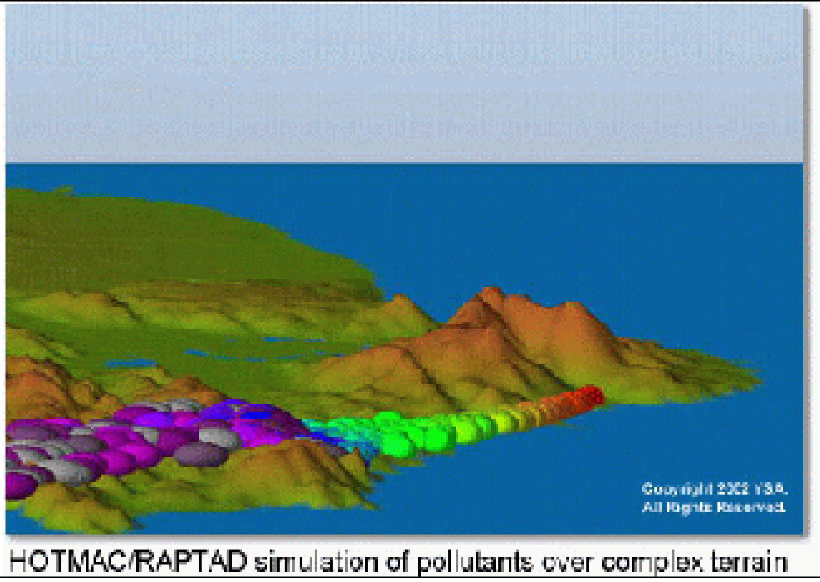

FIGURE C-11. HOTMAC/RAPTAD simulation of the transport and diffusion of pollutants over complex terrain. Contributed by Ted Yamada of YSA Corporation. Rt. 4, Box 81-A, Santa Fe, NM 87501.

and depict transport and diffusion within complex wind regimes (e.g., between buildings or during a frontal passage).

4. A **box model** assumes the modeling domain is one large homogeneous volume (box). Emissions entering this volume are assumed to be uniformly and instantaneously mixed throughout the volume (figure C-13). The top of the box may rise to simulate the rise of the mixing depth after sunrise, and pollutants above this rising lid could then be entrained into the volume. The location of the box can be stationary (to simulate the air over a city), or it can move with the transport wind (to simulate the “aging” of an air mass). Box models have been used to study photochemical problems and to compare alternative chemical kinetics.

5. An **Eulerian grid model** divides the world into a three-dimensional array of rectangular cells (grids) within each of which mixing is considered uniform and instantaneous. Grid models are used to simulate the formation of products through atmospheric chemistry and the removal of products by clouds and precipitation, all of which are usually sufficiently removed from the emissions of immediate concern that the “well-mixed” assumption in each cell is reasonable. Eulerian grid modeling systems have been used to study regional transport and fate of secondarily formed species (e.g., ozone, acid deposition, and fine particulate haze). Figure C-14 illustrates the application of the Community Model of Air Quality (CMAQ) to simulate the effect of reducing nitrogen oxide (NO_x) emissions by 50 percent. Results for ozone and particle matter (PM) with diameters less than 2.5 micrometers (PM2.5) are shown for the original base, the strategy simulation, and the difference (strategy minus base case) between the two for July 14, 1996, at 0100 GMT. Thus, negative

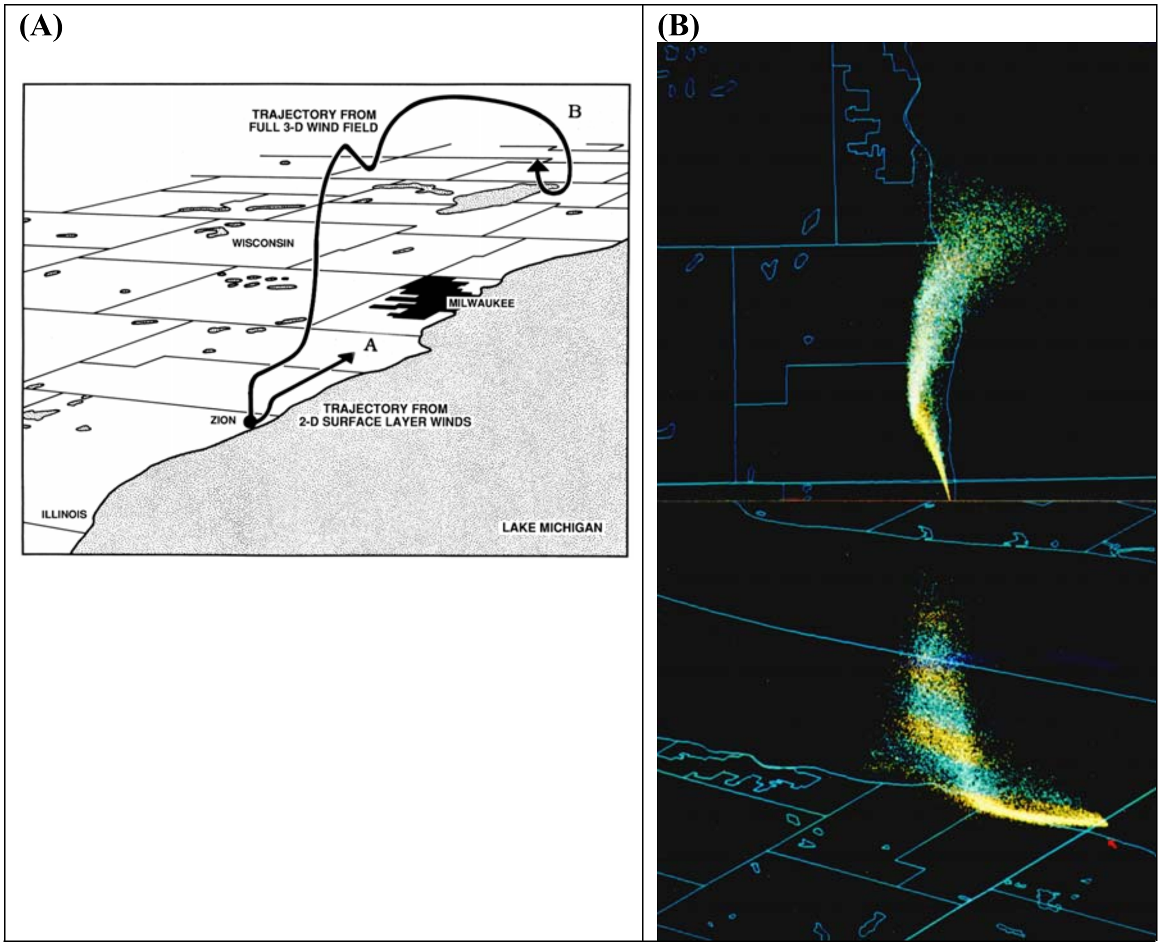

FIGURE C-12. (A) Typical plume trajectories calculated from RAMS output using only surface layer winds (trajectory A) which stays at 50 m altitude and the complete wind field (trajectory B) which rises to 1600 m altitude. (B, Top) Plan view of a simulated plume released from a 50 m high shoreline source into a weak lake breeze along the Lake Michigan shoreline. (B, Bottom) a perspective view of the plume from the southwest showing large quantities of the plume being transported vertically due to the strong upward motions in the lake breeze frontal zone. (Lyons et al. 1995; figures contributed by Walt Lyons.)

differences indicate decreases in ozone and PM2.5 levels, whereas positive differences indicate increases in the pollutants.

6. A **CFD** model is based on the three fundamental principles that govern the physical aspects of any fluid flow:
    - Mass is conserved.
    - Energy is conserved.
    - Newton's second law (the acceleration of an object is a function of the net force acting upon the object and the mass of the object).

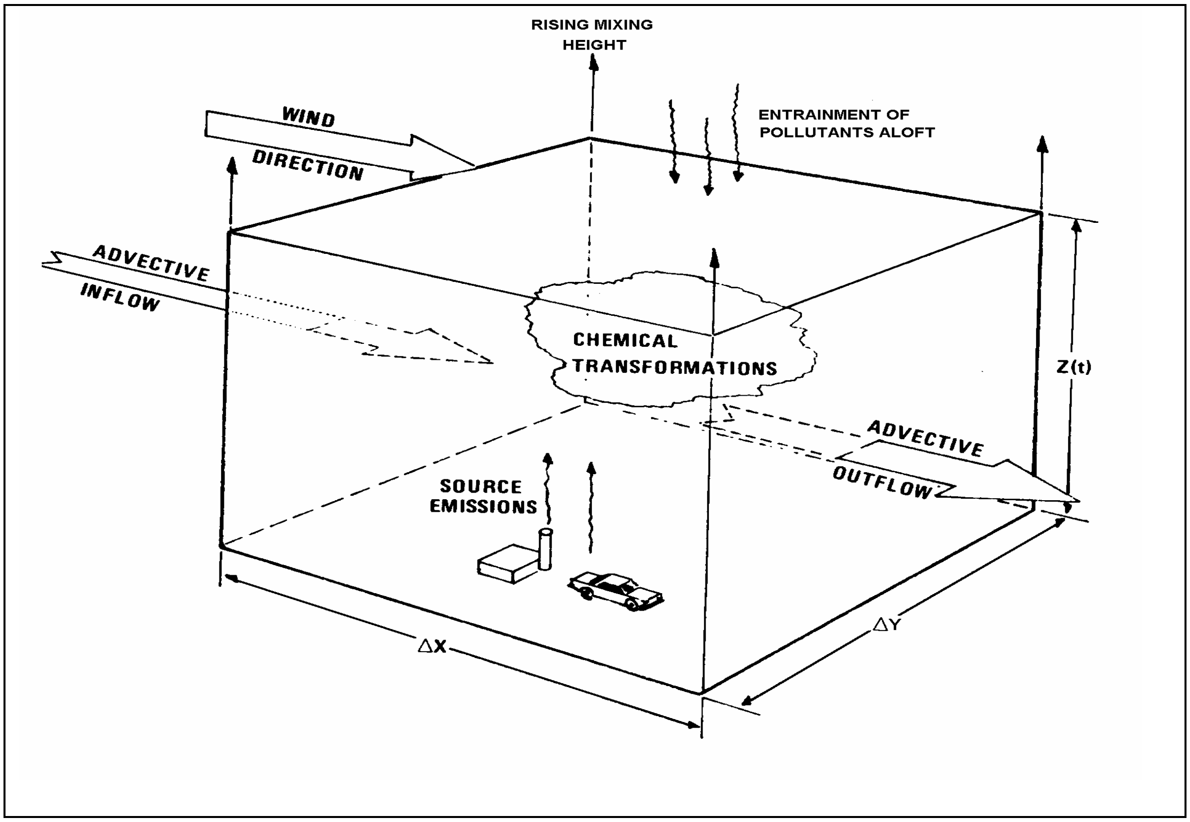

FIGURE C-13. Schematic illustration of a photochemical box modeling domain (Schere and Demerjian, 1984).

These fundamental principles can be expressed in terms of mathematical equations, which in their most general form are usually partial differential equations. CFD is the science of determining a numerical solution to the governing equations of fluid flow while advancing the solution through space or time to obtain a numerical description of the complete flow field of interest. The governing equations for Newtonian fluid dynamics, the unsteady Navier-Stokes equations, have been known for over a century. However, the analytical investigation of reduced forms of these equations is still an active area of research, as is the problem of turbulent closure for the Reynolds averaged form of the equations. For non-Newtonian fluid dynamics, the theoretical development of chemically reacting flows and multiphase flows is at a less advanced stage. CFD has been used to study flows around airplane wings and rockets, air flow through engine parts, and the transport and diffusion of particles around and between hills and buildings (e.g., figure C-15). To date the data requirements, problem definition, and time required to generate results have limited the use of CFD models to studies of special situations.

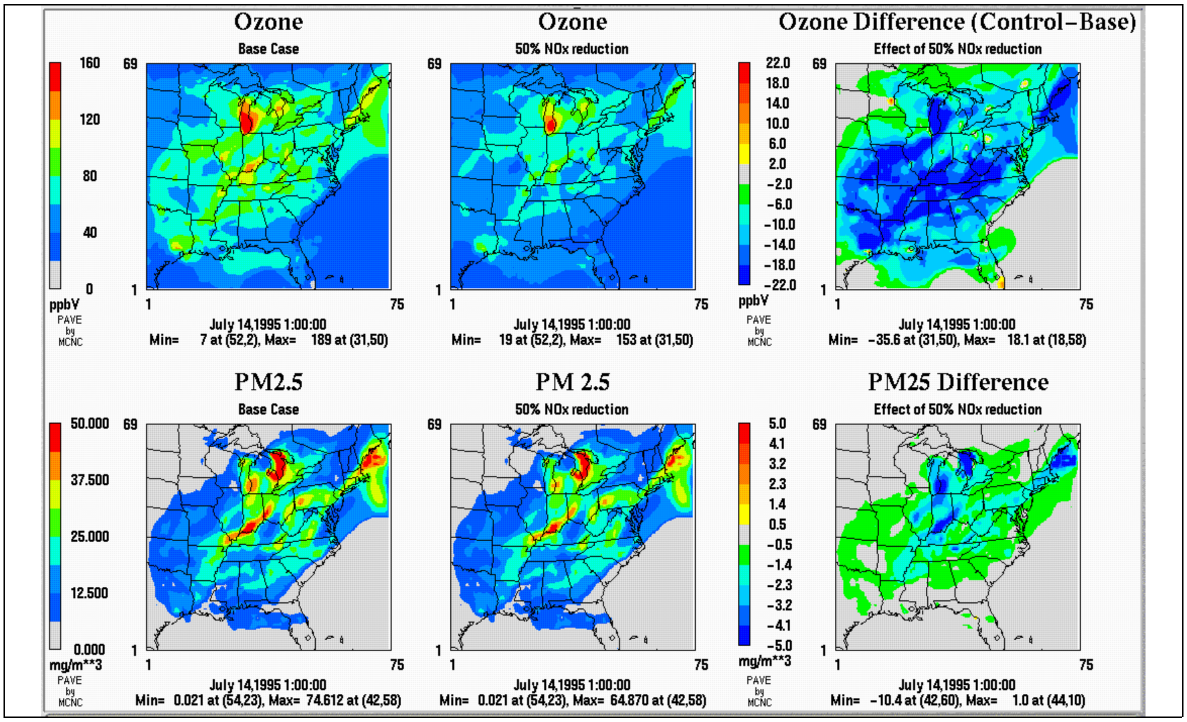

FIGURE C-14. Illustration of the effect of reducing NOx emissions by 50 percent, as computed by the Models3/CMAQ modeling system. “PM2.5” stands for “particle matter with diameter less than 2.5 µm. Source: Leduc, Schere, and Godowitch 2001.

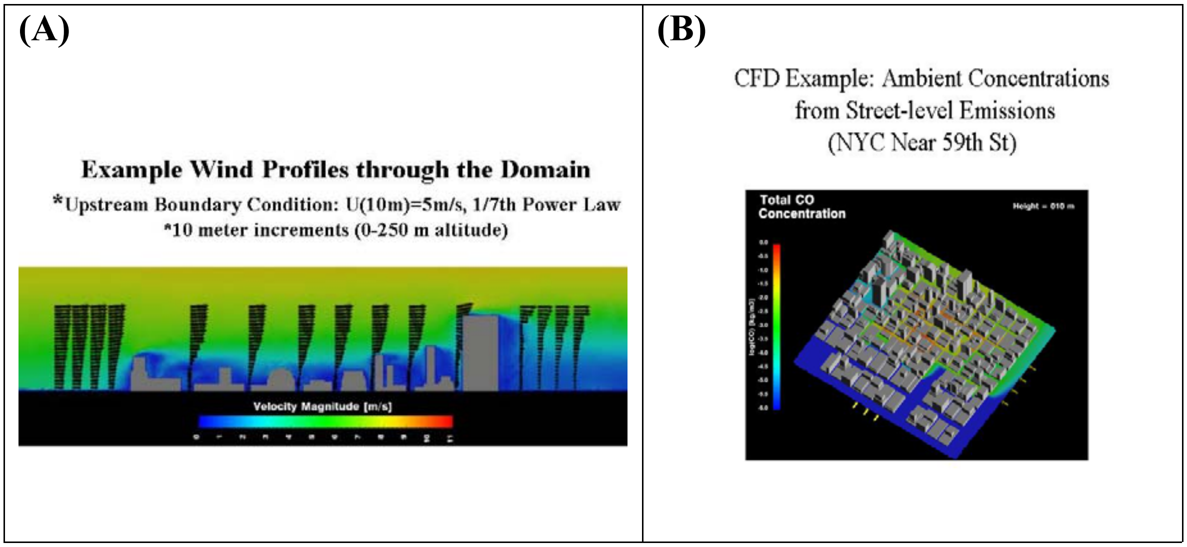

FIGURE C-15. Computational fluid dynamical simulation results for the adjustment of the wind profile to buildings associated with an urban domain (A) and a simulation of ambient carbon monoxide concentration values from street-level emissions (B).

C.6 Diffusion Characterizations

Any contaminant released into the atmosphere is transported by a variety of processes that can be defined generically as either advection or molecular and eddy diffusion (often referred to as turbulent dispersion). Advection is the movement of contaminants as a result of the mean flow. Molecular diffusion is a redistribution of mass (or energy) within a gas by Brownian motion and tends towards uniformity in mass (or energy). Brownian motion is thermal energy and results in random molecular collisions. There is motion in all directions, but there is a tendency for the mass (or energy) to move from areas of high concentration to areas of low concentration. Molecular diffusion is rarely of significance in comparison with eddy diffusion. Eddy diffusion results from turbulent velocity deviations from the mean flow. Turbulent deviations are mechanically generated by friction drag and flow through and around obstacles. Turbulent deviations can be enhanced or suppressed thermally by buoyancy forces arising from relative differences in temperature in air layers next to the ground or other surfaces. In this discussion, the term “diffusion” encompasses both molecular and eddy diffusion.

When reading the ATD literature, one can easily become confused by different usage of the terms “diffusion” and “dispersion.” “Diffusion” is often used without mentioning whether it is meant to include both molecular and eddy diffusion. To further complicate matters, some texts use the term “dispersion” to refer to the combined effects of eddy diffusion and advection, whereas other texts use the term “dispersion” in the sense of “turbulent dispersion” but without the qualifier “turbulent.” For the sake of clarity, this discussion avoids use of the term “dispersion.” It uses “diffusion” to refer to the combined effects of molecular and eddy diffusion.

There are two other considerations to be recognized in characterizations of eddy diffusion. First, there is an implicit averaging time assumed, which is associated with the definition of the “mean flow” of the atmosphere. In atmospheric transport and diffusion models, the mean flow is typically defined at 1-hour intervals, but this choice is not mandated. If the mean flow is defined at 5-minute intervals, then a portion of what would have been characterized as eddy diffusion for 1-hour intervals will instead necessarily be characterized by the time and space variations in the 5-minute mean flow. Second, not all deviations from the mean flow are random; hence, not all eddy diffusion is random. The thermal eddies of a convective boundary layer transport mass from the surface to the top of the convective boundary layer in an organized manner. This convective eddy transport could be thought of as advection, but since it occurs in less than 1 hour and cannot be simulated deterministically, it is typically viewed as a component of eddy diffusion.

C.6.1. Empirical Characterizations of Diffusion

There are many instances when field-data observations of smoke and tracer diffusion have been organized into empirical schemes for the characterization of diffusion. Typically, these schemes rely on the empirical observation that the vertical and lateral crosswind concentration distribution appears to be similar to a Gaussian shape. Hence, these schemes provide characterizations of the vertical and lateral Gaussian parameters (as a function of travel time or distance of transport, stability, and roughness length of the surface). The well-known Pasquill-Gifford diffusion parameters (Pasquill 1961; Gifford 1961) have been used extensively in many of the popular transport and diffusion models. The Pasquill-Gifford diffusion parameters were derived from various experiments over rural terrain. The lateral diffusion parameters have an implied averaging time of 3 minutes and a roughness length of 3 cm for transport distances less than 1 km. For transport greater than 10 km, the lateral diffusion parameters still have an implied averaging time of 3 minutes but a roughness length of 30 cm. The vertical diffusion parameters are likely appropriate for all averaging times up to 30 minutes and have the same variation in roughness as the lateral diffusion. Field studies conducted in the 1960s in St. Louis, Missouri, by McElroy and Pooler (1968) included observations of a tracer released and sampled for 1-hour periods. Their results have been used to develop a characterization of diffusion for urban environs. There are many such studies (Randerson 1985); however, the important consideration in the use of any of these schemes is to recognize that they may be relevant only for the circumstances under which the data were collected.

C.6.2 Similarity Theory and PBL Parameterizations

Useful schemes for the characterization of diffusion have been fashioned though an analysis of field studies of diffusion that incorporate known important variables and governing “scaling” parameters. Such models are called similarity models because they imply “similar” behavior of the atmosphere from one place or time to another, if one assumes that certain scaling parameters are held constant. The important scaling parameters in surface-layer similarity models of diffusion are L, u*, and z_o, where L is the Monin-Obkhov length, u* is the friction velocity, and z_o is the surface roughness length. Examples of surface-layer similarity models of diffusion are provided by Briggs and McDonald (1978); Horst, Doran, and Nickola (1979); and Briggs (1982). The surface layer is nominally the lower of |L| or Zi/10, where Z_i is the mixing height. Scaling parameters for convective diffusion models are L, Z_i, and w*, where w* is the convective velocity scale. Examples of convective diffusion models are Weil and Furth (1981), Misra (1982), and Venkatram (1983).

C.6.3 Statistical Characterizations of Diffusion

Taylor’s (1921) theory for homogeneous and stationary turbulence has served as the basis for several statistical models of atmospheric diffusion. These models imply that the spread is linear with time in the near field, and proportional to the square-root of time in the far field. The transition from near field to far field is typically specified in terms of a Lagrangian time scale. Examples of statistical theory for the characterization of the vertical or lateral extent of a release as it is transported downwind are Draxler (1976) and Venkatram, Strimaitis, and DiCristofaro (1984). The Monte Carlo particle trajectory models of diffusion are statistical characterizations of diffusion.

C.6.4 First- and Second-Order Closure Assumptions

Gradient transport (K-theory) models are derived from the continuity equation with the turbulent fluxes of concentration (C) assumed to be proportional to the mean gradient of C, with K being the constant of proportionality. This is called a "first-order closure" assumption because it retains the prognostic equations for only the zero-order mean variables and parameterizes the turbulent fluxes. K-theory models are typically used with grid models, where the emphasis is often on atmospheric chemistry and regional transport. An important consideration is that gradient transport models of diffusion have implicit time and space scales. The mean wind components represent averages over some time scale and space scale. Velocity fluctuations with time and space scales less than those implicit in the mean wind components are considered turbulence. Therefore, they are implicitly included in the proportionality constant K. However, as discussed by Taylor (1921), the rate of diffusion of a plume depends on the plume size. This limits the applicability of K-theory models of diffusion to instances where the size of the plume is greater than the size of the dominant turbulent eddies so that all of the turbulence implicit in K is taking part in the diffusion. The vertical diffusion of point sources can be modeled using K-theory for sources near the ground, where the turbulent eddies are sure to have scales less than the thickness of the plume. However, K-theory can be used to model elevated releases only when the vertical extent is spread out over several hundred meters (Hanna, Briggs, and Hosker 1982).

There are "higher-order" closure assumptions (e.g., second-order) where the prognostic equations are retained for both the mean and the flux variables and the third moments are parameterized. Second-order closure has been used to develop plume models (Sykes Lewellen, and Parker 1986) and puff diffusion models (Sykes and Henn 1995).

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APPENDIX D. ACRONYM LIST

24/7	24 hours per day, 7 days per week
ABL	atmospheric boundary layer
ACARS	Aircraft Communications Addressing and Reporting System
AEC	Atomic Energy Commission
AFWA	Air Force Weather Agency
ALOHA	Areal Locations of Hazardous Atmospheres [an ATD model]
AMS	Aerial Measuring System [a NIRT asset]
ARAC	Atmospheric Release Advisory Capability
ARL	Air Resources Laboratory [of NOAA]
ASMD	Atmospheric Sciences Modeling Division [of NOAA/ARL]
ATD	atmospheric transport and diffusion
CAMEO	Computer-Aided Management of Emergency Operations [software system]
CBNP	Chemical and Biological National Security Program
CBRN	chemical, biological, radiological, or nuclear
CBRNE	chemical, biological, radiological, nuclear or high-yield explosive
CFD	computational fluid dynamics
CD-ROM	compact disk–read-only memory
CMAQ	Community Model for Air Quality
CMAT	Consequence Management Advisory Team
CSEPP	Chemical Stockpile Emergency Preparedness Program
CTM	chemical transport model
DAS	data assimilation system
DOE	Department of Energy
DHS	Department of Homeland Security
DNA	Defense Nuclear Agency
DNS	direct numerical simulation
DOD	Department of Defense
DTRA	Defense Threat Reduction Agency
EPA	U.S. Environmental Protection Agency
EP&R	Emergency Preparedness and Response [Directorate of DHS]
ESSA	Environmental Sciences Services Administration
FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FEMA	Federal Emergency Management Agency
FRMAC	Federal Radiological Monitoring and Assessment Center
GMU	George Mason University
GIS	geographical information system
GPS	Global Positioning System
HAZMAT	hazardous material
HMRD	Hazardous Materials Response and Assessment Division [of NOAA]

HPAC	Hazard Prediction and Assessment Capability
JAG	Joint Action Group; unless otherwise qualified, the JAG/ATD(R&DP), which is the author of record of this R&D plan.
JAG/ATD(R&DP)	Joint Action Group for Atmospheric Transport and Diffusion Modeling (R&D Plan)
JAG/SEATD	Joint Action Group for Selection and Evaluation of Atmospheric Transport and Diffusion Models
JEM	Joint Effects Model
JTF-CS	Joint Task Force for Civil Support
LES	large eddy simulation
LFA	lead Federal agency
LINC	Local Integration of NARAC with Cities
LLNL	Lawrence Livermore National Laboratory
LOE	level of effort
MAC	Mapping Analysis Center
MADONA	Meteorology and Diffusion over Non-Uniform Areas [field study]
METOC	Meteorology and Oceanography [U.S. Navy]
METREX	Metropolitan Tracer Experiment
MOA	memorandum of agreement
MUST	Mock Urban Settings Test
NARAC	National Atmospheric Release Advisory Center
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NIRT	Nuclear Incident Response Team
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
NORTHCOM	U.S. Northern Command [of DOD]
NRC	Nuclear Regulatory Commission
NTS	Nevada Test Site
NWP	numeric weather prediction
NWS	National Weather Service of the National Oceanic and Atmospheric Administration
OFCM	Office of the Federal Coordinator for Meteorological Services and Supporting Research
OSE	observation system experiment
OSSE	observation system simulation experiment
OWS	Operational Weather Squadron
QA/QC	quality acceptance and quality control
R&D	research and development
RAP	Radiological Assistance Program
RDT&E	research, development, test, and evaluation
READY	Realtime Environmental Applications and Display System
SBIR	Small Business Innovative Research
SBL	stable boundary layer

SDO	standard development organization
SORD	Special Operations and Research Division [of NOAA/ARL]
STTR	Small Business Technology Transfer [program]
UAV	unmanned aerial vehicle
VTMX	Vertical Transport and Mixing [field program]
WMD	weapons of mass destruction
WRF	Weather Research and Forecasting [model]
WSR-88D	Weather Service Radar 1988, Doppler (also Doppler Weather Radar; NEXRAD)

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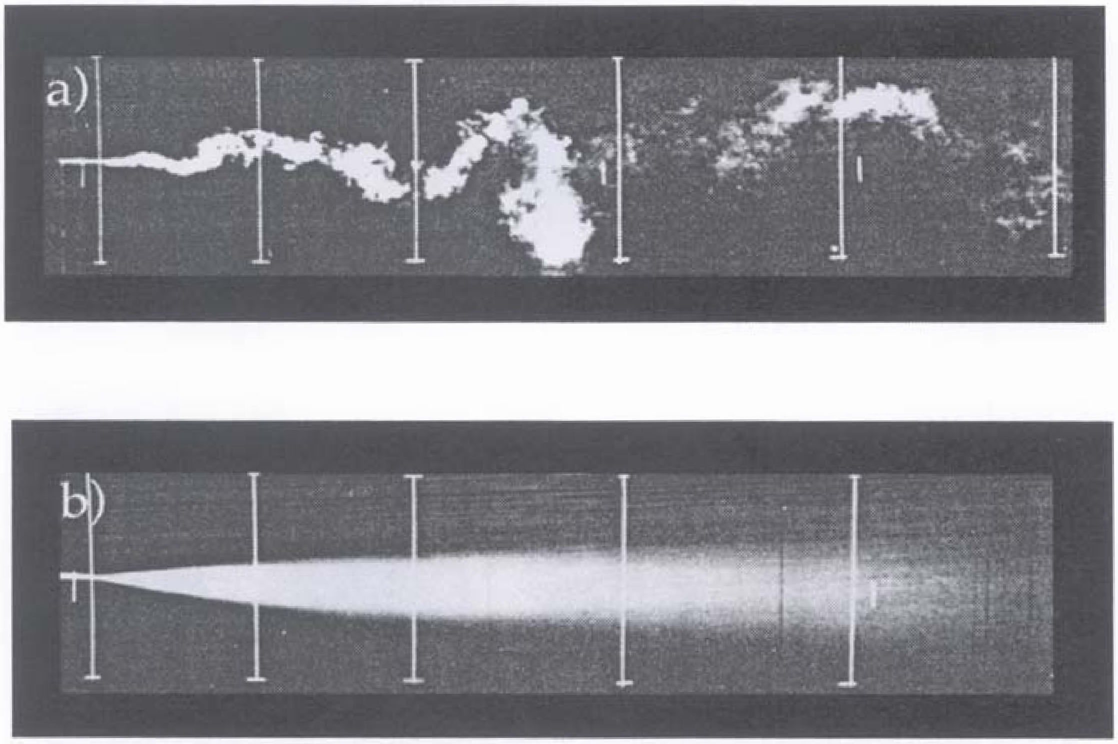

Two images of the same release. In (a) we see a photograph of an instant during a point source release of smoke within a wind tunnel (view is taken looking down on the plume), where large and small swirls have distorted the plume into serpentine twists and turns. In (b) we see a time-average photographic exposure of the smoke release, where the time-average of the individual chaotic swirls are seen to have the “traditional” Gaussian plume shape used in ATD plume dispersion models. (Photographs are courtesy of U.S. EPA/NOAA Fluid Modeling Facility).

Model of World Trade Center site, Manhattan, New York City in the U.S. EPA/NOAA Fluid Modeling Facility.