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Survey and Discussion of Models Applicable to the Transport and Fate Thrust Area of the Department of Energy Chemical and Biological Nonproliferation Program

Argonne National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory

Environmental Energy Technologies Division

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CONTENTS

Foreword ..... *iii*
Executive Summary ..... *v*
1. Introduction **1-1**
1.1 The Threat 1-1
1.2 Responding to the Threat 1-1
1.3 Transport and Fate 1-1
1.4 Model Requirements 1-3
1.5 Data Needs 1-5
1.6 Research Needs 1-6
1.7 Transport and Fate Direction 1-6
2. Subway Transport and Fate Models **2-1**
2.1 Background and Purpose 2-1
2.2 Subway System Modeling 2-2
2.3 Subway Station Modeling 2-6
2.4 Transport and Fate Team Modeling Capabilities 2-11
2.5 Findings and Recommendations 2-11
3. Buildings Interior Transport and Fate Modeling **3-1**
3.1 Overview of Buildings Interior Transport and Fate Modeling 3-1
3.2 Interzonal Models 3-1
3.3 Intrazonal Models 3-7
3.4 Advanced Building Simulation Model 3-10
3.5 Indoor Pollutant Behavior Models 3-10
3.6 Findings and Recommendations 3-12
4. Models for Flow and Transport Around Buildings **4-1**
4.1 Introduction 4-1
4.2 Rationale 4-1
4.3 Computational Fluid Dynamics Models 4-2
4.4 CFD Model Review Studies - Flow Around Building Application 4-3
4.5 Analytical-Empirical Models 4-8
4.6 Field and Wind-Tunnel Experiments 4-10
4.7 Research Issues 4-10
4.8 Findings and Recommendations 4-14
5. Local-Regional Meteorology and Dispersion Models **5-1**
5.1 Introduction 5-1
5.2 Modeling Strategies 5-2
5.3 Diagnostic Wind Field Models 5-3
5.4 Diagnostic Model Surveys and Evaluations 5-3
5.5 Diagnostic Model Findings and Recommendations 5-4
5.6 Prognostic Wind Field Models 5-4
5.7 Prognostic Model Surveys and Evaluations 5-6
5.8 Prognostic Model Findings and Recommendations 5-7
5.9 Local-Regional Dispersion Models 5-7
5.10 Recent Dispersion Model Evaluations 5-9
5.11 User Base of Transport and Fate Team Dispersion Models 5-16
5.12 Dispersion Model Findings and Recommendations 5-16
5.13 Conclusions 5-17
Appendix. Transport and Fate Model Summaries **A-1**

Foreword

This report was the result of a multi-laboratory effort of the Transport and Fate thrust area team of the Department of Energy's Chemical and Biological Nonproliferation Program. The report was prepared for the Office of Nonproliferation and National Security at the request of the following:

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EXECUTIVE SUMMARY

The U.S. Department of Energy (DOE) established the Chemical and Biological Nonproliferation Program (CBNP) to address the threat to national security posed by the proliferation of chemical and biological (C/B)weapons. Transport and Fate (T&F) is one of six thrust areas within the CBNP program. Efforts within the T&F thrust area are directed toward the support of the Incident Response mission to an urban terrorist C/B attack including preplanning and mitigation, real-time response, and post event analysis and reconstruction. Within this mission focus, the T&F team has two general goals: (1) to develop an integrated and validated state-of-the-artatmospheric transport and fate modeling capability for chemical and biological agent releases within the complex urban environment and (2) to apply these modeling capabilities in a broad range of case studies to explore the range of probable consequences.

The first task of the T&F team has been to survey existing modeling capabilities for the various scales that are involved in chemical and biological releases in the urban environment. In the survey, we identify existing modeling capabilities, recommend and justify the selection of models to be used in the transport and fate studies, identify capabilities that should be added to the team's suite of models, and identify areas where research and development is needed to meet the goals of the T&F thrust area. The transport and fate area has been divided into four sub-areas, delineated by scale and by physical considerations. The four sub-areas are: 1) flow through a subway system and through a subway station, 2) flow in the interior of a building, including exchanges through multiple zones in the building, 3) flow around the exterior of buildings, including multi-building complexes, and 4) flow to the local and regional scale, including the effects of urban complexes.

The atmospheric transport and fate area contains many models developed for many different purposes. The criteria for selection of models for this program were based on the following items listed in order of priority:

(1) applicability to user needs,
(2) state-of-the-artscience,
(3) publicly available literature of testing and validation,
(4) national and/or international recognition of use,
(5) preference for publicly available computer codes, and
(6) team experience with the model.

The T&F team chose models that were developed by other federal agencies, international cooperative efforts, private firms, and universities, as well as models developed by the DOE laboratories. The choices in many areas are not unique, but will provide the capabilities needed in a cost-effective manner. Moreover, the choice of models is consistent with the Atmospheric Release Advisory Capability (ARAC) which is the real-time incident response capability planned for use in this program.

In conclusion, the DOE has made significant investments over the past two decades in developing research and operational capabilities in transport and fate modeling and analysis. It is the intention of the T&F team to build on this investment and the DOE commitment to solve complex problems of importance to science and national security using high performance computing capabilities.

Subway Transport and Fate (Chapter 2)

One-dimensional time-dependent modeling of flows, temperature, and humidity has been shown to be adequate for modeling the ventilation within a subway system. The T&F team chose the Subway Environment Simulation (SES) model to be the core model for further studies as it is the de facto standard for modeling subway system behavior. SES was developed for the Department of Transportation (DOT) and it has been used in the design of ventilation systems for over 20 subway systems throughout the world. Capabilities for treating source term behavior, contaminant dispersion, and C/B agent behavior will be added to SES to meet the requirements of the T&F thrust area.

Computational fluid dynamics (CFD) models are appropriate for modeling dispersion within subway stations. A wide variety of models exist with similar capabilities. Many of the CFD models are proprietary, with the proprietary models frequently being more user-friendly. However, the fundamental capabilities of the T&F team models are on a par with the proprietary models and with other non-proprietary models. GASFLOW, a model developed at LANL, will be used for subway station modeling. Capabilities for complex geometry, moving

trains, and C/B agent behavior will be added to GASFLOW. Other CFD models may be used for special niche applications, especially CFX 4.1 (developed by AEA Technologies) which includes aerosol physics and is being adapted for C/B applications by the Department of Defense (DOD).

Building Interior Transport and Fate (Chapter 3)

The survey of interior building flow models is built on a 1992 survey, in which 50 different air flow models were reviewed. The 50 models encompassed a wide range of capabilities and applications, but many are not available to third parties and are not "user-friendly". Only two models, COMIS and CONTAM, meet the requirements of the T&F team. COMIS was developed at LBNL by an international team of scientists from nine countries and was chosen as the core model for most applications. In addition, MIAQ4 (developed at U.C. Berkeley and LBNL) was selected to model aerosol deposition in rooms. Research and development is needed for aerosol deposition in ducts, sorption and re-emission of vapors, and the effect of different surface materials.

Some CFD modeling is also required to address specific research issues that arise in developing lumped parameter models. A number of CFD models are available (see discussion above in Subway Transport and Fate, and below in Flow and Transport Around Buildings) for this purpose, each with certain capabilities and limitations. The CFD model most appropriate for the particular research problem will be utilized.

Flow and Transport Around Buildings (Chapter 4)

The exterior building flow problem ranges from flow around an individual building, to flow around a complex of several buildings, to flow within a domain including many buildings and several city blocks. CFD models are used to calculate the detailed flow fields, and from the detailed flows, parameterizations for simpler analytical/empirical models can be formulated. Several T&F team models, DYNAFLOW and FEM3C (developed at LLNL), and GASFLOW and HIGRAD (developed at LANL) are state of the art, are available and will be used for different aspects of the problem. Each has different strengths, weaknesses and capabilities. Physics modules will be added, as appropriate, for aerosol transport, vapor and aerosol deposition, dense gas dispersion and C/B behavior.

Local-Regional Meteorology and Dispersion (Chapter 5)

Contaminant dispersion on the local-region scale is usually thought of as two separate but coupled problems: 1) developing the wind field, and 2) forecasting the dispersion. The wind field can be derived using either simple diagnostic models (no forecast capability) or more complex prognostic models. Similarly, the dispersion models range in complexity from simple plume models to three-dimensional, time dependent stochastic particle models. In each category of models, a number of models were found to be recognized as state-of-the-art for their ability to simulate various wind field and dispersion scenarios; however, no single model stood above the rest for all applications. Furthermore, the conclusions of earlier surveys and evaluations indicate that familiarity with the models is often the most important factor in successful applications.

Diagnostic wind field models have an important role for real-time incident response due to their speed in calculating a first estimate of the wind field, but are limited by available local observations and are restricted to persistence (constant in time). Prognostic models provide a forecast capability of up to 2 or 3 days; however, the high computational time required to complete a forecast currently restricts their use to applications at specific locations, longer duration or anticipated events, and other special circumstances. Non-hydrostatic prognostic models solve the complete set of atmospheric equations and are applicable at scales from global down to local. Hydrostatic models approximate the vertical momentum equation and are restricted to scenarios where vertical motions are small relative to the horizontal.

On the local-regional scale, spatial and temporal variations in the wind field can be critical and need to be included in the dispersion calculation. Three-dimensional Lagrangian puff and particle models and three-dimensional Eulerian models meet this requirement with the Lagrangian particle models being the most versatile. Several of the T&F team dispersion models are of this type and are recognized by the scientific community as state-of-the-art, contain a range of features directly applicable to C/B releases, have extensive validation and verification, and have performed well in independent reviews such as the recent international ETEX experiments and model evaluation.

Local-regional model suites selected by the T&F team for future application studies and further development are: the current operational ARAC models MATHEW-ADPIC and the future operational ARAC models ADAPT-NORAPS/COAMPS-LODI; the non-hydrostatic wind field and dispersion models RAMS-HYPACT developed by Colorado State University; and the hydrostatic wind field and dispersion models HOTMAC-RAPTAD developed at LANL. The NORAPS and COAMPS wind field models were developed by the DOD's Naval Research Laboratory and are hydrostatic and non-hydrostatic, respectively. The other ARAC codes were developed at LLNL.

Algorithms for simulating some of the physical processes that affect C/B agent transformation need to be added to the regional dispersion models. We also recommend research for including more realistic representations of the source term, developing methods for treating the effects of structures within the urban environment, and characterizing the uncertainty of the contaminant concentration forecast.

Final Comments

Significant challenges exist for the successful prediction of the transport and fate of C/B agents in urban environments. Trade-offs need to be addressed between model sophistication, accuracy and computer power available to specific applications. Innovative research efforts are required in the areas of numerics, turbulence closure methods, gaseous and aerosol dispersion physics and chemistry, and high performance computing.

During the development of the T&F multi-scale capability, attention should also be paid to the validation process. Relevant data from laboratory and field experiments need to be identified and a measurement program to obtain verification data should be encouraged within DOE or partner agencies. In addition, it is also recommended that a collaboration be established with local emergency managers to identify those capabilities of greatest relevance to emergency responders and planners.

1. INTRODUCTION

1.1 The Threat

The availability and easy production of toxic chemical and biological agents by domestic and international terrorists pose a serious threat to U.S. national security, especially to civilian populations in and around urban areas. Testimony to the U.S. Congress has emphasized this point.

"Concern about the proliferation of weapons of mass destruction (nuclear, biological, and chemical - NBC) and terrorism is decades old, but to date, the threat of NBC terrorism has been regarded as low. Accordingly, preparing to meet NBC threats has not been a major focus of U.S. national security planning and policy. Recent developments, from nuclear smuggling out of the former Soviet Union, to the terrorist use of nerve gas in a crowded Tokyo subway, to the rapid diffusion of technologies applicable to the manufacture of biological weapons, have heightened the visibility of the NBC threat to national security. It is essential to better understand and characterize the threat; to analyze the military and especially the civilian vulnerabilities of the United States and its allies; and to assess the policy, technical, and organizational response to the threat. A major R&D effort at the National Laboratories will be needed to meet these challenges.

There are over 20 countries suspected of some form of nuclear, biological, or chemical proliferation. In addition, subnational, organized crime, and other terrorist groups that could gain access to these materials are of growing concern. Events two years ago in Tokyo heighten the gravity and seriousness of the situation and highlight the vulnerability of U.S. civilians and interests. The proliferation of weapons of mass destruction is the most urgent and direct threat to national security. The threat to U.S. civilians and interests is real, and the political, societal, economic, and psychological impacts are potentially devastating. The consequences of failure in countering the threat could be catastrophic. We cannot afford to be surprised, nor, as one senior government official put it, (be) 'exchanging calling cards at the site of an NBC incident.'" - *Congressional Record*

The list of chemical and biological agents accessible to the terrorist is lengthy. Those that have been used (more or less successfully) and those for which the actual material was discovered prior to use include: sarin (GB), cyanide, ricin, botulinum toxin, typhoid, anthrax, and salmonella. Dispersion of chemical or biological agents by the terrorist may be made by very simple means. Aerosols may be generated by insect foggers, pressurized cans with spray nozzles, vacuum cleaners, aspirators, airless paint sprayers, fire extinguishers, etc. Transport and concealment may be as simple as briefcases, lunch boxes, or plain plastic bags. In addition, the potential exists for large agent releases through the use of truck-mounted sprayers or crop dusters provide means to increase the mass of agent.

1.2 Responding to the Threat

To address this threat, the Department of Energy (DOE) has established the Chemical and Biological Nonproliferation Program (CBNP) with the goal of focusing the DOE's technical resources and expertise on capabilities to deny, deter, mitigate and respond to clandestine releases of chemical and biological agents. With the intent to build on DOE core competencies, the DOE has established six technology thrust areas within the CBNP Program: Biological Information Resources; Point Sensor Systems; Stand-off Detection; Transport and Fate; Decontamination; and Systems Analysis and Integration. These technical thrust areas address four national missions: Intelligence and Assessment, Policy and Treaty Support, Incident Response, and Support to Military Operations.

1.3 Transport and Fate

The purpose of the Transport and Fate Thrust is to accurately predict the dispersion, concentration and ultimate fate of chemical and biological agents released into the urban and suburban environments. Transport and Fate primarily supports the Incident Response mission and in so doing will concentrate on release and dispersion in the atmosphere. However, the sophisticated simulation and analysis tools that will be available can readily be employed in support of the intelligence and military operations missions. Support to Incident Response will be multi-faceted with the intent to enhance effective planning and management of emergency response operations and ultimately, to safeguard human health and life. Consequently, the Transport and Fate Thrust Area has two major goals:

(1) to develop an integrated and validated state-of-the-art atmospheric transport and fate modeling capability for chemical and biological agent releases within the complex urban environment from the regional scale down to building and subway interiors, and

(2) to apply this modeling capability in a broad range of simulation case studies of chemical and biological agent release scenarios in suburban, urban and confined (buildings and subways) environments and provide analysis for the incident response user community.

The capability to be developed is unique and will provide customers in the intelligence, law enforcement and emergency management communities a heretofore unrealized ability to better protect the security and lives of our citizens. We will achieve this capability for incident responses to the release of chemical and biological agents through development of documented and validated models of the highly distorted flow, complex chemistry and transport in the immediate vicinity of and within urban buildings and subways, along with improved depiction and communication of results to users.

The Incident Response mission has three phases: 1) pre-incident planning and vulnerability assessment; 2) real-time incident response, mitigation, and damage assessment; and 3) post-incident reconstruction and consequence analysis. The ultimate goal of all three phases is to protect people and property; however, the specific goals and constraints inherent to each phase determines the importance of various model-related activities and the appropriateness of general classes of models.

In the pre-incident planning and vulnerability assessment phase, studies are conducted to identify the range and likelihood of potential events, the consequences of these events, and possible mitigation measures. Model simulation predictions are an integral part of these emergency management planning activities and often lead to improvement of safety procedures, deployment of sensors, modification of facility operations and retrofitting of facilities. In model simulation studies of this type, the source and meteorological conditions are generally specified, so that the focus of model simulations is on the transport of the released agent. Important physical processes include atmospheric dispersion, chemistry, degradation of bio-agent viability, deposition (especially for indoor releases), and resuspension. Since an actual emergency is generally not imminent, the time-constraints on these studies are not severe allowing for the use of physically complete and sophisticated modeling capabilities.

In an actual emergency incident, mitigation of consequences and protection of the public are the primary concerns and time is of the essence. Real-time model predictions of agent dispersion, concentration and deposition can help identify affected areas, estimate exposure levels, and characterize the source. This information can then be used by emergency response managers to notify health officials of potential casualties, inform emergency response teams of hazardous locations, and make a variety of public safety decisions. Emergency response applications require very fast and robust computational tools that can be applied to a multitude of situations. Rapid acquisition and assimilation of relevant geographic and meteorological data and rapid generation of accurate windfields are essential for the development of meaningful simulations of agent dispersion in an actual event. Currently, time constraints during an emergency incident dictate the use of models simpler than state-of-the-art and the use of parameterizations for certain model components. However, in the near future, advances in computer technology will allow for greater use of physically complete, high resolution models in real-time response.

In the post-incident reconstruction and consequence analysis phase, a more complete understanding of the evolution and consequences of the event and the discovery of improved emergency response procedures are sought. Transport and fate model predictions are again a primary tool for source characterization, support of decontamination efforts and continuing medical assistance efforts, and for consequence analysis. As was the case in the real-time incident phase, meaningful reconstruction simulations of the time-history of the dispersing agent are highly dependent on being able to accurately generate the actual meteorological fields that are then used to drive the dispersion calculations (exterior releases). Generally, time constraints are significantly relaxed in the post-incident phase, allowing for the use of more detailed modeling approaches.

The first task of the Transport and Fate Thrust Area is to conduct a survey of models that could be applied to chemical and biological releases within the urban environment in support of the incident response mission. The objectives of the survey are:

(1) to discover and document current applicable modeling capabilities, both in and out of the DOE,

(2) to identify currently available modeling capabilities that should be built upon or added to the DOE suite of models,

(3) to recommend and justify the selection of models with which to begin studies in Transport and Fate, and

(4) to identify technical needs for which further research and model development is warranted to meet the goals of this thrust area.

In addition to an evaluation of the applicability of a model as a whole, specific scientific components or algorithms that represent important modeling capabilities will be reviewed for possible incorporation into the selected suite of models.

A number of specific tasks have been identified in order to fulfill the objectives of this model survey within the directives of the program sponsors. They are:

- Review recent surveys of transport and fate models and identify relevant findings.
- Review recent model evaluation studies and identify relevant findings and recommendations.
- Interview DOD, DOT, EPA and other agencies regarding their modeling capabilities for chemical and biological releases in the urban environment.
- Identify and review transport and fate models available within the DOE laboratories that may be applicable to chemical and biological releases within the urban environment.
- Categorize transport and fate models based on simulation scale (interior, microscale, mesoscale), completeness of physical description, and intended application.

These tasks will provide the necessary information to identify and recommend the modeling capabilities to be used within the DOE CBNP Transport and Fate Thrust Area and to identify research and development efforts to establish an integrated and validated state-of-the-art atmospheric transport and fate modeling capability for chemical and biological agent releases within the urban environment.

1.4 Model Requirements

The transport and fate problem is multi-scale with phenomena that occur at each scale providing boundary conditions or initial conditions for the next scale up or down. The interior of the subway car, the subway station, or the public building may have to be modeled with a fine grid resolution. The few-building microscale might require a resolution of 2-5 meters and the many-building microscale 10-50 meters. The local to regional scale would be modeled with a resolution of one km up to several km. Overlaid across all scales is the need to model the physical and chemical behavior of the gaseous or aerosolized agent. Determination of the fate of the chemical and biological (CB) agent as it is transported requires knowledge and modeling of gas-phase, surface, and multi-phase chemistry, deposition and resuspension, and bio-agent viability as a function of temperature, humidity, and sunlight.

Subway Interiors

There are three main types of releases of a CB agent in the interior of a subway. They are (a) releases in a subway station, (b) release in a subway railcar, and (c) release through the ventilation shaft into the subway tunnel. All of these have the potential, due to train movement and ventilation systems, of dispersing through the subway system or to street level.

Two types of models have traditionally been used to simulate the flows and dispersion in subways. A *subway system model* is a one-dimensional, time-dependent network model that predicts flow and dispersion throughout a network of stations and tunnels. The subway system model accounts for the piston effect of moving trains and air movement resulting from the operation of fans in the ventilation shafts. A very limited number of such models exist.

The *subway station model* is a three-dimensional computational fluid dynamics (CFD) model and is aimed at a more precise understanding of the three-dimensional flow within a station itself. The station might include the subway platform, a mezzanine area, and a street level entrance connected by stairs or escalators. Some transit authorities have insisted on the use of 3-D CFD modeling before the purchase of station emergency ventilation systems. Simulation of the detailed station dynamics can help provide a better understanding of the flows and dispersion from pollutant releases (the typical application is for smoke) and can aid in evaluating evacuation routes. Both public domain and commercial 3-D CFD models are available.

Building Interiors

Buildings are classified into two main categories: residential and commercial. Single family residential buildings would be most impacted by ventilation and infiltration following an exterior release. Commercial and multi-family residential buildings are more likely to be targeted for an interior CB agent release because of their high occupancies. The most likely types of buildings for CB agent releases are probably shopping centers, office

buildings, schools, public assembly buildings, and airports. Many of these buildings have central heating, ventilating and air-conditioning systems (HVAC) in which various proportions of outside and re-circulated air are thermally conditioned and then distributed throughout the building by duct systems.

Several modes for release and subsequent dispersion throughout the building are possible for these major categories of buildings:

(1) release into an outside air intake, with subsequent distribution throughout the building by the ventilation system;

(2) release within the HVAC system, either into the mechanical system or in a duct, with subsequent dispersion throughout the building by the HVAC system;

(3) release within a large central room with high occupancy (e.g., auditorium, airport terminal), with subsequent dispersion within the space and throughout the building by convective and advective air movement and/or by re-circulation by the HVAC system;

(4) release within a room in a building, with subsequent dispersion throughout the building due to interzonal airflows from pressure differenceswithin the building and/or through recirculation by an HVAC system;

(5) release within a stairwell of a multistory building with subsequent dispersion throughout the building due to interzonal airflows and pressure differences.

Predicting the transport and fate of CB aerosols and vapors in building interiors requires *models for interzonal airflows* within the buildings, including duct systems, and infiltration of outside air through building envelopes. There are just a few models which have been developed for this purpose and these have been tested only to a limited degree against measurement data. In addition, because building interiors have large surface-to-volume ratios, models are required to predict the *depositional losses of aerosols and vapors* to interior surfaces and building envelopes (during infiltration of outside air), *and the sorption and re-emission of vapors* from various indoor materials, since these losses can be large. There is one existing model that predicts depositional losses of aerosols to indoor surfaces as a function of particle size and air turbulence, and there is also one model for prediction of depositional losses of aerosols in simple duct systems. Models to estimate sorption losses and re-emission of vapors from indoor surface materials, including ducts, have not been well developed, although this is an active area of research in the indoor air research community.

Around Buildings

Models for predicting air contaminant concentration levels in the vicinity of buildings can be divided into *analytic*, *diagnostic*, and *prognostic* categories. *The prognostic CFD models*, based on physics-based conservation laws for mass, momentum, and energy, are in principle capable of simulating the flow and dispersion fields in detail around individual or multiple buildings. CFD models can be used for a wide range of applications, but are relatively slow and computer intensive. CFD models that have been validated for single building and urban canyon geometries are in general agreement with measured mean flow fields, but there is usually some disagreement in the turbulence fields. There have been few attempts, if any, at detailed 3-D modeling of many-building complexes due to computational limitations.

The *analytic models*, usually based on Gaussian dispersion algorithms, either account for the macroscopic effects of many buildings through modified plume spread coefficients or treat the microscopic effects of one or two buildings individually through dimensional or empirical parameterizations. In the macroscopic case, the plume dispersion is enhanced -- but not obstructed -- by buildings, so that regions of high and low concentrations around buildings are not computed. In the microscopic case, concentration fields are computed around a single building or between buildings, but the effect of many buildings on dispersion is not considered. Analytic models are fast and easy-to-use, but suffer from over-simplification and lack of generality.

Diagnostic models usually begin with an objective analysis (e.g., based on experience we know a vortex develops on the rooftop of a building and a cavity region develops downwind of the building, the sizes of which are determined from empirically-derived equations) and then the flow field is modified to satisfy mass conservation conditions using numerical minimization techniques. Diagnostic models are much slower than analytic models, but faster than prognostic models. Like analytic models, they suffer from over-simplification and lack of generality. However, diagnostic models have been used for modeling flow and dispersion fields around building complexes.

To be completely general, analytic and diagnostic models would require that thousands of carefully-controlled experiments be performed under numerous atmospheric conditions, for many building shapes, spacings, etc., so that empirically-derived parameterizations can be derived for the many real-world conditions that exist. Prognostic CFD models, validated using a few, well-controlled experiments, could be used in lieu of field experiments to develop some of these parameterizations at reduced cost.

Local To Regional

The spatial range of concern for an urban release of a chemical or biological agent on the local to regional scale extends across large areas of the urban environment on out to the surrounding suburbs for tens and even as much as a hundred kilometers. At these spatial scales, the wind field and resultant dispersion pattern are affected by topography, differences in the surface forcing and the presence of weather systems. Buildings are not treated explicitly, so their effectsneed to be parameterized within the local to regional meteorology and dispersion models. While the modeling of dispersion around buildings is usually done with a single model forecasting both the wind field and the dispersion, the atmospheric dispersion and emergency response communities have found it to be more convenient and cost effective to use two separate models on the local to regional scale: one to produce the *wind field* and another to forecast the *dispersion.*

The windfield (meteorological) information may be provided by either *diagnostic* or *prognostic models. Diagnostic models* produce a stationary analysis of atmospheric structure using observations along with topography and simple physical constraints. They are fast and most appropriate for small temporal and spatial scales. Some may provide rough estimates of turbulence, solar radiation and precipitation. These models are well suited for either initial emergency response calculations or post-accident analysis.

Prognostic models produce a time varying analysis of the atmospheric structure, solving a time dependent system of equations which represent a more detailed description of the physics. They work well on small spatial scales and can be extended through the regional scale to global problems if necessary. Prognostic models also provide more detailed meteorological information so that more sophisticated dispersion models may be employed. However, prognostic models are computer intensive and are not presently well-suited for real-time response except for support at specific sites or events where they may be set up before hand.

A *dispersion model* uses winds, temperature and stability, turbulence intensity and solar radiative flux to produce forecasts of contaminant concentration, deposition and exposure. Local to regional scale dispersion models range in complexity from simple Gaussian plume models to puff models to particle models. Algorithms have been added to some dispersion models to treat CB agent related physical processes such as gravitational settling of aerosols, ground deposition, droplet evaporation, chemical reactions, and bio-agent viability degradation. Simpler models have the advantage of ease of use and rapid execution time. However, because of the simplicity they sacrifice accuracy and general applicability. The more complex models, such as particle models, use not only accurate representations of the terrain, but also time-varying, three-dimensional winds and turbulent intensities to produce concentration fields. Also, these models often incorporate more detailed physical processes. Particle models are generally more accurate and have a wider range of applicability. However, they are more computer intensive than the simpler models.

1.5 Data Needs

There are data input needs required to operate all models. These needs are determined by both the model and the particular problem to be addressed. For real-time response, models often draw upon previously assembled data bases and/or default values due to the requirement for rapid predictions. In some cases, a simpler model with fewer data input requirements can be used. However, for pre-incident planning and post-incident analyses, more detailed and data intensive models are likely to be needed and used to provide greater predictive accuracy. The data needs can be met in some cases by pre-assembled data bases. In others, the modeling effort will require assembling some of the input data to fit the specific problem to be addressed. The types of data required for transport and fate modeling, in general, are summarized below. Again, the level of detail required depends on whether the application is pre-planning, incident response, or post-event reconstruction.

Source Data

The accuracy achieved in modeling the transport and fate of chemical or biological agents is greatly dependent upon knowledge of the source information. This not only includes information on the amount of agent released and the method of release, but also on the agent's characteristics as they relate to exposure to ambient conditions. When source data is not available for an incident, simulations may be run to bracket the estimates. When sensor or laboratory data become available, Transport and Fate simulations may be used to reconstruct the strength and location of the source term.

Meteorological Data

Abundant meteorological data including vertical profiles increases the assurance of meteorological modeling and subsequent dispersion modeling. While modern prognostic models may be initialized with a minimum of data, additional data for assimilation will improve the results. An assimilation system is a means to combine observations with model forecasts or analyses to provide the best estimates of the key quantities. There are two modes of operation for assimilating data: cold start and continuous. A cold start means that there is no background, analyzed field into which the latest observations are merged. Available observations are combined with physical constraints to produce estimates of the winds and thermodynamic fields. In continuous assimilation, local observations are used to adjust an existing forecast or analysis, producing detailed fine scale estimates. Generally, continuous assimilation is preferred. However, time pressure or lack of existing analysis may necessitate a cold start assimilation.

Geographic Data

The geographic data needed depends upon the scale of the problem and the sophistication of the modeling system used. The minimum information needed for the regional scale is terrain elevations and surface roughness at the resolution of the model grid. As the sophistication of the model used increases so do the data needs. Additional information needed may include: surface albedo, land/water masks delineating the coast and shore lines, soil type, soil moisture, land use, and vegetation type and phenology.

As one moves down in scale to flow through a city, terrain elevations may or may not be important, but a layout of the city streets and highways as well as general descriptions of and locations of the buildings and green space within the city are necessary. Moving down in scale further to flow around a particular building or a small group of buildings now requires a detailed description of each building's exterior.

Building Data

The need for details of building layout and operation naturally increases with the desired sophistication of the analysis. For real-time or near real-time incident response generic descriptions appropriate to the class of building may have to suffice. For pre-incident planning or post-incident reconstruction complete building plans and HVAC operations plans are necessary. An inventory of surface materials (wall, floor, ceiling) and furniture is also needed. External windfields, cross-building pressure differentials, and external source terms are needed to evaluate infiltration into a building from an external release.

Subway System Data

Characterization of a subway system for CB agent modeling requires considering the physical characteristics, of the system, physical and performance characteristics of the trains, and subway operations data. Physical characteristics of the system include details on subway alignment (plan and profile) together with (1) the location of stations, ventilation shafts and fan shafts; (2) the cross-section information of tunnels and stations; and (3) the dimensions of the fan shafts, ventilation shafts, dampers, gratings, etc. Architectural drawings of the subway system provide much of this information. Physical and performance data of the trains include physical dimensions of cars, train configurations (number of cars per trains), and train performance data (includes deceleration rate and maximum acceleration rate). Finally, subway operations data includes train scheduling parameters such as headways, station stops, and dwell times, as well as changes in passenger loading. The operations data also includes information concerning the mechanical ventilation system such as fan performance curves for supply/exhaust fans during normal and/or emergency operations. For subway station modeling, details of the geometrical configuration of the multi-level system including platform, mezzanine and street level along with escalator and stair configurations is required.

1.6 Research Needs

Research needs and areas in which existing models should be improved are documented within each chapter for the models at their respective scales.

1.7 Transport and Fate Direction

The DOE has been a world-leader in developing and using high-performance computing capabilities for the solution of problems of national interest. Some current programs include:

- Accelerated Strategic Computing Initiative (ASCI)
- DOE Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP),

- High Performance Computing and Communications projects.

Further, the DOE has made a commitment to enable the solution of complex problems of importance to science, national defense, industry, and society and to be a leader in developing and using computational and information technologies. Over the past two decades, the DOE has also made significant investments in operational and research transport and fate modeling and analysis capabilities. The intention of the Transport and Fate Thrust Area team is to build on these complementary investments to develop an integrated and validated state-of-the-artatmospheric transport and fate modeling capability for chemical and biological agent releases within the complex urban environment from the regional scale down to building and subway interiors using models that incorporate the best science available.

In the following chapters a survey and review of models is given, with recommendations for the models to be used within the DOE CBNP Program and a description of research needs that can be identified at the start of the program. Chapter 2 covers models for subway systems, Chapter 3 discusses building interior models, Chapter 4 covers models for exterior flows and dispersion around buildings, and Chapter 5 describes local to regional meteorology and dispersion models.

2 SUBWAY TRANSPORT AND FATE MODELS

2.1 Background and Purpose

Statement of the Subway Problem

Subway transport and fate modeling refers to both the modeling of flow and dispersion in individual subway stations as well as the entire subway system containing multiple subway stations, tunnels, and ventilation shafts. Figure 2-1 presents a sketch of the subway transport problem. Here, a chemical or biological incident results in the release of a C/B agent within a subway station. The piston action of the train movement together with the flow generated by the ventilation system acts to disperse the agent within that station as well as to stations along the subway line and possibly to other subway lines at crossover stations. For analysis of this problem, we require a model to predict the dispersion, deposition, resuspension, and fate of the agent. In general, release types fit three categories: (a) releases in stations, (b) releases in subway tunnels (such as down a ventilation shaft), and (c) releases in subway train cars. A subway transport model needs to address all three release possibilities. In addition, modeling tools need to be identified and/or developed to simulate all reasonable scenarios and their consequences both throughout the subway system and within individual subway stations of interest since a single incident can affect the entire subway system.

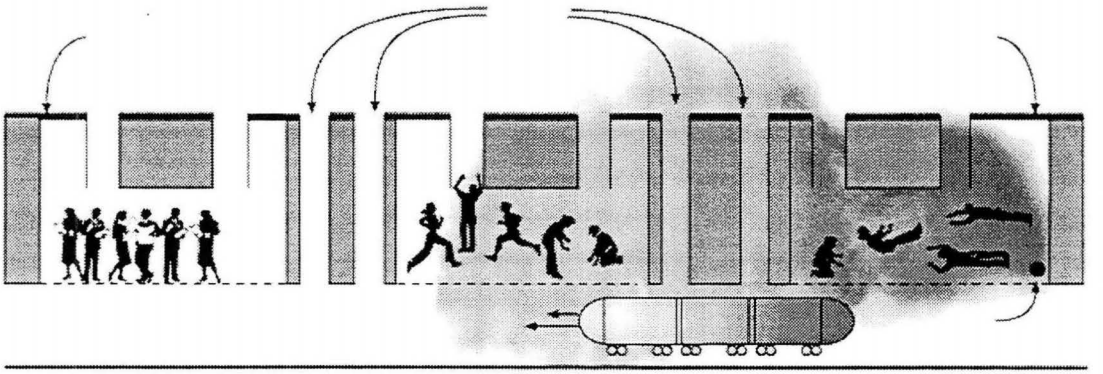

Figure 2-1. Sketch of chemical agent release in subway system with associated transport and dispersion by piston action of a train.

In order to meet the above objectives, it is necessary to identify two classes of models:

(1) subway *system* models that can simulate dispersion through an entire subway system due to release(s) within a station, a tunnel, or a train car, and

(2) subway *station* models that can predict more detailed dispersion characteristics within a particular subway station of interest.

Existing subway system models handle the combination of stations and tunnels. Subway system models treat subway stations in a parameterized manner so that the basic features of subway stations can be considered while allowing the entire subway system to be modeled in real time. As a result, subway system models can be run for both pre-planning, incident response, and post-event analysis.

Existing subway station models are simply specialized applications of more general purpose 3-D CFD models. It is important to emphasize that no 3-D CFD model has been developed specifically for the analysis of subway station flows. This class of models is useful in pre-planning and post-event analysis for a specific station but is not applicable for real-time incident response due to the considerable computational requirements of the codes. In real-time applications, the subway system models are used to predict impacts within stations, albeit in a less detailed manner.

Basic Characteristics of Subway System and Station Models

The principal difference between the subway system and subway station models is that subway system models are variants of one-dimensional network models and subway station models are usually 3-D computational fluid dynamics (CFD) models. Clearly, more detail is provided by the 3-D models for station flows, and such models can be used for locating agent sensors and providing guidance on effectiveevacuation routes. On the other hand, only subway system models predict the dispersion of pollutants through subway tunnels and the impact of the pollutants on the other stations in the system. Subway system models also can predict the emissions to the street level from ventilation shafts as well as provide boundary conditions to 3-D CFD models for individual subway station simulations. Each type of modeling is discussed in turn in Sections 2.2 and 2.3.

General use of Models and Accuracy Considerations

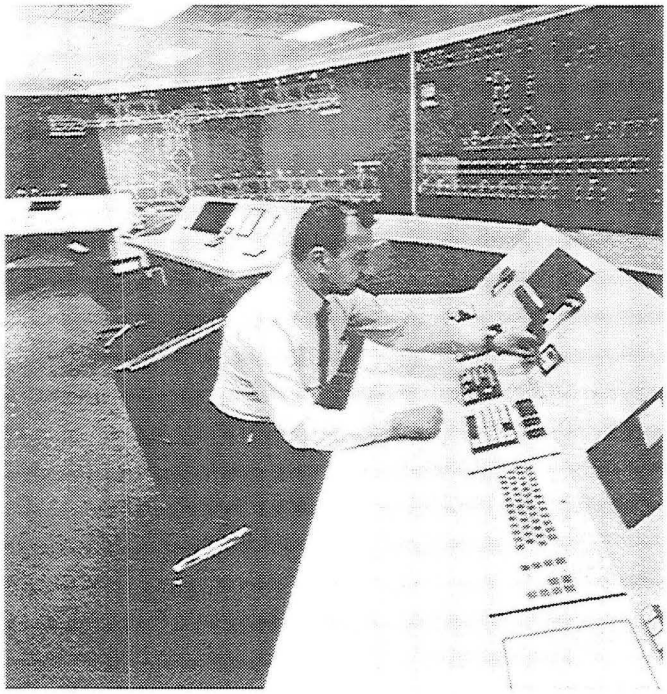

Figure 2-2. Layout of operational control center (OCC) of the BART (Bay Area Rapid Transit) subway system.

As indicated above, the subway system model can be applied in both planning, real-time incident response, and post-event reconstruction. Figure 2-2 shows an operational control center (OCC) of the BART (Bay Area Rapid Transit) subway system. The C/B subway system model developed as part of the current program can be placed on a PC in the OCC and linked to the control system so that the position of all trains in the system at any time can be instantaneously fed into the model. Upon entry of the location and some basic information about the agent release, the subway system model can be used as a decision analysis tool to assess (and optimize) emergency response alternatives and their consequences based on the estimated distribution of people in the subway system and at street level. Such systems are in operation for decision analysis for fires and smoke release in many subway systems today.

The subway station model can be used in pre-planning for point sensor location and for evacuation planning. Additionally, it can be used for post-event analysis to identify the areas of greatest impact in the stations known to be affected by the release.

In the context of the above applications, the issue of model accuracy becomes very important. In considering real-time analyses with subway system models, both the location of contaminated areas and their levels of concentration must be accurately determined so that emergency response and decontamination personnel can be properly deployed. In considering subway station models, the general flow patterns need to be accurately resolved for both point sensor placement and assistance in evacuation planning. However, details such as the accurate prediction of vortices in corner areas are typically unimportant.

2.2 Subway System Modeling

Subway System Fundamentals

A subway system includes multiple tunnels, stations, and ventilation shafts. Releases of C/B agents into a subway system can easily contaminate a large area within the subway system. The piston action of train movements and flows to and from the tunnels from the ventilation shafts provide a natural means of spreading the contamination to other parts of the system. Moreover, deposition to the ground and impaction onto walls and ceiling surfaces can lead to contamination which can resuspend the chemical or biological agents as trains continue to move through the contaminated areas.

A sketch of a typical subway system is presented in Figure 2-3. Due to train movement, hourly passenger number variations, and the presence of ventilation shafts to the outside, the temperature, humidity, and air flow in a subway system is inherently transient. The predominant cooling load is due to electrical and mechanical energy dissipation. In addition, the presence of passengers in train cars and stations adds latent and sensible heat to the thermal energy balance. As a result, the cooling system includes individual train-car cooling systems as well as station cooling systems. The ventilation flow system is governed by the presence and operation of (1) ventilation shafts, stairs and station entrances within the stations; (2) tunnel entrances; (3) street-level and other elevated vents, (4) single and multi-speed fans that are used for either routine or emergency operation; (5) dampers (automatic or electro-pneumatic for system-wide control); and (6) buoyancy-driven flow that is often present within ventilation shafts. Even from this simplified description, it is clear that the modeling of a subway system is very complicated and requires considerable amounts of input data.

Modeling the flow, temperature, and moisture within an entire subway system is commonly done by subway design engineers. They are able to predict the flow, temperature, humidity, and pressure environment as a function of time for the entire system of tunnels, stations, and ventilation shafts. Such computer modeling is typically done for the design of new subway lines and in designing emergency ventilation systems that are aimed at managing smoke during a fire incident. The objective is to assure the physical comfort of passengers in both the train cars and the stations. It is also done to assure that emergency ventilation systems will work well during fire and smoke incidences. Currently, emergency ventilation systems are being upgraded in Chicago, New York, and other cities. The Washington D. C. Metro already has a state-of-the-art ventilation systems in place for both routine and emergency operation. Emergency ventilation systems are advantageous in that they provide the subway control center with a means of employing forced air flow to help manage an emergency situation. The protocol for such emergency ventilation operation has not been set for any subway system in the U.S. at this time for chemical or biological incidents. Clearly, our efforts in this project can provide valuable assistance in this direction.

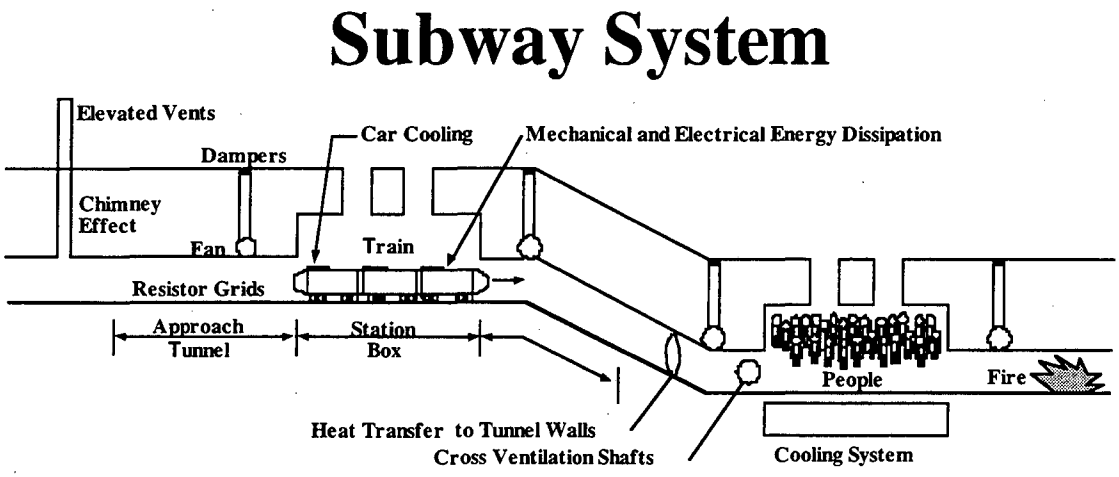

Figure 2-3. Major components and features of subway system required for subway system environmental impacts.

Subway System Models

Subway system models are required because the heat energy released by the cooling systems of the trains and the sensible and latent heat emitted by the passengers lead to elevated temperatures in the subway stations, tunnels, and train cars. Natural ventilation from the subway stations (for those that are of open design) and ventilation shafts are usually not sufficient to cool the stations and tunnels in summertime. Individual train cars require separate ventilation and cooling systems which must be accurately sized. Although the available models were developed for ventilation and cooling system design, they also predict air velocity, temperature, humidity and pressure as a function of time in the subway system once the train schedule and other train performance and system design parameters are specified. It is the predictions of flows and velocities due to the

piston action of train movement and the ventilation fans that are of critical importance in determining C/B agent dispersion and impacts.

Models for subway systems are few in number and are very similar to each other. All are one-dimensional models for the subway tunnels with one-dimensional parameterizations of the stations. The most prominent and successful model is the Subway Environmental Simulation (SES) Model developed for the U.S. DOT. This model has been used in the design of over 20 subway systems around the world including those in Atlanta, Baltimore, Boston, Buffalo, Caracas, Chicago, Dallas, Hong Kong, Los Angeles, Minneapolis, Montreal, New Jersey, New York City, Philadelphia, Pittsburgh, San Francisco, Shanghai, Singapore, Taipei, and Washington D.C. SES was developed from one-dimensional integral theory with considerable empiricism based on laboratory and field data. One consulting firm, Mott and MacDonald in the U.K., has a competing model that yields very similar predictions but uses one-dimensional compressible flow theory. The two models provide very comparable results except in the case of long tunnels where trains travel at high speeds (> 60 mph). In this case, the compressible model often provides improved results. However, this special case is rare in the U.S. The SES approach is valid for nearly all sections of all U.S. subway systems. An additional problem with the Mott-MacDonald model is that it is proprietary and cannot be purchased or used outside that firm. The SES and Mott-MacDonald models are mainly used in the evaluation of proposed ventilation and cooling systems to determine if they will be meet requirements of passenger comfort (for routine use) and the removal of smoke from subway fires (for emergency ventilation use). In addition, the Mott-MacDonald model is often applied for evaluation of proposed subway train schedules in the U.K. The general characteristics of subway system models are presented in Table 2-1.

Future development for chemical/biological applications requires the addition of dispersion modeling algorithms that account for specific chemical and biological agent features such as half lives, physical degradation, effect of light, deposition, impaction, and resuspension. No subway station or system model has any chemical or biological reaction capability at this time. Validation for subway system models that has been carried out to date has encompassed testing the model against laboratory and field data for pressures, velocities, and temperatures only. No dispersion experiments have been performed. Consequently, no model/data comparisons have been made for a release with subsequent dispersion through the entire subway system. Since velocity and temperature predictions have been shown to be reasonably accurate, it is expected (though not proven) that dispersion predictions should also be accurate.

Table 2-1. Subway System Models

Past Applications	-Vary from design of ventilation systems to scheduling of trains to choice of emergency ventilation systems in case of fires.
Predictive Capability	-Predict velocity, temperature and humidity in subway system as function of time. -Vary in output from ventilation system characteristics to time-dependent history of air characteristics.
Model Approach	-One-dimensional parameterized models used for modeling entire subway systems including stations. -Design predictions for ventilation systems for station sometimes performed using 1-D or 3-D CFD models, depending on level of detail required. -Fire impact predictions and ventilation system design done with both 1-D and 3-D models.
Key Features	-Account for train performance and heat released during (1) train motion (aerodynamic drag a nd tunnel skin friction) and (2) short-term and long-term heat sinks.
Dispersion	-Either predict no dispersion or predict ventilation requirements of emergency ventilation systems aimed at preventing smoke (pollutant) from advancing into tunnel from fire. -Modification of original code or addition of post-processor easily adds simple dispersion capabilities. -Near-field dispersion of pollutant not predicted.
Chemistry	-None handle chemical transformations.
Mesh	-All models one-dimensional in nature; however each model uses varied level of complexity in dividing up subway alignment.
Input	-Manual input or graphical user interface. -Data requirements are considerable involving performance data, geometric data, ventilation information, and environmental conditions.
Output	-Hardcopy and diskfile only. -All data must be post-processed by other graphical visualization programs available to user separate from models.
Platforms	-These one-dimensional models are quick running and use PC.

The SES (Subway Environment Simulation) Model

The SES computer model provides a dynamic simulation of the bi-directional operation of a multiple-track subway and permits continuous predictions of the air velocity, temperature, and humidity throughout any arrangement of stations, tunnels, ventilation shafts, and fan shafts. As previously discussed, the model has mainly been used to design station cooling and heating capacities necessary to satisfy given environmental criteria, as well as the percentage of time during which specified environmental criteria are exceeded. Although a simulation can extend over any period of subway operations, the primary focus of SES has been on short-term simulations such as the peak rush hours, when the load on the environmental control system is the greatest. Although the main application of the model has been the design of cooling and ventilation systems, the model is capable of predicting velocities as a function of time for any moving train scenario – a necessary requirement to simulate the consequences of a chemical or biological agent release.

Figure 2-3 presents an overview of the physical components included in the simulation using the SES model. The SES model has a number of subprograms that make up the final computer model. The train performancesubprogram determines the speed, acceleration, position, and heat rejection of all trains in the system on a continuous basis. The aerodynamic subprogram uses these computed train parameters, coupled with the geometric arrangement of the system and the ventilation performance data to compute continuous values for the air velocity in all stations, tunnels, and ventilation shafts. In turn, the temperature/humidity subprogram uses these computed airflow parameters together with the train heat-release data generated in the train performancesubprogram to compute the convective dispersal of sensible and latent heat throughout the system. It is thereby able to continuously determine the temperature and humidity at all locations. Finally, the air velocities computed in the aerodynamic subprogram are used by the train performance subprogram to determine the airflows adjacent to the trains, providing the means to compute the vehicle aerodynamic drag. The subway ventilation and heat load data from these subprograms, together with information on daily and annual changes in outside conditions, are used by the heat sink/environmental control subprogram to compute the long-term conduction of heat between the subway air and the structure and soil surrounding the subway as well as the heating and cooling capacities required to satisfy design conditions in specified areas of the subway. The integrated calculation procedure makes possible continuous simulation of the complex interactions among the dynamic phenomena operative in a subway system. Table A-1 of the Appendix presents the main characteristics of the SES model. Since the SES model is widely recognized throughout the world as the preeminent model in the field, it will be used by the Transport and Fate thrust team in the study of subway-system agent releases.

Since the SES model does not predict dispersion at the level required for our purposes, a separate program will be used to post-process the SES output. This program (not part of SES) will provide the time dependent concentrations field. We note that the SES model does have a fire model component to study the impact of fire and smoke emissions. However, that subprogram is not used to predict the time-dependent smoke concentrations throughout the system but is available solely to determine whether there is a backing up of smoke against the ventilating air stream (backlayering). The occurrence of backlayering indicates that the ventilation system is not adequate to handle the fire scenario under consideration.

Laboratory and Field Testing of SES

The SES model was developed from a series of laboratory tests and then validated with small-scale and large-scale field tests. Confirmation of the basic mathematical models was achieved through comparisons with scale model tests (Parsons, 1973a, 1973b), and later with controlled full-scale field tests conducted at the Bay Area Rapid Transit (BART) District's Berkeley Hills Tunnel (Parsons, 1974a), and the long-term temperature measurements in the Toronto subway (Parsons, 1974b). Final confirmation of the SES program required comprehensive field testing program in an operating subway system, the Montreal METRO (Parsons, 1975). The METRO tests have validated the computer program as a design tool to predict the flow, temperature, and humidity of air throughout a multiple-track system. The validation of the SES program as a whole implicitly validates within engineering accuracy the component theories, formulations, and scale model tests comprising the SES program.

The original lab tests were carried out at the Caltech Jet Propulsion Laboratory where the piston effectof trains was studied using a moving small model train car in a tube representing a tunnel. Developmental Sciences, Inc. carried out the Vent and Station (VST) Facility tests which evaluated how ventilation shafts worked, and they carried out the Subway Aerodynamic and Thermodynamic (SAT) Test facility studies which verified the basic theory using a 1/3 scale model of a subway system.

Field validation in the Toronto subway system has shown that the predicted long-term temperature are predicted within 9% of actual measurements. Predicted temperatures were within plus or minus 3 degrees F of

the measured average air temperatures which could range from 50-95 degrees F in the system. Tunnel air velocities are also predicted very well. Figure 2-4 presents a comparison of velocities measured for the Montreal METRO field study. In that field test, train coming from opposite directions passed and the velocities were measured before, during, and after the train passage. The SES-predicted airflows in those tests provided excellent agreement with the measured airflows, especially when considering the manner in which the system air leaks were approximated, and considering the large differences in cross-sectional area between the tunnel and the fan shaft. The SES-predicted air velocities at site was always within 100 feet per minute (fpm) of the measured air velocities for three tests. Velocities measured in the fan shafts showed good agreement as well.

Although velocities and temperatures are predicted quite well for single-point measurements, there have been no validation tests of any kind for pollutant dispersion. No data exist for following a pollutant as it disperses through a subway system. The SES model along with a separate dispersion model should perform well; however, there are no

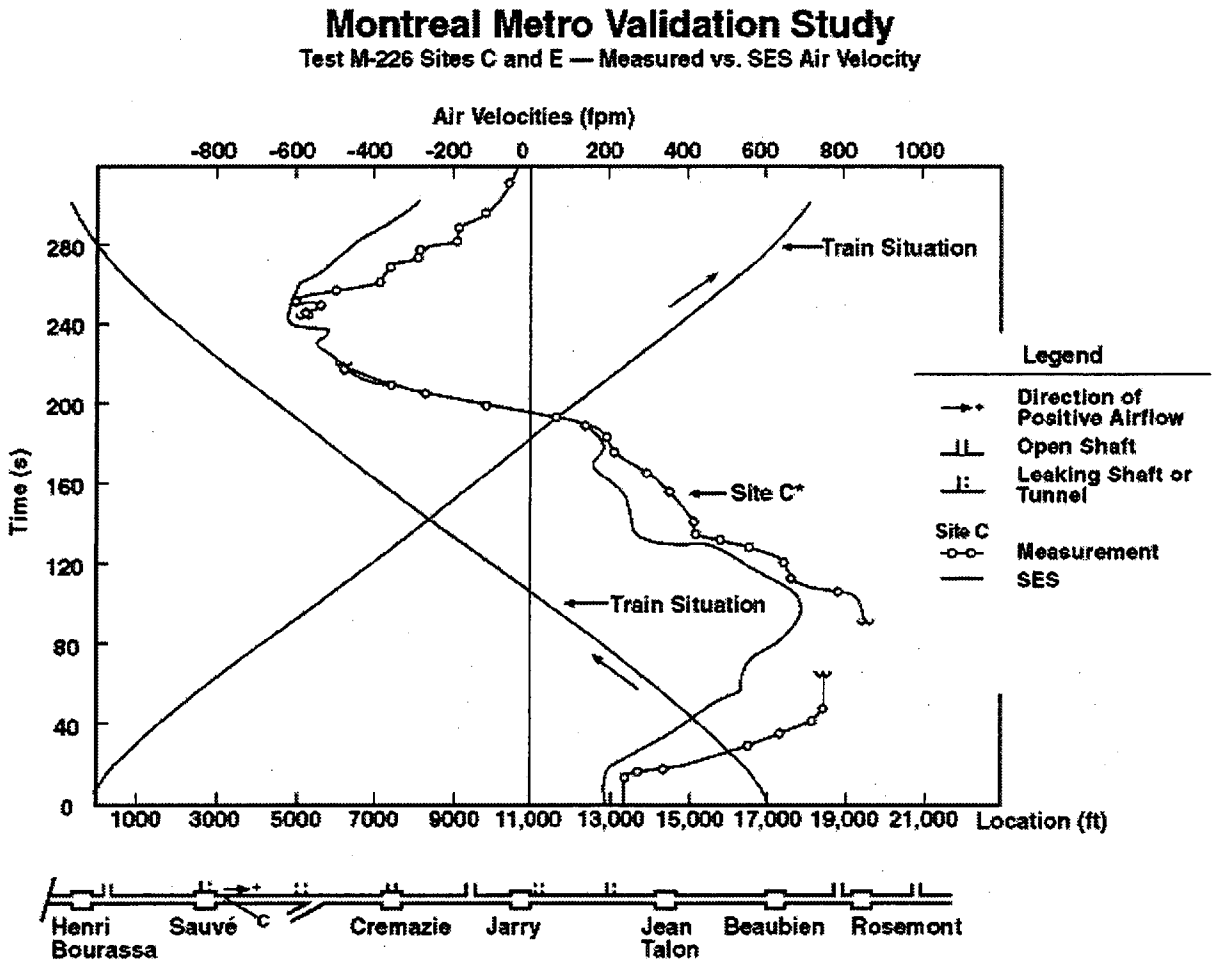

Figure 2-4. Comparison of SES-predicted air velocities with measured data at Site C (Test M-226) due to crossing of trains in the Montreal METRO field study

data available to test that expectation. Additionally, the SES model does not currently treat deposition, evaporation, and resuspension of pollutants whether they be chemical and biological agents or other pollutants. Those physical phenomena need to be added in the future.

2.3 Subway Station Modeling

The analysis of subway station air flows has recently been advanced through the use of CFD models which afforda greater accuracy and level of detail of simulation than simpler integral based approaches. The

objective of using CFD methods in subway design is to determine if (a) the planned routine ventilation system will provide comfort to passengers under ordinary conditions, and (b) if emergency ventilation systems for the station will protect people in case of a fire. Considering that the fire may occur on the train car or in the station, multiple runs are typically made to determine if the exits are clear from smoke and at a temperature that is tolerable to people making an exit (i.e., usually less than 60 °C.). There are several general-purpose commercial packages commonly used for such studies although no one model has gained acceptance over the others and very few validation studies have been done to date.

A typical simulation involves the use of a one-dimensional model (such as the Subway Environmental Simulation Model) to determine boundary conditions at the tunnel/station interface from which a steady state, or less often, a time-dependent calculation could be made with the 3-D CFD model. Some transit authorities insist on the use of such 3-D CFD models for subway design whereas other transit authorities are satisfied with the predictions of the SES model for the stations despite its simplified station-flow parameterization. The use of a CFD model to evaluate the performance of emergency ventilation systems for a station allows the same model to be used to determine the impacts of a chemical or biological agent incident in that station. The use of the 3-D model can help in the location of point sensors for agent detection and possibly assist in identifying the safe exit routes depending upon the agent released and its source term and location. That all can be done as part of pre-planning.

Table 2-2 summarizes the key elements of a variety of 3-D models that can be used for subway stations. Several sample candidate models are identified which fit the model descriptions presented in the table. Although there are some differences among the models in terms of physics and ease of use, their basic approach is the same and their output options are similar as well.

Table 2-2. Computational Fluid Dynamics Models for Subway Stations

differentiators	comments
POPULAR AND PROMISING CANDIDATE MODELS: Proprietary Codes –CFX (AEA Technology Engineering Software, Inc.; Pittsburgh, PA) _FIDAP (Fluid Dynamics, International, Inc.; Evanston, IL) –PHOENICS (CHAM, Inc.; London, U.K.) –STAR-CD (Computational Dynamic Ltd.; London, U.K.) –TASCflow (Advanced Scientific Computing Ltd.; Waterloo, Ontario, Canada) Non-Proprietary Codes –FEM3C (Lawrence Livermore National Laboratory, Livermore, CA) –DYNAFLOW (Lawrence Livermore National Laboratory, Livermore, CA) –GASFLOW (Los Alamos National Laboratory; Los Alamos, NM) –TEMPEST (Pacific Northwest National Laboratory, Richland, WA) –NIST Fire Model (National Institute for Standards and Technology, Gaithersburg, Md.)	Each fluid dynamics code can be applied to subway stations due to their general-purpose development. Models may provide similar predictions in cases where radiation of heat is not a significant factor - i.e., nonfire cases. CFX is later version of FLOW3D which was used to model King Cross Station fire in London. CFX, PHOENICS, STAR-CD, and TASCflow models have been used previously for model ventilation in subway stations. Commercial models are available for annual fees that are in the $10K-$40K range. Non-proprietary models developed by the U.S. government (FEM3C, see Appendix, Table A-2; DYNAFLOW, see Appendix, Table A-3; GASFLOW, see Appendix, Table A-4; TEMPEST, and the NIST Fire Model) are free and have source code available for inspection and modification.
PHYSICS: –fluid type and flow regimes -incompressible vs. compressible -Newtonian vs. non-Newtonian	Flows in subway stations are incompressible, non-hydrostatic and Newtonian. Compressible flow in subways only occurs during long stretches of tunnel with train traveling about 60 mph and higher. That is not the case in subway station. Candidate models may allow for more general flow types than needed for subway station simulation.

Table 2-2. Computational Fluid Dynamics Models for Subway Stations (cont.)

–turbulence closure scheme	Candidate models typically have variety of turbulence models for user choice. Models have such closure schemes as k-epsilon turbulence model, low Reynolds number k-epsilon model, RNG k-epsilon model, algebraic Reynolds stress model, differential Reynolds stress model, and differential Reynolds flux model. k-epsilon model has been typically used for subway station modeling in past.
–flow and conservation equations	Past runs for subway stations involved solution of mass, momentum, energy, and traceable scalar (typically smoke for fire applications). That traceable scalar represented particulates emitted from fire. For CB applications, tracer can represent CB agent but specifics of decay and transformation should more properly be added to codes.
–boundary conditions -inflow and outflow -pressure at open boundaries -fan inlets and outlets	Each has variety of possible boundary conditions for each surface and inlet/outlet. Past subway station modeling has revealed that assumed pressure boundary conditions in interface between tunnel and station are critical to accuracy of results inside station. Adjustment of pressure coefficients at tunnel/station interface is one method of treatment to account for tunnel and trains not included in model.
–dispersion capability -Lagrangian vs. Eulerian -Dense, neutral, and buoyancy gases -deposition and resuspension	For releases of chemical or biological agent, models can represent those processes as tracer with no deposition or resuspension. Most models use moving particles to determine dispersion. Inclusion of density of agent gases should be able to be handled by models in current framework. Including specific deposition and resuspension algorithms is possible in most commercial codes due to flexible user routines in which users can provide the special coding needed.
–chemistry	Chemical reaction mechanisms for chemical agents in gas or aerosol form beyond simple formulas is not currently warranted based on current state of art. One exception is mustard gas. Inclusion of sunlight effects on biological agents can be done at this time for some agents. Increased complexity of degradation formulations for biological agents may be available next year. These mechanisms can be entered into from user routines in commercial codes. All models do handle general chemical reactions in parameterized manner with input from user.
NUMERICS: –mathematical representation of governing equations -finite volume (finite difference) -finite element -finite element-based finite volume	Finite element models and the competing finite volume models can represent complex tunnel/station geometries. Finite volume models (e.g., STAR-CD) permit use of hexahedral and also prismatic and tetrahedral cell volumes to constitute computational domain in more accurate manner. A challenge in subway station modeling is still to match circular tunnel and rectangular station platform within same grid structure without losing accuracy.
–numerical scheme -implicit -semi-implicit -explicit	Each type has its advantages and disadvantages for subway station applications in terms of rate of convergence, accuracy, time step, etc. Good CFD model can be any of these types. Subway station applications usually require large number of grid points and hours to days of computer time for detailed run. Schemes that allow linear increase in run time with linear increase in number of grid points have advantages for complex station simulations.

Table 2. Computational Fluid Dynamics Models for Subway Stations (cont.)

–grid (mesh) type -Cartesian/cylindrical with/without orthogonality of grid -grid embedding -unstructured multiblock (can expand or deform) -transient (moving) grid -sliding grid (e.g., moving vehicles like train)	Sliding mesh capability can be advantage to simulations where train is moving into or out of station. Some CFD models have dynamic cell deletion which allows removal of cells displaced by moving train from calculation.
USER AMENITIES: –graphical user interface	Can reduce data input time considerably if CFD code can be applied directly to problem without coding changes.
–ease of input: -preprocessor linking CAD and CFD •direct access to CAD databases from CAD packages •complex geometry creation •interactive assignment of boundary conditions	Grid generation time can be much reduced with these utilities while vastly extending range of geometries that can be modeled with such tools as multiblock meshing.
–output post-processing and visualization: -advanced visualization such as animation, ISO-surfaces, probes, shaded contours, and vectors	Wide range of output and post-processing of output can make it possible to develop insights rapidly and present those results more easily to laymen.
–platforms and run times: -IBM-PC's; single-processor workstations, minicomputers; multi-processor workstations, servers, mainframes;vector mainframes, minisupercomputers; supercomputers	Competing models available on variety of platforms of this type - some on all and some on only one or two. Models as applied to subway station flows and dispersion have run times on order of hours for single case when run on workstations. Including time for model setup, these models are practical for pre-planning but not real-time incident response.

Previous Subway Station 3-D CFD Simulations

The reader can learn more about past application of these models by studying the papers identified below on some of the models and their past use in subway station model applications. None of those models has been used to predict chemical/biological agent releases at this time. However, the 3-D model types can be used for that purpose quite easily and without change in the model structure if those agent releases are treated as a scalar tracer. The addition of specific chemical/biological agent degradation and conversion is an effort that has not yet been undertaken for any of the models.

The addition of chemical/biological agent physics in the models should involve not only physical degradation (if any) but also deposition and resuspension of either the vapor or aerosol released. In fact, once droplet aerosols are released for a chemical agent, there is time-dependent evaporation of aerosol to vapor. This conversion for most agents typically takes place on time scales on the order of hours. Deposition and impaction of aerosol and vapor can lead to resuspension at a later time when decontamination might be occurring. Some 3-D models identified in the table can treat these effects by means of flexible user-prepared routines (for the commercial codes) or through usual coding changes for any of the non-proprietary codes of the group.

A sample application of TASCflow is given in Elias, Bostwick, and Raw (1996) in which the consequence of a train car fire is predicted for a Toronto subway station. The efficacy of the proposed ventilation system was being evaluated to determine if passengers could escape the fire through the subway station.

An example of the use of CFX is provided in a videotape available from AEA Technology Software Engineers, Inc. in Pittsburgh. The earlier version of CFX (called FLOW3D) was used to evaluate the fire in the Kings Cross Station in the U.K. on November 18, 1987. In that fire, 31 people died because they were not able to escape on an escalator rising from the station. The fire started on the escalator and hugged (through a so-called trench effect) the escalator. Consequently, the fire and smoke did not rise to the ceiling as the station designers had expected. The video shows the modeling done and visualization of the results as well as 1/3 scale laboratory tests that validated the model predictions.

An example application of the STAR-CD model is presented in Mendoza and Drake (1996) illustrating the use of a 3-D code to evaluate the comfort of passengers in the station as a decelerating train enters the station. Predicted air velocities were low enough so that passenger comfort would not be affected. That STAR-CD model was also applied to a section of the proposed London Underground extension to provide information on backlayering of smoke from a fire and to identify a simpler method (use of critical velocity concept) for evaluating emergency ventilation systems. That work is described in Meeks, Drake, and Leong (1997).

An example of the use of the PHOENICS 3-D model application for a subway is given in Eckford, Pope, Tan, and Michel (1995). This case involves a study of the behavior of smoke generated by a fire on a train in a tunnel in the presence of a longitudinal forced ventilation flow. The model predictions coupled with data visualization revealed a realistic view of the smoke in the tunnel around the train from the viewpoint of people evacuating along a tunnel walkway. It was found in that case that the smoke exhibited a high degree of stratification.

Capabilities of Commercial and Non-Proprietary 3-D CFD Models

In this section, the possible use of CFD models for subway stations is discussed, with five commercial codes and five non-proprietary codes cited as promising candidate models. The commercial codes have the advantages of many years of development, ability to deal with complex geometries, and experience in application to complex geometry subway station problems. Some of the models treat dispersion of aerosols but usually for combustion applications. Most models such as CFX and TASCflow can be modified to handle C/B agents. A wide variety of turbulence models can be applied and excellent user amenities are available such as programs that transfer CAD representation of the station directly to a computational mesh. State-of-the-art visualization tools are available for output study and presentation. Generally, the CFD codes need 1-2 months of learning and are costly for an annual license.

Most of the non-proprietary codes presented here have been developed by DOE laboratories. Each of the non-proprietary models reviewed all have relevant capabilities and, in principle, could be adapted for modeling air flow and dispersion of C/B agents in subway stations. The applicable DOE models include, DYNAFLOW (see Appendix, Table A-3), FEM3C (see Appendix, Table A-2), GASFLOW (see Appendix, Table A-4), the NIST Fire Model, and TEMPEST. All except the NIST model are also discussed in Chapter 4 and compared in Table 4.3. Each of the five models has its unique capabilities and limitations. For example, DYNAFLOW has the most advanced turbulence model and unstructured grid capability best-suited for treating complex irregular geometries. However, development is required to extend it to simulate the dispersion of C/B agents. FEM3C is also capable of simulating complex irregular geometries and has been validated in many studies for the dispersion of heavy gases. However, the dispersion capabilities for C/B agents also remain to be developed. GASFLOW has the most complete physics of dispersion and can treat complex regular geometries; however it lacks the ability to handle complex irregular geometries effectively. TEMPEST has been validated to some extent against flow and dispersion data from a cubical building but it does not have C/B dispersion physics and is very similar to GASFLOW in numerics and grid capability. The NIST Fire Model and CONTAIN are discussed in more detail below.

The NIST Fire Model is a 3-D large eddy simulation (LES) model that simulates fire incidents in 3-D enclosures. The model has high spatial resolution and employs efficientflow solving algorithms. It predicts combustion products from fires and follows their transport in configurations ranging from a single-room to multi-room enclosures. The computational mesh is gridded uniformly in the horizontal directions, with an option of non-uniform gridding in the vertical direction. The model can be used to predict dispersion in a simply-designed subway station using the orthogonal grid system required in the model. As with the other non-proprietary models, the model cannot handle moving trains. Although the subway station problem was not the purpose for the original model development, the model can be easily adapted to treat the general flow patterns in such a system including the effectsof fans and blowers. The code also follows the trajectories of tracer material but does not predict deposition at this time. As with the other DOE models, the NIST Fire Model is a candidate for running simple subway configurations; however, the model documentation is still in preliminary form. Additional details on the NIST Fire model as well as comparisons with experimental data on enclosure fires can be found in McGrattan, Baum and Rehm (1997, a, b and c).

The only non-CFD model considered for subway stations is the CONTAIN model (see Murara, et al., 1989). This model is a lumped parameter model that assumes full mixing within each control volume. CONTAIN has been developed and used for reactor containment vessels and has been used to handle similar closed environments. It has limited capability for treating blowers, fans, and filters but the model does treat multiple aerosol and gases dispersion as well as deposition. Hydrodynamic simplifications made in the lumped parameter modeling make this approach less preferablethan the CFD models considered for subway stations, especially considering the fact that some of the models have already been applied to subway stations.

CONTAIN, as well as all the non-proprietary CFD models, has the additional limitation in that it cannot handle moving trains.

As a group, the four DOE CFD models and the NIST Fire Model have relatively sophisticated numerics and cover a range of gas dispersion applications including aerosol deposition and resuspension. These models can provide the basic capabilities for the CBNP program to build on in terms of modeling C/B-agent transport and dispersion in subway stations.

2.4 Transport and Fate Team Modeling Capabilities

The Transport and Fate Team has both the SES model (at ANL, see Appendix, Table A-1) and DYNAFLOW, FEM3C (see Appendix, Table A-3 and Table A-2 respectively), and GASFLOW (see Appendix, Table A-4) codes. These can be the basic tools to carry out studies of transport and dispersion of chemical and biological agents in both subway systems and subway stations. ANL, LANL and LLNL are very knowledgeable concerning their respective models (LANL developed the GASFLOW model, see Appendix, Table A-4; and LLNL developed the DYNAFLOW and FEM3C models, see Appendix, Tables A-3 and A-2, respectively) and this expertise will be very valuable in future years as these models get modified to handle the specific aspects of chemical and biological agent behavior. One of the ANL team members was a developer of SES and has applied the model to numerous subway systems. GASFLOW has been applied by LANL to over a dozen problems analyzing gases, aerosols, and flames in and around facilities. The all-purpose 3-D nature of the model should allow LANL to apply GASFLOW to the simulation of subway station flows and dispersion and LLNL the DYNAFLOW and FEM3C models as needed.

2.5 Findings and Recommendations

The Subway Environment Simulation (SES) Model is clearly the superior model for *subway system* flow predictions and has become the de facto standard in the field. It is the only real candidate for possible use in this project for subway system modeling. It has been developed over a 10-year period and has been used for over 20 years by transit authorities all over the world for the evaluation of ventilation systems. The model can predict the flow, temperature and humidity at all points in the subway system as a function of time. The model has shown good results in previous validation tests at the Toronto and Montreal METRO systems. The model has no open-literature competitors and has been funded and is the recommended model for subway system dynamic calculations by the U.S. Department of Transportation. That model can be the fundamental building block onto which the dispersion of chemical and biological agents can be added. That model is available at ANL.

Our DOE team plans to expand the capabilities of that model for C/B applications by adding (a) C/B source term algorithms, (b) a state-of-the-artdispersion algorithm so that agent concentrations can be followed throughout the subway system and to the shaft exits to street level (dispersion is not predicted in SES), (c) droplet/vapor partitioning including droplet evaporation during transport through the subway system including the effects of turbulence on droplet and vapor motion, (d) deposition, resuspension and physical/chemical degradation of the agents (both droplet and vapor forms) as available data permit, (e) improved treatment of flow within the stations from the 1-D parameterization that currently exists, and (e) the addition of input/output to support the C/B user whether his purpose is pre-planning or real-time incident response. The revised model will be run for case studies to illustrate and exercise its capabilities for preplanning and real-time incident response. It is planned to also have a version prepared for easy application within the operational control centers of the subway systems in the U.S.

Concerning the separate issue of modeling of *subway station* impacts as part of a C/B pre-planning exercise, 3-D CFD modeling was found to be most appropriate for representing the true three-dimensional nature of the C/B plume as it disperses within a station. The typical station has three levels: platform, mezzanine level, and street level along with multiple entrances, exits, and vents. A number of non-proprietary 3-D CFD models are good candidates for consideration of the problem of modeling subway station flows. Many of the non-proprietary models have been developed by the DOE laboratories. The prominent candidate models from the DOE labs are GASFLOW (available at LANL), DYNAFLOW (available at LLNL), FEM3C (available at LLNL) and TEMPEST (available at PNL). The NIST Fire Model is also a prominent candidate and was developed at the National Institute for Standards and Technology. Although none of them has yet to be applied to a subway station scenario, their general-purpose nature allows any one of them to be applied to this problem. Each of the non-proprietary codes reviewed all have relevant capabilities and, in principle, could be adapted for modeling air flow and dispersion of C/B agents in subway stations. Presently, none of them can handle a moving train, but each can be modified to be able to do so in the future. None of the candidate models is clearly superior to the others for this application. Validation of models for subway station flows and dispersion is very limited and no model/data comparisons covering multiple models considered has been made. No CFD model evaluated has been excluded by our team for future application. However, our team currently

plans to use GASFLOW for general subway station modeling due (a) its ability to treat the problem as do the other candidate CFD models, (b) the fact that it has the most complete physics of dispersion and is able to treat complex regular geometries, and (c) the familiarity of GASFLOW to researchers at LANL as they are working on that 3D subways station problem for our team. Use of a non-proprietary model can (1) allow greater flexibility in output type and format, (2) ensure the continued availability of the code, and (3) result in a model package that will be available at no cost to all interested parties.

Although non-proprietary codes are favored for this problem, there may be occasions in which a special niche can be filled by using one of the commercial codes. For instance, an immediate need to model a very complex geometry station might be better served by using CFX 4.1 due to its capability of treating unstructured grids for complex geometry applications and moving trains using the sliding mesh technique. Although the other commercial codes may be able to run such a case, we believe that the CFX 4.1 model has the greatest number of special capabilities for this subway station application. That model has also been applied previously to the Kings Cross station in the U.K. with results that were validated with lab and field data. Previous application to subway stations is indeed an advantage. The disadvantage is the annual cost of the code to a DOE laboratory and lack of access to the source code. There is also the need to add C/B to CFX 4.1 for detailed C/B impact predictions. Currently, the Naval Surface Warfare Center is adding C/B algorithms into CFX 4.1 and those additional algorithms can be made available to the DOE labs upon official request when work is completed after the end of FY 1997.

The proprietary codes are all general-purpose commercial codes with annual fees to the vendor of between $10-40K per year. Although some of those commercial models allow user programming and flexibility of additional development for a particular application, the coding of all those candidate models remains proprietary. Finally, for long-term use of such a subway station model, a non-proprietary model would be preferable for general use. A non-proprietary code allows a wide range of coding additions to be made, allowing increased flexibility in output type and format and greater certainty that the code will continue to be available.

In summary, GASFLOW and CFX are the prime candidates for our *subway station* applications, but other CFD codes will be considered based on special application needs.

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3 BUILDINGS INTERIOR TRANSPORT AND FATE MODELING

3.1 Overview of Buildings Interior Transport and Fate Modeling

The U.S. population, on average, spends about 85 to 90% of the time indoors, about 60% of the time in their homes, and 25% at work and other indoor locations (Szalai, 1972; Jenkins, *et al.,* 1992). Thus, buildings, particularly those with high occupancies (e.g., office buildings, auditoriums, airports) pose attractive targets for CB agent release by terrorists. In addition, high exposure levels can be achieved for a given quantity of material released in a building or subway because of the enclosed volume and low air exchange (dilution and removal) rates. For outdoor releases, buildings can offervarying degrees of protection from exposures to CB agents, depending upon outdoor concentrations and rates of outdoor air exchange.

Accurate predictions of the indoor concentrations of CB agents and their temporal and spatial variability require several different types of models, some of which exist already, and some of which require more research and development. The core model which is required for the purposes of this Program is an interzonal airflow and pollutant transport model. Models to calculate air flow and pollutant transport in buildings include *interzonal nodal models* (single-zone and multizone) describing transport mechanisms between zones and the outside, as well as *intrazonal* models to describe air flow and dispersion patterns within zones.

The air-mass flow distribution in a given building is caused by pressure differencesevoked by wind, thermal buoyancy, mechanical ventilation systems, or a combination of these. But air flow is also influenced by the distribution of openings in the building shell and by the inner pathways. Actions by the occupants can also lead to significant differences in pressure distribution inside a building (see Figure 3-1).

Processes other than air flow must also be modeled in buildings in order to predict the temporal and spatial distributions of CB agents in indoor settings. Because of the high surfaceto volume ratio of building interiors and of the duct systems which transport ventilation air throughout many buildings, both particles (e.g., bioaerosols) and vapors are removed from the transported air as it moves through building envelopes, and throughout buildings and duct systems. In addition, particles can be resuspended, although this appears to be a relatively small effect, and vapors sorbed on indoor surface materials can be re-emitted to varying degrees as the concentrations in air change. Thus, models to address these removal and re-emission processes are required for accurate predictions of air concentrations. This additional group of models to be included in the analysis of buildings are generally termed *deposition and adsorption/desorption models.* Although some of the interzonal models include deposition and/or adsorption/desorption components, these are very simplified. For example, aerosol deposition in these models is handled with a single deposition constant which does not take into account the large differences in deposition rates for different sizes of particles. More accurate and detailed models for these processes in buildings, where available, are described in the section Indoor Pollutant Behavior Models.

Indoor air flow models typically use source emissions terms, in units of mass emitted per unit time, rather than a source emissions model. For many of the buildings models, the source term can be varied over time, thus simulating a more complex release process. However, either experimental data or a source emissions model, for example, NUSSE-4 (Pennsyle, 1991), will be needed to provide this input data for the air flow model.

3.2 Interzonal Models

Air flow models can be divided into two main categories, single-zone models and multizone models. Single-zone models assume that the structure can be described by a single, well-mixed zone. The major application for this model type is the single-story, single-family house with no internal partitions (e.g., all internal doors are open). As this is a limited application, models were developed which can simulate the interzonal flows of buildings with more than just one well mixed zone. In reality, most buildings do not consist of a single well-mixed zone and, therefore, have to be characterized as multizone structures. This is true even for buildings where no internal partitions are present (e.g., airplane hangers, stadiums).

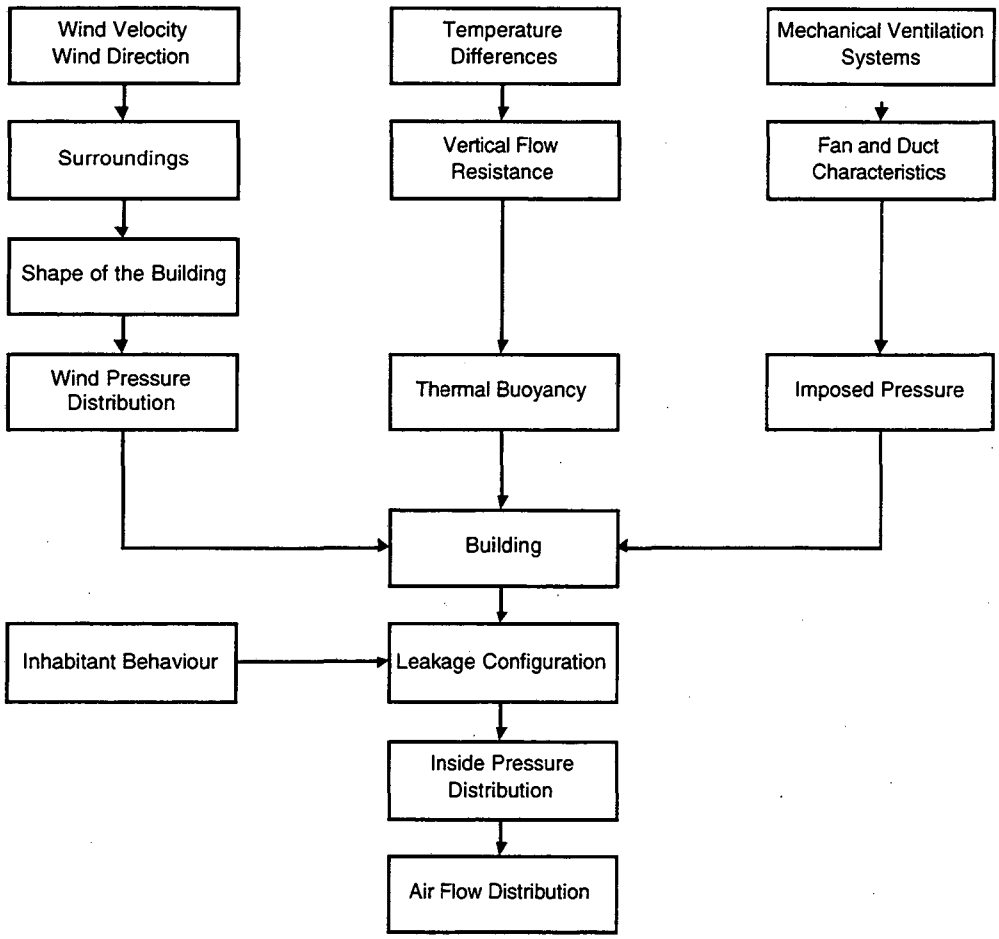

Figure 3-1. Influences on the Air Flow Distribution in Buildings (Feustel 1984)

In terms of air-mass flow, buildings represent complicated interlacing systems of flow paths. In this grid-system the joints represent the zones of the building and the connections between the joints simulate the air flow paths. These include the flow resistances caused by open or closed doors and windows and air leakage through the walls. The boundary conditions for the pressure can be described by grid points outside the building.

Multizone infiltration network models deal with the complexity of flows in a building by recognizing the effectsof internal flow restrictions. They require extensive information about flow characteristics and pressure distributions. As for their single-zone counterparts, these models are based on the mass balanced equation.

A large number of papers describing multizone air flow models have been published (Jackman 1970, Walton 1989, Herrlin 1987, Feustel 1984). However, even more papers describing the applications of such numerical tools are available (*e.g.*, Diamond, *et al.,* 1995, Esdorn, *et al.,* 1977, Matson, *et al.,* Nazaroff, *et al.,* 1985, Sextro, *et al.,* 1993).

A survey of multizone air flow models published in 1992 produced descriptions of 50 differentmodels Feustel and Dieris, 1992). The first of these models developed was probably the BSRIA-model LEAK (Jackman) which was published in 1970. Since that time many more models have been developed but, most of them have been written as research tools and are not available to third parties. As a consequence, they are difficult to use and are, at best, "user-tolerant" rather than "user-friendly". For details of these multizone air flow models, please referto Feustel and Dieris (1992). Several of the more widely used air flow and pollutant transport models, which are readily available and have been tested to varying degrees, are described below.

COMIS

The latest development in interzonal air flow modeling is the COMIS model (Feustel 1996) (see Appendix, Table A-5). In a twelve month period ten scientists from nine countries developed a multizone model on a modular base at Lawrence Berkeley National Laboratory. Because of its modular structure COMIS is designed to expand its capability to simulate buildings. COMIS can be used as a stand-alone infiltration model with input and output features or as an infiltration module for thermal building simulation programs. It also serves as a module library. Due to its international character, COMIS may become a standard in multizone air flow modeling. So far, the program is being used in more than 15 countries.

In 1990, the International Energy Agency's (IEA) adopted a working group on multizone air flow modeling ("Annex 23"). The objective of this working group was to study physical phenomena causing air flow and pollutant transport (e.g., moisture) in multizone buildings and to develop modules to be integrated in a multizone air flow modeling system. Several modules were implemented to include air flow equations for large vertical openings, single-sided ventilation, and different opening situations for various window constructions. The input data requirements for COMIS include: wind speed and direction, pressure field around the building (in terms of pressure coefficients as function of wind direction), outside temperature, inside temperature distribution, leakage and leakage distribution of the envelope, internal leakages between zones, dimensions of large openings (e.g., windows, doors), fan characteristics, layout of duct work (will be transferred into flow resistances), pollutant source strength inside the building and pollutant concentration field outside the building.

Special emphasis was given to providing data necessary to use the system (e.g., calculation of the wind pressure distribution) (Feustel, 1996). A series of events or a time schedule can be defined for the time variation of many individual parameters, such as temperature, window opening, fan operation, and source emissions and sinks (for up to five pollutants). Many of these parameters are readily obtainable (e.g., meteorology) or can be estimated based on measurements of existing buildings. For example, for single family residential buildings, there is now a large database of air leakage measurements available (Sherman and Dickerhoff, 1996) and some limited measurement data for infiltration of air for large multistory commercial buildings (Grot and Persily, 1986; Turk, *et al.,* 1989).

Several interfaces were developed for COMIS. The simplest is the FORTRAN program COMIN, which reads and writes COMIS input files and allows the addition, change and deletion of input data. COMERL offers an alphanumeric, DOS™-oriented user interface allowing the creation or modification of COMIS input files using a specific task adapted editor. A data base for air flow components (e.g., cracks, windows, or HVAC components) is integrated into COMERL (Dorer, *et al.*, 1995).

COMIS Evaluation

Because of the difficulty of measuring infiltration in buildings under controlled boundary conditions, none of the models had been validated properly, if at all (Scartezzini, *et. al.*, 1987). The possibility of doing piecemeal validations of certain algorithms has been considered: *e.g.*, the algorithms for air flow through open doorways or air flow through cracks have been tested separately. Measuring a few cells of the whole structure could still provide a severe test for existing models.

Measurement data are important not only for validation purposes but also as a means of further understanding air movement in large multizone buildings. We need to identify the critical variables in different building types in order to develop more accurate input data and, ultimately, more accurate models. Wind pressure coefficients, for example, represent a factor that needs further study, and the collating of existing data should help our efforts in simplifying data requirements.

The goal of Annex 23[1] was to provide a reliable, practical, and user-friendly multizone air flow model. The user should be able to have confidence in the results of the simulations performed with the program. Therefore, a variety of tests were performed to make sure that the program contained no numerical errors. COMIS simulation results were compared with more than fifty benchmarks for which either an analytical or a numerical solution was obtained. Each of these test cases was developed to check a particular feature of the COMIS program. These tests were repeated for each individual program update to be sure that a "model improvement" did not interfere with already tested program features.

1 International Energy Agency's Energy Conservation in Buildings and Community Systems implementing agreement, Annex 23 "Multizone Air Flow Modeling"

Furthermore, two user tests were developed. The first user test represents a very simple network in which all openings and pressure boundary conditions were defined. This test and the comparison of simulation results with analytical solutions, enabled inconsistencies and problems in the code to be quickly identified and rectified. A second user test was performed to evaluate the user influence; assumptions were necessary to be able to simulate "user test 2". This helped very much to further develop the COMIS documentation, particularly the COMIS User's Guide. The results, however, showed clearly that the ability of the user was critical in securing reliable predictions (Liddament, 1996).

COMIS was also checked by means of inter-model comparison. Fourteen other simulation programs[2] were used by the five research stations involved to compare results between different simulation tools. As different programs have different features, the objectives for each inter-model comparison had to be adapted in a way, that both models to be compared were able to simulate a particular physical phenomena. As the programs all use similar algorithms and simulations were performed with identical input data, the results are within a very narrow dispersion band (Fürbringer, *et al.*, 1996).

An important part of the effort of the IEA Working Group was the comparison of results between the model and in-situ tests. Nine studies were performed, using results from tracer gas tests for single-family houses, test cells, flats as well as small office buildings. These results were compared with results obtained by numerical simulation. For each case, a sensitivity analysis was performed, not only to learn about the uncertainties on the measurements, but also the confidence intervals of the simulations, which result from uncertainties in the input data.

Additional evaluation of COMIS was performed by Haghighat and Megri (1996). In this study, experimental data for two multizone objects were compared with results from COMIS and CONTAM. Both models predicted the experimental data very well.

CONTAM

CONTAM is a multizone air flow and pollutant transport model developed at the National Institute for Standards and Technology. Details about the operation of and algorithms used in the computer model CONTAM are presented in the CONTAM93 user Manual (Walton, 1993). CONTAM93 is designed for the simulation of large buildings using the simulation capabilities of CONTAM88 and the airflow analysis methods of AIRNET (Walton, 1989). CONTAM96 is the latest version of the CONTAM program series and is available over the internet. It includes a significantly revised user interface and expanded capabilities as compared to the original CONTAM93 program. CONTAM96 is a DOS program which can also be run in a DOS window under Windows 3.1 and Windows 95.

Non scale building drawings are produced by a graphic user interface. Symbols are placed to indicate flows, ducts, room conditions, etc. Input parameters are then added by clicking on the appropriate symbols. The input requirements for CONTAM are the same as for COMIS, i.e., wind speed and direction, pressure field around the building, outside temperature, inside temperature distribution, leakage and leakage distribution of the envelope, internal leakages between zones, dimensions of large openings (e.g., windows, doors), fan characteristics, layout of duct work, pollutant source strength inside the building and pollutant concentration field outside the building. Although CONTAM does not include a source model per se, the pollutant source strength terms (mass emitted per unit time) can be varied over time.

Air flows and contaminant concentrations are calculated for each zone in the building. Factors which are considered include the influence of the HVAC systems, the possibility of contaminant removal, and the possibility of chemical reaction, radio-chemical decay, or sorption of contaminants. All equations for contaminant concentration fractions are solved simultaneously for all zones and contaminants. CONTAM allows for the definition of contaminant sources and sinks using several models including pressure models, volatile organic compound models, and filtering device models.

To solve for the migration of contaminants through the building and its systems, a flow analysis has to be performed. Quasi-steady state conditions are assumed such that the sum of flows into and out of each zone is equal to zero. The flow through each flow path is assumed to be a function of the pressure differential from one side of the flow path to the other. As these flow functions are usually non linear, the Newton-Raphson method is used to solve by iteration. The flows for each zone are solved simultaneously (Upham 1997).

[2] Models compared include AIDA, AIRNET, ASCOS, BREEZE, BREVENT, CBSAIR, CONTAM93, ESP, LBL, MZAP, NORMA, PASSPORT AIR, TURBUL and VENCON.

During the working phase of Annex 23, an inter-model comparison was performed. One of the models being tested was CONTAM. For the features tested in this comparison, CONTAM and COMIS provide very similar results.

BREEZE

BREEZE is a suite of integrated computer programs designed to run on IBM PCs and compatible machines operating under Microsoft MS-DOS (version 3.0 or later). It is a modeling tool for those concerned with the ventilation of buildings. The floor plans are drawn on the computer display screen, along with the location of openings and their characteristics. Running the program helps to determine air movement and/or the dispersal of a contaminant (or tracer gas).

BREEZE includes a data base of cracks, windows, doors, ducts and fans. Large openings (e.g. open doors and windows) include two-way flow calculation procedures. Fans require coefficients for the cubic fan characteristic. The BREEZE flow/pressure analysis program applies methods of network flow computation to calculate balanced mass flows and pressure differences throughout the building.

The network analysis model employs a Newton-Raphson procedure. The contaminant analysis program employs an adaptive step-length Runge-Kutta method to determine cell concentration histories.

The inclusion of design variables greatly accelerates studies of the ventilation characteristics of different building designs. Whole sets of parameters may now be linked to case-specifiers. For example, the open areas of a large set of vents, and/or their heights can be varied in step, with analysis being invoked automatically after each variation. Results may be displayed on the floor plans and, for more detailed study, summaries and full results may be stored in output files.

Some of the features of BREEZE include:

- Heat-gains (rather than fixed temperatures) in selected cells
- Remote cell connections
- Cell area & volume displays
- Many on-screen information pages
- Built-in Wind Pressure Coefficient (Cp) database of common building configurations

BREEZE is a commercial program which has been developed by the Building Research Establishment in the UK. The source code of the program is not available.

EPA Models

Within the mass balance model category, EPA has developed two major indoor air models to meet their needs, Exposure, based on the INDOOR model described by Sparks, *et al.* (1991, 1993), and MCCEM (Geomet, 1989; Koontz and Nagda, 1991). They have also supported development of the IAQM model developed by SAI (Hayes, 1991).

The first two EPA models were developed to estimate inhalation exposures to indoor air pollutants from indoor sources and intended for application to residential buildings (because most of the population spends 70% of the time, on average, in their homes). IAQM also addresses residential buildings but it's initial application was for indoor exposures to an outdoor air pollutant, ozone. The emphasis of all three models is on estimating human exposures to air pollutants but they all calculate pollutant concentrations over time. The models require specification of a *single air exchange rate* for the whole building for the modeling period, rather than a calculation of the infiltration rate as a function of meteorology. Pollutant concentrations in the infiltrating outdoor air must be specified and it is generally assumed that these penetrate through the leakage pathways with no losses (as do other models) and are constant. Similarly, interzonal airflows are specified once by the user. The models assume that the air in a room is instantaneously and completely mixed. These models were not designed to model indoor concentrations in more complex buildings with multiple zones and floors and HVAC systems but are useful for single family residential buildings. A particularly attractive feature of the Exposure model is that time-activity data for the population can be easily used with indoor concentration data to estimated distributions of exposures for the population. Each of these models is described below in more detail.

Exposure

Exposure (Version 2), is an EPA model for calculating individual exposure (as opposed to distributions of population exposures) to indoor air pollutants from indoor sources in a single family residential building. The model requires input data on source emissions, room-to-room air flows, air exchange rate with the outdoor air, and indoor (reversible) sinks to predict concentration-time profiles for all rooms. The building information includes number of rooms, room dimensions and the arrangement of rooms. The concentration time profiles are then combined with individual activity patterns to estimate an individual's exposure. The model allows analysis of the effectsof air cleaners located in both the central air circulating system or individual rooms on indoor air concentrations. Differenttypes of sources can be modeled: long-term steady state sources, on/off sources, and decaying sources. Several sources are allowed for each room. The model can also be for analysis of the effects of sinks and re-emissions on indoor air quality. The model has been compared to measured data for vapors in a test house; measurements agreed well with model predictions (Sparks, *et al.*, 1991) In the model called RISK, the Exposure model has been extended to incorporate calculations of health risks due to the pollutant exposures.

MCCEM

The Multi-Chamber Concentration and Exposure Model (MCCEM) was developed by GEOMET for use by the US EPA Office of Pollution Prevention and Toxics (Geomet, 1989; Koontz and Nagda, 1991). It is a user-friendly computer model that calculates indoor concentrations and individual exposures to chemicals released from products used in homes. Concentrations of a single pollutant can be modeled in as many as four zones in a house. The user can input time-varying emission rates for a contaminant in each zone of the residence, outdoor concentrations, and the location of the individual, in a spreadsheet environment. Users can select input values from a library, e.g., infiltration and interzonal air flow rates for different types of residences in various geographic areas, or input a specific choice. The current version includes a one-way sink but is currently being upgraded to include a reversible sink. Time varying exposure profiles can be developed. Monte Carlo simulation of some input parameters is available for estimating output distributions. Output includes summary statistics (mean, standard deviation, percent of cases at or above a user-specifiedlevel of concern) for the contaminant concentrations in each zone of the residence and for consumer exposure. Existing measurement data bases were used to test the model in the initial development. Scale-up from an environmental chamber experiments on a flooring tile adhesive to a research house have also been used to test the model (Nagda, *et al.*, 1995). The software is in the public domain and available from EPA.

The current version of MCCEM is written in Microsoft QuickBasic for PC use. It is now being upgraded to operate on Windows 95 (Koontz, Personal Communication to J.M. Daisey).

IAQM

IAQM is a PC-based multicompartment indoor air quality model, developed by SAI (Hayes, 1991), for calculating distributions of pollutant concentrations in various building types, e.g., home with open windows, home with closed windows, air conditioned home, energy-efficienthome, officeventilated with 100% outdoor air, etc. It was developed for estimation of the indoor exposures of the population to ozone from outdoor air for EPA, but can be used to model other pollutants as well, one at a time. The user inputs outdoor concentrations and indoor emission rates for each averaging period; indoor sources can be continuous or intermittent. Sinks are a function of surface; re-emission rates must be incorporated into the emission rates by the user. For each building type, the user must specify a mixing factor (a parameter used to specify air mixing), infiltration, recirculation rate of indoor air, and indoor volume. The model formulation is based on a recursive solution of the mass continuity equation for a reactive pollutant in a single compartment.

Other Related Models

There are a number of other models which have been developed for very specific problems (e.g., explosions or nuclear reactor failures), rather then as general models for typical buildings and building operating conditions. Two of these are described below as examples.

Multi-Chamber Blowdown Model

This code is a physics-based interior flow engineering code that calculates time-varying conditions within a rigid-walled, multichamber system. Because this code was designed principally for use in simulating the effects of explosive or rapid-burning events, much attention is paid to heat and mass transfer and to combustion physics. Each chamber is treated as a single computational zone using (what appears to be) a finite differencemethodology. However, advective transport between rooms is done through integrated solution to

quasi-steady gas flow equations. Thus, the user specifies the size of such connections (doors, hallways, ventilation ducts, etc.) and a roughness parameter for each connection.

The principal driver for the heat and mass transfer is the explosion or rapid combustion (such as a rocket fuel burn). Thus, the pressures and temperatures are significantly different than are typically found in buildings under ordinary "ambient" conditions (several atmospheres versus a few Pascals; several thousand degrees Centigrade versus about 20 degrees Centigrade). Presumably the code could incorporate such "ambient" pressure and temperature conditions as the principal drivers for advective transport. However, as presently constituted, the code does not appear to directly include these effects (Maxwell, 1997).

CONTAIN

CONTAIN is an integrated code designed and developed for predicting the contaminant behavior (chemical, physical, and radiological) in a severe accident (e.g., explosion) in a nuclear reactor facility by Sandia National Laboratories under U.S. Nuclear Regulatory Commission (NRC) sponsorship (CONTAIN, 1993). It models the thermal hydraulics as well as the aerosol and fission products behavior inside the containment. The vessels modeled can be cubic, spherical or cylindrical. Since it is designed for containment accidents in nuclear facilities, the CONTAIN code addresses the extremes of pressures (e.g., tens of MPa) and temperatures (e.g., 700°K) that would be associated with such an accident (Washington and Stuart, 1996). CONTAIN models transport between rooms but, since it was designed for containment facilities (closed systems), does not include infiltration of outside air which is an essential feature of buildings models. CONTAIN does include a ventilation system but with limited fan/blower models available (Spore, et al., 1996). Thus, it was not designed to address the complex HVAC systems (with ducts and controls) typical of multistory officebuildings and the subtle effects of interactions of wind pressures and HVAC imbalances.

The CONTAIN code does include aerosol deposition. There are four aerosol mechanisms modeled in the CONTAIN code: settling, diffusion to surfaces, thermophoresis, and diffusiophoresis. In general, the settling and diffusion are the most important. Comparison of the CONTAIN deposition rate expression with a general and more accurate rate expression (Fernandes and Loyalka, 1996), has shown that for most geometries, the code overestimates the deposition of small particles, mainly because of an assumption regarding the thickness of the boundary layer on particle size. Fernandes and Loyalka (1996) recommended a modification of the code to address this.

The CONTAIN model has recently undergone a rigorous peer review which has qualified it for use by the NRC in its check analysis for vendors and utilities (Boyack, et al., 1995). As would be expected, CONTAIN has not been experimentally tested for buildings and conditions typical of the U.S. building stock. Although it is appropriate for the use for which it was designed and developed, its use to model dispersion of CB agents in a wide range of conventional building types under their typical operating conditions would require substantial modification of the code as well as the kind of experimental testing that the models specifically developed for this purpose have already undergone.

3.3 Intrazonal Models

Indoor CFD Models

Computational fluid dynamics (CFD) models are necessary when local effectswithin rooms need to be resolved (e.g., relationship between a source, detectors, and vents) and when effects across rooms, such as stratification and plumes, depend on phenomena whose scale is small compared to room size. CFD models provide more accuracy than can be obtained from interzonal codes, but at a greater cost in computing time. CFD intrazonal and lumped parameter interzonal models complement each other as transport and fate tools. CFD models are often used to help parameterize lumped parameter models.

CFD models are now commonly employed for predicting the behavior of contaminants (gases and aerosols) in the indoor environment under *high-value situations* (since they are very computer-intensive). For example, CFD models are now routinely used to predict and improve the transport and removal processes for aerosol contaminants in cleanroom environments. There now exists extensive research literature on the use of CFD to predict air flows (and the resulting thermal comfort environment) in indoor spaces which would be expensive to retrofit to "fix" errors: e.g., atria of large buildings (Kato, *et al.,* 1995), stadiums, ice-skating rinks, and auditoriums, although these do not generally include any pollutant deposition to surfaces. Although there have been a number of applications of computational fluid dynamics to building interiors, each application has addressed only one part of the problem, e.g., heat transfer or air flow, and typically in only one or two rooms, and specification of the boundary conditions controlling the CFD simulation have generally been simplified.

For air flow in buildings, turbulence must be a key feature of interior CFD modeling because air flow is rarely laminar. The k-epsilon turbulence model (usually a low Reynolds number version) is the generally accepted standard for modeling turbulent flows inside buildings (e.g., Baker, *et al.*, 1994; Chen, 1997). The world's leading group in modeling turbulent air flow in buildings is probably the Kato and Murakami group at the University of Tokyo. Although most of the publications are in Japanese, there are some English literature reports of that work (e.g., Kato, 1995). In Europe, the most advanced work is from the University of Strathclyde (Clark, *et al.*, 1996) which integrates building thermal simulation with a CFD capability.

LBNL has also developed a series of CFD codes specifically for buildings research applications. The first of these, developed in the early 1980s, was the CONVEC2 model for heat transfer in a single building zone by natural convection (Bauman, *et al.*, 1983; Gadgil, *et al.*, 1984). The CONVEC2 model solves the three dimensional Navier-Stokes equation using the method of false transient to rapidly reach convergence to a quasi-static solution. The building air is modeled as an incompressible Boussinesq fluid. Two equation turbulence models (k-epsilon / k-omega), modified for low Reynolds number turbulence, are used. Arbitrary sources and sinks of fluid mass and heat in the space and on the bounding surfaces are modeled based on Patankar-Spalding differencingusing the SIMPLE and SIMPLER algorithms developed at Imperial College and University of Minnesota.

The CONVEC2 model was tested against careful benchtop convective heat transfer experiments in enclosure flows. Accurate prediction of local Nusselt numbers is a good test of the accuracy of a CFD model for interior spaces. The agreement between CONVEC2 model predictions and measurements of local Nusselt numbers was very good (Gadgil and Gobin, 1984).

More recently, LBNL has led the effort to model generation, transport and deposition of ultra-fine aerosols under natural convection in room sized enclosures with realistic building thermal boundary conditions using the more advanced CONVEC9 (see Appendix, Table A-6) version of the model (Gadgil, *et al.*, 1992; Nazaroff,*et al.*, 1992). CFD modeling of aerosol transport must include an acceptably accurate model of the turbulence in the air flow. This is because Brownian diffusion of most aerosols is far slower than turbulent diffusion, which is determined by local kinetic energy of the air stream. Important sources of turbulence generation in the indoor environment are thermal plumes (lamps, equipment, people, computers, direct solar radiation gain on a surface element) and mechanical (fans, HVAC) systems. Turbulent eddies can also be shed into the air from flow disruptions and detachment of boundary layers from abrupt surface edges. For modeling this latter feature, it is important that the model should have the ability to address architectural details and furnishings. CONVEC9 includes all of these features and also includes radioactive decay and generation of radionuclides. It has been used to investigate deposition of unattached ^{218}Po and ^{212}Pb to enclosure surfaces under laminar natural convection (Nazaroff, *et al.*, 1992). The CONVEC code has also been used to investigate the deposition of ozone to indoor surfaces for laminar convective flow field typically observed in buildings (Cano-Ruiz, *et al.*, 1993). Because CONVEC9 was developed as a research model, it does not have a user manual.

GASFLOW (2.0) (see Appendix, Table A-4) is a CFD model developed at LANL (Travis, *et al.*, 1994; Lam, *et al.*, 1994) to model geometrically complex containment buildings around nuclear reactors, including ventilation systems with multiple compartments and internal structures. It can calculate gas and aerosol behavior of low-speed buoyancy-driven flows, diffusion dominated flows, and turbulent flows during deflagrations. It has been used primarily to model flows inside facilities and around obstacles. Unique features include combustion and transport of flammable gases, chemical reactions, entrainment and deposition of aerosols, and heating/cooling of material surfaces. Because the model uses structured and orthogonal grids rather than unstructured or composite grids, it is not optimal for modeling complex HVAC duct systems or interior spaces with non-orthogonal geometry. Also, GASFLOW models some of these complex phenomena with correlations based on empirical data rather than from models of fundamental underlying processes. Since the empirical data are often based on nuclear reactor accident experiments, it is not clear how applicable these correlations are to other types of buildings and conditions.

GASFLOW has been validated against data from many international experiments, from benchtop tests to 10-story high facilities using mixtures of different gas species and aerosols in a wide variety of conditions from quiescent to highly turbulent (Royl, 1995). At LANL GASFLOW has been used to calculate a plutonium processing facility glovebox fire: temperature profiles and aerosol dispersion; multiroom ventilation system flow patterns and releases (Lam, 1996); experimental program for placement of Continuous Air Monitor (CAM) monitors (Whicker, et al., 1996). Another application was for the Hanford Tank 101-SY ventilation system aerosol and flame transport. GASFLOW was coupled with ABACUS to model structural response in the tank. It was used to reconstruct the Tomsk-7 accident, a runaway chemical reaction and explosion. GASFLOW was used at the Savannah River ITP Tanks to calculate gas mixing, aerosols, and deflagration.

There are also two CFD models which were developed at LLNL for outdoor air modeling, FEM3C (see Appendix, Table A-2) (*e.g.,* Ermak, *et al.*, 1982; Chan, *et al.*, 1984; Koopman, *et al.*, 1989, Chan, 1992) and DYNAFLOW (see Appendix , Table A-3) (*e.g.,* Gresho and Chan, 1990, 1997; Craft, *et al.*, 1997) which might be used for indoor air flow modeling and analysis. These are described in more detail in other parts of this report. FEM3C is a three-dimensional finite element model for simulating the dispersion of heavier-than-air and trace gas releases in the atmosphere. It solves the fully three-dimensional conservation equations of mass, momentum, energy, and species. It can handle instantaneous, finite-duration, and continuous sources and the released materials can be in the form of pure vapor or vapor/droplet. The model also treats variable terrain and obstructions. A modified k-epsilon model based on similarity theory and an advanced model based on the k-ε transport equations are available for turbulence parameterization. Both of these models are finite element based and thus are best-suited for problems with complex geometry. FEM3C has been validated to a large extent for atmospheric flow and dispersion problems. DYNAFLOW is a newer model with many prominent features, including advanced turbulence modeling, modern and efficientnumerics, and unstructured grid, etc. It is likely that both models could be adapted to model the indoor flow and dispersion problem. They would also have to be modified to include removal processes such as aerosol deposition.

There are also a number of general purpose CFD codes available offthe shelf, such as FIDAP (Sohn, 1988), FLUENT (FLUENT, 1993), and FLOVENT (FLOVENT, 1996) which have been used for buildings in research applications. However, their main applications have been in modeling air flows in highly engineered systems, such as aerospace technologies, airflows in clean rooms, cooling of critical pieces of electronic equipment, etc. Recent developments in general purpose CFD methods include COMPGRID and the OVERTURE system (Brislawn, *et al.*, 1996), developed at LANL, and OVERFLOWS (Jespersen, *et al.*, 1997), developed at NASA-Ames.

In summary, there are a number of CFD models (commercial, research type, and publicly available government codes) available to address research problems that are likely to arise during this project, each with certain capabilities and limitations. In general, the commercial codes have capabilities similar to the research and government codes, and none of them is clearly superior to the others. Validation of models for interior dispersion has been very limited and no model/data comparisons covering multiple models has been made. It should also be noted that none of the CFD models developed to date integrate energy use and thermal simulation (e.g., DOE-2), building interior airflow (e.g., CONVEC9, GASFLOW), duct air flow, and nodal modeling of multiple interconnected zones in multistory buildings (e.g., COMIS, CONTAM). Until recently, such integration was hampered by computer speed and capacity limitations. The University of Strathclyde group has recently integrated a convection code (TEACH) with a building thermal model (ESP); however, it lacks a duct model and a nodal model for multiply connected zones (Clark, *et al.*, 1996). LBNL98, a buildings model which is under construction, will integrate all of the pieces (See Section 3.4) but is not yet available.

For the CNBP Transport and Fate modeling and analysis project, we will select CFD models for in-buildings air flow and pollutant transport and fate research problems based on the nature of the research problem to be addressed.

Lumped Parameter In-Room Dispersion Models

In many studies of indoor air pollutant behavior, the assumption is commonly made that pollutant concentrations are well-mixed within a single zone or room. The validity of this assumption strongly depends upon the system under study, the presence or absence of mechanical mixing (such as an HVAC system), the size of the space(s) involved, the ventilation time constant, etc. In some circumstances, pollutant mixing times may be long (see, for example Baughman, *et al.,* 1994), in which dispersion times should be considered in estimating short-term exposures. Even when mechanical systems are present, the location of inlet and outlet ducts or other openings through which airflows occur can set up local concentration gradients within a zone (see, for example, Yamamoto *et al.*, 1990).

There are several methods for estimating the short-term concentration gradient and mixing time, usually relying upon empirical or lumped parameter estimates of diffusion coefficientsfor use with an analytical model (see, for example Drivas, *et al.*, 1996) or, in some cases, coupling diffusion with estimates of airflow in a numerical simulation model (Kim, *et al.*, 1990). In the case of the former approach, it is valid only for cases where there is no strong internal air motion. This is a fairly severe limitation, for even without mechanical mixing, thermally-driven convective cells within a room can provide rapid air motion and hence mixing (Baughman, *et al.*, 1994). In the case of the latter approach, unlike a CFD model, one has to have semi-empirical knowledge about the air flows.

3.4 Advanced Building Simulation Model

As noted in Section 3.3, current models of airflows in buildings are inadequate because they only address one or two pieces of the full problem, with sketchy or non-existent linkages to other full pieces of the problem of heat, air and pollutant transport and fate. The ability to predict transport and fate of airborne pollutants in a complex multizone building requires the ability to model (and interlink) the behavior of the building in terms of:

(1) *Thermal behavior*: modeling the influences of surface temperatures on boundary layers on walls (boundary layers are a significant factor in pollutant transport). Thermal simulation includes the modeling of conduction, convection and radiation transport of heat through the building shell, thermal exchanges of various building elements through these mechanisms, and also the response of the building engineering systems (heating, ventilation, cooling plants, fans and duct works, and sensor and control systems) to the thermal exchanges with the outside and heat flows inside the building. This simulation is routinely undertaken with building thermal models such as DOE2, BLAST, etc.

(2) *Intrazonal air flow:* modeling air flows in large open spaces in the building (such as atria, auditoriums, open plan offices, large entrance spaces, etc.) under the influence of natural convection, mechanical ventilation and infiltration and exfiltration. This modeling must include the critical gas and particulate phenomena of interest, namely, diffusion, advective transport, coagulation, various removal mechanisms including deposition on surfaces, exhaust through duct systems and exfiltration, volatilization and condensation (interactions between gas-phase and aerosol phase materials for semivolatile compounds), etc. This task is routinely handled with CFD models. There have been some recent attempts to integrate CFD models with thermal models. However, existing CFD models have not yet been integrated with large multi-zone network models and duct models.

(3) *Ducts*: modeling the intake, transport, exhaust and removal processes for aerosols and gases through the duct systems in the building, including the details of removal phenomena, e.g., deposition on various duct surfaces and on fan blades, removal by filters in the duct systems, as well as resuspension.

(4) *Multizone transport*: modeling of transport of air into and out of various zones in the building driven by the pressure differencesand flow resistance of doorways and windows, mechanical ventilation, thermal stratification, exfiltration and wind-infiltration. This requires modeling the building as a nodal network of sparsely interconnected zones. This simulation is commonly undertaken with models such as COMIS and CONTAM. (A typical large commercial building may have 200 zones each modeled as a node. The most that current CFD codes can directly model in detail is a couple of interconnected zones.)

No simulation model exists today that integrates these diverse phenomena, each of which is separately a crucial piece of the full problem, although fast and accurate simulation models for each of these pieces were available a couple of decades ago. The major reason for the lack of such integration is that sufficient computer power was not available to solve this problem. Only now, with the rapid increase in computing power, has such an integration become feasible.

LBNL has an ongoing funded project to develop such an integrated building model, designed to operate using the computing power of the NERSC (National Energy Research Scientific Computing Center) at LBNL. However, even early versions of this model, tentatively titled LBNL98, will not be available until late in 1998. A summary of salient features of the LBNL98 code has been included the Appendix (Table A-9) for completeness. It should also be noted that, although input and output modules of LBNL98 will be user-friendly, like existing CFD models, LBNL98 will be very input data intensive and computationally intensive. Thus, it will be used for simulation modeling to address specific research problems for buildings and will not replace multizone air flow models such as COMIS or CONTAM.

3.5 Indoor Pollutant Behavior Models

Aerosol Deposition Models

The behavior of aerosols has received considerable attention, particularly with respect to outdoor (ambient) concentrations, the downwind transport and fate of aerosols in plumes, their interaction with surfaces, etc. In addition, analytical equations for the deposition of aerosols, under the influence of diffusion, gravitation, etc. have been derived. However, indoors the presence of surfaces can alter the behavior of aerosols. For

example, aside from the influence of ventilation (which interacts with almost all airborne species uniformly), deposition is often the largest removal process for aerosols. However, this is very size dependent, with a minimum deposition velocity for particles in the range of 0.1 to 0.5 μm equivalent aerosol diameter. For particles smaller than 0.1 μm, the deposition velocity rapidly increases as the particle size decreases, due to the increasing particle diffusion rates. Similarly, for particles larger than ~0.5 μm, deposition velocities rapidly increase with size, as gravitational settling becomes increasingly important.

Models for aerosol behavior indoors have often treated airborne species with a single deposition velocity (or equivalently, a single loss rate due to deposition). For some applications, this approximation is adequate, e.g., for aerosols within a narrow size range. For polydisperse aerosols, it is not very useful. In addition to deposition, it is sometimes important to incorporate terms such as coagulation or gas-to-particle conversion, which can also alter the concentrations and size distribution of the indoor aerosol.

MIAQ4

There are few models that provide the basis for calculating the deposition rate (velocity) as a function of particle size. Of these, the particle deposition theory of Crump and Seinfeld (Crump and Seinfeld, 1981) is among the best known and used. This model, based on the approach by Corner and Pendlebury (1951) for homogeneous turbulence, derives deposition coefficients, which are related to the turbulence intensity, K_e, for various surface orientations. When combined, as in the case of a room with vertical surfaces (walls), a downward-facing surface (ceiling) and an upward-facing surface (floor), the overall particle deposition coefficient or rate shows a strong particle size dependence. Depending upon the turbulence intensity used, the minimum deposition coefficient (rate) is for particles in the size range from 0.2 to 0.5 μm.

Comparison with experimental data is limited, especially for room-size enclosures. In two cases, the model predictions were examined against measured environmental tobacco smoke (ETS) loss rates in a room-size chamber (Nazaroff and Cass, 1989a; Xu, *et al.*, 1994). In both cases, the data and the model predictions show a similar behavior with respect to particle size. However, in neither case is there excellent agreement. It is likely that inhomogeneities in the turbulence within the room and/or imperfect mixing might account for the differences.

A more complete treatment of aerosol behavior indoors has been developed by Nazaroff and Cass (1989b). This model, named MIAQ4 (see Appendix, Table A-7), uses a multicomponent sectional representation of the aerosol size distribution in which the concentration and size distribution of the aerosol are given by a series of contiguous size sections or bins. Within each of these, the aerosol behavior is represented by differential equations accounting for the effects of ventilation, filtration, deposition onto surfaces, resuspension, direct emission or entry into the indoor space, and coagulation.

Of particular importance to this work, the model addresses particle deposition on surfaces in considerable detail, including the effects of surface temperature, surface orientation and flow conditions within the enclosure. A series of equations describing the different deposition regimes has been derived and used iteratively in the model. Alternatively, the user may specify the deposition velocities for each particle size section as a substitute for those derived from these detailed calculations.

The model can be used to predict the time-dependent behavior of airborne aerosols, specifying both the concentrations and the size distributions at any given time. Mass loading on the various indoor surfaces - also as a function of time and aerosol size bin - is also predicted. The model can incorporate a variety of source terms -usually provided as emission profiles and total mass - and removal terms, such as ventilation.

The model was validated against environmental tobacco smoke data obtained in a single room-size chamber (Nazaroff and Cass, 1989b). The model has been used to develop emissions profiles for indoor aerosol sources (Sextro *et al.*, 1991). MIAQ4 has also been used to examine the behavior of aerosols indoors, from estimating exposures to environmental tobacco smoke (Miller-Leiden, *et al.*, 1993) and evaluating engineering controls for ETS (Miller-Leiden and Nazaroff 1996) to the soiling of museum artwork by deposition of indoor aerosols (Nazaroff, *et al.*, 1990).

LBNL Simplified Duct Model

This model (see Appendix, Table A-8) is based on a set of analytical equations describing aerosol deposition in (or alternatively, penetration through) ducts as a function of several key parameters, including duct dimensions, flow, aerosol size and density, and whether or not the flow is turbulent. The model was first formulated to examine the efficiency for delivery of aerosol particles through a duct system for use as sealants for duct leaks (where the overall sealing efficiency is a product of the aerosol penetration through the duct and the deposition efficiency in the leaks themselves) (Carrie and Modera, 1995) The model can be used for first-order

estimates of the loss of aerosols in ducts in single family residential buildings, which when coupled with an air flow model like COMIS and room deposition modeling with MIAQ4, helps form a more complete picture of aerosol behavior in indoor environments. This model does not address depositional losses of aerosols in more complex duct systems found in commercial buildings, nor does such a model yet exist.

Models for the Deposition/Re-Emission of Vapors from Indoor Surfaces

Buildings and ducts have large surface-to-volumeratios so airborne vapors (e.g., sarin, tabun) can be expected to be removed from the air by sorption onto various indoor surfaces, and to be subsequently re-emitted to some degree. Thus, sorption and desorption can be expected to have a very substantial effecton indoor air concentrations and on human exposures to vapor-phase chemical warfareagents. There have been only a very limited number of models developed to describe the sorption and re-emission of vapors in indoor environments (e.g., Dunn and Tichenor, 1988; Dunn and Chen, 1993; b 1989a; Axley, 1991; Axley and Lorenzetti, 1993; Van Loy, *et al.*, 1997), and even less work on model validation (Guo, 1993).

Dunn and Tichenor (1988) described a linear reversible sorption model for the sorption and desorption of volatile organic compounds (VOCs)[3] in indoor air at partial pressures which are low relative to their saturation vapor pressure. This model assumes a Langmuir-type of interaction between adsorbate and adsorbent. At low partial pressures, the Langmuir isotherm reduces to a linear partitioning coefficient. Mass transfer between the gas- and sorbed-phase is first order in both directions. Dunn and Tichenor (1988) achieved good agreement between modeled and measured concentrations in indoor air for emissions from moth cake crystal (1,4-dichlorobenzene) and mixed emissions from latex caulk. This model was later refined by Tichenor, *et al.*, (1991) to incorporate a non-linear, power-law desorption rate into the linear reversible model. They achieved good agreement between measurement and model for emissions from wood stain in a model house used for indoor air quality research.

In ongoing research at LBNL, we are investigating the sorption and desorption of nicotine, a semi-volatile organic compound (SVOC), in a 20 m^3 environmental chamber, without and with carpet, painted wallboard, etc., in order to further the development of such models (Van Loy, *et al.*, 1996, In press). In the empty chamber, approximately 80 to 90% of the emitted nicotine is lost from air via deposition to the walls within about 30 minutes of emission and reaches a plateau within about 45 minutes. Some of the sorbed nicotine is re-emitted after the chamber is ventilated with outdoor air. Three differentmodels were tested to determine how well the each model predicted the experimental data - a linear reversible sorption model and a nonlinear reversible sorption model with linear deposition (Tichenor model), and a nonlinear reversible sorption model with nonlinear deposition and re-emission. All three models gave reasonable fits to the gas-phase concentration data for the first 3 hours of the experiments at a low air exchange rate. However, only the fully nonlinear model gave a good fit to the full experimental data set, which includes both sorption and re-emission.

Experiments on nicotine sorption and desorption in a carpeted chamber have been completed and are being analyzed. Experiments are planned on the sorption and desorption of nicotine on painted wallboard in the environmental chamber. A second series of experiments with another SVOC, phenanthrene, will then be undertaken in the chamber without added surfaces and with carpet, and painted wallboard. This ongoing research will advance our modeling capabilities for sorption and desorption processes. However, almost nothing is known about the specific interactions of various compounds with differentkinds of indoor surfaces that are commonly found indoors, e.g., painted wallboard, vinyl flooring, carpeting, and duct linings. Thus, more research will be needed to develop adequate models for vapor-phase agents for the purposes of the Fate and Transport Modeling and Analysis Thrust area.

Bill Blewitt (Aberdeen Proving Ground, DOD) is currently conducting experiments on sorption losses to surfaces within a building structure and across the building envelope using mustard simulant and sarin (Personal communication to A. Policastro). This experimental work is expected to be of considerable value in our efforts to model such losses in buildings.

3.6 Findings and Recommendations

Accurate prediction of the temporal and spatial variability of concentrations of CB agents in buildings requires several different types of models, some of which exist already, and some of which require more research

[3] VOCs are generally defined as organic compounds with saturation vapor pressures greater than about 0.1 Pa. Examples include benzene, toluene, hexanal and pentanal. Semi-volatile organic compounds (SVOCs) are defined as compounds with saturation vapor pressures between about 0.1 to 10-5 Pa. Examples of the latter include p-dichlorobenzene (mothballs), nicotine (from cigarettes), phenanthrene from combustion sources, and, based on its physical properties, probably tabun.

and development. The core model which is required is an interzonal (multizone) airflow and pollutant transport model that can be used for a wide range of building types and conditions. Because buildings have large surface-to-volume ratios, models to estimate depositional losses of aerosols and vapors to interior surfaces, building envelopes, and HVAC systems are also required..

A recent survey (Feustel, H.E. and J. Dieris, 1992) of multizone air flow models produced descriptions of 50 differentmodels. More models have been developed since. However, most of these models have been written as research tools and are not available to third parties. As a consequence, they are difficult to use and are, at best, "user-tolerant" rather than "user-friendly". Some are proprietary commercial rather than public access codes, and thus less suitable. The following criteria were used to select a core model:

(1) publicly available code;

(2) substantial field validation in a range of building types;

(3) capable of addressing a wide range of building types (e.g., residential, small and large commercial, stadiums, etc.).

Two models met these criteria best: COMIS and CONTAM. COMIS was selected as the core model for most applications. It has been evaluated extensively by the International Energy Agency (IEA) and in inter-model comparisons with 14 other models and showed good agreement between model predictions and experiments. Furthermore, a recent validation study of COMIS and CONTAM (Haghighat and Megri, 1996) showed that the results of the two models were virtually identical under the conditions which were modeled. COMIS was originally developed at Lawrence Berkeley National Laboratory with DOE funding, and COMIS related research efforts within the frame of the International Energy Agency were directed and coordinated by the Berkeley Laboratory. In addition, there is no reason to prefer another existing model and we are very familiar with COMIS and its codes. If appropriate, we will also use some of the simpler models such as Exposure or MCCEM.

We expect that both in-room dispersion models and CFD models may be required in this effortto help address discrepancies between experimental measurements and airflow model predictions. We will use the most suitable and easily applied CFD model, as needed, to address specific research issues in the development of parameterized model components to be integrated into COMIS, e.g., the development of a model for aerosol deposition losses in complex duct systems.

To address the physical and chemical behavior of CB aerosols and vapors with interior surfaces (i.e., deposition, re-suspension, re-emission), additional model modules must be integrated into COMIS. MIAQ4 was selected to model deposition of aerosols in rooms. MIAQ4 is (to the best of our knowledge) the only model that has been developed and tested to predict deposition of aerosols in rooms, in buildings operating under standard conditions of temperature and pressure, we plan to use this model for most applications. This model takes into account particle size and air flow conditions within buildings and has been tested against measured data. We plan to integrate this model with the COMIS air flow model to predict air concentrations of CB aerosols in buildings and their temporal and spatial variability.

For aerosol deposition in complex duct systems typical of multistory commercial buildings, there are no existing models that are adequate. To meet this modeling need, we plan to conduct an integrated program of experimental research and modeling to develop a parameterized model for deposition losses of aerosols in duct systems as a function of particle size, air flow rates, etc. It is likely that CFD modeling will be required for parameterization of the duct model for complex HVAC systems. The developed model will be integrated with the core COMIS multizone airflow model for indoor air modeling in buildings.

There have been only a very limited number of models developed to describe the sorption and re-emission of vapors in indoor environments (e.g., Dunn and Tichenor, 1988; Dunn and Chen, 1993; Nazaroff and Cass, 1989a, b; Axley, 1991; Axley and Lorenzetti, 1993; Van Loy, *et al.*, In press), and even less work on model validation (Guo 1993). Furthermore, we do not currently have information on the sorptive interactions of toxic chemical agents that might be used in a terrorist attack with key indoor materials which constitute the largest indoor surface areas, e.g., painted wallboard, carpets, vinyl flooring, duct liners, although there is some ongoing DOD research in this area (B. Blewitt, Aberdeen Proving Ground, Personal Communication to A. Policastro).

Our current plan is to work on vapor deposition and re-emission modeling in Years 4 and 5 of the CBNP Program and to build upon and utilize the results of ongoing research in this area at LBNL and several other research laboratories, e.g., U.S. EPA, Aberdeen Proving Ground (DOD). Experiments to determine how strongly selected toxic chemicals sorb on selected indoor materials (*e.g.*, determinations of deposition

velocities) will be needed. Once some measured data have been generated on deposition velocities for representative vapors, it should be possible to use structure-activity relationships to infer deposition velocities for related compounds.

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4 MODELS FOR FLOW AND TRANSPORT AROUND BUILDINGS

4.1 Introduction

In this section, we review numerical and analytical models that could be applied to predicting concentration fields in the vicinity of buildings. Our review emphasizes numerical models due to the complexity of the problem, but analytical-empirical models are considered as well due to their computational efficiency and relative ease of application. We limit our numerical model review to Computational Fluid Dynamics (CFD) codes that have been developed within the DOE, but include several others that have been widely used or have unique features. Since many of the CFD codes are used in conjunction with separate dispersion models, we have concentrated our efforts on the numerical modeling of the flow dynamics and mention only briefly the pollutant transport and dispersion capability of these models. We begin with a short description of how fluid dynamics models could be used in the context of a chemical and biological warfare (CB) agent release in an urban environment and why it is important to explicitly model the flow around buildings in an urban environment. Tables of the major features of the CFD codes are reviewed in the Appendix. These including information on model attributes, referencesto application and model comparison studies, and contacts for each CFD model. Due to the importance of model validation, we also provide a condensed referencelist for field and wind-tunnel experiments of flow and dispersion around buildings. We conclude this chapter with research needs and recommendations.

4.2 Rationale

A major concern of the DOE CBNP Program will be the release of chemical and biological warfare agents by terrorists into urban areas. Flow and transport models will necessary for three main reasons: 1) pre-incident planning and vulnerability assessment, 2) real-time emergency response, mitigation, and damage assessment, and 3) post-incident reconstruction and consequence analysis. *Pre-incident planning and vulnerability assessment* requires knowledge of the path taken by hazardous materials moving through a city. Understanding of the dispersion, chemistry, and deposition of the agents through use of CFD models can be used to design precautionary measures for specific targets or the population at-large. Real-time *emergency response, mitigation, and damage assessment* within an urban environment requires fast computational tools that can be applied to a multitude of situations. In the near future, it may be possible to model proactively, using faster than real-time CFD models to predict localized effectsand concentration hot spots. Currently, however, even with state-of-the-art computers, real-time response is only possible with simpler, parameterized models. These simpler models can be enhanced by using CFD models to design better parameterizations. *Post-incident reconstruction and consequence analysis* will be enhanced in urban environments by use of CFD codes. Source strength, location, and the time history of the agent release can be reconstructed. From this, decontamination and medical-assistance efforts can be improved by determining where the agent traveled and what the exposure levels were for different segments of the population.

The transport and fate problem subdivides into several conceptual areas of effort delineated by scale: mesoscale, many-building microscale, several-building microscale, and indoor microscale. The outdoor microscale is the focus of this chapter, and can be divided into the "many-building" and "several-building" study problems. The former involves modeling of flow around ten to twenty buildings with adequate resolution—perhaps tens of meters—to simulate the major recirculation features. The latter involves detailed modeling of flow around one or two buildings with computational grid cells on the order of a few meters in size. At this resolution buildings possess sharp corners and obstruct the flow. Vortices, or zones of recirculation, form on all sides of the buildings—including the rooftop—with the largest generally forming downwind of the building. CB agents can be trapped in the vortices between structures and concentrations can build up significantly there. Groups of buildings act to enhance the horizontal diffusion of the CB agent (see Fig. 4-1), thus resulting in a larger area of plume impact. In addition, CB agents can actually travel in a direction opposite to the prevailing wind direction through vortex transport and can lead to non-zero concentrations upstream of the source. Enhanced turbulent mixing caused by building elements can loft CB agents higher into the atmosphere where the winds are stronger, thus resulting in greater distances covered by the CB agent in a given amount of time. Moving objects, like automobiles, and heating and shading of the building and street surfaces add another dimension to the problem by contributing to the turbulent mixing process at street level. Clearly, accounting for the influence of buildings is critical to the accurate description of transport and fate on urban up to regional scales.

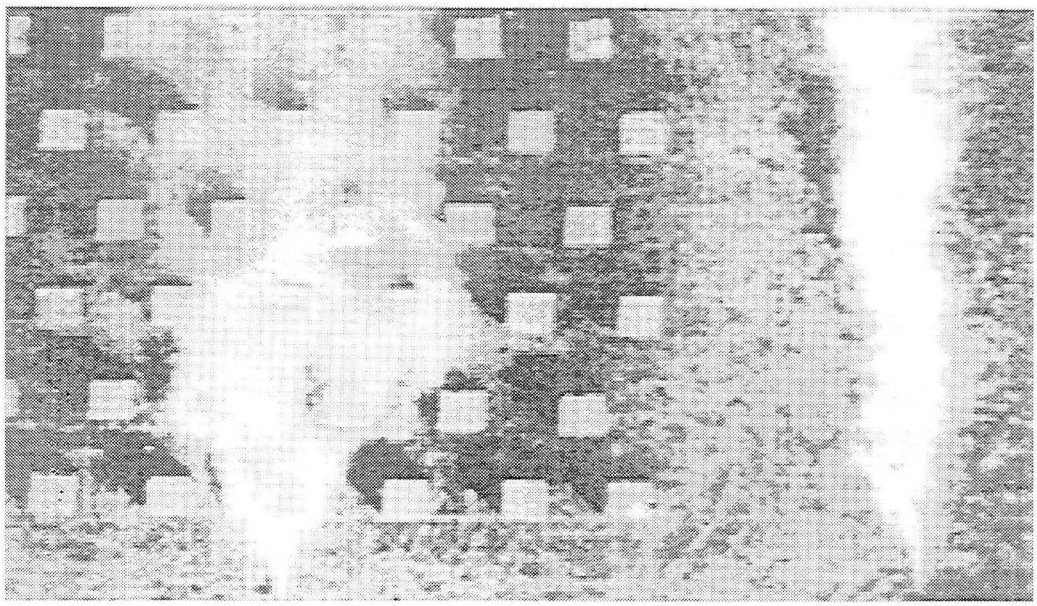

Figure 4-1. Plan view of reduced-scale dispersion experiments showing plume dispersal through group of buildings on left and over unobstructed terrain on the right (Davidson et al., 1995). The concentration fields become even more difficult to predict when the relative sizes, shapes, heights, and spacings of the buildings change or when the wind is not perpendicular to the building face.

4.3 Computational Fluid Dynamics Models

In this section we will give a brief review of DOE and other popular CFD codes that have been or could be applied to simulating flow around buildings, building complexes, and street canyons. To keep the number of codes reviewed manageable, we will not consider CFD codes that are used primarily for aerodynamic, combustion, metal casting, heat transfer, and other non-building related applications (i.e., models that would require significant recoding for building flow applications). We begin with a list of the major features found in CFD models (Table 4-1). They are divided into physics, numerics, and user amenity categories. Many of the entries are similar to those given for the mesoscale models (see Appendix—Prognostic Meteorological Models) since the conservation equations describing the fluid dynamics are nearly the same on both scales. Like the mesoscale, how to specify the subgrid-scale turbulence is important. For the microscale, however, modifications to turbulence closures have been made to account for sharp-edged and streamline curvature effects. Simulations of flow around obstacles show strong sensitivity to the turbulent diffusion representation. Table 4-2 lists many of the turbulent parameterization techniques being incorporated into CFD models and gives a short overview of their advantages and limitations.

On the microscale, the hydrostatic approximation is never valid in the vicinity of buildings. In other words, the vertical velocity is computed prognostically and cannot be deduced solely from mass conservation considerations. Also, the Coriolis effectis generally neglected on the microscale. For real-world applications, stratification and surface heating effects need to be accounted for in the CFD code.

Table 4-1. Features of CFD models applied to flow around buildings

differentiators	comments
PHYSICS: ➤ fluid type and flow regimes - compressible vs. incompressible - sub- vs. supersonic - Newtonian vs. non-Newtonian	Atmospheric flow around buildings will be non-hydrostatic, incompressible, sub-sonic and Newtonian. Some codes have broader applicability, however.
➤ turbulence closure scheme	Range from simple to complex. Generally, trade-off between representativeness and computational efficiency. Simple empirical schemes generally not valid in flows around buildings. Some argue that gradient diffusion schemes too simple.
➤ temperature conservation equations	Atmospheric and building-induced stratification may have important effect on flow around buildings.
➤ moisture conservation equations	Not certain if moisture effects important; perhaps for aerosol chemistry or condensation formation (which affects the surface energy balance)
➤ surface heating schemes	Range from simple boundary condition specification to surface energy budget calculations. May need to account for solar heating of walls and streets, shadow effects, heat conduction into and out of buildings, etc.
➤ boundary conditions - inflow & outflow - top & bottom	Different b.c. options (e.g., zero gradient, cyclic, pressure, slip, no-slip) are required for correct flow field representation and allow the user flexibility and potential short-cuts in modeling.
➤ dispersion capability - Lagrangian vs. Eulerian - dense, neutral, and buoyant gases - deposition and resuspension	Trade-offs between Eulerian and Lagrangian methods. Codes can have built-in dispersion or be linked to dispersion models. Gas/aerosol density, deposition, and resuspension may be important for CB agents.
➤ chemistry	Chemical reaction mechanisms for gases and/or aerosols may be important for CB agents.
NUMERICS: ➤ mathematical representation - finite difference or volume - finite element - spectral	Different mathematical approaches for obtaining numerical solution have advantages and disadvantages. Trade-offs in speed, stability, accuracy, complexity, and problem representation.
➤ numerical scheme - implicit vs. explicit time integration - advection scheme - pressure solver	Schemes have differences in accuracy, speed, timestep size, solution damping, robustness, rate of convergence. Generally, no one scheme is best.
➤ mesh type - coordinate system (cartesian, cylindrical, spherical) - structured vs. unstructured - orthogonal vs. non-orthogonal - variable grid size - multi-block capability - adaptive mesh capabilities	High resolution in near-wall regions is needed for flow around obstacles. This can be achieved in different ways, ranging in complexity, accuracy, and efficiency. Methods that can achieve high resolution in localized areas are advantageous from a computational standpoint.
USER AMENITIES: ➤ graphical user interface	Can reduce learning-curve, but can make code changes more difficult to implement.
➤ input format - pre-processor - grid generator	Some codes require manual input of mesh points, initial conditions, etc. Others can automate some of the input.
➤ output formats	Is data format fixed or user-specified?
➤ graphics packages	Is graphics capability built into code? Data output for specific graphics packages? Real-time graphics? 1-d, 2-d, and 3-d visualization essential.
➤ platforms	IBM-PC, Mac, UNIX Workstation, Supercomputer (vector and/or parallel) compatible? 3-d simulations will require lots of CPU time.

Table 4-2. Some Turbulence Schemes Used in CFD Modeling

type	comments
➤ **K-theory gradient diffusion**	* equates the unknown Reynolds turbulent shear stress to the product of the turbulent diffusivity and mean velocity gradients * this closure method has been used in many applications; lots of validation studies * gradient diffusion is known to incorrectly represent turbulent mixing, but in practice works relatively well
➤ 1st order - empirical formulae	* not universal; performs poorly in complex, inhomogeneous flow fields * doesn't provide full-suite of turb. parameters for dispersion models (i.e., no tke or dissipation) and spatial variation oversimplified
➤ $1^1/_2$ order - 1-eqn k model	* more universal than 1st order closures * one prognostic eqn. (for tke) and 1 emp. formula (usually for the mixing length)
➤ $1^1/_2$ order - 2-eqn k - ε, k-l and k-ω models	* more universal than 1st order and 1 eqn. $1^1/_2$ order closures * two prognostic eqns. (for tke and either dissipation, mixing length, or vorticity) * provides more complete description of turb. parameters for dispersion modeling
➤ $1^1/_2$ order - non-linear 2-eqn k -ε model	* terms added to gradient diffusion relationship to overcome perceived limitations of traditional 2-eqn k -ε approach
➤ $1^1/_2$ order - RNG 2-eqn k -ε model	* derived from 2nd order models using renormalization group theory * thought to be more universal than traditional 2-eqn k -ε models
➤ $1^3/_4$ order - non-linear 3-eqn k -ε–A model	* includes 3rd prognostic eqn. for anisotropy invariant * thought to be more universal than traditional 2-eqn k -e models
➤ **2nd order closure** ‰ algebraic stress model ‰ Reynolds stress model	* solves approximated prognostic equations for the Reynolds turbulent shear stresses * used mostly for research purposes * may give better results than 1.5 order models for specific cases, but overall results are inconclusive * difficult to parameterize 3rd order moments * adds significant computational requirements
➤ **Large-eddy simulation (LES)**	* solves space-filtered conservation equations; produces turbulence directly on the large-scale and uses closure for the sub-grid scale * used mostly for research purposes * difficult to use in stable (nighttime conditions) or with variable grid size * very computationally intensive
➤ **Direct numerical simulation (DNS)**	* solves conservation equations; produces turbulence directly * applied to idealized flows only, not real atmosphere * extremely computationally intensive

This requires the temperature (and possibly moisture) conservation equations and surface radiation budget equations to be explicitly modeled. Building shading effectsand surfacemoisture might play a significant role in energy budget partitioning and hence affect the flow field. Finally, for release of toxic agents, the CFD code should be linked to or have a built-in Eulerian or Lagrangian transport and dispersion capability, and possibly the capacity of handling gaseous and aerosol chemistry, as well as deposition and resuspension physics.

CFD codes usually solve the fluid dynamics conservation equations using either finite difference,finite element, or spectral numerical methods (although no spectral models are reviewed here). Each have their advantages and disadvantages in regards to accuracy, stability, computational efficiency,complexity, and range of application. Likewise, the numerical schemes for solving the conservation equations generally have trade-offs between accuracy, speed, stability, robustness, conservativeness, and solution damping. A large number of numerical schemes exist (e.g., see Roache, 1985; Ferziger and Peric, 1996) and to say which are "best" is often problem dependent and user defined. Similar trade-offs exist for the pressure solver, which must be instituted for a non-hydrostatic flow problem. For flow around buildings, special numerical techniques are often adopted to avoid the instabilities arising at sharp corners.

Grid meshes are either structured or unstructured. Unstructured grids offer flexibility in terms of cell shape and refinement, and are well suited for flows around complex geometries. They suffer from higher computational

requirements and more complex solver coding. Structured meshes are more commonly found in CFD codes and a number of techniques have been developed to utilize them efficiently in flows with obstacles of complex geometry (e.g., nested grids, non-orthogonal grids, volume fraction techniques). Since high resolution is needed near walls when modeling flow around buildings, variable mesh size capability is very important to combat computational requirements. For orthogonal structured meshes, multi-block methods are useful for providing high resolution in specific regions.

User amenities, such as a graphical user interface(GUI), are sometimes required depending on the user audience. GUI interfaces are found on commercial CFD codes, but few government or university research codes. These interfaces can reduce the learning curve and often reduce the problem set-up time. A run-time interface is found on several commercial codes, and provides graphical or text-based feedback on the status of a simulation. All CFD codes require 1-d, 2-d, and 3-d graphics packages for visualization of data. Some codes offerbuilt-in graphics packages, while in others the data is exported to an external package. Most of the CFD codes have been designed to work on workstations or supercomputers. Several have been modified to work on vector or parallelarchitectures.

A short description of the major features, referencesto model descriptions and application studies, and contact persons are given for the DOE-team CFD models (see Appendix Tables). The models are in different stages of development, have been applied to a broad range of applications, and each have their unique advantages, limitations, and "bells and whistles". For example, the GASFLOW code (Table A-4) has unique combustion, particle deposition and resuspension, and chemical kinetics capabilities. HIGRAD (Table A-10) has an advanced monotone numerical scheme and radiative energy balance equations. FEM3C (Table A-2) has strengths in dense and buoyant gas dispersion and phase change processes and its finite element approach allows for complicated geometries to be handled. DYNAFLOW (Table A-3) has the most advanced turbulence model and complex geometries are easily handled with its unstructured mesh capability. TEMPEST (Table A-11), although having few unique features, has been successfully validated against experimental building flow data (Zhang et al., 1996). Each code is capable of modeling flow around buildings with varying amounts of success, although multiple building complexes will certainly stress computer resources and specifics of the flow field may contain errors (e.g., cavity size, turbulence intensity). Table 4-3 summarizes the features of these models. For comparison, we present several popular commercially-available CFD codes in Table 4-4 and list their unique features. These codes are on par with the DOE-team codes in numerical and physics capabilities, but generally have stronger graphical user interfaces (GUI's).

4.4 CFD Model Review Studies - Flow Around Building Applications

In general, CFD model review studies of low-speed turbulent flows around bluff bodies have attempted to validate turbulence closures or numerical schemes rather than specific CFD codes. Although there is some consensus about CFD model limitations, it is often difficult to separate the numerics, physics, and boundary condition issues (e.g., Bradshaw et al; 1994). The backward facing step has been a traditional flow problem by which to test models for application to flow around obstacles. For example, Rodi (1994) found somewhat better agreement with experimental data for the mean and turbulent flow fields using a 2-layer k-ε compared to the traditional k-ε approach. Speziale (1991) showed that the non-linear k-ε approach predicted the reattachment point and turbulence intensity better than the traditional k-ε approach. Friederich and Arnal (1993) found good agreement between experimental data and LES model results for most mean and turbulence flow components, although the results were not vastly superior to advanced traditional k-ε approaches. Reviews of traditional CFD modeling studies is given by Bradshaw et al. (1994), Lumley (1990), and Patel et al. (1985).

Although most of the DOE-team models have been applied to flow around obstacles, only TEMPEST has been validated for flow around a building through comparison of results with experimental data in a peer-reviewed article. Zhang et al. (1992) found reasonable agreement for the mean flow around a single building in neutral stratification. For stable stratification, Zhang et al. (1996) showed that TEMPEST wind fields were in reasonable agreement with measurements, but found differences in the concentration fields. The other DOE-team models should perform equal to or better than the TEMPEST code, however, due to more advanced numerical, turbulence, and dispersion schemes.

Table 4-3. DOE-Team CFD Model Attributes

	PHYSICS							NUMERICS						
	Fluid Eqns.	Turb. Scheme	Heat Eqns.	Moist. Eqns.	Shear Stress B.C.	Surface Temp. B.C.	Bldg. Shade	Math. Scheme		Solver Method	Accuracy time	Accuracy space	Pressure Solver	Vector/ Parallel
Dynaflow	I	3 eqn. k-e-A2	T	no	wall integrated	U & F	no	FE	I &E	PM	2nd O	2nd O	I	V
Fem 3c	I	K-theory +2 eqn. k-e	T	no	law-of-wall	U & F	no	FE	E	MFE-BTD	2nd O	2nd O	I	V
Gasflow	C	K-theory + 2 eqn. k-e	IE	no	law-of-wall	U & C	no	FD	I/E	ICEd-ALE	1st O	1st O + 2nd O	I	V
Higrad	C & I	K-theory + 1 eqn. k-l	IE	yes	none	R	no	FD	E		2nd O	2nd O	D & I	V & P
Tempest	I	2 eqn. k-e	T	no	law-of-wall	U & C	no	FD	E/I	SMAC		1st O	I	V

Key:

Fluid Equations:
I = Incompressible
C = Compressible

Heat Equations:
T = Temperature
IE = Internal Energy

Surface Temperature B.C.:
U = User specified
C = 1-D Conduction
R = Radiation Scheme
F = Specified Flux

Mathematical Scheme:
FE = Finite Element
FD = Finite Difference or Volume
E = Explicit
I = Implicit

Solver Method:
PM = Projection Method
MFE-BTD = Modified Forward Eulerian - Balanced Tensor Diffusion
ICEd-ALE = Implicit Continuous-fluid Eulerian - Arbitrary-Lagrangian- Eulerian
SMAC = Simplified Marker & Cell

Pressure Solver:
D = Diagnosed (Direct, Explicit)
I = Iterative (Indirect, Implicit)

Table 4-3. DOE-Team CFD Model Attributes (cont.)

	MESH				DISPERSION								USER AMENITIES		
	Grid Type	Vari-able Mesh Size?	Multi-block?	Adap. Mesh?	Built In or Linked?	Model Type	Source Type	Depo-sition	Resus-pension	Dense Gas	Aerosol Physics	Chem.	GUI Interface?	Run-time Interface?	2-d & 3-d plots?
Dynaflow	U-N	Yes	Yes	No	Built-in	E	None	No	No	No	No	No	No	No	Yes
FEM 3C	S-N	Yes	No	No	Built-in	E	M-A & V	No	No	Yes	No	No	No	No	Yes
Gasflow	S-O	Yes	No	No	Built-in	E	M-A & V	Yes	Yes	Yes	Yes	Yes	No	No	Yes
Higrad	S-N-T	No	No	No	Could be Linked	x	x	x	x	x	x	x	No	No	Yes
Tempest	S-O	Yes	No	No	Built-in	E	M-A & V	No	No	No	No	No	No	No	Yes

Key:

Grid Type:
S = Structured
U = Unstructured
O = Orthogonal
N = Non-Orthogonal
T = Terrain-following

Type:
E = Eulerian
L = Lagrangian

Source Type:
P = Point
L = Line
A = Area
V = Volume
M = Multiple Sources

Table 4-4. Some Commercially-available CFD Models

Model Name	Applications and Unique Features
CFD-ACE 2.0 CFD Research Corp. Huntsville, AL 205-536-6576	• Interior flows, turbine combustors, turbomachinery, heat transfer, multi-phase flows. • Multi-block mesh; 3rd order accurate spatial scheme option; chemical kinetics models; 2-phase spray models.
CFX 4.1 AEA Technology Bethel Park, PA 412-833-4820	• Interior flows, car/train aerodynamics, turbomachinery, heat transfer, multi-phase flows. • Menu-driven GUI pre-processor; grid generator; multi-block mesh; 2nd order turbulence closure option; chemical kinetics models; solar radiation scheme.
FLOW-3D Flow Science, Inc. Los Alamos, NM 505-662-2636	• Interior flows, spacecraft and missile aerodynamics, heat transfer, porous media flow, nozzle flow, natural convection and free surface flows. • Menu-driven GUI pre-processor; grid generator; fractional area volume obstacle representation; RNG and LES turbulence options.
FLUENT & FLUENT/UNS Fluent, Inc. Lebanon, NH 603-643-2600 800-445-4454	• Interior flows, electronics systems, turbomachinery, heat transfer, free surface and multi-phase flows. • Menu-driven GUI pre-processor; run-time interface; grid generator; multi-block and hybrid meshes; dynamic mesh adaptation, RNG k-e turbulence closure option.
PHOENICS 2.2 CHAM London, England 44-0-181-947-7651	• Interior flows, electronics systems, turbomachinery, heat transfer, free surface and multi-phase flows. • Menu-driven GUI pre-processor; run-time interface; grid generator; multi-block mesh; RNG k-ε turbulence closure option; chemical kinetics models; shareware version available.
STAR-CD Computational Dynamics Limited London, England 44-0-181-969-9639	• Interior flows, building flows, ventilation, turbomachinery, heat transfer, electronics systems and multi-phase flows. • Menu-driven GUI pre-processor; grid generator; multi-block mesh; chemical kinetics models.

4.5 Analytical-Empirical Models

References for analytic-empirical models used to compute concentrations in the vicinity of single or multiple buildings are given in Table 4-5. These models are generally based upon Gaussian concentration solutions, dimensional analysis, and/or empirical data-fitting. Methods are sub-divided into macroscopic and microscopic viewpoints. In the former case, the effect of many buildings on the larger-scale plume evolution are parameterized, but concentration variations between buildings are not accounted for. In the latter case, the impact of an individual building or urban canyon on the near-field concentration distribution is approximated. Much of the analytical-empirical model development has been sponsored by the USEPA, NRC, and state air quality agencies for regulatory purposes. Models developed for traffic dispersion purposes often include emissions sub-modules or links to emissions models. We review only those that account for building or urban canyon effects on plume dispersion.

From the macroscopic viewpoint, the simplest and most popular approach has been modification of the Gaussian plume spread parameters σ_y and σ_z to account for enhanced mixing due to the urban canopy. In general, the modifications do not account for different building densities, shapes, and heights, and the approaches are saddled with the limitations of the Gaussian plume methodology. Several models utilize urban turbulence and heat flux parameterizations for determining the plume spread parameters, which makes them applicable over a broader range of meteorological conditions.

Table 4-5. Analytic-Empirical Models for Urban Environments and Buildings

Method	Reference(s)	Description
Macroscopic-Many Buildings		
Gaussian dispersion model w/ urban plume spread parameters	see Hanna et al. (1987), Boubel et al. (1994), Pasquill and Smith (1983)	urban s_y and s_z parameters are input into the Gaussian eqn. They are larger than the rural plume spread parameters and were determined from a limited number of urban tracer experiments.
CRSTER and MPTER (USEPA)	Wilson (1993)	Regulatory Gaussian plume models with option for urban plume spread parameters. Intended for tall stacks, no building downwash.
Hybrid Plume Dispersion Model (HPDM)	Hanna and Chang (1992)	Uses Gaussian, PDF, Low-wind, and Lofting models for different met. conditions. Uses urban plume spread parameters and also includes urban turbulence and heat flux parameterizations and building downwash algorithms.
Microscopic-SingleBuilding		
Gaussian w/ Building Amplification Factors	Thompson (1993)	Concentrations computed by Gaussian eqn. for flat terrain are multiplied by factors to account for buildings. Factors are empirically determined.
Gaussian w/ Building Downwash Method	Huber and Snyder (1982)	Gaussian plume spread parameters modified to account for enhanced mixing in building wake. This formulation incorporated in several EPA and commercial models.
	Ramsdell and Fosmire (1995)	Incorporates spread parameters with three components: standard diffusion, meander, and building wake correction. Building wake correction is function of building area and wind speed.
ISC-Industrial Source Complex Model (USEPA)		EPA regulatory model that uses building downwash algorithms.
Minimum Dilution Model	Wilson and Chui (1994)	Only estimates upper bound on concentration. Function of wind speed, building area, and downwind distance.
Microscopic-Urban Canyon		
CAR Model	Eerens et al. (1993)	Purely empirical model. Background urban concentrations are modified based on wind-tunnel parameterizations for 4 urban canyon street types.
CALINE 4 (California Air Resources Board)	Benson (1992)	Regulatory street intersection/highway model. Uses Gaussian line source model with urban canyon wall reflection and vehicle-wake induced mixing options. Has traffic emissions sub-modules.
CAL3QHC (USEPA)		EPA regulatory model. Similar to CALINE.
Box Model	Nicholson (1975)	Gives average concentration within urban canyon based on volume and ventilation rate.
Microscopic-Urban Canyon		
Upwind/Downwind Model-APRAC w/ STREET sub-module	Dabberdt et al. (1973)	Gaussian plume model with urban canyon sub-model. Conc. increases/decreases on downwind/upwind side of canyon as fn. of wind speed, building ht, and street width.
- Intersection Midblock Model	Benesh (1978)	Uses STREET sub-module with minor modifications.
- MAPS Model	Sobottka & Leisen (1980)	Uses STREET sub-module with minor modifications.
Canyon-Plume-Box (CPB3) Model	Yamartino and Wiegand (1986)	Accounts for non-vortex and vortex dispersion using Gaussian plume model and box model. Plume dispersion parameters determined from the Hotchkiss & Harlow (1973) urban canyon wind profile formulation and turbulence profiles based on wind-tunnel experimental data (fn. of wind speed, building ht, and street width). Also vehicle-induced dispersion accounted for.

Several approaches have been devised to account for individual buildings on the mixing process. The building amplification factor method uses the Gaussian dispersion equations for flat terrain and then modifies the computed concentration by a factor representing the ratio of concentrations with and without buildings. The building amplification factors are functions of space, building shape, and source position and must be determined from experiments or CFD modeling. The building-downwash approach is used to simulate releases on top of buildings that are entrained into the wake downwind of buildings. A modified Gaussian model with enhanced plume spread parameters is used if the ratio of wind speed to effectivestack height is larger than a critical value. Several analytical-empirical approaches have been devised for computing concentrations in urban canyons. Most account for pollutant trapping in the urban canyon by specifying a ventilation velocity parameter. Several of the analytic models are based on the seminal numerical CFD modeling work of Hotchkiss and Harlow (1973) in which the numerically predicted vortex between the buildings is parameterized.

The analytic models are relatively fast and easy to use, but they are not applicable to a broad range of conditions. In general, the models are not able to handle a wide variety of building shapes, spacings, differences in building heights, oblique angle approach winds, non-ideal stratification, and unsteady meteorological conditions. Since most of the models rely on empirical data for specifying parameterizations, the models are only as good as the data and can only cover the range of conditions found in the experiment. An evaluation study of plume dispersion around nuclear facilities found that nearly 50% of the concentrations computed by the best current analytic models are off by more than a factor of 4 and 15% off by more than a factor of 10 (Ramsdell and Fosmire, 1995). Forty percent of the concentrations computed by the current NRC Regulatory model were

off by a factor of 10. State-of-the-art CFD modeling could be used to improve predictions by generating flow and concentration fields over a wide range of conditions and using them to generalize analytic model parameterizations.

4.6 Field and Wind-Tunnel Experiments

Because of the complexities of flow and transport around buildings, use of experimental data for validation purposes is essential. In this section, we present references to field and wind-tunnel experiments that may be useful for verification of microscale model physics. Table 4-6 lists referencesfor recent or often-cited field studies and is divided into dispersion and flow-fieldexperiments. Relatively few field experiments have been performed due to cost, the large number of instruments needed, the difficulty in repeating experiments with similar atmospheric conditions (in order to obtain data with statistical significance), and the problem of generalizing results due to site-specific complexity (e.g., buildings of different heights, shapes and spacing, variable terrain, trees). Notice that several of the dispersion experiments used tracers, while others measured pollutant concentrations emanating from cars, buses, and nearby industrial sources. For the latter cases, it is often difficult to quantify the source position and strength. Also, notice that some of the experiments are performed in built-up urban areas while others were performed with only one or two buildings in the vicinity. In general, we expect very different results for the two cases.

Table 4-7 gives referencesfor recent or often-cited wind-tunnel studies. Many studies around buildings have been performed in wind-tunnels and, in general, the flow and dispersion fields are measured with higher resolution and accuracy than in field studies. Additionally, an idealized and systematic arrangement of buildings is possible and the wind speed and direction can be controlled. However, the broad range of conditions that occur in real atmospheres cannot be simulated in wind tunnels, as they are usually limited to simulating neutral stability flows. We note a few studies have been performed in towing tanks that allow for stable stratification, but no wind shear. For more information, see reviews by Hosker (1984) and Hosker (1987).

4.7 Research Issues

Significant research efforts are called for in the modeling of flow and transport around buildings. Fluid and plume dispersion physics research is needed in both the prognostic and analytic modeling arenas. Unique research efforts can be identified based on scale, going from mesoscale, to urban scale, and down to building scale. Table 4-8 lists some of the areas in which models need to be improved and/or validated. A major contribution to the end-user community could be made by improving the universality of the analytical-empirical models. Many of these improvements could be accomplished using CFD modeling results. Another important research contribution can be made in the many-building transport and fate problem. Few efforts, if any, with CFD models have been attempted due to the computational resources necessary to address the problem. Cutting-edge research on numerics, physics, fidelity, and high performance computing issues will be necessary. Critical research efforts will need to be undertaken in gaseous and aerosol chemistry on the small scale, including deposition and resuspension physics. Finally, investigation of appropriate urban canopy sub-grid parameterizations needed in mesoscale models should be performed in collaboration with the mesoscale modeling team.

Table 4-6. Field Experiments

Reference	Description
Dispersion Studies	
Higson, Griffiths, Jones, and Hall, 1996. Flow and dispersion around an isolated building, At. Env., v 30, p 2859.	Tracer study. Point source releases upstream of isolated model building. No met measurements reported. Includes concentration fluctuations.
MacDonald, Griffiths, and Cheah, 1997. Field experiments of dispersion through regular arrays of cubic structures, At. Env., v 31, p 783.	Tracer study. Point source releases upstream of array of model buildings. Limited met measurements.
Davidson, Mylne, Jones, Phillips, Perkins, Fung, and Hunt, 1995. Plume dispersion through large groups of obstacles- a field investigation, At. Env., v29, p3245.	Tracer study. Point source releases upstream of array of model buildings. Vertical profiles of met measurements reported.
Ramsdell and Fosmire, 1995. Atmospheric dispersion estimates in the vicinity of buildings, Rep. No. PNL-10286.	Tracer study. Point source releases in vicinity of nuclear reactors. Arcs of concentration data around reactors or measurements on buildings. Limited met measurements. Multiple stability classes reported.
Kitabayashi, 1992. A field study of airflow and tracer gas diffusion in a model street canyon, 9th World Clean Air Cong., Montreal, Canada.	Tracer study. Point source releases in urban street canyon in Tsukuba, Japan. Multiple met and turbulence measurements on masts.
Depaul and Sheih, 1985. A tracer study of dispersion in an urban street canyon, At. Env., v19, p 555.	Tracer study. Line source release in "typical" urban street canyon in Chicago. Limited met measurements.
Dabberdt, Ludwig, and Johnson, 1973. Validation and applications of an urban diffusion model for vehicular pollutants, At. Env., v 7, p 603.	Auto emissions. Multiple CO and met measurements on masts in urban street canyons in St. Louis.
Luria, Weisinger, and Peleg, 1990. CO and NO_x levels at the center of city roads in Jerusalem, At. Env., v 24B, p 93.	Auto emissions. Moving CO and NO_x measurements in city of Jerusalem. No met measurements.
Qin and Chan, 1993. Traffic source emissions and street-level air pollution in urban areas of Guangzhou, At. Env., v 27B, p 275.	Auto emissions. Multiple CO and NO_x measurements on masts in city of Guangzhou. Limited met measurements.
Qin and Kot, 1993. Dispersion of vehicular emissions in street canyons, Guangzhou, At. Env., v 27B, p 283.	Auto emissions. Review of other experiments. Found contradictory conclusions, indicative of problem complexity.
Zamurs and Conway, 1991. Comparison of intersection air quality models' ability to simulate CO concentrations in an urban area, Trans. Res. Rec. 1312.	Auto emissions. Ground-level CO measurements at intersections in NY City. Limited met measurements.
Nakamura and Oke, 1988. Wind, temperature, and stability conditions in an east-west oriented urban canyon, At. Env., v 22, p 2691.	Detailed met. measurements on masts in an urban canyon in Kyoto, Japan. Includes temperature field within canyon.
Oikawa and Meng, 1995. Turbulence characteristics and organized motion in a suburban roughness sublayer, Bound. Layer Met., v 74, p 289.	Detailed met. and turbulence measurements on masts downwind of suburban area in Sapporo, Japan. Includes power spectra.
Rotach, 1995. Profiles of turbulence statistics in and above an urban street canyon, At. Env., v 29, p 1473.	Detailed met. and turbulence measurements on masts in urban canyon located in Zurich city center.
Rotach, 1993. Turbulence close to a rough urban surface, Part I: Reynolds Stress, Part II: Variances and Gradients, Bound. Layer Met., v 66, p 1.	Detailed met. and turbulence measurements at rooftop in Zurich city center.

Table 4-7. Wind-Tunnel Experiments

Reference	Description
Dispersion Studies	
Lee, Call, Lawson, Clements, Hoard, 1996. A video image analysis system for concentration measurements and flow visualization in building wakes, At. Env., v 25A, p 1211.	Single building(s). Point source releases at numerous locations on variable size buildings. No flow measurements reported. Includes real-time concentrations.
Thompson, 1993. Building amplification factors for sources near buildings: a wind-tunnel study, At. Env., v27A , p 2313.	Single building(s). Point source releases at numerous locations on variable size buildings. No flow measurements reported. Neutral stratification.
Huber and Snyder, 1982. Wind-tunnel investigation of the effects of a rectangular-shaped building on dispersion of effluents from short adjacent stacks, At. Env., v 16 , p 2837.	Single building(s). Point source releases at numerous locations on variable size buildings. No flow measurements reported. Neutral stratification.
Snyder, 1994. Some observations of the influence of stratification on diffusion in building wakes, in *Stably Stratified Flows*, Clarendon Press.	Single building. Point source release downstream of building. Concentration measurements and flow visualization. Stable stratification (towing tank).
Ohba and Lawson, 1993. Physical modeling of concentration distributions around two high-rise buildings, AMS 8th Appl. of Air Poll. Met. Conf., Nashville, TN.	Two buildings. Point source releases downstream of buildings. Concentration fields. Flow and turbulence measurements in separate report. Neutral stratification.
Lee and Hoard, 1992. Wind-tunnel experiments on plume dispersion in clusters of buildings, LA-12229-MS.	Multiple buildings. Point source releases at several locations. Video image analysis, includes real-time concentration measurements. Neutral stratification.
Hoydysh and Dabberdt, 1994. Concentration fields at urban intersections: fluid modeling studies, At. Env., v 28, p 1849.	Building arrays. Line source releases in urban canyons. Concentration fields and flow measurements reported in several papers. Neutral stratification.
Flow Field Studies	
Martinuzzi and Tropea, 1993. The flow around surface-mounted, prismatic obstacles placed in a fully-developed channel flow, J. Fl. Eng.., v 115, p 85.	Single building. High resolution flow and turbulence measurements around single block-shaped obstacle. Neutral stratification.
Castro and Robins, 1977. The flow around a surface-mounted cube in uniform and turbulent flows, J. Fl. Mech., v79, p307.	Single building. Flow visualization studies. Neutral stratification.
Counihan, Hunt, and Jackson, 1974. Wakes behind 2-d surface obstacles in deep boundary layer flows, J. Fl. Mech., v 64, p 529.	Single building. Flow visualization and mean field measurements. Neutral stratification.
Kothari, Peterka, and Meroney, 1979. Stably stratified building wakes, NRC NUREG/ CR-1247.	Single building. Mean flow field measurements. Stable stratification.
Snyder, W.H. and Lawson, R.E., 1994: Wind-tunnel measurements of flow fields in the vicinity of buildings, AMS 8th Joint Conf. on Appl. of Air Poll. Met., Nashville, TN.	Single building(s). Mean and turbulence flow field measurements. Neutral stratification, multiple approach flow angles.
Theurer, Baechlin, and Plate, 1992. Model study of .the development of boundary layers above urban surfaces, J. Wind Eng.., p 437.	Building array. Detailed flow and turbulence measurements around several building array arrangements. Neutral stratification.

Table 4-8. Research Issues for Modeling of Flow and Transport in Urban Areas

Analytic-Empirical Models
Urban Scale - Determine Gaussian plume spread parameters as function of building spacing, height-to-width ratio, etc. Currently, there are plume spread parameters for rural and urban cases only. - Account for building effects (e.g., trapping, reflection off walls) in Gaussian plume models. Currently buildings are invisible to plume except for enhanced spread.
Building Scale - Improve flow descriptions (e.g., wake size, velocity profiles) and dispersion parameterizations for larger set of conditions (e.g., variable wind angles, building heights, height-to-width ratios, stability) through experiment and CFD modeling. Current model-data comparisons show low correlation.
Prognostic Models
Plume Dispersion Modeling - For Eulerian modeling, need to address near-source resolution issues for point source plumes. Otherwise, numerical diffusion of the plume can be significant. - For Lagrangian modeling, need to determine internal parameters (e.g., Lagrangian timescale) for complex flows. Relations linking these parameters to k-e model output need to be validated for complex flows. - Small-scale gaseous and aerosol plume chemistry capabilities need to be expanded. - Deposition and resuspension physics need to be improved. - Concentration fluctuation capabilities need to be added in cases where peak concentrations are important. - Linking plume dispersion models across scales may be problematic.
Fluid Dynamics Modeling-Mesoscale - Parameterizations accounting for the sub-grid scale effect of the urban canopy on the mean and turbulent flow fields, as well as the surface radiation budget, need to be developed or improved. - Appropriate feedback mechanisms with the urban scale need to be identified.
Fluid Dynamics Modeling-Urban Scale - Modeling flow around large number of buildings will require tradeoffs in resolution and computational speed. Innovative numerical schemes may need to be developed and fidelity issues will need to be resolved. - The advantages and limitations of different turbulent closures for many building applications should be investigated. Tradeoffs between turbulence closure sophistication and computational speed may be necessary. - Need to investigate whether atmospheric phenomena at this scale are still important. For example, CFD models generally do not account for many atmospheric processes (e.g., surface radiation budget, moisture transport), turbulence constants are different for atmospheric and engineering boundary-layer flows, and topography may be difficult to treat in traditional CFD models. - Appropriate feedback mechanisms with the mesoscale and building scale need to be identified.
Fluid Dynamics Modeling-Building Scale - Modeling flow around a few buildings may require tradeoffs in resolution and computational speed. Ultra high resolution simulations on high performance computing platforms may be necessary for resolving fidelity issues. - The advantages and limitations of different turbulent closures for single building and urban canyon applications should be investigated. Comparison with detailed wind-tunnel experiments is warranted. - The impact of off-axis wind, stratification, and surface heating effects should be determined. - Appropriate feedback mechanisms with the urban scale need to be identified.

4.8 Findings and Recommendations

The DOE suite of CFD models are all capable of modeling flow around buildings and differentaspects of plume transport and dispersion. The DOE models are on par with university and commercial codes, except in the area of graphical user interfaces and automatic mesh generation where commercial codes have a decided advantage. Which model is "best" is problem dependent. For example, one model may more accurately simulate flow around a group of rectangular buildings while another does better for a few buildings of odd shape and size. Which model is "best" also depends on the user's needs. For example, does the end-user need to know the concentrations to within ±5% accuracy or is ±25% acceptable? Does the end-user need the answer in a few seconds or will several days suffice? If the former is true, then analytical-empirical models are necessary.

We recommend that a suite of CFD models be used for CB transport and fate issues, as no one model can claim to be superior in all areas. The modeling suite should include both prognostic and analytic models, and perhaps even diagnostic codes. This would provide a modeling system capable of dealing with the entire range of Incident Response Issues. These CFD models should be evaluated against experimental data of flows around idealized obstacles (e.g., backward facing step, single building, two building urban canyon) in order to test numerics, turbulence closures, and other parameterizations.

Below are summarized the main points of this chapter:

1. Relatively sophisticated CFD models can play a vital role in all phases of CB transport modeling, including pre-incident planning, real-time emergency response, and post-incident analysis. For pre-incident planning and post-incident analysis, CFD models can provide the detailed flow fields required for the accurate simulation of CB agent dispersion inside and around buildings, and in subway stations as well. For real-time emergency response, relatively computer-intensive CFD models can be used in designing improved parameterizations for the simpler, but faster analytical-empirical models.

2. The five DOE CFD models reviewed in this section all have relevant capabilities and, in principle, could be adapted for modeling air flow and the dispersion of CB agents around buildings and in subway stations. As a group, the models have relatively sophisticated numerics, cover a range of turbulence closures, and can model neutral, buoyant, and dense gas dispersion, as well as aerosol deposition and resuspension. These models can provide the basic capabilities for the CBNP program to build on for modeling CB agent dispersion inside and around buildings, and in subway stations.

3. Each of these models has its unique capabilities and limitations. For example, DYNAFLOW has the most advanced turbulence model and unstructured grid capability best-suited for treating complex geometries. However, development is required to extend it to simulate the dispersion of CB agents. FEM3C is also capable of treating complex geometries and has been validated in many studies for the atmospheric dispersion of heavy gases. However, the dispersion capabilities for CB agents also remain to be developed. GASFLOW has the most complete dispersion physics; however, it has first-order-in-time numerics and lacks the ability to treat non-orthogonal geometries effectively. HIGRAD has an advanced monotone numerical scheme and radiative energy equations, but its turbulent parameterizations are incomplete and its CB dispersion capabilities remain to be developed. TEMPEST has been validated to some extent against flow and dispersion data from a cubical building, but it does not have CB dispersion physics and has less sophisticated numerics and grid capabilities.

4. The DOE-suite of CFD codes are on par with the best commercial and university codes. It is preferable and advantageous to build on the DOE CFD models, instead of investing in proprietary codes, for CB dispersion modeling. Besides having substantial capabilities to build on, the National Laboratories are one of the few places in the world that have the expertise in all related disciplines and the computer power needed for tackling the complex CB transport and fate problem.

5. From an end-user perspective, relatively fast and easy-to-use analytical-empirical models may be necessary for real-time emergency response scenarios. Research efforts to improve their range of applicability needs to be performed. Use of CFD models may help in this purpose.

6. During the development of the CFD and analytical-empirical models continuous validation should be carried out. References to relevant field and wind-tunnel experiments around buildings have been presented in Tables 4-6 and 4-7.

7. Significant challenges exist for the successful prediction of the transport and fate of CB agents in urban environments. Trade-offs between model sophistication, accuracy, and computer requirements need to be addressed. Innovative research efforts are required in the areas of numerics, turbulence closure methods, gaseous and aerosol dispersion physics and chemistry, and high performance computing.

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5 LOCAL-REGIONAL METEOROLOGY AND DISPERSION MODELS

5.1 Introduction

In this chapter, we are concerned with the transport of a terrorist release of a chemical or biological agent that moves across large urban areas and on out to the surrounding suburbs. The size of the release could vary from a small hand-held container of agent released by a single terrorist to a large transportation or storage vessel of hazardous materials that is released as a result of sabotage. Smaller scale models (reviewed earlier) address the dispersion in the immediate vicinity of the source. Here, we are reviewing models for simulating the transport and the subsequent effect on downwind sections of urban areas, and the surrounding suburbs several kilometers or even a hundred kilometers away. At these larger scales, topography, differencesin surface forcing or weather systems affect the wind pattern. Hence, in general, models used at these scales must account for these features.

To predict dispersion in the atmosphere at scales up to 100 kilometers, one must account for the effects of many different and competing processes such as: advection by the mean wind field including the effectsof wind variations in space and time, turbulent diffusion caused by the random eddies present in the wind field, transport by coherent structures such as the thermals in the convective boundary layer, and interactions with the surface including vegetation canopy effects and urban building effects. Many additional processes may also be involved depending upon the specific characteristics of the contaminant. For example, gravitational settling and deposition complicate the dispersion of aerosols, and buoyancy effects are important for heavier-than-air contaminants. Chemical agents can undergo important chemical transformations and the viability of bio-agents can be influenced by factors such as ultraviolet light exposure.

Because the mean position of the contaminant and the mean wind are closely related, an accurate representation of the mean wind field is the primary requirement for an accurate dispersion simulation. For predictions within a few kilometers and in regions of flat terrain, using the value of the wind at the release point may be sufficient. However, in regions of complex terrain or for larger scales, one must account for the wind variations in both time and space. Therefore, such simulations require a full three-dimensional description of the wind field at a number of different times.

A second requirement for an accurate dispersion simulation is to predict the spread correctly. The plume's shape will be strongly dependent upon transport by both the turbulent eddies and the coherent structures in the atmosphere. How accurately these phenomena must be modeled depends upon the time and space resolution desired. To predict the instantaneous concentration field, one would have to predict every turbulent eddy the plume encountered. However, to predict the hourly integrated concentration, one need only predict the hourly average effectof the turbulent eddies on the plume. A similar relationship is seen when predicting point values rather than volume averages.

We are interested in models for: 1) pre-incident planning and vulnerability assessment, 2) real-time emergency response, and 3) post-event reconstruction and analysis. The requirements for emergency response, where time is essential, are significantly different from those for planning or reconstruction. We review a broad spectrum of models used to produce winds, from simple diagnostic models to complex prognostic models. Similarly, we review a range of dispersion models, from simple plume and puff models, to more complex particle models. Modeling systems that can be rapidly executed are necessary for emergency response, while models with more complete and accurate representation of the physics (and generally longer execution time) would be desirable for planning, analysis, or reconstruction.

5.2 Modeling Strategies

Since dispersion and the wind field are intimately connected, the prediction of the wind field and the dispersion would, ideally, be done concurrently within the same model. However, for reasons of efficiency, these operations are often split between a wind field model and a dispersion model that are run serially. Therefore, one must understand not just the dispersion model, but also, the model that provides the wind fields to the dispersion model. (See Fig. 5-1)

The simplest wind model is one in which the wind field is constant in space determined by a single wind observation or wind profile near the source. This is the approach used in plume dispersion models and is one reason that they are very limited in application, i.e.. to areas of flat terrain and short distances.

Diagnostic models are the next step in complexity. Diagnostic models create steady-state, three-dimensional atmospheric wind fields. They combine interpolation/extrapolation of observations with the application of a physical constraint (usually conservation of mass) to produce the wind field. Thus, the availability of observations determines the fidelity of the information provided. The major disadvantages of diagnostic models are that they have no forecast ability, and unless an unusually dense observation network exists, they do not accurately represent complex flow patterns. Their major advantages are simplicity, and an ability to provide information very rapidly. This can be vital for an initial emergency response.

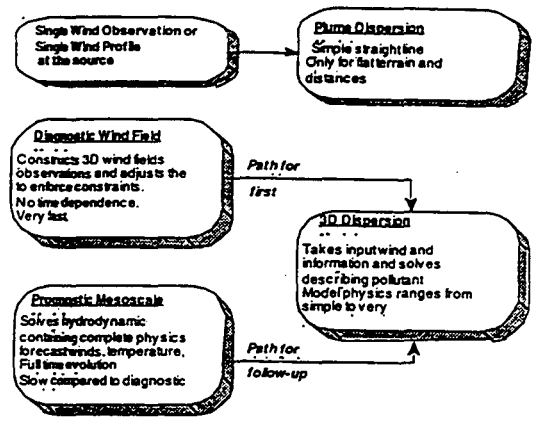

Figure 5-1. Relationship between wind field and dispersion models.

Prognostic models, on the other hand, are remarkably complex, solving a full set of hydrodynamic equations and often including cloud and precipitation processes. They combine observations and analyzed data, with topographic forcing, to produce a forecast of the full three-dimensional representation of the winds and thermodynamic structure over time. These models provide turbulence information as well as forecast wind and temperature fields that are not available from diagnostic models. They have the advantage of being able to represent complex flows for long time periods over long distances. Their major disadvantage is the time necessary to provide information.

Once the wind field model has run, the dispersion model uses its results plus information about the source to simulate the movement of a pollutant through the atmosphere and produce forecasts of pollutant concentrations as a function of time and space. Dispersion models have a wide range of complexity ranging from simple plume models to complex stochastic particle model and will be described in more detail later in the chapter.

Since it often takes a series of models to predict the pollutant concentrations, these models often come as complete modeling suites. While parts of these suites may be mixed and matched, it is usually not cost effective to do so. Fig. 5- 2 lists the modeling suites currently available to this project.

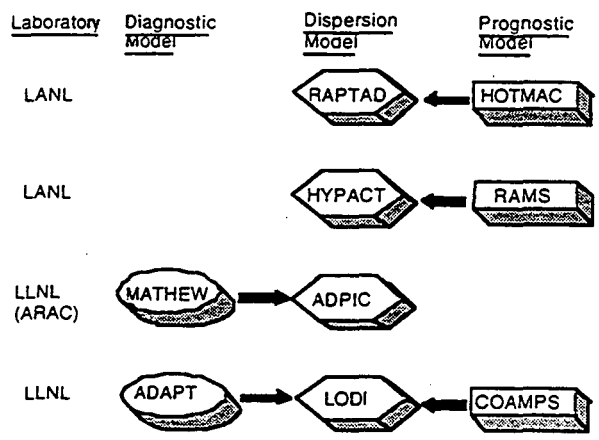

Figure 5-2. Dispersion modeling suites currently available to the CBNP Transport and Fate thrust area scientists.

In the remainder of this chapter, we will be describing and comparing the various models that could be adapted to a modeling suite whether they are actually part of a dispersion modeling suite or not. The goals of this comparison are to 1) verify that the scientific community recognizes the CBNP Transport and Fate models as a basis for an emergency response system, 2) identify capabilities, techniques or resources that may be acquired to aid in development of the DOE CB emergency response system, and 3) identify areas of research that need to be undertaken. We will first examine wind field models both diagnostic and prognostic and follow this with an examination of dispersion models.

5.3 Diagnostic Wind Field Models

Diagnostic wind field models are used to provide rapid estimates of atmospheric winds, and to a lesser extent the thermal structure of the atmosphere. Diagnostic models rely on steady state physical constraints, most frequently mass conservation. These models produce gridded wind fields using data from a variety of sources (surface, towers, upper air, radar, sodar, etc.). These models interpolate data from the various sources, producing gridded data fields, using terrain forcing at the lower boundary and physical constraints throughout the domain. The winds are passed to dispersion models for calculating transport of the released agent. Because of their simplicity, advantages and disadvantages exist. They execute very rapidly on any platform, providing quick answers for emergency response. However they are limited by the number of observations, providing better estimates as the number of observations increases. This is especially true when the circulation is complex. They are limited to short time estimates (1 to 2 hours), since they have no forecast capability and must assume persistence.

Table 5-1. Diagnostic Wind Field Models

	ADAPT	MATHEW	MINERVE
Constraint	Mass Conservation	Mass Conservation	Mass Conservation
Vertical Coordinate	Option (Terrain Following)	Constant z, block terrain	Terrain Following
Stability	Temperature Lapse Rate, f(terrain)	Pasquill Stability Classes	Pasquill Stability Classes
Interpolation (x,y)	Option (Barnes, $1/r^2$, linear)	$1/r^2$	Option (Cressman)
Interpolation (z)	Option (linear, cubic spline, power law)	power law, linear	Option (3-d, linear)
Winds	(u,v) or (s,d)	(s,d)	(u,v)
Temperature	Yes	No	No
Terrain Influence on Winds	Yes	Yes	Yes
Contact	Gayle Sugiyama, ASD, LLNL	John Nasstrom, ASD, LLNL	James Hodge, DSWA

Two diagnostic models available to the CBNP Transport and Fate researchers, ADAPT and MATHEW, as well as the MINERVE model are summarized in Table 5-1. ADAPT is currently being developed at LLNL as part of an upgrade to the ARAC system. MATHEW is the current diagnostic model in the ARAC system, and together with the dispersion model ADPIC, has been used for several years, and independently evaluated by several agencies. MINERVE, included for comparison, was developed in France and has been used for DOD applications as part of the HPAC/HASCAL system.

In Table 5-1, when the entry is "option", examples of the option follow in parenthesis. For example, the vertical coordinate in ADAPT may be terrain following as an option, but ADAPT can use one of several vertical coordinate options, according to the user's preference.The stability entry refers to whether the vertical weights vary for the vertical interpolation. All three models weigh the vertical wind differently than the horizontal, and all choose the weights differently. For the winds, (u,v) refers to interpolation of components, (s,d) to interpolation of speed and direction. ADAPT also interpolates the temperature as well as the winds, although univariately. Neither of the other models currently has this capability.

5.4 Diagnostic Model Surveys and Evaluations

Ratto et al. (1994) recently completed a survey of diagnostic models. The survey included models that are constrained by conservation of mass, as well as those that also use a simplified form of the momentum equations, i.e. linear dynamic models (LDM). Approximately fifteen models were reviewed.

Diagnostic models, by nature, are very simple with very basic physics. While that can be advantageous, they are limited in how much detail in the wind field they can represent. Any feature in a flow field must be observed, otherwise the feature will not be represented. Therefore, for more complex flow, more observations are necessary.

Due to their simplicity, diagnostic wind field models tend to be very similar in capabilities, ease of use and computational requirements. Diagnostic models can differ in the choice of vertical coordinate and terrain representation, physical and dynamic constraints, and interpolation techniques. The representation of the wind field is most sensitive to the choice of interpolator. Adjustments due to the constraints tend to be small and the vertical coordinate choice and terrain representation also lead to differences.especially near the surface when the terrain is complex.

Besides the Ratto et al. survey, there have been two recent evaluation studies of diagnostic models. Kamada (1992) evaluated six diagnostic models (NUATMOS, CALMET, PGEMS, WOCSS, LINCOM, MATHEW), but also included dispersion models. The purpose of his evaluation was for spills at Vandenberg AFB, California, and included computational requirements and portability. The conclusions of the study were: 1) there is no undisputed winner among diagnostic wind flow models, and 2) each flow model displays limitations.

Finardi et al. (1993) evaluated four diagnostic models: two mass consistent models (MATHEW and MINERVE) and two linear dynamic models (MS3DJH/3R and FLOWSTAR). Model simulations were compared against wind tunnel data. A primary weakness of LDM is the choice of horizontal scale of the topography, i.e. the aspect ratio. They do a better job than mass consistent models for sparse data cases, as they represent more physics. A primary weakness of the mass consistent models is the dependence on properly sited input data. Comparisons with wind tunnel data representing flow over isolated hills showed that all models described the flow to within 20%, excluding the wake region, and are therefore suitable for practical applications, with caveats.

5.5 Diagnostic Model Findings and Recommendations

Diagnostic models have an important role in the CBNP program for real time emergency response, due to their speed in calculating a first estimate of the wind field. Due to their simplicity, the overall performanceof diagnostic wind field models is similar and no single model is clearly superior. The DOE laboratories, especially through the ARAC system (MATHEW and ADAPT), have a long history in the use of diagnostic models. At the same time, it is recognized that diagnostic wind field models are limited. Because they have no forecast capability, they are limited to short duration (1 to 2 hours) where persistence is reasonable. Also, due to the lack of physics, they are less useful for reconstruction calculations where time is not limiting and more detailed calculations are warranted. The same is true for pre-event or planning calculations. It is recommended that existing CBNP Transport and Fate models be used in the CBNP research and model development program, in particular MATHEW and ADAPT. As new diagnostic techniques, physics capabilities, or more efficient computer algorithms emerge, the DOE labs should add these to the existing models.

5.6 Prognostic Wind Field Models

Prognostic models (commonly referredto as mesoscale meteorological models) solve three-dimensional time-dependent equations for atmospheric circulation. In simpler terms, they predict the evolution of the winds, thermodynamic structure, and moisture in the atmosphere for periods out to two or three days. Most of these models also predict other physical values of possible interest, such as precipitation and radiative fluxes. These models can be run at very fine spatial scales but also can be used for very large domains. In short, prognostic models create a realistic representation of the winds and other important variables at the time and space scales necessary for the CBNP program.

Prognostic models also have their limitations. Surface elements (e.g. buildings) at very short spatial scales are crudely represented. There is a "spin-up" problem at very short time scales (1 to 2 hours) and a "predictability" issue at longer time scales (after2 to 3 days). A method for addressing both of the time scale issues is time-dependent data assimilation, where observations are included with the model equations without destroying the balance in the equations. This is an increasingly difficult task as spatial resolution is increased and is an area for active research. The computational time required to complete a forecast is another limitation of these models, making current prognostic models of limited value for real-time emergency response.

Prognostic wind field models can be divided into two general classes: hydrostatic and non-hydrostatic. Hydrostatic implies that the mass and pressure are in approximate balance in the vertical, or equivalently that vertical accelerations are small relative to gravitational acceleration. Hydrostatic models solve a reduced set of equations, the primitive equations, where the vertical momentum equation is replaced by a balance between the gravitational acceleration and the vertical pressure gradient. The implication is that the vertical velocity and scale of motion is small relative to the horizontal. For large horizontal scales, the approximation is valid and hydrostatic models are adequate for representing atmospheric flow. In fact, hydrostatic models are used for weather prediction at all major forecast centers worldwide, predicting winds, temperature and precipitation. However, as the horizontal scale decreases, the approximation is less valid and hydrostatic models are inadequate. Since we are dealing with problems at the low end of the forecast model scale, non-hydrostatic models will be more appropriate in general.

Non-hydrostatic models solve the full set of the atmospheric Navier-Stokes equations. In particular, an equation for vertical acceleration is included. All non-hydrostatic models solve the same fundamental set of equations. Like the hydrostatic models, non-hydrostatic models forecast weather, including winds, temperature

and precipitation. There are no fundamental limiting assumptions in these models and they are applicable at scales from global down to very small scales.

Both hydrostatic and non-hydrostatic models are used by the CBNP Transport and Fate researchers. NORAPS (see appendix, Table A-12), a hydrostatic weather forecast model is used in research at LLNL and is being incorporated into the ARAC emergency response system. COAMPS (see appendix, Table A-13), a non-hydrostatic model, is also used in research at LLNL, with plans to include it in the operational ARAC system as well. HOTMAC (see appendix, Table A-14), a hydrostatic model, and RAMS (see appendix, Table A-15), a non-hydrostatic model are used at LANL for various programs. HOTMAC has been used in a variety of complex terrain situations. RAMS has been applied to a variety of atmospheric conditions by various institutions, is widely documented in the open literature and is well respected in the scientific community. With this combination of models, DOE has the capability to deal with most conceivable atmospheric disturbances or weather conditions.

Differences among models arise from grid structure, sub-grid approximations, physical parameterizations, numerical methods, etc. Five models, used by various agencies are reviewed in this report. COAMPS is developed by the Navy, and is used at LLNL. RAMS has been developed at Colorado State University and is used at LANL. ARPS is a model developed at the University of Oklahoma, MM5 is a joint development effort of NCAR and Penn State University. ARPS and MM5 are included in the comparison as they are well known in the scientific community and scored well in the survey discussed in section 5.7. Omega is being developed at SAIC under contract with DSWA and is included to represent the DOD. Some of the attributes of the five models are summarized in Table 5-2.

Table 5-2. Prognostic Meteorological Models

Attribute	COAMPS	RAMS	MM5	ARPS	OMEGA
Data Assimilation	Intermittent Insertion	Newtonian Nudging	Newtonian Nudging	none	none
Mesh Refinement	up to 7 nests	infinite nests	infinite nests	none	static grid adaptation
Clouds	explicit bulk microphysics 5 species (Rutledge and Hobbs)	explicit bulk microphysics (Cotton et al.)	several options explicit bulk microphysics	explicit bulk microphysics 5 species (Kessler, Lin et al.)	simplified bulk microphysics 5 species
Cumulus Parameterization	Kain-Fritsch	simplified Kuo	option	none	Kuo-Anthes
Vertical Grid	variable, sigma-z	variable, sigma-z	variable, sigma-p	analyticf(z)	variable, z
Time-Integration	Klemp-Wilhelmson time splitting	time splitting	Klemp-Wilhelmson time splitting	Klemp-Wilhelmson time splitting	Smolarkiewicz semi-Lagrangian
Turbulence Closure	TKE-e	TKE	TKE-e	TKE-e	TKE-e

Besides differencesdelineated in the table, other differencesexist among the models. For example, the first four models all have regular, rectilinear grids in the horizontal with nesting (finer resolution grids imbedded within outer grids) capabilities. The variable grid structures in the vertical are summarized in the table. The OMEGA model has an unstructured grid in the horizontal, although structured in the vertical.

The model attributes detailed in the table are among those that most affectthe forecast of wind vectors and sub-grid scale turbulence. A data assimilation capability allows incorporation of observations that are not coincident in time with the initialization, or of local observations not included in the normal initialization procedure. Mesh refinement captures greater horizontal detail in vicinities of interest, usually near a strong gradient of some type or possibly near the source release point. Cloud physics and cumulus parameterization schemes forecast precipitation which may be important for wet deposition, but also simulate the latent heating which often critically forces mesoscale circulation. All of the models have a variable vertical grid, allowing finer detail in the simulation near the surface. The turbulence parameterization affects the mesoscale simulation through the boundary layer and surface processes. but maybe more importantly, provides the diffusion parameters for the dispersion models. The time integration comparison is included solely to accentuate the inherent similarities in most of the models. All of the structured grid models use a small time step for the fast

moving sound waves, but a larger time step for the slower moving inertia-gravity and large scale waves of meteorological interest. The structured grid models typically use a second order, centered finite difference scheme. The unstructured grid model, OMEGA, uses the flux form of a second order, positive definite algorithm for advection (Smolarkiewicz and Grabowski, 1990).

A key point illustrated by the table is the similarities in the models. There are differences in the details of the physics included, the gridding or the numerical methods used, but the models are essentially similar. Most of the models are documented in the peer-reviewed open literature. It is impossible to state, based on the description of the models, that one particular model is far superior to the others (or conversely, far inferior).

5.7 Prognostic Model Surveys and Evaluations

The Dynamics Research Corporation, at the request of the Air Force, recently completed a comprehensive survey of prognostic wind field models (DRC, 1993). The Air Force commissioned the survey in their effort to choose a model for theater forecast operations.

The starting point for the survey was the open literature, where almost 40 different candidate prognostic wind field models were identified. To narrow the list before further evaluation, "filters" were applied to the models. These filters included how well the model had been documented in the open literature and whether the source code was available for inspection. Also, models which originated in organizations outside the United States or which were proprietary were eliminated. Finally models which were designed for a specific purpose or which had a small support base were eliminated. These last criteria eliminated several high quality models developed at universities, but the Air Force felt that models with a history of operations and wide applicability would be more cost effective.

Once the initial culling process was complete, eleven models were chosen for further evaluation. A subjective rating system was established and the models ranked according to the criteria in the system. The criteria included pre- and post-processing options, data assimilation capabilities, applicability world wide, utility over a wide range of scales, and many more. The existing Air Force model was chosen as a baseline to establish minimum requirements. All evaluated models exceeded the minimum requirements.

A major finding of the survey was that no single model was far superior to the other models. Conversely, no model was far inferior. Any of the candidate models would have been an acceptable choice. However, the recommendation from the report was that the Air Force choose one of the following: the Colorado State University RAMS , the Pennsylvania State University/National Center for Atmospheric Research MM5, or the Naval Research Laboratory (NRL) NORAPS. The recommendation was based on the utility and applicability of these models, their history in operational use, and the strong support base which exists for each of them. Finally, the report states that the NORAPS model may be the most cost effective choice.

There were a few reasons for recommending NORAPS as the possible best choice. NORAPS is the Navy's operational model at the Fleet Numerical Meteorological and Oceanographic Center, providing a strong support base for the model. It is easily run on workstations, the Air Force's planned platform for theater operations. And finally, COAMPS, a non-hydrostatic model under development at NRL at the time of the report, is a planned replacement for NORAPS. COAMPS extends the applicability to the smaller scales that non-hydrostatic models allow.

There have been very few attempts to evaluate different prognostic wind field models. These models are very expensive to run, largely because of personnel costs, but also due to computer resources. Generally, trained scientists and programmers are necessary for executing these models. Also, different design criteria, different initialization techniques and different verification methods make it difficult to compare models with common data sets. However, the Army attempted such a study (Pielke and Pearce, 1994) in Project WIND (Winds In Non-uniform Domains). Project WIND was designed to collect meteorological data in a network of nested domains corresponding to the Orlanski (1975) mesoscale classification system. The data were collected over four observation periods, one for each season, lasting 15 days. The data were provided to the modeling groups for comparison to their model runs.

Four models were evaluated: MM4 (Mesoscale Model, version 4), FITNAH (Flow over Irregular Terrain with Natural and Anthropogenic Heat sources), CSU RAMS (Regional Atmospheric Modeling System), and HOTMAC (Higher Order Turbulence Model for Atmospheric Circulation). The models were run on the common data sets and evaluated using a common set of statistics, such as correlation coefficient, relative mean bias, percentage of cases within a factor of 2, and the mean difference. All models demonstrated skill, no model was clearly superior, all models had relative strengths and relative weaknesses. There was no definitive conclusion from the evaluation.

5.8 Prognostic Model Findings and Recommendations

The CBNP Transport and Fate models, including COAMPS, NORAPS, RAMS and HOTMAC are state of the science models, with capabilities similar to those that exist in any other models. It is clear from the Air Force survey and the Army evaluation, as well as review of the open literature, that no particular model is superior to all others. A major cost associated with a model is personnel cost; learning new models is not trivial. The CBNP Transport and Fate models are among those that are state of the science, consequently it would be cost effective to use these models. The DOE laboratories use these models for other programs and as advances in the science occur, new features will be added to the models. These might include improved representation of the physics, new numerical techniques, or methods to improve efficiency. For these reasons, it is recommended that the CBNP Transport and Fate models be used to provide prognostic wind fields. Additional development of the CBNP team models is recommended. The recommended research associated with this program includes data assimilation techniques, methods for representing surface structures such as buildings, and methods for making the models execute more efficiently. Also, the DOE has considerable investments in computing resources and will continue to invest in computing resources over the next several years. The CBNP Transport and Fate models should be adapted to take advantage of the computing power.

5.9 Local-Regional Dispersion Model

Once the wind fields have been constructed, the dispersion model uses that information together with the source information to predict the concentrations of the agent in both space and time. Within the atmospheric science community there are a vast number of atmospheric dispersion models. These models range from those developed to solve a very specific problem to those that attempt to simulate a very wide range of problems. There are many documents that list and describe various dispersion models: *Guidelines on Air Quality Models (Revised)* for U.S. Environmental Protection Agency, *Atmospheric Dispersion Modeling Resources*, U.S. Department of Energy; *Directory of Atmospheric Transport and Diffusion Models, Equipment, and Projects*, Office of the Federal Coordinator for Meteorological Services and Supporting Research, NOAA, U.S. Department of Commerce.

A subset of these models is currently available to the CBNP Transport and Fate researchers. At Lawrence Livermore National Laboratory (LLNL), ARAC, the Atmospheric Release Advisory Capability, has been developing and using the ADPIC (see appendix, Table A-16) dispersion model operationally for about 20 years. In a major ARAC upgrade, a new dispersion model, LODI (see appendix, Table A-17), is being developed to replace ADPIC as the operational dispersion model in 1999. LLNL also has developed models, SLAB (see appendix, Table A-18) and FEM3, to predict the dispersion of heavier than air gases. Los Alamos National Laboratory, has developed and used the RAPTAD (see appendix, Table A-19) dispersion model for a number of years in support of projects such as ASCOT, Atmospheric Studies in Complex Terrain, and the Mexico City Air Quality Initiative. They have also used the HYPACT (see appendix, Table A-20) dispersion model (or its predecessor, LPDM) to support ASCOT and other DOE projects. In the remainder of this chapter, we will compare the features of these models with other well-known dispersion models, examine the results of published evaluations, and appraise the user base of the models.

Dispersion Model Types

The first and most basic categorization of dispersion models is the method chosen to treat the basic dispersion process. The basic choices are: a simple plume, a set of puffs, a large number of marker particles, or as an Eulerian variable. The first part of this survey is then represented in Table 5-3 which lists the general advantages and limitations of each method with the name of some models in that category. It must be noted however, that rather than a strict categorization, these categories list major sections of a continuum of methods. To evaluate a particular model one must examine the documentation for that model.

As stated before, we are interested in transport away from the source into the suburbs tens of kilometers away. For this scale, the dispersion model must be flexible enough to handle not only simple scenarios, but also scenarios involving winds that change in time and space. Thus, the ability to use three-dimensional wind fields is a minimum requirement for the dispersion model. As can be seen from the above table, this requirement limits plume and simple puff models to special purpose use. Therefore, the complex puff, stochastic puff, particle, and three-dimensional Eulerian models which can use three-dimensional wind fields which change in time and modeling complex terrain effectswill be the primary focus of this review for C/B applications in the CBNP Transport and Fate thrust area.

Table 5-3. Dispersion modeling methodology

Model Classification	Advantages	Limitations	Examples
Gaussian Plume	very, very fast requires very limited computer resources easy to understand little input required	utilizes only one wind speed and direction. does not handle terrain or highly parameterized simplistic turbulence and diffusion parameterizations	HPS RAM CTDM
Non-Gaussian Plume	very, very fast requires very limited computer resources easy to understand handles vertical wind shear via power law	utilizes only one wind direction but can simulate vertical speed sheer at one point, i.e., horizontally homogenous wind. terrain not accounted for or highly parameterized	SLAB DEGADIS
Simple Puff	very fast can model variable wind speed and direction	trouble handling wind shear as puff gets large over time terrain/puff interactions can be complicated simplistic turbulence and diffusion parameterizations	AFTOX RTVSM
Complex Puff	fast can model complex terrain can model fully 3D wind fields can use more sophisticated turbulence information/parameterizations can model shear flow by using puff splitting	dispersion within a puff often very simplified terrain/puff interactions can be complicated follows mean wind field streamlines puff splitting algorithm critical to accuracy in highly sheared flow modeling effects of particle size distributions complicated	SCIPUFF
Random-walk puff	fast to moderate can model complex terrain can model fully 3D wind fields can use more detailed turbulence information random process allows puffs to get off mean wind streamlines	dispersion within a puff often very simplified terrain/puff interactions can be complicated modeling effects of particle size distributions complicated must have a priori knowledge of the Lagrangian time scale	RAPTAD
Stochastic Particle	moderate can model complex terrain can model fully 3D wind fields can use detailed turbulence information (modeled, measured, or parameterized) can simulate aerosol size distribution effects	must track a large number of particles to get good statistics must have a priori knowledge of the Lagrangian time scale	ADPIC ERAD LADM LODI LPDM
Eulerian Advection/ Diffusion model	moderate to slow can model complex terrain can model fully 3D wind fields can have sophisticated turbulent diffusion modeling usually directly coupled with dynamic model. when coupled with dynamic model can model heavy gas effects accurately.	does not treat point sources well. numerical diffusion can be a problem coupled models very expensive to run particle size distribution effects complicated to model	FEM3C UAM

Capabilities of Major Dispersion Models

In addition to the dispersion methodology, the models can also be categorized by the various phenomena that they simulate. To keep this report from growing unbounded, we will present a more detailed look at the models currently used by the CBNP Transport and Fate researchers together with a few well-known models: RTVSM , U.S. Army Dugway Proving Ground; UAM, Environmental Protection Agency; VLSTRACK, Naval Surface Warfare Center; SCIPUFF, Defense Special Weapons Agency; ERAD, Sandia National Laboratories.

As can be seen from Table 5-4, the current models used by the CBNP Transport & Fate researchers have a wide range of features. All but one, SLAB, are fully three-dimensional and allow terrain. ADPIC, HYPACT, and LODI treat aerosol size distributions and dry deposition while ADPIC and LODI also treat wet deposition. SLAB and ADPIC also treat heavier-than-air gas effects. However, none of these models were specifically developed for the CB problem and therefore lack some CB specific features such as droplet evaporation and important chemical reactions. Thus, part of the model development program would be to add such features plus heavier-than-air gas effects to the three-dimensional models. In addition to adding the CB features. methods of modeling the effects of the urban environment, especially building enhanced turbulence, must be developed and incorporated into the models. Also, forecast uncertainty is a quantity requested by many decision makers. The developers of the SCIPUFF model have made an initial thrust into this arena by predicting the variances of the concentration field. While this addresses one aspect of the uncertainty question, it does not address many of the major factors in forecast uncertainty such as how errors in observations propagate through a forecast and what effecterrors in the mean wind will have on the concentration forecast. To actually be able to quantify the uncertainty in any forecast requires the development of techniques not yet available and should be part of the model development program.

Table 5-4. Model features

MODEL / Feature	RTVSM	VLSTRACK	SLAB *	UAM	SCIPUFF	ADPIC *	ERAD	HYPACT *	LODI *	RAPTAD *
Dispersion class	plume / puff	puff	plume	Eulerian	complex puff	particle	particle	particle / Eulerian	particle	random walk puff
Terrain	n	n	n	y	y	y	n	y	y	y
Time dependent winds	y	y	n	y	y	y	y	y	y	y
Full 3D wind fields	n	y	n	y	y	y	y	y	y	y
Neutral gas	y	y	y	y	y	y	y	y	y	y
Buoyant gas effects	y	y	n	y	n	y	y	n	y	y
Heavy gas effects	n	y	y	n	n	y	n	n	n	n
Building effects	n	n	n	n	n	n	n	n	n	n
Decay / degradation	y	y	n	y	y	y	y	y	y	n
Concentration variances	n	n	n	n	y	n	n	n	n	n
Aerosol size distribution	y	y	n	n	y	y	y	y	y	n
gravitational settling	y	y	n	n	y	y	y	y	y	n
dry deposition	y	y	n	y	y	y	y	y	y	n
wet deposition	y	y	n	n	n	y	y	n	y	n
droplet evaporation	y	y	n	n	y	n	n	n	n	n
secondary evaporation	y	y	n	n	y	n	n	n	n	n

* model currently used by the CBNP Transport & Fate researchers

5.10 Recent Dispersion Model Evaluations

In the following section we summarize the results of model evaluations conducted by a number of differentagencies for a number of differentpurposes. We have included an Environmental Protection Agency (EPA) evaluation of air quality models to be used to meet numerous government statutes, an EPA evaluation of hazardous chemical models for industrial use, a joint American Petroleum Institute (API) and USAF evaluation of hazardous gas models, a review of CB dispersion models conducted by the DOD, a DOE Officeof Defense Programs review of chemical and radiological dispersion models.

EPA Evaluation of Air Quality Models

The Environmental Protection Agency (EPA) has evaluated urban air quality models for use in meeting the numerous government statutes dealing with the protection of urban air quality. In this capacity, the EPA has listed nine air quality models (Appendix A models) as preferred: BLP, CALINE3, CDM 2.0, RAM, ISC3, UAM, OCD, EDMS, and CTDMPLUS. Of the nine models, seven are variants of a simple Gaussian plume model: BLP, CALINE3, CDM 2.0, RAM, ISC3, OCD, and EDMS. CTDMPLUS is a refined point source Gaussian air quality model for use in all stability conditions and in complex terrain.

UAM, the urban airshed model, is a three-dimensional, Eulerian grid type model for the urban scale. It is designed specifically for computing ozone concentrations under short term, episodic conditions lasting one or two days and typically calculates one hour average concentrations. While UAM has many of the features desired for an urban emergency response model (such as the ability to utilize three-dimensional, time-varying winds, terrain effects and dry deposition), it was not designed to treat the short-term exposures associated with instantaneous, acute releases.

In addition to its preferred models, the EPA also lists 19 alternative air quality models. Notable among these 19 models are AVACTA II, HOTMAC/RAPTAD, and PANACHE as they are the only models that

accept a full three-dimensional wind field. Two other models are also noteworthy for their treatment of heavier-than-air gases. These are DEGADIS and SLAB. DEGADIS and SLAB both are plume models that are applicable for periods of less than two hours.

API/USAF and EPA Hazardous Gas Model Evaluations

The American Petroleum Institute and the United States Air Force sponsored a hazardous-gas model evaluation in the early 1990's. The study was conducted by Sigma Research Corporation and led by Dr. S. R. Hanna. The final evaluations were published in "Hazardous Gas Model Evaluation with Field Observations" by Hanna et al. in *Atmospheric Environment Vol. 27a*, 1993. The final study involved two simple analytic models and 13 plume models of varying complexity and eight field study data sets. The observational data sets came from the following eight field experiments: Burro, Coyote, Desert Tortoise, Goldfish, Hanford, Maplin Sands, Prairie Grass, and Thorny Island. The 15 models were: AFTOX, AIRTOX, Britter and McQuaid (BM), CHARM, DEGADIS, FOCUS, GASTAR, GAUSSIAN PLUME MODEL (GPM), HEGADAS, HGSYSTEM, INPUFF, OB/DG, PHAST, SLAB, AND TRACE.

An evaluation of plume centerline concentration predictions showed that "the BM, CHARM, GASTAR, SLAB, HEGADAS, HGSYSTEM, PHAST, and TRACE models produced the most consistently good performance in simulating plume centerline concentrations for the continuous and the instantaneous dense gas data sets, with relative mean biases of about ± 30-50% and relative scatters that are about equal to the mean". The evaluation of plume width predictions revealed that "the better models for the dense gas releases were the AIRTOX, HGSYSTEM, PHAST, and SLAB models whose prediction of plume width were about 30-50% too large on average. The HEGADAS model predictions of plume width were about a factor of three high, while GASTAR and DEGADIS predictions were about a factor of two high."

The EPA conducted its own independent evaluation and issued a report entitled *Guidance on the Application of Refined Dispersion Models to Hazardous/Toxic Air Pollutant Releases*, EPA-454/R-93-002. The report lists five differentplume models to be used by industry for safety analysis and accident response: ADAM, ALOHA, DEGADIS, HGSYSTEM, and SLAB.

These models include some capabilities applicable for the CB problem, such as heavier-than-air gas dispersion. However, as plume models their simplistic treatment of transport and diffusion does not allow for the utilization of time-varying, three-dimensional winds.

DOD Review of CB Models

In 1996 a major Chemical and Biological (CB) model review (Prociv and Hollis, 1996; Glasow and Miller, 1996; Glasow, 1996, and Gibbs and Miller, 1996) was carried out by DOD in which models were critically reviewed and compared with DOD user needs. Recommendations were made identifying three models for interim use. Also recommended was a long-term plan for a single or suite of NBC models to be developed to meet all of DOD needs. More details of this review and recommendations are described below.

In 1996, the DOD formed a Process Action Team (PAT) for CB modeling with the objective "to evaluate current modeling effortsand to provide the Officeof the Secretary of Defense with a consolidated and integrated CB modeling program where possible harmonizing individual Service and Agency work into joint programs and eliminating duplication and overlapping projects." The PAT was composed of two subgroups: Requirements and Modeling. The Requirements subgroup aimed at identifying the CB modeling needs of the members of the DOD user community. The Modeling subgroup was asked to: identify organizations with CB modeling missions; identify all models in use; correlate solutions to those operational requirements identified by the Requirements subgroup; where necessary; make recommendations for resolution of overlapping or duplicative efforts; and make recommendations for satisfying requirements for which there is no current solution."

Presented in Table 5-5 is a listing of the major players in the development of CB models in DOD (and elsewhere) as well as the names of the models developed or under development, and whether the models apply to chemical agent impacts, biological agent impacts or both. Those models are also ranked in terms of the level of computer requirements they require to operate them. Table 5-6 presents a matrix breakdown of model capabilities so that they can be inter-compared. New funding is being put into the MESO Model which some believe may become, in several years, the future standard NBC hazard prediction model for DOD.

Table 5-5. Summary of Major Players in C/B Modeling and Simulation in DOD (Adapted from a Viewgraph of Major Jerry Glasow of US Army Concepts Analysis Agency)

The Players			
DNA	**OMEGA/MEDOC(FR)	CW/BW	CRAY
LLNL	MATHEW/ADPIC	CW/BW	CRAY / Workstation
ARL-BED	**ABCSIM	CW/BW	CRAY / Workstation
NSWC	**ADVEDS	CW/BW	Workstation
UASNCA	**CBD-IMPACT	CW/BW	Workstation
NSWC	CWNAVSIM	CW	Workstation
ARL-BED	**LAGRANGIAN	CW/BW	Workstation
BMDO	**MESO	CW/BW	Workstation
ARL-BED	**ABCSIM-PC	CW/BW	Workstation / 486
DNA	**HPAC;HASCAL	CW/BW	Workstation / 486
NSWC	**VLSTRACK 2.X	CW/BW	486
NSWC	VLSTRACK 1.X	CW/BW	486
ERDEC	NUSSE4	CW	486 / 386
DRES(CA)	**CANPUFF	BW	486 / 386
CBDE(UK)	BIOL	BW	386
			** = Under Development

Results of the Modeling Subgroup were included in the overall recommendations. Differentmodels were chosen to handle each of the three major hazard prediction areas of concern at this time. They are (a) CB attack hazards, (b) NBC hazards from destruction of NBC facilities, and (3) hazards from industrial chemical accidents. The following models were designated as Standard Hazard Prediction Models for these applications:

1. VLSTRACK for hazards caused by CB attacks (i.e., counter proliferation passive defense applications),

2. HPAC for NBC hazards caused by the destruction of NBC facilities (i.e., counter-proliferation counter force applications), and

3. D2PCw for industrial/chemical hazards caused by accidents/incidents. This model is already in use at the eight depots planned for the destruction of the chemical agent stockpile.

A description of the CB agent related features (deposition, degradation, etc.) of the two newer DOD designated models SCIPUFF (HPAC / HASCAL) and VLSTRACK, is given in Tables 5-7 and 5-8, respectively. (The ability of ten major dispersion models to simulate a range of phenomena affecting CB agent dispersion is presented in Table 5-4 and discussed in section 5.4.2 Capabilities of Major Dispersion Models.)

An additional finding of the Requirements group was that there were efforts at model development going on that did not meet user requirements and, at the same time, some user requirements were not being met at all. Greater coordination of user needs with model development needed to be made and integrated into a coordinated model development effort reducing duplication and overlap where possible.

Table 5-6. Summary of Capabilities for the major CB Models of Interest to DOD. (Source: Gibbs and Miller, 1996)

		Under Development	Operational	Analytical	Research	Terrain	3D Wind	Time Varying Wind	Weapon Source	Large Release Source	CW	BW
HPAC / HASCAL /	DSWA	x	x		x	x	x	x	x	x	x	x
MATHEW / ADPIC	LLNL		x			x	x	x	x	x	x	x
CWNAVSIM	NSWC			x		s	x		x		x	
ADVEDS	NSWC	x		x		s	x	?	x		x	?
MESO	BMDO	x		x			x	x	x	x	x	x
ABCSIM	ARL-BED	x			x			?	x		x	x
CBD-IMPACT	USANCA	x	x			x	x	x	x		x	x
VLSTRACK 1.X	NSWC		x	x				x	x		x	x
VLSTRACK 2.X	NSWC	x	x			x	x	x	x		x	x
NUSSE4	ERDEC			x					x		x	
CONFLUX	DRES/(a)	x		x	x			?	x			x

s = Ship Geometry

Table 5-7. Description at CB related features of the SCIPUFF Model

Deposition: 1.Dry Deposition mechanisms	Mechanisms included are interception, impaction and Brownian motion using Slinn's methodology. These mechanisms are added to gravitational settling. Parameters include aerosol size, turbulence, intensity, and nature of surface (vegetative, desert, etc.). Vapor and aerosols are dispersed in the atmosphere within each puff as the puff spreads due to turbulent diffusion. Vapor deposition based on deposition velocity concept. No inclusion of stomatal resistances or solubility at this time.
2.Wet deposition mechanism	Washout rate is proportional to rain rate for particles. Precipitation categories are used-light, medium, heavy, snow, rain.
3.Resuspension	None
4.Changing meteorological conditions	Changing meteorological conditions are included as aerosols and vapor move downwind.
Chemical Agents:	
1.Agents Considered	Treatment based on physical and chemical property parameters. DSWA has data base of chemical agents for inclusion with parameters identified.
2.Evaporation	Droplet evaporation equation used from input of saturation vapor pressure, aerosol density, etc. (like NUSSE4). Droplets and vapor are tracked separately as droplet plume can settle but vapor plume does not.
3.Change in Meteorological Conditions During Evaporation	Yes.
4.Reaction Types Included	Nonlinear chemical capability only for air pollutants for industrial use. No first or second order reactions for chemical agent application.
5.Decay Equations	No.
6.Secondary Re-evaporation	Yes, built on lab work of Baines and James in Canada. Droplets are assumed to be on impermeable surface where evaporation rate is a function of droplet size, Nusselt and Sherwood Numbers.
7.Ground Cover/Canopy Effects	Included only in terms of deposition algorithm.
8.Reaction with Soil before Evaporation	No. There are plans to include this phenomenon based on models of dispersion in porous media including evaporation.
9.Coagulation in Soils	No.
Biological Agents:	
1.Decay in Time	Exponential decay allowing for different rates in daytime and nighttime. DSWA provides rates in CB data base included with model.
2.Other mechanisms	Dry deposition of biological agents included with no resuspension. No coagulation, clumping. Wet spores treated as dry with no evaporation from initial distribution. No resuspension.

Table 5-8. Description of CB related features of the VLSTRACK Model Version 1.6.2

Deposition:	
1.Dry Deposition mechanisms	Only droplets/particles >10 microns in dia. are deposited; no vapor deposition. New Version: Dry deposition of droplets/particles based on stripping mass from cloud bottom with mass reduction only from cloud bottom. Above methodology used for droplets/particles >250 microns in dia. No vapor deposition.
2.Wet deposition mechanisms	None
3.Resuspension	None
4.Changing meteorological conditions	Meteorological conditions change in both time and space.
Chemical Agents:	
1.Agents Considered	Treatment based on physical parameters. NSWC has data base of chemical agents for inclusion with parameters identified. The data file currently lists 39 chemical agents and simulants.
2.Evaporation	Droplet evaporation based on NUSSE mass transfer equations. VLSTRACK adds background concentration. Agents forming dense vapor clouds also have a settling velocity for the vapor clouds which is computed along with evaporation of any remaining droplets. New Version: User-defined surface type allows specification of surface roughness, porosity, and tortuosity to define a variety of different surfaces such as concrete, glass, horizontal vehicle surfaces, etc.
3.Change in Meteorological Conditions During Evaporation	Yes.
4.Reaction Types Included	No first or second order reactions for chemical agent applications.
5.Decay Equations	Exponential decay permitted using different daytime and nighttime decay rates.
6.Secondary Re-evaporation	Yes. Droplets are assumed to be on impermeable surface where evaporation rate is a function of droplet size as included in Nusselt and Sherwood Numbers.
7.Ground Cover/Canopy Effects	New Version: Transport and diffusion within a forest canopy or an urban region is included.
8.Reaction with Soil before Evaporation	Agent is assumed to hydrolyze at a constant rate in water otherwise, no surface reaction is assumed.
9.Coagulation in Soils	No.
Biological Agents:	
1.Decay in Time	Agent impurities are addressed in the agent purity record and only particles of 10 microns or less in dia. contribute to dosage output. New Version: Biological slurry calculations start with combined water and agent and evaporate down to dry particles.
2.Other mechanisms	Dry deposition of biological agents included with no resuspension. No coagulation, clumping. Biological agents are disseminated in either a dry form or from a wet slurry. Only viable and respirable biological agent material is normally tracked -- water droplets, filler material, agent impurities, and non-respirable particles are not treated. Evaporation of the slurry solvent is not computed for biological agents. Particles remaining after solvent evaporation are what exists at time equals zero. Deposition onto water is treated in model. The model currently uses 9 biological agents and simulants.

DOE Review And Evaluation of Chemical and Radiological Dispersion Models

Under the sponsorship of the Office of Defense Programs of the US Department of Energy the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program has been established to identify and evaluate methodologies and computer codes to support accident phenomenological and consequence calculations. Two working groups were relevant to this report: the Chemical Dispersion and Consequence Analysis (CDCA) working group and the Radiological Dispersion and Consequence (RDC) working group.

The CDCA working group was charged with establishing guidance for the selection and application supporting DOE facility safety documentation. It set out to identify and evaluate appropriate computer models for this use. The group began with a list of 135 models which was reduced to a list of 25 models via a screening process. A further screening process split the 25 models into a Tier I set of 13 models for in-depth review and a Tier II set of 12 models which were subject to the same technical review as the Tier I models but were not run on the test problems. As a result of this evaluation, the CDCA working group recommended five models: ALOHA, DEGADIS, HGSYSTEM, TSCREEN, and SLAB. They also conditionally recommended four other models: ADAM, CALPUFF, FEM3C, and INPUFF. HOTMAC/RAPTAD, CASRAM-SC, and SCIPUFF are said to be suitable for further review and VLSTRACK was not recommended.

In addition to its model review, the CDCA working group recognized a continuing need for model development. They identified some key areas needing improvement: (1) release aerosolization and evaporation, (2) increased surface roughness effects typically associated with industrial plants, (3) short duration releases, and (4) the aerodynamic effects of buildings and surrounding terrain on near surface releases.

Similar to the CDCA working group, the RDC working group was charged with evaluating and identifying models to support DOE safety analysis and emergency management organizations. The RDC examined 15 different models. Each model was evaluated in three areas: software quality / user interface, technical adequacy, and source term type. Based upon these evaluations the models were placed into one of five levels. The MATHEW/ADPIC model pair was the only model ranked at the highest level (1), 3 models, COSYMA, MACCS2, and TRAC RA/HA, were ranked in level 2, one model, RSAC-5, was in level 3, two models were in level 4 and the remaining 8 were in level 5.

The DOE reviews included models of several levels of sophistication from Gaussian plume models to three-dimensional dispersion models. Several of the CBNP Transport and Fate models (SLAB, FEM3C, HOTMAC/RAPTAD, MATHEW/ADPIC) were recommended or conditionally recommended for use in chemical or radiological releases. Of these, HOTMAC/RAPTAD and MATHEW/ADPIC are three-dimensional wind field and Lagrangian dispersion models and are suitable for emergency response applications.

ETEX Dispersion Model Comparison

The European Tracer Experiment (ETEX) was organized to evaluate the capability in Europe to respond to an emergency such as the Chernobyl accident. The experiment design called for two separate releases of inert tracer gases, sampling of the releases by an extensive network of detectors, and a statistical analysis of the model predictions with the sampler measurements. The releases were conducted in October and November, 1994. The model evaluation was conducted in two phases. In Phase I participating organizations were notified that the release was taking place and were required to have their results to the ETEX committee within six hours using whatever data they had. This tested a complete emergency response system. In Phase II, conducted in the spring and summer of 1996, participants had access to the same gridded meteorological data in order to allow direct comparison of the dispersion modeling systems.

For Phase II, forty-seven organizations submitted results including six groups from the United States. The US participants included two groups from NOAA, the ARAP Group of Titan Research and Technology, Science Applications International Corp. (SAIC), LLNL, and Savannah River Laboratory (SRL). The results of the comparison (Mosca et al., 1997) show that the LLNL group using MATHEW/ADPIC was first in three out of 10 statistical measures, eleventh overall and first of the U.S. groups. The other U.S. groups ranked from 31 to number 45.

Dispersion Model Evaluation Conclusions

As is evidenced from the various conclusions reached by the different model reviews and evaluations, there are a number of good models for various purposes, however, there is no one model that is best for all situations or for all applications. The best model for use is often determined by the restrictions placed on its use. For example, the DOD values completely portable stand alone systems because the model must operate in battlefield conditions where communications may be unreliable. The hazardous chemical models reviewed by the API and the EPA are simple to use and have limited computational requirements since these models must

be used by companies ranging from large corporations to small businesses that have a wide variety of proficiency and resources.

The current models used by the CBNP Transport and Fate researchers are recognized as excellent models in various independent surveys. Both the SLAB model and FEM3C developed at Lawrence Livermore National Laboratory are cited by the DOE APAC CDCA working group. The SLAB model is recognized by both the EPA and the API/USAF study. The HOTMAC/RAPTAD code developed at Los Alamos National Laboratory is recognized by the EPA as an alternative air quality model and the CDCA working group has listed it as suitable for further evaluation. The MATHEW/ADPIC model pair was cited by the DOE APAC RDC working group as the "best overall computer model for most source types."

5.11 User Base of Transport and Fate Team Dispersion Models

Another useful method of evaluating a dispersion model is to examine its user base. A broad base of independent user's is an indication of the model's acceptance by the community. The ARAC operational dispersion model, ADPIC, is used by organizations in Italy, Japan, Sweden, Brazil, Switzerland and Spain as well as the Fleet Numerical Meteorological and Oceanographic Center of the United States Navy. A commercialized version of RAPTAD is used by a wide range of organizations including utility companies, United States Army research laboratories, and leading Japanese universities. Likewise, HYPACT and/or it predecessor LPDM are used at Savannah River National Laboratory, Batelle Northwest Laboratory, Kennedy Space Center, and a wide range of universities. All three models are being used by the U.S. Air Force Atmospheric Sciences Division. In other words, all of these models have been accepted by a wide range of independent organizations.

5.12 Dispersion Model Findings and Recommendations

There are a large number of available atmospheric dispersion models within the scientific community. The transport dynamics for these models range in completeness and sophistication from simple Gaussian plume models to coupled wind field-dispersion models with three-dimensional, time-dependent meteorological capabilities. They also include a range of physics and chemistry capabilities to address specific emission release issues. In the local-regional scale dispersion problem, we are interested in transport out to distances of up to a hundred kilometers from the source and durations ranging from tens of minutes to many hours, depending upon the size, rate, and toxicity of the release and the meteorological conditions. At these scales, temporal and spatial variation in the wind field will be critical factors in the transport of a release and need to be included in the dispersion calculation. Simple plume- and puff-type models can be used for special purposes, such as source models. However, the dispersion models to be developed and applied on the local-regional scale must be able to utilize three-dimensional, time-dependent wind fields.

One of the major conclusions reached by the different dispersion model reviews and evaluations covered in this section is that there are a number of good models for various purposes; however, there is no one model that is superior to all others, in all situations or for all applications. Generally a number of models were recommended for use in each study or if a single model needed to be selected, the choice was determined by restrictions placed on the models' use or other parochial interests and concerns. For example, the DOD valued completely portable stand-alone systems for operations in battlefield conditions where communications may be unreliable. In addition, the experience of the atmospheric dispersion modeling community suggests that the level of model performance tends to be correlated with the user's familiarity, understanding and experience with the model. Therefore, seeking the "best" dispersion model is an elusive goal. A sounder approach is to identify state-of-the-art models and to conduct further research and development as appropriate for the intended applications.

The models being used by the CBNP Transport and Fate researchers are well recognized by the scientific community, have extensive validation and verification, and have been shown to perform well.

The CBNP team models contain a wide range of features and capabilities that are directly applicable to chemical and biological releases on the local-regional scale. The ADPIC, HYPACT, LODI, and RAPTAD dispersion models are all fully three-dimensional, include representations of terrain, and utilize time-varying winds. ADPIC, HYPACT, and LODI are able to treat aerosol size distributions and dry deposition of particles and gases. ADPIC and LODI also include treatment of wet deposition. In addition, ADPIC possesses a heavier-than-air dispersion modeling capability.

These models have also been recognized as excellent models in a variety of independent reviews and model evaluations. For example, the HOTMAC/RAPTAD wind field-dispersion model pair is recognized by the EPA as an alternative air quality model and the DOE APAC CDCA working group has listed it as suitable for further evaluation. The MATHEW/ADPIC model pair was cited by the DOE

APAC RDC working group as the "best overall computer model for most source types" and was the top performing US model in the international ETEX experiment.

In addition, the CBNP Transport and Fate team models have been accepted by a wide range of independent organizations and possess a strong user base. ADPIC is the current ARAC operational emergency response dispersion model and is used for this and other purposes by organizations in several countries as well as by the US Navy's Fleet Numerical Meteorological and Oceanographic Center. The LODI model is currently under development and is scheduled to replace ADPIC as the ARAC operational dispersion model within the next two years. A commercial version of RAPTAD is used by a wide range of organizations including utility companies, US Army research laboratories, and leading Japanese universities. Similarly, HYPACT (or its predecessor, LPDM) is used at several DOE laboratories, Kennedy Space Center, and a number of universities.

Thus, it is recommended that the ADPIC, HYPACT, LODI, and RAPTAD models form the modeling base for further dispersion research and model development by the CBNP Transport and Fate team.

Recommended areas for the development of the CBNP team models can be separated into two categories: upgrades which can be adapted using community recognized methodologies and developments requiring significant research activities. In the former group are several capabilities of specific relevance to chemical and biological releases such as the treatment of droplet evaporation, chemical reactions specific to certain agents, and biological degradation processes within the atmosphere. In the latter category are two areas of recommended research. The first is the development of methods for treating the aerodynamic and thermodynamic effects of structures within the urban environment. These effects tend to enhance turbulence and alter the mean structure of the wind field and subsequent dispersion pattern. The results of CFD calculations and wind tunnel simulations of the flow over buildings (discussed in the previous chapter of this report) will be useful aids in the development of parameterizations for this purpose. The second recommended research area involves characterizing the uncertainty within concentration forecasts, a quantity often requested by decision makers. Uncertainty in predicted concentration and exposure is due to the inherent statistical nature of turbulence and errors in both the emission source characterization and the meteorological observations used to initialize the forecast wind fields. Small changes in the initial conditions can lead to significant changes in the resultant dispersion pattern due to the chaotic dynamic nature of the atmosphere. These changes in the dispersion pattern can be quantified through the production and analysis of ensembles of forecasts. Such studies, while computationally intensive, can be made tractable by exploiting the massively parallel computing capabilities within the DOE.

A final recommendation is made in regard to the need for coordination between the local-regional model development efforts of this program and the needs of local emergency managers. The Requirements Group of the DOD Process Action Team for Chemical and Biological modeling recommended greater coordination between model developers and users to reduce deficiencies and duplication. A similar recommendation is made here for the DOE CBNP regional modeling effort. Specifically, it is recommended that a collaboration be established with local emergency managers to identify those capabilities of greatest relevance to emergency responders and planners. Potential collaborators include representatives from one or more of the emergency management teams from the major US cities such as Denver, Los Angeles, New York and San Francisco.

5.13 Conclusions

Three major conclusions can be drawn from this examination of local to regional scale wind and dispersion modeling systems: 1)while there are a number of "good" models that are recognized for their ability to simulate various wind and dispersion scenarios, no single system stands above the rest for all applications; 2) often the "best" model is determined by constraints such as available computer power, anticipated communications links and capabilities, the expertise level of the intended user, or the need to function in a specific environment; and 3) the CBNP Transport and Fate researchers have proven expertise in and access to recognized high quality models both for wind field generation and dispersion modeling.

There is an opportunity within the CBNP to develop a local-regional dispersion modeling capability that would set the standard for the emergency response community. Achieving this goal will require building upon and coupling the ARAC operational emergency response capability, the atmospheric modeling expertise of the CBNP Transport and Fate researchers, and the computational resources of the DOE in a structured model development program. The CBNP Transport and Fate models include: the MATHEW and ADAPT diagnostic wind field models, the HOTMAC, RAMS, NORAPS, and COAMPS prognostic wind field models, and the RAPTAD, HYPACT, ADPIC, and LODI dispersion models. The dispersion models would be expanded to include features particular to chem-bio agent problems using adaptations of available technology. Research would be required to enhance the models in several areas including meteorological data assimilation, representation of surface structures such as buildings, and the quantification and characterizations of the

uncertainty associated with model predictions. Adapting the models to massively parallel computers would enable fast response time without sacrificing model physics or necessary spatial resolution, and would also enable the study of uncertainty in model predictions of plume concentration and exposure. Finally, coordination of these efforts with representatives from major urban area emergency management teams would identify those capabilities of greatest relevance to the emergency response community and facilitate integration into an operational capability.

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Table A-1. (SES) Subway Environment Simulation Model

Past Applications	-Used in design of subway lines in following subway systems: Atlanta, Baltimore, Boston, Buffalo, Caracas, Chicago, Dallas, Hong Kong, Los Angeles, Minneapolis, Montreal, New York City, Philadelphia, Pittsburgh, San Francisco, Singapore, Taipei, and Washington DC.
Predictive Capability	-Predicts time-dependent history of temperature, humidity, and air velocity throughout entire subway system including tunnel, station, and ventilation shafts including effects of moving trains.
Model Approach	-one-dimensional. -based on conservation equations of mechanical energy, mass, and heat energy applied to individual control volumes representing segments of subway system. -control volume relationships form a set of linear ordinary differential equation that are solved as function of time.
Key Model Features: 1. Train Performance	Predicts: -total heat released by trains, passengers, and ancillary equipment such as air conditioning as function of time for entire system. -location of each train in system as function of time including acceleration and braking. -power demand, line current, and energy consumption (including tractive effort for each train and segment) for each train as function of time.
2. Aerodynamic Effects	-predicts time-dependent aerodynamic drag acting on each train in the system as function of specific train location and speed. -pressure changes caused by trains, fans, and buoyancy in vent shafts; viscous and minor losses computed.
3. Temperature/Humidity Effects including Heat Sink Effects	Accounts for: -localized heat/humidity sources and sinks (including train and station heat loads). -long-term heat conduction between subway and surrounding earth. -passenger sensible and latent heat included in analysis.
Dispersion	-No algorithm for dispersion of pollutants, but ANL has developed algorithm to predict dispersion using SES-predicted air flows. -Fire effects algorithm in SES predicts adequacy of emergency ventilation including buoyancy in tunnels, throttling at fire site, wall temperature, radiation effects, and modified viscous losses.
Chemistry	-No chemistry of pollutants accounted for at this time.
Mesh	-Entire subway system divided into line segments, each with cross-sectional areas and perimeters. -Subway alignment includes multiple track areas, junctions, portals, and nodal points. -Fan and ventilation shaft locations, lengths, cross-sectional areas, and perimeters used along with dimensions of dampers and gratings.
Input	-Graphical user interface to be available from U.S. DOT in March 1997. -Otherwise input is manual and includes general system data, train performance data, aerodynamic data, and temperature/humidity data.
Output	-Detailed printout of all dynamic parameters at specific time intervals is made to file and hard copy. -Time-dependent variables available. -No plots or visualization available at this time.
Platforms	-Runs on PC in real time.
References	-1. Subway Environmental Design Handbook (1980), Volume I. Principles and Application, 2nd Edition; Volume II. Subway Environmental Simulation (SES) Computer Program, Volume II, Part 1: User's Manual; and Volume II. Subway Environmental Simulation (SES) Programmer's Manual, U.S. Department of Transportation, 1980.
Comments	-Used throughout world for new subway design and emergency ventilation design and planning. -Code is in public domain since it was funded by U.S. DOT and city transit authorities. -Recommended by U.S. DOT for subway system flow and smoke studies.
Contact Person	-At DOE labs, contact is: Tony Policastro EAD/Building 900 Argonne National Laboratory 9700 South Cass Avenue Argonne, Illinois 60439 630-252-3235; policastro@anl.gov

Table A-2. FEM3C: Computational Fluid Dynamics Model

Model Name	FEM3C
Past Applications	This CFD code has been applied to small-scale atmospheric flow and transport/diffusion of pollutants in which the effects of terrain and obstruction are important and/or the coupling between pollutants and flow field must be considered.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- Similarity-based K-theory (1st order) - 2 eqn. k-epsilon (1.5 order)
Wall Shear Stress	Traditional law-of-wall approach and specified turbulence stresses
Heat Transport	Solves temperature eqn.
Moisture Transport	No moisture transport.
Surface Heating	User-specified through B.C.'s
Dispersion	Eulerian dispersion algorithms are second-order accurate and used for solving the conservation equations of species -area and volume sources defined by grid cells. - multiple sources possible - dense or buoyant gas dispersion possible - phase change allowed (droplet/vapor) - no deposition or resuspension physics
Chemistry	- No internal chemistry modules.
Numerics	- finite element - explicit (modified forward Euler) - 2nd order accurate in time and space - pressure is determined by solving an implicit pressure equation (direct solver or pre-conditioned conjugate gradient method) - variables computed on staggered grid
Mesh	- structured grids (non-orthogonal) - variable grid spacing - irregular domains allowed - obstacles handled by "no flow" grids
B.C.'s	zero gradient, free-slip, no-slip, and specified flux
Input	- ASCII input files; no graphical user interface
Model Name	**FEM3C**
Output (Graphics)	- Wind, concentration, and dosage fields for selected times are post-processed by a graphics code called GRIZ. Time history data of wind components and concentration for preselected locations are readily processed by a X-Y plotting routine. - 3-d visualization (GRIZ) - no run-time interface
Platforms	- UNIX-based workstations and supercomputers (Cray Y-MP, DEC ALPHA , SGI) - vectorized version available
References model description: flow around obstacles: evaluation studies:	Chan, S.T., 1994, "FEM3C-An improved three-dimensional heavy-gas dispersion model: User's manual," UCRL-MA-116567 Rev. 1, LLNL, Livermore, CA. Chan, S.T., 1992, "Numerical simulations of LNG vapor dispersion from a fenced storage area," Journal of Hazardous Materials, 30:195-224. Ermak, D.L., S.T. . Morgan, and L.K. Morris, 1982, "A comparison of dense gas dispersion model simulations with Burro series LNG spill test results," Journal of Hazardous Materials, 6:129-160. Chan, S.T., D.L. Ermak, and L.K. Morris, 1987, "FEM3 model simulations of selected Thorney Island phase I trials," Journal of Hazardous Materials, 16:267-292.
Comments	The FEM3C model has recently been used to simulate the dispersion of a line-source of trace gas (to simulate the release of C/B agents by terrorists from a moving truck) in the vicinity of the Capitol Building. Very plausible results have been obtained.
Contact Person(s)	Stevens T. Chan, L-103 Atmospheric Science Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94551 Phone: (510) 422-1822 E-mail: schan@llnl.gov

Table A-3. Dynaflow: Computational Fluid Dynamics Model

Model Name	Dynaflow
Past Applications	This CFD code has been applied to flow and transport problems that involve arbitrarily complex geometry and require sufficiently fine-grid resolution and robust solution techniques. With some further development, the code could also be a highly useful tool for simulating local-scale atmospheric flows and the transport/diffusion of pollutants.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient and Steady State Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- 3 eqn. k-epsilon-A2 w/ non-linear anisotropic eddy viscosity (1.75 order)
Wall Shear Stress	No slip. Eqns. integrated to the wall.
Heat Transport	- solves temperature eqn.
Moisture Transport	- no moisture transport eqn.
Surface Heating	user-specified through B.C.'s
Dispersion	No internal dispersion modules. Flow fields can be used to drive Lagrangian dispersion models. Scalar advection/diffusion equation, but no source set-up
Chemistry	- No internal chemistry modules.
Numerics	- finite element - second-order projection method for time integration - modified forward Euler explicit scheme also available - 2nd order accurate in time and space - implicit pressure equation solved by direct solver or preconditioned conjugate gradient method - variables computed on staggered grid
Mesh	- unstructured grids (non-orthogonal) - variable grid spacing - irregular domains allowed - obstacles handled outside of computational domain
B.C.'s	specified in-flow, zero gradient, free-slip, no-slip, and specified flux
Input	- ASCII input files; no graphical user interface
Output (Graphics)	- velocity and scalar fields are post-processed (plotting package used is GRIZ). Time history data can be post-processed by a X-Y plotting routine. - 3-d visualization by GRIZ - no run-time interface
Platforms	- Unix-based workstations and supercomputers (Cray Y-MP, DEC ALPHA , SGI) - vectorized version available
References model description: flow around obstacles: evaluation studies:	 Gresho, P.M. and S.T. Chan, 1990, "On the theory of semi-implicit projection methods for viscous incompressible flow and its implementation via a finite element method that also introduces a nearly consistent mass matrix, part 2: implementation," Int, J. for Num. Meth. in Fluids, 11:621-659. Christon, M.A., 1995, "HYDRA-A finite element computational fluid dynamics code: User's manual," UCRL-MA-121344, LLNL, Livermore, CA. Gresho, P.M. and S.T. Chan, 1997, "Projection 2 goes turbulent--and fully implicit," Int. J. Comp. Fluid Dyn. (in press). Craft, T.J., B.E. Launder, and K. Suga, 1997, "Development and application of a cubic, non-linear eddy-viscosity model of turbulence," Int. J. Heat & FluidFlow (in press).
Comments	The code was developed mainly for solving engineering-type problems and thus some development is necessary in order to use it to simulate atmospheric flows and the transport/diffusion of pollutants. The current code derives from the Hydra CFD code.
Contact Person(s)	Stevens T. Chan, L-103 Atmospheric Science Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore, CA 94551 Phone: (510) 422-1822 E-mail: schan@llnl.gov

Table A-4. GASFLOW: Computational Fluid Dynamics Model

1	Model Name	GASFLOW 2.0
2	References Model description: Flow around obstacles: Evaluation studies:	Lam et al., 1994, Hydrogen Mixing Studies User's Manual, NUREG/CR-6180. Travis et al., 1994, GASFLOW: Theory and Computational Model, Vol. 1, LA-UR-94-2270. Lam et al., 1993, Hydrogen Mixing Studies Assessment Manual, NUREG/CR-6060. Lam et al., 1993, Hydrogen Mixing Studies Assessment Manual, NUREG/CR-6060. Breitung, W., P. Royl, J.R. Travis, and H. Wilkening. (1996) Analyses of hydrogen dispersion-GASFLOW computer program for determination of hydrogen distribution in pressurized water reactors. *ATW-International Zeitschrift fur Kernergie*, **41** (N6):411-416. P. Royl, J. R. Travis, E. A. Haytcher, and H. Wilkening, "Analysis of Mitigating Measures during Steam/Hydrogen distributions in Nuclear Reactor Containments with the 3D Field Code GASFLOW," presented at the OECD/NEA CSNI Workshop on the Implementation of Hydrogen Mitigation Techniques, Winnipeg, Canada, May 13–15, 1996. Whicker, Y. Yang, J. Rogers, and J. Spore, "Experimental characterization and computational modeling of indoor aerosol dispersion and their applications in optimization of continuous air monitor placement, " LA-UR-95-4174, presented at the ASME Fluids Engineering Division Summer Meeting, July 1996. P. Royl, C. Müller, J. R. Travis, T. Wilson, "Validation of GASFLOW for Analysis of Steam/Hydrogen Transport and Combustion Processes in Nuclear Reactor Containments," Procs 13th Conference on Structural Mechanics in Reactor Technology, August 13-18, 1995 Porto Alegre, RS, Brazil C. Müller and J. R. Travis, "GASFLOW comparisons with Bureau of Mines Experiments," LA-UR-94-2020, presented at the American Nuclear Society 1994 Winter Annual Meeting, November 13-17, 1994.
3	Abstract	This CFD code has been developed and used primarily to model flows inside geometrically complex nuclear containment facilities and around obstacles, such as walls, cabinets and other structures. Unique features include combustion and transport of flammable gases, chemical reactions, entrainment and deposition of aerosols, and heating/cooling of material surfaces.
5	Contact Person(s)	George Niederauer Los Alamos National Laboratory, Group TSA-10, MS F575 Los Alamos, NM 87545 505-665-2538; georgen@lanl.gov
6	Applications	Applicable to containment buildings, tanks, single rooms with and without ventilation systems. Applicable to multi-species gas mixing and transport problems, as well as aerosol transport problems
7	Limitations	Major assumptions include: each cell is well mixed, each gas species has the same velocity at cell boundaries; agglomeration is currently ignored in the aerosol model; diffusion of species is based on mixture diffusion equations; gases assumed to behave as ideal gases; choking is currently not considered in the ventilation system components.
8	Sponsors	LANL, U.S. Department of Energy; Nuclear Regulatory Commission
9	Computer Requirements	- UNIX-based workstations and supercomputers - Vectorized form available, but no parallel version
10	Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Compressible Form w/ buoyancy production)
11	Fluid Type and Flow Regimes	- Compressible or Incompressible - Newtonian - Sub or Supersonic - Laminar or Turbulent
12	Turbulence Scheme(s)	- Algebraic K-theory (1st order) - 2 eqn. k-epsilon (1.5 order)

Table A-4. GASFLOW: Computational Fluid Dynamics Model (cont.)

1	Model Name	GASFLOW 2.0
13	Wall Shear Stress	- traditional law-of-wall approach, but modified with 1/7 power law - laminar sub-layer law-of-wall very close to sfc.
14	Heat Transport	- solves internal energy equation
15	Moisture Transport	Modeling of flow through multiple species transport and of condensation and vaporization on structures and droplet "rainout", with feedback through source or sink terms in mass and energy equations
16	Surface Heating	- 1d heat conduction through specified boundary conditions - hardwired radiation heat transfer model for simple geometries can easily be added easily by Fortran programming
17	Dispersion	Eulerian: -through multiple gas species transport can have single or multi-grid source(s) - dense or buoyant gas dispersion possible - no deposition/resuspension Lagrangian: - discrete particle (aerosol) transport determined by fluid drag forces and Monte Carlo diffusion - deposition/resuspension through particle bounce threshold velocity - entrainment through fluid drag/frictional force balance approach
18	Chemistry	- gaseous: one-step global chemical kinetics (H2, NH3, CO, CH4 w/ O2 or NO2); foundation for programming other chemical kinetics - no aerosol chemistry
19	Numerics	Finite volume; implicit/explicit (ICEd-ALE scheme); 1st order donor cell or 2nd order Van Leer advection schemes; Preconditioned Conjugate Residual method for solving Poisson pressure eqn.; variables computed on staggered grid
20	Mesh	Orthogonal mesh (rectangular & cylindrical); variable grid size capability; rudimentary automatic mesh generation; obstacles defined by "no-flow" grid cells
21	Boundary conditions	- zero gradient, cyclic, pressure, velocity, slip, no-slip
22	Input	- ASCII input file; initial graphical user interface coming in summer 1997 - no CAD interface (planned for FY98)
23	Output (Graphics)	- binary files for LANL-developed PSCAN (x-y, line contour, vector, grid mesh plots), plot types specified in input file; ascii column output for general plotting packages (e.g., XMGR, Spyglass), but no conversion codes; no run-time interface - initial graphical user interface coming in summer 1997
24	Evaluations	Validated against data from many international experiments, from benchtop tests to 10-story high facilities using mixtures of different gas species and aerosols in a wide variety of conditions from quiescent to highly turbulent conditions
25	Comments	- DOE-DP recommended in-facility CFD code - NRC recommended containment (in-facility) CFD code - derives from LANL family of CFD codes (e.g., SOLA, K-FIX, KIVA) - includes combustion physics

Table A-5. COMIS: Interzonal Airflow Model

1	Name	COMIS (Conjunction of Multizone Infiltration Specialists)
2	References	Feustel, H. E.: Annex 23-An International Effort in Multizone Air Flow Modeling, In: *Proceedings, ROOMVENT '96*, July 1996, Yokohama H.E. Feustel, A. Raynor-Hooson (Editors): COMIS Fundamentals, Air Infiltration and Ventilation Centre, Technical Note 29, Lawrence Berkeley Laboratory Report, LBL-28560, 1990 - Feustel, H.E., F. Allard, V.B. Dorer, M. Grosso, M. Herrlin, M. Liu, J.C. Phaff, Y. Utsumi, and H. Yoshino: The COMIS Infiltration Model, In: *Proceedings, Building Simulation '89*, The International Building Performance Simulation Association, Vancouver, 1989 Dorer, V. and A. Weber: Output Options for COMIS, Internal Annex Report, EMPA Dübendorf, 1995 Fürbringer, J.M., C.-A. Roulet, and R. Borchiellini: Annex 23 Subtask II&III Report-Evaluation of COMIS, Vol. 1 and Vol. 2, EPFL Lausanne, Switzerland, 1996
3	Abstract	COMIS is a multizone air flow and transport model. In terms of air-mass flow, buildings represent complicated interlacing systems of flow paths. In this grid-system the joints represent the zones of the building and the connections between the joints simulate the air flow paths. These include the flow resistances caused by open or closed doors and windows and air leakage through the walls. The boundary conditions for the pressure are described by grid points outside the building. Because of the nonlinear dependency of the flow rate on the pressure difference, the pressure distribution for a building can be calculated only by using a method of iterations.
4	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3074 Berkeley, CA 94720, USA
5.	Information Contacts	Helmut E. Feustel Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3074 Berkeley, CA 94720, USA
6	Application	Air flow distribution and pollutant transport mechanism in single-zone and multizone buildings.
7	Limitations	Availability of flow characteristics of zone envelopes and outside pressure distribution and outdoor concentration data. Zones are defined as fully mixed volumes with a constant concentration level of the enclosed gas mixture representing a uniform pressure.
8	Sponsors	Department of Energy, International Energy Agency
9	Computer Requirement	FORTRAN 77 source code runs on all computer platforms if FORTRAN compiler is available.
10	Source-Receptor Relationship	Sources can be specified anywhere on a three-dimensional grid. Zones are handled as fully mixed.
11	Emission Rate	Each zone can have one source/sink for up to five airborne contaminants.
12	Chemical Composition	N/A
13	Plume Behavior	N/A
14	Wind Field	Complicated wind pressure distributions have to be provided by the user.
15	Dispersion Algorithms	N/A
16	Chemical Reactions	N/A
17	Removal Process	Sink terms can be specified for each zone
18	Boundary conditions	Pressure field around the building, temperature field, outdoor concentrations
19	Meteorological Requirements	Wind speed at reference height for pressure coefficients, outdoor temperature, outdoor humidity, barometric pressure.
20	Evaluation	Model has successfully been evaluated by the Energy Conversation in Buildings and Community Systems implementing agreement. Analytical evaluation, inter-model comparison, user-tests, and comparison with in-situ experiments were performed.
21	Output	COMIS output include all interzonal air flows, nodal pressures, driving pressures for air flows, distribution of concentrations
22	Genealogy	COMIS was initially developed by the COMIS Workshop. Evaluation and further development took place in the frame of IEA ECBCS's Annex 23. COMIS now has the following features: Several air flow components, including cracks, large vertical openings, ducts, passive stacks, fans, flow controllers. Variable time step for air flow modeling, fixed time step based on time constant of critical zone for pollutant concentrations. Zone layers Schedules for leakage distribution, fan operation, and source/sink terms. Calculation of pressure coefficients for simple buildings.
23	Availability	see 5.

Table A-6. CONVEC9: Computational Fluid Dynamics Model

1	Model Name	CONVEC9
2	References:	Bauman, F., A. Gadgil, R. Kammerud, E. Altmayer, and M. Nansteel. (1983) Convective heat transfer in buildings: Recent research results. *ASHRAE Transactions*, **89**:1A, 215-233. Gadgil, A.; Bauman, F.; Altmayer, E.; Kammerud, R.C. (1984) Verification of a numerical simulation technique for natural convection. *Transactions of the ASME. Journal of Solar Energy Engineering*, **106**, (no.3): 366-9. Gadgil, A.. and D. Gobin. (1984) Analysis of two-dimensional melting in rectangular enclosures in presence of convection. *Transactions of the ASME. Journal of Heat Transfer*, **106**, (no.1): 20-6. Nazaroff, W.W., D. Dong, and A. J. Gadgil. (1992) Numerical Investigations of the Deposition of Unattached 218PO and 212PB from Natural Convection Enclosure Flow, Journal of Aerosol Sciences, 23(4): 339-352.
3	Abstract	Series of CFD codes developed and used to model natural and forced convection, for internal and external flows, in two and three dimensions, for complex interiors of rooms (e.g., internal partitions, furniture); includes heat and pollutant sources and sinks, and velocity sources and sinks (e.g., fans, windows). Simulation of laminar and turbulent flows for typical building conditions.
4	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3058 Berkeley, CA 94720, USA
5	Contact Person(s)	Ashok Gadgil Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program; Building 90, Room 3074 Berkeley, CA 94720, USA
6	Applications	Heat transport and air flow in a room; accurate calculation of heat transfer coefficients; deposition of radon progeny on interior surfaces of an enclosure; investigation of ozone deposition on interior surfaces of a room.
7	Limitations	Research model. No user's manual. No user-friendly input/output interfaces. Limited to rectilinear details on walls and partitions.
8	Sponsors	U.S. Dept. Energy
9	Computer Requirements	Developed for single processor machines. Code language is FORTRAN
10	Conservation equations	Energy and mass transport and conservation. Arbitrary sources and sinks of fluid mass and heat in the space and on the bounding surfaces can be modeled
11	Emissions rates	User-specified emission rates for surfaces and inside space
12	Fluid Equations	3 Dimensional Navier Stokes Solver
13	Fluid properties	Building air modeled as an incompressible Boussinesque fluid
14	Turbulence Scheme(s)	Two equation turbulence models (k-epsilon / k-omega) modified for low Reynolds number turbulence
15	Heat Transport	Transport by convection only, no radiation model
16	Dispersion	- dense or buoyant gas dispersion possible - deposition modeled in detail
17	Chemistry	Not available
18	Numerics	Based on Patankar-Spalding differencing using the SIMPLE and SIMPLER algorithms developed at Imperial College and University of Minnesota; Alternating Direction Implicit solver
19	Mesh	Non-uniform rectilinear Cartesian grids, staggered for velocity and pressure solutions. Can easily incorporate blockages and "frozen off" solid sections in the fluid space
20	Boundary conditions	Periodic, pressure, pressure-gradient, velocity, slip, no slip
21	Input	ASCII input file No user friendly graphical interface
22	Output (Graphics)	ASCII column output for general plotting packages but no conversion codes; no run-time interface
23	Evaluations	CONVEC2 model predictions and measurements of local Nusselt numbers compared

Table A-7. MIAQ4: Aerosol Deposition in Rooms Model

1	Name	MIAQ4
2	Reference	Nazaroff, W. W. and G. R. Cass. (1989) Mathematical Modeling of Indoor Aerosol Dynamics, *Environmental Science and Technology*, **23**: 157-166.
3	Abstract	MIAQ4 is a model of aerosol behavior within interior spaces, accounting for the effects of ventilation, filtration, deposition, coagulation and direct emission. It permits the tracking of the aerosol concentration and size distribution as a function of time, along with the accumulation of deposited materials on surfaces with various orientations. The model has been evaluated with data from experiments using environmental tobacco smoke and reasonable agreement was obtained.
4	Location	LBNL and UC Berkeley
5	Information Contact	Richard Sextro, LBNL William Nazaroff, UC Berkeley (and LBNL)
6	Application	Indoor aerosol behavior, permitting estimates of inhalation exposures to aerosols as a function of size and the accumulation of materials on surfaces as a secondary source of exposure
7	Limitations	The model treats indoor aerosol concentrations as being spatially uniform (well-mixed) and thus does not account for aerosol dispersion from sources. Interior airflow conditions are not treated as a continuum, but are assumed to fall into three different regimes.
8	Sponsors	Original work done as part of Nazaroff Ph.D. dissertation at Caltech (Nazaroff and Cass 1989); current and recent uses funded by a variety of sponsors, including U.S. DOE.
9	Computer requirement	Source code is in FORTRAN; will run on workstation or fast PC platforms
10	Source-receptor relationship	The model can treat multiple rooms, specifying air flow between the rooms as the transport process, along with the filtration efficiency for filters incorporated in an HVAC system. Sources may be located within any of the rooms, subject to the previously noted assumption that the interior concentrations are well mixed.
11	Emission rate	Emissions are treated as constant per unit time, with specification of the appropriate start and stop time, or as time varying, done as discrete steps each with a constant source rate for a given time period.
12	Chemical composition	The model currently treats the aerosols as spheres of uniform composition and assumes that the interaction between the aerosols and the surfaces (including other aerosols) is physical (and inelastic).
13	Plume behavior	N/A
14	Wind Field	Interior air flows along surfaces are treated as either 1) natural convection, 2) homogeneous turbulence or 3) forced laminar flow parallel to the surface of interest.
15	Dispersion Algorithms	N/A
16	Chemical reactions	The current model version does not explicitly account for chemical behavior but such a module could easily be added to the present model
17	Removal processes	As noted, the interaction with surfaces is assumed to take the form of inelastic collisions (if surface chemical effects can be specified, this interaction could be incorporated into the model. Coagulation, ventilation and surface deposition are accounted for. Surface deposition depends upon surface orientation and their thermal condition with respect to the room interior.
18	Boundary conditions	Dimensions of surfaces; initial conditions include specification of starting aerosol size distribution and concentration (if any) for indoors or for outdoors when infiltration is included in the problem
19	Meteorological requirements	Interior air and surface temperatures (or alternatively temperature differences)
20	Evaluation	MIAQ4 has been validated against ETS data (Nazaroff and Cass 1989).
21	Output	Tabular outputs (flat ASCII files) which can be ported to various graphics programs to provide time series plots, 2-D concentration plots, etc.
22	Genealogy	See 8 above. MIAQ4 has been used to examine the behavior of aerosols indoors, from estimating exposures to environmental tobacco smoke (Miller-Leiden *et al.* 1993) and evaluating engineering controls for ETS (Miller-Leiden and Nazaroff 1996) to the soiling of museum artwork by deposition of indoor aerosols (Nazaroff *et al.* 1990).
23	Availability	See 5 above.

Table A-8. LBNL Simplified Duet Model: Aerosol Deposition in Ducts Model

1	Name	LBNL simplified duct model
2	Reference	Carrie, F. R. and M. P. Modera. Particle Deposition in a Two-Dimensional Slot from a Transverse Stream, *Aerosol Science and Technology* (Submitted); LBL Report LBL-34829 (1995)
3	Abstract	The LBNL simple duct model is based on a set of analytical expressions for different air flow regimes, treating the problem in steady-state. It computes the deposition losses in-or alternatively the penetration through-ducts as a function of aerosol size and density, duct dimension, and air flow rate. It was designed for duct systems in single family residential buildings.
4	Location	LBNL
5	Information Contact	Richard Sextro, LBNL Mark Modera, LBNL
6	Application	Aerosol transport and deposition in straight duct sections
7	Limitations	The model treats indoor aerosol concentrations as being spatially uniform, with two flow regimes. Current model implementation does not account for effects of duct bends, changes in shape, size, etc.
8	Sponsors	Sponsors include California Institute for Energy Efficiency and the U.S. Department of Energy
9	Computer requirement	The model is currently implemented as either a spreadsheet or coded in FORTRAN and will run in a Mac or PC environment or on a workstation.
10	Source-receptor relationship	The model assumes that the aerosol concentration in the duct flow is well-mixed upon entrance.
11	Emission rate	N/A
12	Chemical composition	The model currently treats the aerosols as spheres of uniform composition and assumes that the interaction between the aerosols and the surfaces is physical (and inelastic).
13	Plume behavior	N/A
14	Wind Field	Linear velocities are computed from the duct dimensions and the air flow rate and are compared with the duct Reynolds number to distinguish the flow regime.
15	Dispersion Algorithms	N/A
16	Chemical reactions	N/A
17	Removal processes	As noted, the interaction with surfaces is assumed to take the form of inelastic collisions.
18	Boundary conditions	Dimensions of surfaces; initial conditions include specification of aerosol size and flow.
19	Meteorological requirements	N/A
20	Evaluation	The model has not yet been validated.
21	Output	Tabular outputs (flat ASCII files) can be ported to various graphics programs to provide time series plots, 2-D concentration plots, etc.
22	Genealogy	The model was first formulated to examine efficiency for delivery of aerosols through a duct system as sealants for duct leaks (where the overall sealing efficiency is a product of the aerosol penetration through the duct and the deposition efficiency in the leaks themselves) (Carrie and Modera 1995).
23	Availability	See 5 above.

Table A-9. LBNL98: Advanced Building Simulation Model

(This advanced building simulation model is under development and will not be available until late in 1998.)

1	Name	LBNL98
2	References	Not yet available
3	Abstract	Advanced building simulation model which will calculate thermal behavior, intrazonal air flow, ducts and multizone air flow and the generation, transportation and removal of pollutants in complex buildings.
4	Location	Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3058 Berkeley, CA 94720, USA
5	Contact	Ashok Gadgil Lawrence Berkeley National Laboratory Environmental Energy Technologies Division Indoor Environment Program, Building 90, Room 3058 Berkeley, CA 94720, USA
6	Applications	Heat transfer, air flow distribution and pollutant transport mechanisms in single-zone and multizone buildings.
7	Limitations	Not available until late 1998
8	Sponsors	LBNL Laboratory-Directed R&D Program
9	Computer Requirements	Parallelized for multiple processor platforms, and UNIX workstations
10	Conservation Equations	Energy (convection, conduction and radiation heat transfer) and multiple species (generation, transportation and removal)
11	Fluid Equations	3 dimensional, transient, Reynolds averaged, incompressible, Navier-Stokes with buoyancy production.
12	Boundary Conditions	Any combination of flux, known property and radiation boundary conditions variable in space and time.
13	Fluid Properties	Determined from CHEMKIN program
14	Chemicals	Multiple species tracked separately. Chemical interactions possible through CHEMKIN program.
15	Origins of Model Approach	Developed by Prof. Harry Dwyer at U.C. Davis (H.A. Dwyer. "Calculation of Droplet Dynamics in High Temperature Environments". Progress in Energy and Combustion Science,. 15, pg. 131, 1989.) based on NASA Ames OVERFLOW code (P.G. Bunning et al, OVERFLOW User's Manual Version 1.7u, 1997)
16	Solution Method	Finite volume, ADI, Predictor – Corrector solution method, 2nd order in time and space, Pressure projection method used to solve Poisson's equation
17	Turbulence Models	Two equation turbulence models (k-ε and k-ω) modified for low Reynold's number flow
18	Radiation Models	Both long wave (thermal infrared) and short wave (visible and solar infrared)
19	Meshing Method	Overset (Chimera) meshing strategy. Background Cartesian with overlapping generalized curvilinear meshes as needed to capture details of the geometry
20	Mesh Generators	Public domain hyperbolic (HYPGEN) and elliptic (GRIDGEN) mesh generators as needed.
21	Output	Output in format for use with TECPLOT

Table A-10. HIGRAD: Computational Fluid Dynamics Model

Model Name	HIGRAD
Past Applications	This CFD code has been used to generate potential flow over a sphere; resolve a flow field in the vicinity of buildings and/or steep hills; simulate small cumulus clouds; and resolve boundary-layer eddies over the Pacific warm pool.
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations (Transient Compressible or Incompressible Forms w/ buoyancy production))
Fluid Type and Flow Regimes	- Compressible or Incompressible - Newtonian - Sub or Supersonic - Laminar or Turbulent
Turbulence Scheme(s)	- Smagorinsky K-theory (1st order) - 1 eqn. k-l (1.5 order)
Wall Shear Stress	No current parameterizations are present in the code.
Heat Transport	Solves internal energy eqn.
Moisture Transport	A conservation equation for moisture transport is included and condensational effects are handled.
Surface Heating	- surface energy budget eqns., including both long and shortwave radiation, are currently being added; but no building shadow effects - no heat conduction through building materials
Dispersion	No internal dispersion modules. Flow fields can be used to drive Lagrangian dispersion models.
Chemistry	No internal chemistry modules.
Numerics	- finite volume - explicit - employs MPDATA advection scheme with monotone behavior or semi-Lagrangian scheme - second order accurate in time and space - pressure is diagnosed (compressible option) or is determined by solving an implicit pressure equation (pre-conditioned conjugate gradient method) (anelastic option)
Mesh	- nonorthogonal terrain following coordinate system (can easily incorporate orthogonal transformations) - numerics can handle expanding mesh - zero flow at obstacle grid points
B.C.'s	- side boundary conditions can either be cyclic, gradient equal to zero, or set to relax to specified environmental profiles - an absorbing layer can be activated at the top and either non-slip or free-slip boundary conditions can be imposed at the bottom.
Mesh	- nonorthogonal terrain following coordinate system (can easily incorporate orthogonal transformations) - numerics can handle expanding mesh - zero flow at obstacle grid points
B.C.'s	- side boundary conditions can either be cyclic, gradient equal to zero, or set to relax to specified environmental profiles - an absorbing layer can be activated at the top and either non-slip or free-slip boundary conditions can be imposed at the bottom.
Input	- ASCII input file; no graphical user interface - input can include atmospheric sounding data and/or data interpolated from other models.
Output (Graphics)	- output has been fed into graphics packages such as NCAR graphics and AVS - no run-time interface
Platforms	- UNIX-based workstations and supercomputers - Fortran 90 and Fortran 77 versions of the code exist - runs on both vector and parallel machines.
References model description: flow around obstacles: evaluation studies:	Smolarkiewicz, P.K., and L.G. Margolin, 1995: On forward-in-time differencing for fluids: An Eulerian/semi-Lagrangian nonhydrostatic model for stratified flows. LA-UR-94-4357.
Comments	
Contact Person(s)	Jon Reisner Los Alamos National Laboratory Group EES-8, MS D401 Los Alamos, NM 87545 505-665-1889; reisner@lanl.gov

Table A-11. TEMPEST: Computational Fluid Dynamics Model

Model Name	TEMPEST
Past Applications	This CFD code has been used primarily to model heating and cooling of reactor components and flows in complex terrain, around buildings, and inside residential structures.
Fluid Equations	Reynolds-Averaged Navier-Stokes (Transient Incompressible Form w/ buoyancy production)
Fluid Type and Flow Regimes	- Incompressible - Boussinesq - Newtonian - Laminar or Turbulent
Turbulence Scheme(s)	- 2 eqn. k-epsilon (1.5 order)
Wall Shear Stress	- traditional law-of-wall approach
Heat Transport	- solves potential temperature eqn.
Moisture Transport	no moisture transport eqns.
SurfaceHeating	- 1d heat conduction through specified B.C.'s - no solar radiation, bldg. shadow, and surface radiation budget calculations

Dispersion	- Eulerian
	  - through single-species concentration eqn. (can have single or multi-grid source(s))
	  - dense or buoyant gas dispersion possible
	  - no deposition/resuspension
	- Lagrangian
	  - flow fields can be used to drive Lagrangian dispersion models.

Chemistry	- no internal chemistry modules.
Numerics	- finite volume - explicit for momentum eqns., implicit for other eqns. (SMAC scheme) - 1st order donor cell for advection - finite difference methods for solving Poisson pressure eqn. - variables computed on staggered grid
Mesh	- orthogonal mesh (rectangular & cylindrical) - expanding grid capability - rudimentary automatic mesh generation - obstacles defined by "no-flow" grid cells
B.C.'s	zero gradient, cyclic, velocity, slip, no-slip
Input	- ASCII input file; no graphical user interface - no CAD interface
Output (Graphics)	- ASCII output files for x-y, line contour, vector, grid mesh plots - no run-time interface
Platforms	- UNIX-based workstations and supercomputers - vectorized form, but no parallel version
References model description: flow around obstacles:	Trent and Eyler, 1989, TEMPEST, A 3-d Time Dependent Computer Program for Hydrothermal Analysis, PNL-4348. Zhang, Arya, and Snyder, 1996, A comparison of numerical and physical modeling of stable atmospheric flow and dispersion around a cubical building, Atm. Environ., v30, pp 1327-1345. Guenther, Lamb, and Stock, 1990, 3-d numerical simulation of plume downwash with a k-e turbulence model, JAM, v 29, p 633.
Comments	Currently not actively used at PNNL.
Contact Person(s)	Pacific Northwest National Laboratory Richland, WA

Table A-12. NORAPS: Prognostic Meteorological Model

Model Name	**NORAPS** (Navy Operational Regional Atmospheric Prediction System)
Applications	regional atmospheric weather forecasting
Fluid Equations	Reynolds-Averaged Hydrostatic Primitive Equations in s coordinates
Fluid Type and Flow Regimes	Fully compressible - hydrostatic - Newtonian
Turbulence	TKE-epsilon (1.5 order)
Wall Shear Stress	
Heat Transport	Solves Thermodynamic Energy Equation
Moisture	Nonconvective precipitation occurs when supersaturation occurs at a grid point. Cumulus Parameterization of Kuo
Surface Treatment	Surface Layer Parameterization of Deardorff Ground temperature calculated from surface energy budget of Blackadar
Dispersion	None
Chemistry	None
Numerics	Split-explicit time integration scheme of Madala
Mesh	Staggered Grid (Arakawa-C grid) nesting capability for up to 3 grids
B.C.'s	From large scale weather prediction model or gridded analysis
Input	Namelist driven Binary (IEEE 32 bit standard) input/output
Output (Graphics)	NCARGRAPHICS post-processor Vis-5d capability
Platforms	UNIX-based workstations and supercomputers (vectorized and parallel)
References	Hodur, R.M., 1982: Description and evaluation of NORAPS: The Navy operational regional atmospheric prediction system. *Mon. Wea. Rev.*, **100**, pp 1591-1602. Hodur, R.M., 1987: Evaluation of a regional Model with an update cycle. *Mon. Wea. Rev.*, **115**, pp 2707-2718.
Comments	Has been running operationally at the Fleet Numerical Meteorological and Oceanographic Center for a number of years.
Contact Persons	Martin Leach Lawrence Livermore National Laboratory L-103 Livermore CA, 94550 510-422-5192; mleach@llnl.gov

Table A-13. COAMPS: Prognostic Meteorological Model

Model Name	**COAMPS** (Coupled Ocean/Atmosphere Mesoscale Prediction System)
Applications	micro to mesoscale atmospheric weather forecasting (cloud scale to extratropical cyclone scale)
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations
Fluid Type and Flow Regimes	Fully compressible - Nonhydrostatic - Newtonian
Turbulence	TKE-epsilon (1.5 order) Large Eddy Simulation Capability
Wall Shear Stress	Vertical Mixing length at Earth's surface according to Mellor and Yamada (1974) or Therry and Lacarrere (1983)
Heat Transport	Solves Thermodynamic Energy Equation
Moisture	Explicit moist physics with Cumulus Parameterization
Surface Treatment	Surface Layer Parameterization Heat and Moisture Transfer into the soil
Dispersion	None
Chemistry	None
Numerics	2nd order centered finite difference time splitting semi-Lagrangian in LES mode
Mesh	Staggered Grid (Arakawa-C grid) nesting capability for up to 7 grids
B.C.'s	From large scale weather prediction model or gridded analysis
Input	Namelist driven Binary (IEEE 32 bit standard) input/output
Output (Graphics)	NCARGRAPHICS post-processor Vis-5d capability
Platforms	UNIX-based workstations and supercomputers (vectorized)
References	Hodur, R. 1997: Mo. Wea. Rev. in process Haack, T., 1996: Software User's Manual for the COAMPS , NRL
Comments	A state of the science operational and research model capable of simulating a broad spectrum of atmospheric circulation.
Contact Persons	Martin Leach Lawrence Livermore National Laboratory L-103 Livermore CA, 94550 510-422-5192; mleach@llnl.gov

Table A-14. HOTMAC: Prognostic Meteorological Model

Model Name	HOTMAC
Applications	Complex mesoscale flow in coastal, mountainous, and urban areas
Fluid Equations	Incompressible hydrostatic Navier-Stokes Equations
Fluid Type and Flow Regimes	Incompressible - Hydrostatic - Newtonian Terrain Following
Turbulence	2 equation q2-l closure (1.5 order) (similar to k-e) 1 equation q2 closure (1.5 order) (empirical equation for l)
Wall Shear Stress	
Heat Transport	Solves potential energy equation
Moisture	Yes, condensation effects are also included Statistical description of clouds based on moisture content.
Surface Treatment	Surface heating: long and shortwave radiation, sensible, latent, and soil heat flux are accounted for with 13 different land classes available. Urban canopy: model has parameterizations for canopy-induced momentum drag, turbulent kinetic energy production, and longwave/shortwave attenuation, as well as urban landclass properties.
Dispersion	RAPTAD model
Chemistry	None
Numerics	ADI (alternating direction implicit) numerical algorithm. Relatively fast compared to most numerical schemes since it allows for a 1 to 10 minute timestep.
Mesh	Rectilinear terrain following coordinate system with expanding mesh in the vertical direction (typically use Dz = 2 m near surface) and nested grids in the horizontal (typically Dx=1, 3, 9 km or 2, 6, 18 km)
B.C.'s	I.C's: Typically use rawinsonde for vertical profiles of T, ws, wd, rh, and assume horizontal homogenity. Need 6-12 hour spin-up time to overcome initialization approximations. Also have the capability to use multiple vertical profiles. Nudging: Uses simple 4-d data assimilation scheme for winds. Can use single or multiple vertical profiles and define a horizontal cone of influence.
Input	ASCII file
Output (Graphics)	Formats for NCAR graphics, Spyglass 2D and 3D software, AVS and Deltagraph software.
Platforms	Fortran77 version of the code exist for UNIX and IBM platforms
References	Model description: Yamada and Bunker, 1989: A Numerical Model study of Nocturnal Drainage Flows with Strong Wind and Temperature Gradients, *JAM, 28*, pp 545-554 Urban Canopy-Brown and Williams, 1997: the Effect of Urban Canopy Parameterizations on Mesoscale Meteorological Model Simulations in the Paso del Norte Area, 90th AWMA Conf., Toronto, Canada.
Comments	
Contact Persons	Mike Williams or Michael Brown Energy & Environmental Analysis Group Los Alamos National Laboratory Los Alamos, NM 87545 (505) 667-1788

Tabel A-15. RAMS: Prognostic Meteorological Model

Model Name	**RAMS** (Regional Atmospheric Modeling System)
Applications	micro to mesoscale atmospheric weather forecasting (cloud scale to extratropical cyclone scale)
Fluid Equations	Reynolds-Averaged Navier-Stokes Equations
Fluid Type and Flow Regimes	Fully compressible - Nonhydrostatic - Newtonian Terrain Following
Turbulence	First Order K theory, 1.5 order TKE Deardorff for large eddy simulations
Wall Shear Stress	Louis (1979) surface layer parameterization vertical mixing Mellor and Yamada (1981)
Heat Transport	Solves thermodynamic energy equation
Moisture	Bulk microphysics for 7 condensate species cumulus parameterization
Surface Treatment	Prognostic surface energy balance Vegetation, heat and moisture into soil
Dispersion	HYPACT model
Chemistry	None
Numerics	Second or sixth order centered finite difference Hybrid forward scheme Leapfrog momentum Time splitting
Mesh	Staggered grid (Arakawa-C grid) Nesting capability for n grids
B.C.'s	From large scale weather prediction model or gridded analysis and single sounding
Input	Namelist driven Binary (IEEE 32 bit standard) input/output
Output (Graphics)	NCAR GRAPHICS post-processor AVS capability
Platforms	UNIX-based workstations and supercomputers vectorized and parallelized
References	Many but Pielke et al. (1992) is most general
Comments	A state of the science operational and research model capable of simulating a broad spectrum of atmospheric phenomena
Contact Persons	James E. Bossart Los Alamos National Laboratory Mail Stop D-401 Los Alamos, NM 87545 (505) 667-6268 or Craig Tremback ASTER division Mission Research Corporation Box 466 Fort Collins, CO 80526 (970) 282-4400

Table A-16. ADPIC: Lagrangian Particle Dispersion Model

Name	ADPIC
References	Atmospheric Release Advisory Capability, 1997, "User's Guide to the CG-Mathew/ADPIC Models, Version 5," Lawrence Livermore National Laboratory Report UCRL-MA-103581 Rev.5. Lange, R., 1978, "ADPIC--A Three-Dimensional Particle-in-cell Model for the Dispersal of Atmospheric Pollutants and it Comparison to Regional Tracer Studies," *J. App. Meteor., 17*, pp 320-329. Lange, R., 1989, "Transferability of the Three-Dimensional Air Quality Model Between Two Different Sites in Complex Terrain," *J. Climate and App. Meteor., 28,* pp 665-679. Sherman, C.A., 1978, "A Mass-Consistent Model for Wind Fields Over Complex Terrain," *J. App. Meteor., 17,* pp 312-319. Sullivan, T.S., J.S. Ellis, C.S. Foster, K.T. Foster, R.L. Baskett, J.S. Nasstrom, and W.W. Schalk, III, 1993, "Atmospheric Release Advisory Capability: Real-Time Modeling of Airborne Hazardous Materials," *Bull. Amer. Meteor. Soc. 74,* ppÊ343-2361.
Abstract	The MATHEW model generates a mass conservative three-dimensional gridded mean wind field including terrain effects from available interpolated meteorological data and topography by variational methods. ADPIC is a three-dimensional, numerical diffusion and transport model capable of simulating the time- and space-varying dispersal of atmospheric pollutants under complex conditions. MATHEW/ADPIC are the core models for the DOE Atmospheric Release Advisory Capability (ARAC) Program.
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Source code available from: DOE Energy Science and Technology Center P.O. Box 1020 Oak Ridge, TN 37831
Information Contacts	John S. Nasstrom L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 423-6738 E-mail: jnasstrom@llnl.gov Connie Foster Phone: (510) 422-1867 E-mail: cfoster@arac.llnl.gov Hoyt Walker Phone: (510) 422-1840 E-mail: hwalker@arac.llnl.gov
Application	Atmospheric transport and diffusion of radioactive and nonreactive toxic chemical releases. MATHEW/ADPIC is the core model used in the Atmospheric Release Advisory Capability which provides DOE HQ, several federal agencies, and numerous DOE and DOD sites with a real-time emergency response modeling service.
Limitations	MATHEW is a diagnostic model that uses persistence, manual inputs, or gridded wind data for forecasted winds. ADPIC has no reactive chemistry.
Sponsor	Department of Energy
Name	**ADPIC**
Computer Requirements	LLNL runs MATHEW/ADPIC on a VAX/VMS systems (85550, 6610, and 7000 Alphas) It also runs on UNIX workstations. FORTRAN-77 source codes available from ESTSC have been compiled on a variety of systems with more than 3MB of memory.
Emission Rates	Up to nine releases or species may be specified in a run. Optionally, an unlimited number of nuclides may be specified using the hybrid-particle source term. Emission rates are given in g/s or CI (Becquerel) per second for either gases or particulate matter. Particle size distributions (minimum, mean, maximum and standard geometric deviation off the diameter) must be specified for particulate matter.
Chemical Composition	N/A

Table A-16. ADPIC: Lagrangian Particle Dispersion Model (cont.)

Name	ADPIC
Plume Behavior	Release options include the following: • Static source geometry (user specified dimensions) • Plume rise for stack releases using modified Briggs time-dependent buoyant and momentum equations • Explosive cloud rise using Boughton's time-dependent integral plume rise technique • Fires • Reactor accidents involving mixed fission products(an unlimited number of nuclides may be specified using the hybrid-particle source term) • Spills
Wind Field	Three-dimensional vector winds computed by MATHEW
Dispersion Algorithm	Two basic K-theory parameterization dispersion options are available: • Hybrid Eulerian-Lagrangian gradient diffusion • Lagrangian Monte Carlo random displacement diffusion
Chemical Reactions	N/A
Removal Processes	Dry and wet deposition based on deposition velocities and rain rates and gravitational settling base on particle size distribution.
Boundary Conditions	Constant flux in/out flow or reflection at boundary.
Meteorological Requirements	Wind speed and direction at the surface and for at least one vertical profile. Standard deviation of wind direction (s_q), Monin-Obukov length, mixing height, surface roughness (to compute friction velocity), optional temperature profile.
Validation	MATHEW/ADPIC has been extensively evaluated with over a dozen experimental data sets with a wide variety of terrain types, tracer release scenarios, and meteorological conditions. For a summary of validation reports see, Lange(1989) or Sullivan et al. (1993)
Output	Pollutant air concentrations (instantaneous, averaged, or time-integrated) and doses at desired heights and ground-level deposition are written as gridded, two-dimensional arrays. (None of the machine-dependent graphical products are provided with the public-domain ESTSC version.)
Genealogy	MATHEW was initially developed by Christine Sherman and ADPIC by Rolf Lange as the core models for regional-scale dispersion problems in 1975-1978. Since the initial 1979 implementation into the LLNL ARAC emergency response system many improvements have been made including the following: • Controlling the initialization of the wind profiles by either measurements or a parameterized method. • Interpolated three-dimensional wind vectors between meteorological input periods (usually 15 minutes or 1 hour) for each ADPIC time step. • Four-deep nested grids in ADPIC for near-source resolution of concentration and deposition. • Optional K-profile initialization method using sigma theta profile data (validated during DOE Atmospheric Studies in Complex Terrain (ASCOT) program). • Monte Carlo random displacement diffusion option.
Additional Remarks	none

Table A-17. LODI: Lagrangian Particle Dispersion Model

Name	LODI (Livermore Operational Dispersion Integrator)
References	Leone, J.M., Jr., J.S. Nasstrom, and D.M. Maddix, 1997: A First Look at the New ARAC Dispersion Model, to be presented at the ANS Sixth Topical Meeting on Emergency Preparedness and Response, San Francisco CA, April 22-25, 1997
Abstract	LODI is a three-dimensional, time-dependent, numerical transport and diffusion model capable of simulating the time- and space-varying dispersal of atmospheric pollutants over regions of complex terrain and under complex conditions. This model solves the turbulent, advection-diffusion equation via a Lagrangian particle, Monte-Carlo method. Within a simulation, particles representing the pollutant are moved through the domain using a random displacement method to model the turbulent diffusion and a Runge-Kutta method to model the advection.
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551
Information Contacts	John M. Leone, Jr. L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 422-6449 E-mail: jleone@llnl.gov
Application	Atmospheric transport and diffusion of radioactive and nonreactive toxic chemical releases. This model is designed to be used in an emergency response mode.
Limitations	No reactive chemistry. Use of advection-diffusion random displacement method limits accuracy for times less than the Lagrangian time-scale.
Sponsor	Department of Energy
Computer Requirements	Model requires only a computer with a valid Fortran-90 compiler. However, the size of memory will determine the number of particles that can be released during any simulation. LODI has been run on Sun Sparc II, SGI Indy and Indigo 2, desktop workstations, on DEC alpha servers, and Cray C-90.
Emission Rates	Releases may be from either static or time dependent source geometries. Either instantaneous or time dependent continuous releases are modeled. An unlimited (subject to computer memory) number of species may be specified. Emission rates are given in g/s or Ci/s for either gases or particulate matter. Particle size distributions must be specified for particulate matter.
Chemical Composition	N/A
Plume Behavior	Non-Gaussian plume described by a large number of marker particles which move through the domain.
Wind Field	Three-dimensional, time-dependent gridded winds (can be on nested grids) are model input.
Dispersion Algorithm	Lagrangian Monte-Carlo random displacement turbulent diffusion
Chemical Reactions	N/A
Removal Processes	Dry and wet deposition and gravitational settling.
Boundary Conditions	Reflection at boundary or deposition velocity flux boundary condition
Meteorological Requirements	Gridded (u, v, w) wind fields, turbulence parameters depending upon which option chosen e.g. ustar, boundary layer depth, Obukov length, Lagrangian time scale
Validation	Just beginning-code under development.
Output	Pollutant air concentrations (instantaneous or time-integrated) at desired heights and ground-level deposition are written as gridded, two-dimensional arrays in netCDF files. Three dimensional air concentrations (instantaneous or time-integrated) may also be written to netCDF files. Visualization is done via a post-processor.
Genealogy	This a new model currently under development.
Additional Remarks	Requires FORTRAN-90 compiler and netCDF file handling library.

Table A-18. SLAB: Dense Gas Dispersion Model

Name	SLAB
References	DOC OFCM Modeling Resources.
Abstract	The SLAB model, developed by Lawrence Livermore National Laboratory, was enhanced by LLNL under support of AFESC. The model treats denser-than-air releases by solving the one-dimensional equations of momentum, conservation of mass, species, and energy and the equation of state. SLAB handles release scenarios including ground-level and elevated jets, liquid pool evaporation, and instantaneous volume sources. The model accounts for user-selected averaging timeeffects.
Location	Atmospheric Sciences Division Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551
Information Contacts	Don Ermak L-103 Lawrence Livermore National Laboratory P.O. Box 808 Livermore CA 94551 Phone: (510) 423-0146 E-mail: ermak1@llnl.gov
Application	Denser-than-airdispersion
Limitations	Plume model with straight line wind field.
Sponsor	
Computer Requirements	IBM PC-compatible in MS_DOS operating environment; FORTRAN-77 language.
Emission Rates	Point, area, instantaneous, and continuous
Chemical Composition	Ground-level/elevated jets, liquid pools of hazardous chemicals.
Plume Behavior	Gaussian plume
Wind Field	Straight line
Dispersion Algorithm Chemical Reactions	K-diffusivity,heavier-than-airdispersion None
Removal Processes	None
Boundary Conditions	
Meteorological Requirements	Temperature and point winds
Validation	Approved by EPA as a hazardous chemical dispersion model. Recognized in API hazardous chemical model evaluation.
Output	Concentrations
Genealogy	
Additional Remarks	Aerosol two-phase release

Table A-19. RAPTAD: Lagrangian Random Walk Puff Model

Name	RAPTAD
References	Williams and Yamada, 1990: A microcomputer-based forecasting model: potential applications for emergency response plans and air quality studies, *JAWMA, 40,* pp 1266-1274. Williams, Brown, Cruz, Sosa, and Streit, 1995: Development and testing of meteorology and dispersion models for Mexico City, *At. Env., 29,* pp 2929-2960.
Abstract	RAPTAD is a three-dimensional, time-dependent, numerical transport and diffusion model. It uses a computationally efficient combined random-walk/puff approach which allows it to release a smaller number of puffs (particles) than a traditional random-walk method and still obtain smooth, continuous concentration profiles.
Location	Energy & Environmental Analysis Group Los Alamos National Laboratory Los Alamos, NM 87545
Information Contacts	Mike Williams or Michael Brown (505) 667-1788
Application	Complex dispersion in coastal, mountainous, and urban areas. Models point, line, or area sources.
Limitations	Must be able to specify Lagrangian time-scale. No dense gas capability
Sponsor	Department of Energy
Computer Requirements	Fortran77 versions of the model exist for Unix and IBM platforms.
Emission Rates	Either instantaneous or continuous releases of neutral or buoyant pollutants are modeled for both ground-level and elevated sources.
Chemical Composition	N/A
Plume Behavior	Lagrangian, random-walk puff. Puffs are released one after another. They grow with time due to entrainment and travel on a random-walk using an externally supplied mean wind field and an internally computed Monte-Carlo turbulent wind.
Wind Field	Three-dimensional, time-dependent gridded winds are model input.
Dispersion Algorithm	Lagrangian Monte-Carlo random-walk and puff growth using random-force theory.
Chemical Reactions	Version called RAPBOX has carbon-bond chemistry.
Removal Processes	Deposition
Boundary Conditions	Reflection at ground. Reflection or partial penetration at boundary layer top according to stratification and turbulence intensity.
Meteorological Requirements	Gridded wind, temperature, and turbulent kinetic energy fields; usually from Mesoscale model HOTMAC, but data from other models accepted.
Validation	Mexico City Air Quality Research Initiative-reported in Williams et al., 1995 (see above.) U.S. Army, Toole Depot Study, reported in Williams and Yamada, 1990 (see above.) Cross Appalachian Tracer Experiment-Kao and Yamada, 1988: Use of the CAPTEX data set for evaluations of a long-range transport numerical model with a 4D data assimilation technique, *MWR, 116,* p 293. DOE ASCOT-Brush Creek-Yamada and Bunker, 1988: Development of a nested Grid 2nd Moment Turbulence Closure Model and Application to the 1982 ASCOT Brush Creek Data Simulation, *JAM, 27,* p 562. DOE ASCOT-Geysers -Yamada, 1985: Numerical Simulation of the Night 2 Data of the 1980 ASCOT experiments in the California Geysers Area, *Arch. Met. Geoph. Biocl. Ser. A., 34,* p 223.
Output	Pollutant air concentrations in file formats for NCAR graphics, Spyglass 2D and 3D software, AVS, and Deltagraph software.
Genealogy	

Table A-20. HYPACT: Lagrangian Particle Dispersion Model

Name	HYPACT
References	Lyons, W.A. and C.J. Tremback, 1993: A prototype operational mesoscale air dispersion forecasting system using RAMS and HYPACT, Preprints, 86th Annual AWMA Meeting, Denver, CO, 14-18 June 1993.
Abstract	The HYbrid PArticle-Concentration Transport model (HYPACT) simulates the motion of atmospheric tracers. The tracer transport is determined from atmospheric flow and turbulence data, typically RAMS model output. HYPACT incorporates a hybrid Lagrangian/Eulerian treatment for tracer transport. The Lagrangian treatment enables the specification of small scale source regions when compared with the grid spacing of the wind model. The hybrid Lagrangian/Eulerian approach represents a tracer by Lagrangian particles near the source region where concentration gradients are large. HYPACT converts particles to Eulerian concentrations at large distances downwind, where the plume is broad and well mixed and grid resolvable.
Location	Atmospheric and Climate Sciences Group Los Alamos National Laboratory, Mail Stop D-401 Los Alamos, NM 87545
Information Contacts	General: Craig J. Tremback ASTeR Division of Mission Research Corporation P.O. Box 466 Fort Collins, CO 80522-0466 (970) 282-4400 DOE: James E. Bossart Los Alamos National Laboratory, Mail Stop D-401 Los Alamos, NM 87545 (505) 667-6268
Application	Transport and dispersion of non-reactive atmospheric plumes from small scale sources out to hundreds of kilometer distances downwind.
Limitations	Requires a large number of particles be released to adequately define the concentration field. No reactive chemistry or wet deposition.
Sponsor	Primarily Department of Defense
Computer Requirements	Any high-end Unix based work station with FORTRAN and C compilers. Needs sufficient memory and CPU to track large number of particles.
Emission Rates	Releases can be from a specified point, area, or volume anywhere within the domain. Particle releases can be instantaneous, continuous, or over a specified time interval. Any number of particles can be released to represent a known emission rate from a given source. Concentration fields from a known emission are calculated via a particle in cell method.
Chemical Composition	none
Plume Behavior	Non-Gaussian plume described by a large number of tracer particles that are transported by the mean wind and turbulence data.
Wind Field	Three-dimensional, time-dependent winds from a nested grid.
Dispersion Algorithm	Lagrangian first order Markov chain random displacement turbulent diffusion
Chemical Reactions	none
Removal Processes	Dry deposition, gravitational settling, implicit chemical transformation and radiological decay
Boundary Conditions	Reflection or deposition velocity flux boundary condition
Meteorological Requirements	Grid resolved three-dimensional wind field, wind component variances, Lagrangian time scale of wind components
Validation	Ongoing as part of the Emergency Response Dose Assessment System (ERDAS). See Monobianco et al., 1996, *Bulletin of the Amer. Meteor. Soc.* pp 653-672.
Output	Three-dimensional particle positions and air concentrations at any specified time. Post-processing with NCAR graphics includes multicolor plumes from sources over terrain.
Genealogy	RAMS Lagrangian Particle Dispersion Model (LPDM)
Additional Remarks	

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