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Construction Engineering Research Laboratory

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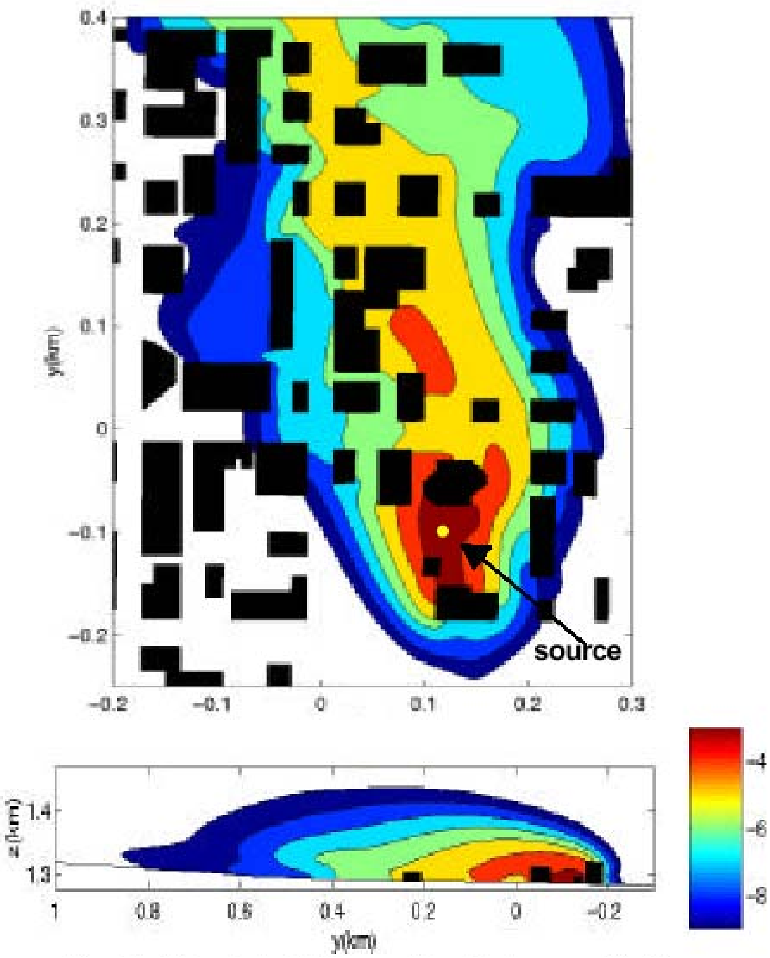
Analysis of Numerical Models for Dispersion of Chemical/Biological Agents in Complex Building Environments

Chang W. Sohn, Andrew Solberg, and Taylor Gonsoulin

November 2004



Simulated patterns for a tracer gas release

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Analysis of Numerical Models for Dispersion of Chemical/Biological Agents in Complex Building Environments

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Final Report

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ABSTRACT: This project reviewed existing technologies that could protect the supply air systems of buildings from chemical/biological (chem/bio) contaminants. This CH2M HILL research: (1) analyzed existing filtration technologies for building heating, ventilating, and air-conditioning (HVAC) systems, and (2) examined numerical models for predicting air flows in and around buildings during a release of chemical or biological agents. This report gives the results of the research into numerical models.

Researchers identified modeling products that would depict the results of a chem/bio release, and rated the models on resolution, cost, convenience, and accuracy. Four models were examined in depth, two for external and two for internal releases. The results provide a modeling approach that can be used to simulate the dispersion of contaminants inside buildings. Such a numerical simulation will help designers and managers evaluate possible ways to reduce occupant exposures to chem/bio contaminants.

Contents

List of Table and Figures

Table

Figures

Conversion Factors

Non-SI* units of measurement used in this report can be converted to SI units as follows:

Multiply	By	To Obtain
acres	4,046.873	square meters
cubic feet	0.02831685	cubic meters
cubic inches	0.00001638706	cubic meters
degrees (angle)	0.01745329	radians
degrees Fahrenheit	(5/9) x (°F – 32)	degrees Celsius
degrees Fahrenheit	(5/9) x (°F – 32) + 273.15.	kelvins
feet	0.3048	meters
gallons (U.S. liquid)	0.003785412	cubic meters
horsepower (550 ft-lb force per second)	745.6999	watts
inches	0.0254	meters
kips per square foot	47.88026	kilopascals
kips per square inch	6.894757	megapascals
miles (U.S. statute)	1.609347	kilometers
pounds (force)	4.448222	newtons
pounds (force) per square inch	0.006894757	megapascals
pounds (mass)	0.4535924	kilograms
square feet	0.09290304	square meters
square miles	2,589,998	square meters
tons (force)	8,896.443	newtons
tons (2,000 pounds, mass)	907.1847	kilograms
yards	0.9144	meters

***Système International d'Unités* ("International System of Measurement"), commonly known as the "metric system."

Preface

This study was conducted for the Engineer Research and Development Center, Construction Engineering Research Laboratory (ERDC/CERL), U.S. Army of Corps of Engineers under the Project 009XGG, "ERASP (Environmental Response and Security Protection)/HVAC (Heating, Ventilating and Air Conditioning)." The technical monitor was Dr. John M. Cullinane, CEERD-EM-J. This study was also supported in part by the Project GD1KGD "Bldg Chem-Bio Protection Modeling & Simulation." The technical monitor was Dr. Paul Howdyshell, CEERD-CV-ZT.

The work was performed by the Energy Branch (CF-E) of the Facilities Division (CF), Construction Engineering Research Laboratory (CERL). The CERL Principal Investigator was Dr. Chang W. Sohn. Part of this work was done by the CH2M HILL at Atlanta, GA under General Services Administration (GSA) Contract GS-10F-0027M, "Analysis of Chemical and Biological (Chem/Bio) Filter Technologies and Numerical Models for Dispersion of Chem/Bio Agents in Complex Building Environments." The technical editor was William J. Wolfe, Information Technology Laboratory. Dr. Thomas A. Hartranft is Chief, CEERD-CF-E, and L. Michael Golish is Chief, CEERD-CF. The associated Technical Directors were Dr. Paul A. Howdyshell, CEERD-CF-F, and Dr. John M. Cullinane, ERDC-EL-MS. The Director of CERL is Dr. Alan W. Moore.

CERL is an element of the U.S. Army Engineer Research and Development Center (ERDC), U.S. Army Corps of Engineers. The Commander and Executive Director of ERDC is COL James R. Rowan, and the Director of ERDC is Dr. James R. Houston.

1 Introduction

1.1 Background

Standing Department of Defense (DOD) policy states that:

> It is the policy of the Department to protect personnel on military installations and DoD-owned or leased facilities from chemical, biological, radiological, nuclear and high-yield explosive (CBRNE) attacks, to respond to these attacks with trained and equipped emergency responders, and to ensure installations are able to continue critical operations during an attack and to resume essential operations after an attack (Huber et al. 2001).

Sohn (2004) addresses the issue of protection of building inhabitants from an accidental or intentional release of the toxic industrial chemicals (TIC) including chemical and biological (C/B) agents. Such aerosolized contaminants released within or near a building could be introduced into the building's heating, ventilating, and air-conditioning (HVAC) system and dispersed throughout the building via normal HVAC operation. This vital issue affects both the public and private sectors. Critical military facilities must meet much higher security standards than typical private-sector buildings. For the millions of buildings in the private sector, the cost of protection makes providing full protection at a level similar to that required for a critical military facility nearly impossible. However, reasonable measures can increase buildings' resistance to the chemical and biological threats; such measures should be incorporated into building design, construction, and operation. The ability to accurately predict potential contaminant dispersion inside a building is critical information in effectively creating and implementing such protective measures.

Lee (2001) discusses a number of passive and active measures that could be taken to protect people inside affected buildings. This work concluded that implementation of an effective C/B protection system would involve two salient technical areas: (1) filter technology, and (2) tools to predict contaminant dispersion inside the building. Gonsoulin (2004) discusses the current state of the filter technologies. This work focuses on the prediction of contaminant dispersion, specifically on the development of numerical tools to simulate contaminant dispersion inside a building, whether the source of contaminant originates outside (i.e., via external release) or inside the building (i.e., via an internal contaminant release).

1.2 Objective

The objectives of this research were to:

1. Identify current simulation models available for determining dispersion of chem/bio agents in and around the building, and conduct a critical review of capabilities and limitations of selected models
2. Review methodologies for accurate simulation of dispersion of chem/bio agents in the complex building environment including building HVAC systems
3. Provide technical direction for future research and development in prediction of contaminant dispersion inside a building.

1.3 Approach

Researchers drew from numerous sources of information on existing modeling technologies, including manufacturers' data, internet content, telephone conversations with industry experts, technical journals, and past experience. This study identified current simulation models available for determining contaminant dispersion in and around buildings. Two models each for external and internal release of contaminants were selected for a critical review. The models included: (1) large-scale environmental simulation (e.g., air pollution from a smoke stack) for concentration of contaminant around the external envelope of a building, and (2) room-scale Computational Fluid Dynamics (CFD) simulation of a concentration profile of contaminant drawn in by convection via building HVAC system or released inside a building.

1.4 Scope

A limited run of selected simulation software was conducted to compare the capability and limitation of selected internal dispersion models. Refinement or development of the simulation software is beyond the scope of this stage of research.

1.5 Mode of Technology Transfer

It is anticipated that the findings from this report will provide technical direction for future research and development in simulation software for prediction of contaminant dispersion inside a building. This report will be made accessible through the World Wide Web (WWW) at URL: http://www.cecer.army.mil

2 Numerical Simulation Models

The simulation programs identified in this work were used to model contaminant migration within buildings, around the exterior of buildings, or preferably both. The approach taken was to identify relevant software, to determine general attributes of each software, and to select the software for further critical review.

Table 1 lists the programs identified, their attributes, and sources for further information. The research revealed four categories of simulation software:

1. Computational Fluid Dynamics (CFD)
2. Real-Time Dispersion-Deposition-Causality Models (Operational Models)
3. Environmental Regulatory Models
4. Multizone Models for internal release.

2.1 Computational Fluid Dynamics Modeling

CFD is a mathematical modeling procedure whereby the fluid parameters of velocity, temperature, pressure, turbulence, and contaminant concentrations are calculated by solving the governing partial differential equations for fluid flow, heat transfer, and conservation of species. These differential equations describe a three-dimensional viscous fluid flow field. Due to the non-linearity of these equations, they cannot be solved analytically. The CFD approach is to transform these differential equations into a set of discrete algebraic equations and solve the algebraic equations by an iterative procedure.

Researchers have used CFD since the early 1970s. Its use has increased dramatically in the last decade as a result of advances in the computing power. In the 1980s, Cray supercomputers typically were used to process CFD simulations, with solution times taking days (which followed a long wait to even gain access to use the supercomputer). The same simulations may now be run on a personal laptop computer in a matter of hours. CFD modeling has been continually validated since its inception against many known fluid phenomena. It is considered a very useful tool for engineers and scientists working on fluid flow problems across many disciplines.

Table 1. Numerical modeling programs for the prediction of contaminant dispersion in complex building environments.

Modeling Package Name		Author	Numerical Simulation Description	Model Size Range	Typical Resolution	Hardware Required	Commercially Available/Cost	Technical Support Available
A. Computational Fluid Dynamics (CFD) Airflow Modeling Packages - Internal/External Modeling								
A1	Flovent	Flomerics Incorporated	CFD - Specific to the built environment (internal/external flows)	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A2	Airpak	Fluent Incorporated	CFD - Specific to the built environment (internal/external flows)	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A3	Star CFD	Adapco Group	CFD - Multi-purpose code	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A4	CFX	ANSYS	CFD - Multi-purpose code	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A5	Flow 3D	Flow Science Incorporated	CFD, Specializes in free surface flows	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A6	Phoenics	Cham Ltd.	CFD - Multi-purpose code	Site (1 km) - Room (10m)	1m - 1cm	PC (High End)	General public $20K - 25K/yr	Yes
A7	FEM3MP	Lawrence Livermore National Laboratory (LLNL)	CFD - High Resolution, specialized code that incorporates meteorological physics, developed solely for the prediction of external flow and contamination migration	City (10km)- Site (1km)	10m - 1cm	Computer Array (100+ processors)	Available through Consultation with LLNL development team	N/A
B. "Real-Time" Dispersion-Deposition-Causality Programs - External Modeling								
B1	Hazard Prediction and Assessment Capability (HPAC)	Defense Threat Reduction Agency (DTRA)	Secondary Closure Integrated Puff SCIPUFF) model and also incorporates urban T&D with Urban Dispersion and Urban Wind Field models.	Region (100km) - Site (1km)	100m - 10m	PC	Available only to the U.S. government, government contractors and educational institutions for non-commercial research (No cost to user)	Yes

Modeling Package Name		Author	Numerical Simulation Description	Model Size Range	Typical Resolution	Hardware Required	Commercially Available/Cost	Technical Support Available
B2	The National Atmospheric Release Advisory Center (NARAC)	Lawrence Livermore National Laboratory	Gaussian Plume for quick response, Modified Steady State CFD, and Modified Transient CFD for advanced analysis	Region (100km) - Site (1km)	100m - 10m	PC for Gaussian, computer array for advanced analysis	Limited to use to Emergency Managers - currently in a trial period. (No cost to users)	Yes
B3	Real-time Environmental Applications and Display sYstem (READY)	NOAA Air Resources Laboratory (ARL)	Hybrid Single-Particle Lagrangian Integrated Trajectory Model	Region (100km) - Site (1km)	100m - 10m	PC	Available only to NOAA and other Federal Agencies, (No cost to users)	Yes
C. EPA Preferred Exhaust Dispersion Modeling Programs - External Modeling								
C1	AERMOD ver. 2222 BETA	AMS/EPA	Modified Gaussian Plume - Steady State - Currently in BETA Testing	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost. Software companies sell graphical add-ons	Limited-User Group, Online Manual
C2	ICS3 (Industrial Source Complex Model)	Pacific Environmental Services - EPA Funded	Gaussian Plume - Steady State	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost. Software companies sell graphical add-ons	Limited-User Group, Online Manual
C3	BLP (Buoyant Line Point Source Model)	Environmental Research Technologies	Gaussian Plume - Steady State	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
C4	CALINE3	California Dept of Transportation	Gaussian Plume -Steady State	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
C5	CALPUFF	Earth Tech	Multi-layer, multi-species non-steady-state puff dispersion model	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
C6	CTMPLUS (Complex Terrain Dispersion Model)	National Technical Information Service (NTIS)	Gaussian Plume -Steady State-Complex Terrain	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual

Modeling Package Name		Author	Numerical Simulation Description	Model Size Range	Typical Resolution	Hardware Required	Commercially Available/Cost	Technical Support Available
C7	OCD (Offshore and Coastal Dispersion Model)	Dept of Interior Funded	Gaussian Plume -Steady State-Complex Terrain-Ocean Terrain	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
C8	10 Different Screening Programs	Various	Gaussian Plume -Steady State-Complex Terrain-Ocean Terrain	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
C9	34 Different “Alternative” Models	Various	Gaussian Plume -Steady State-Complex Terrain-Ocean Terrain	Region (100km) - Site (1km)	10m - 1m	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
D. Indoor Air Quality Internal Models - Internal Modeling								
D1	CONTAM 2.1	National Institute of Science and Technology (NIST)	Nodal Analysis - Multizone indoor air quality and contaminant transport analysis.	Building(100m) - House(10m)	Size of Room or Zone	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
D2	RISK	EPA	Nodal Analysis - Multizone indoor air quality and contaminant transport analysis.	Building(100m) - House(10m)	Size of Room or Zone	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
D3	IAQX	EPA	Add on to RISK for particulate, sources, spills	Building(100m) - House(10m)	Size of Room or Zone	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
D4	COMIS	LBNL	Conjunction of Multizone Infiltration Specialists	Building(100m) - House(10m)	Size of Room or Zone	PC	Source Code Available at no cost.	Limited-User Group, Online Manual
D5	Integration of CFD and Conjunction of Multizone Infiltration Specialists (COMIS)	LBNL	Current research area for LBNL Airflow and Pollutant Transport Group	Building(100m) - House(10m)	1m – 1cm	PC	May be available through consultation	N/A

A number of CFD software programs are available in the current market (Table 1). The differences between these programs exist primarily in the graphical interface between the user and the source code. All source code is based on the same fundamental governing equations. Only slight differences exist in the numerical methods used to solve the equations. Some programs are specifically set up for a particular industry or problem. For example, FLOVENT (by Flomerics) and Airpak (by Fluent) are both tailored to the built environment. These programs may be used to solve flow problems both within and around buildings. Other programs on the list may also be used to solve problems in the built environment, but the user may find their graphical interfaces to be more difficult or time consuming.

The degree of accuracy of a CFD model generally depends on the correct representation of boundary conditions, the solution grid, and the level of transient characteristics. Boundary conditions are the set points at the boundaries of the model, such as wall temperature, flow characteristics at the face of a supply register, characteristics of contamination sources, velocity profile of an approaching wind, and so on. For instance, in C/B protective building design, the proper definition of contamination sources and release mechanism is essential. This might include determining an evaporation rate of a hazardous liquid spill for input to the model, or the definition of a particle release incident including the particle size, total mass, and release scenario.

The solution grid consists of many small volumes that make up the entire volume of the simulation domain. This grid is generated automatically in some programs, or in cases with complex geometry a separate program generates the grid. These volumes may be different shapes (rectangular or triangular) depending on the geometry of the problem being modeled. To obtain a solution that best corresponds to reality, it is necessary to obtain "grid independence," which equates to having enough grid to properly resolve the flow field. Without enough grid, the model is not properly defined and accurate solutions are difficult to obtain. Examples of transient characteristics are flow turbulence, changing temperatures, varying supply jet velocities, a sudden contamination release, or pulsating shifting winds. CFD models can solve for transient conditions, but because of the computational overhead involved, most models are solved for steady-state conditions only.

Most programs come with several options for turbulence modeling. The turbulence models most often used in the built environment are variations of the standard K-epsilon (KE) model. This model is a time average representation of turbulence that is considered very robust, and that provides accurate results with low computational overhead. State-of-the-art models such as FEM3MP by Lawrence Livermore

National Laboratories (LLNL) incorporate a transient turbulence model commonly known as Large-Eddy-Simulation (LES) to increase solution accuracy. The complexity of this model dictates that it is currently run only on a computer array with more than 100 processors.

Commercially available CFD packages that operate on a desktop workstation can handle steady-state models in the size range from 10 meters (m) (single room) to 1 kilometer (km) (small industrial site). A model greater than 1 km is not practical to run on a desktop workstation in less than 1 day per run. FEM3MP is specifically designed to handle external flows over large areas such as the city environment (10 km).

2.2 Real-Time Dispersion-Deposition-Causality Models

The models listed in this category are designed to be used by emergency managers, warfighters, and scientists to limit the loss of life in actual chemical release scenarios. They link real-time weather data, topographical data, dispersion modeling, and population data in one program. They provide human dosage levels at areas of interest within the model.

The numerical engines for the contaminant dispersion portions of these programs are based on statistical dispersion methods rather than the fundamental equations of fluid flow. Hazard Prediction and Assessment Capability (HPAC) and National Atmospheric Release Advisory Center (NARAC) use different mathematical and numerical solutions. HPAC uses a second-order closure equation and a Gaussian puff method, while NARAC uses the diffusion equations and a Lagrangian-Monte Carlo particle method. Computational time for these models is designed to be brief to enable users to make decisions regarding human health as quickly as possible after the release.

Both of these models have been tested extensively by the U.S. government, and are considered the best tools for their intended use. HPAC has been identified by the Department of Defense as a preferred dispersion model (Johnson-Winegar 2003). The model sizes considered with these programs range from the regional scale (100 km) to the site scale (1 km). A paper comparing HPAC and NARAC considered a 10 m grid cell to be fine resolution, and a 40 m grid cell to be coarse resolution. These models are not suitable for modeling indoor air conditions.

2.3 Environmental Regulatory Models

Environmental regulatory models are numerous with approximately seven preferred models, 10 simplified screening models, and 34 alternative models. Slight variations exist among these models, but all are generally based on statistical Gaussian plume numerical engines. They are capable of determining contaminant concentrations within the air, and deposition. Most do not incorporate aerodynamic effects of buildings and terrain.

The latest preferred model listed by the U.S. Environmental Protection Agency (USEPA) is AERMOD, which is considered the most accurate regulatory model available. AERMOD is an improvement over ISCST3 (Industrial Source Complex) with increased accuracy of terrain depiction, vertical and horizontal turbulence modeling, atmospheric convective mixing, and inclusion of building aerodynamic effects. The model sizes considered with these programs range from the regional scale (100 km) to the site scale (1 km). Typical grid resolution is approximately 1 m. These models are not suitable for modeling indoor air conditions.

2.4 Multizone Models

Multizone models are used to determine indoor air quality (IAQ) in compartmentalized buildings and residences. The building is represented as a network of well-mixed spaces, or zones, connected by discrete flow paths such as doors, windows, wall cracks, fans, ducts, hallways, and so on. The model predicts the system's behavior based on the interaction of the assembled components and the conservation of mass.

The two most popular multizone models are CONTAM 2.1 and COMIS. COMIS was developed by the Lawrence Berkeley National Laboratory (LBNL), and LBNL's Airflow and Pollutant Transport Group continues to develop and use this model. CONTAM 2.1 is a product of the National Institute of Standards and Technology (NIST). Both programs have similar capabilities and similar shortcomings.

Multizone models cannot determine detailed zone airflow, and thus they cannot determine whether a zone is poorly mixed. This may result in an over-prediction or under-prediction of the exposure to occupants in the zone, as well as an over-prediction or under-prediction of the rate at which contamination is transferred to the adjacent zone. Other shortcomings are the inability to model bi-directional floor-to-floor flows, duct junctions, and transport delays. Current research by

LBNL's Airflow and Pollutant Transport Group is aimed at combining COMIS and CFD technology to reduce these shortcomings of multizone models.

A full-size office building of 100,000 sq ft (9,295 m^2) may be modeled with a multizone model. However, exterior contaminant concentrations at air handling unit intakes and window openings must be determined with separate software such as a program from one of the other categories.

2.5 Summary of Modeling Types

CFD modeling stands out as the most accurate approach of the modeling technologies considered. A CFD model is able to resolve the fine details of airflow and contamination movement required for an accurate prediction of contamination movement. CFD modeling, however, is not a panacea. Its application is currently limited by its high computational overhead. A large site or city cannot be modeled with commercially available CFD software, and modeling an entire building with a CFD model is a very arduous task. For example, it is estimated it would take 8 to 10 work weeks to completely model and analyze the airflow within a 60,000 sq ft (5577 m^2) four-story office building using a commercial CFD package. A model such as this would involve 3-4 million grid cells with a grid resolution of approximately a foot, and may be executed on a high performance workstation (dual processor, 6 GHz clock speed, 2 gigabytes RAM). Each simulation for a model this size would run for approximately 12 hours. To model a large site or city, use of a modified CFD code such as FEM3MP by LLNL is necessary. Use of FEM3MP, in turn, requires the use of an array of processors (100 processors) for simulation run times of less than 24 hours.

Real-Time Dispersion-Deposition-Causality Models are optimized for speed, and user friendliness, so users with differing technical backgrounds may implement them. However, accuracy may be improved. Dr. Bob Lee at LLNL states that FEM3MP CFD code has shown significant improved contaminant concentration predictions in the urban environment over both the HPAC and NARAC models. Additionally, some of its capabilities (such as the use of real-time weather data and human population databases) may not be required for design purposes. The Department of Defense currently lists HPAC as a preferred dispersion model.

Environmental regulatory models appear to be the most loosely defined group, with a large number of models used to predict contaminant dispersion. Models are based on a statistical Gaussian plume numerical engine similar to that used for HPAC and NARAC. The latest AERMOD release by EPA may be superior to HPAC or

NARAC, but because it has not been compared directly with these models its superiority is uncertain.

Multizone models clearly offer the advantage of being able to model an entire building much more quickly than CFD modeling. However, the shortcomings of multizone models (such as the assumption of a perfectly mixed zone) need to be addressed if greater accuracy is to be achieved. The latest research by LBNL is attempting to combine CFD and the multizone model COMIS to address this problem.

3 Review of External Dispersion Models

The characteristics of the current external models were studied by in depth review of two typical models; one for the real time dispersion-casualty program and the other for the CFD based high resolution program. The two programs selected for in depth review for external release modeling were FEM3MP (a specialized CFD program tailored external flow analysis), and HPAC (a real-time operational model used by emergency managers, warfighters, and scientists to limit the loss of life in actual chemical release scenarios). FEM3MP was selected for its availability in the public domain (i.e., it is not commercial software), and HPAC was selected for its preferred status within DOD.

FEM3MP is a sophisticated CFD-based model with high order turbulence modeling capabilities. It is not available to the general public and must be run on a parallel array computing platform at LLNL. It represents what can be done with CFD at the state-of-the-art level. The national laboratories do very limited consulting work, since they are not intended to compete with industry. To execute an external simulation of a building cluster, the approximate estimated cost would be $100,000.

HPAC is a tool produced by the Defense Threat Reduction Agency (DTRA) to be used by a wide range of users with limited scientific or engineering backgrounds. It is available free, but only to U.S. governmental employees on a case-by-case basis. HPAC has a dedicated technical support staff. HPAC is one of two programs that have been identified by the Department of Defense as a preferred dispersion model (Johnson-Winegar 2003).

Because neither of these programs is available to the general public, the following review is based on information available through literature search and general discussions with primary researchers.

3.1 FEM3MP Overview

LLNL has developed FEM3MP for simulating the transport and dispersion of chemical and biological agents in airflow around buildings. FEM3MP has been used to model various urban sites and downtown areas with hundreds of buildings. Models involving up to 10 million computational cells (grids) have been successfully executed. Validation studies have been conducted with field experiments, as well as with wind tunnel experiments.

A model includes separate sub-models that enable tracking of chemical and biological agents. The sub-models include:

- treatment of neutrally-buoyant and heavier-than-air gases
- aerosol physics including deposition
- surface heating
- tree canopy and vegetation
- ultraviolet degradation
- simple or Sophisticated turbulence models (e.g., nonlinear eddy viscosity, large eddy simulation models).

The program is based on CFD fundamentals, but employs a different approach to solving the Navier-Stokes equations. Rather than solving the coupled set of momentum and continuity equations, the model uses a segregated approach in which the continuity equation is replaced by a consistent Poisson equation. This method is computationally more efficient and enables the program to handle larger problems and higher order turbulence models. Additional efficiency is gained with a modified finite element technique to allow arbitrary grading of the grid mesh.

The program has four turbulence model options: three RANS turbulence models, and one Large Eddy Simulation (LES) model. The RANS models include a simple K-theory model, a two equation K-Epsilon model, and an advanced three-equation model that eliminates the need for wall functions. The LES model is a full transient simulation of turbulence, limited only by the scale of the computational grid (both time and space). However, a turbulence sub-model is still used with a LES model to calculate the effects of motions that cannot be resolved by the grid. Figure 1 shows predictions of a tracer gas release for a LES instantaneous, LES mean, and RANS model. For this example, the RANS simulation required approximately 25 hours (2-processor workstation, clock speed unknown), and the LES simulation required approximately 18 hours (64 parallel IBM processor platform). Thus, comparing these two simulation times, the LES calculation requires approximately an order of magnitude more simulation time than the RANS simulation.

FEM3MP has been compared to field and experimental measurements with good correlation. Figure 2 shows FEM3MP's airflow predictions for a building on the LLNL campus. Model results agreed well with the measured data: within 10 percent for wind directions, and within 15 percent for wind speeds. The model was also able to predict many other detailed flow features, such as the shedding of vortices from building corners and blockage effects from neighboring trees.

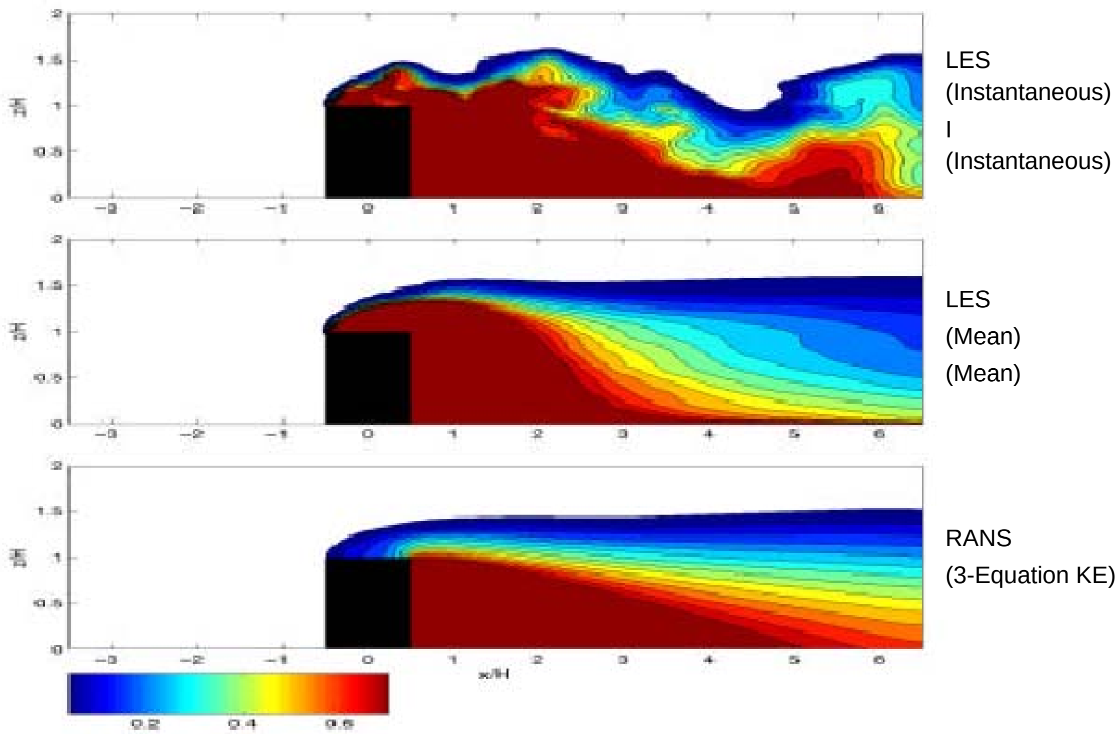

Figure 1. Tracer gas comparison between RANS (advanced KE) and LES turbulence models used in FEM3MP.

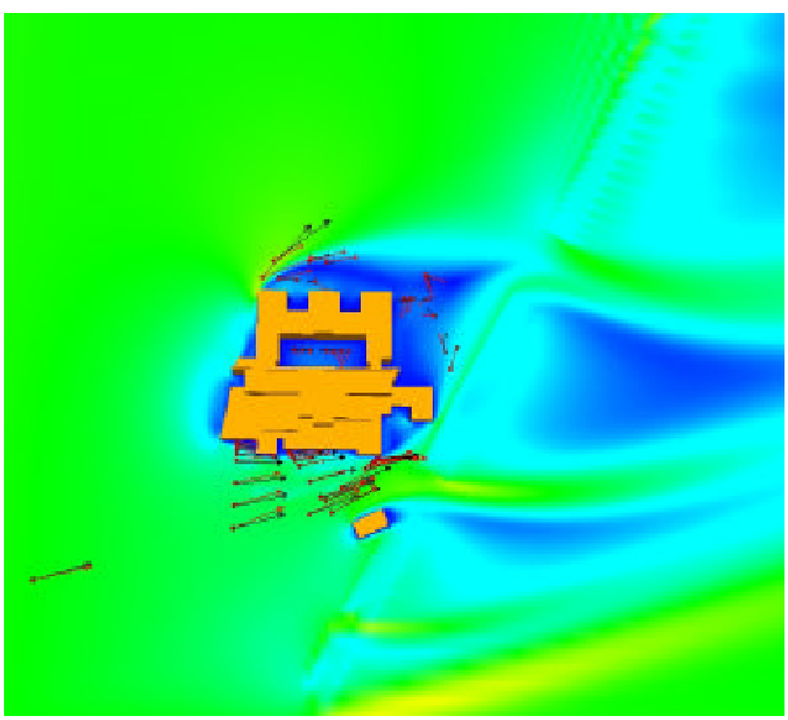

Figure 2. FEM3MP output -validation of wind patterns for an onsite building at LLN (source: Bob Lee, LLNL)

The Department of Energy's Chemical Biological National Security Program (CBNP) supported a field experiment campaign in Salt Lake City in which data were collected for atmospheric flow and dispersion of a tracer gas around the downtown area. FEM3MP was used to recommend locations for tracer gas release point and measurement locations.

Measurements taken during the release showed good correlation (within a factor of 5) with predictions if real-time wind information was used as a driving boundary condition (Chan 2003). Figure 3 shows an example of model results for the Salt Lake City analysis. A wind tunnel dispersion study performed with Los Alamos National Laboratory (LANL) provided additional validation. In this study, experiments focused on the modeling of flow and dispersion of releases within multiple block arrangements. Results were in good agreement using both the RANS and LES turbulence models.

3.2 HPAC Overview

HPAC software is designed to predict the dispersion of a hazardous material release into the atmosphere. It uses integrated source terms, high-resolution weather forecasts, and particulate transport algorithms to determine areas of high hazard, and to estimate collateral effects on population centers. The software was initially developed to assist warfighters in destroying targets containing weapons of mass destruction and responding to hazardous agent releases.

HPAC features as publicized include:

- ability to model nuclear, biological, chemical, radiological, and high explosive collateral effects resulting from conventional weapon strikes against enemy weapons of mass destruction (WMD) production and storage facilities
- prediction of downwind hazard areas resulting from a nuclear weapon strike or reactor accident, with the capability to model nuclear, chemical and biological weapon strikes or accidental releases
- easy user access to and real-time weather (observations) and forecast data by using a variety of DTRA-supported Meteorological Data Server systems
- user access to historical weather data for use when planning incidents beyond the normal time associated with credible weather forecast data
- 1-km terrain data and supporting wind-flow models that calculate the local wind field in the area of concern
- calculation of the areas of hazard impact and the degree of confidence of the prediction, based on weather uncertainty and turbulence effects on possible plume trajectories.

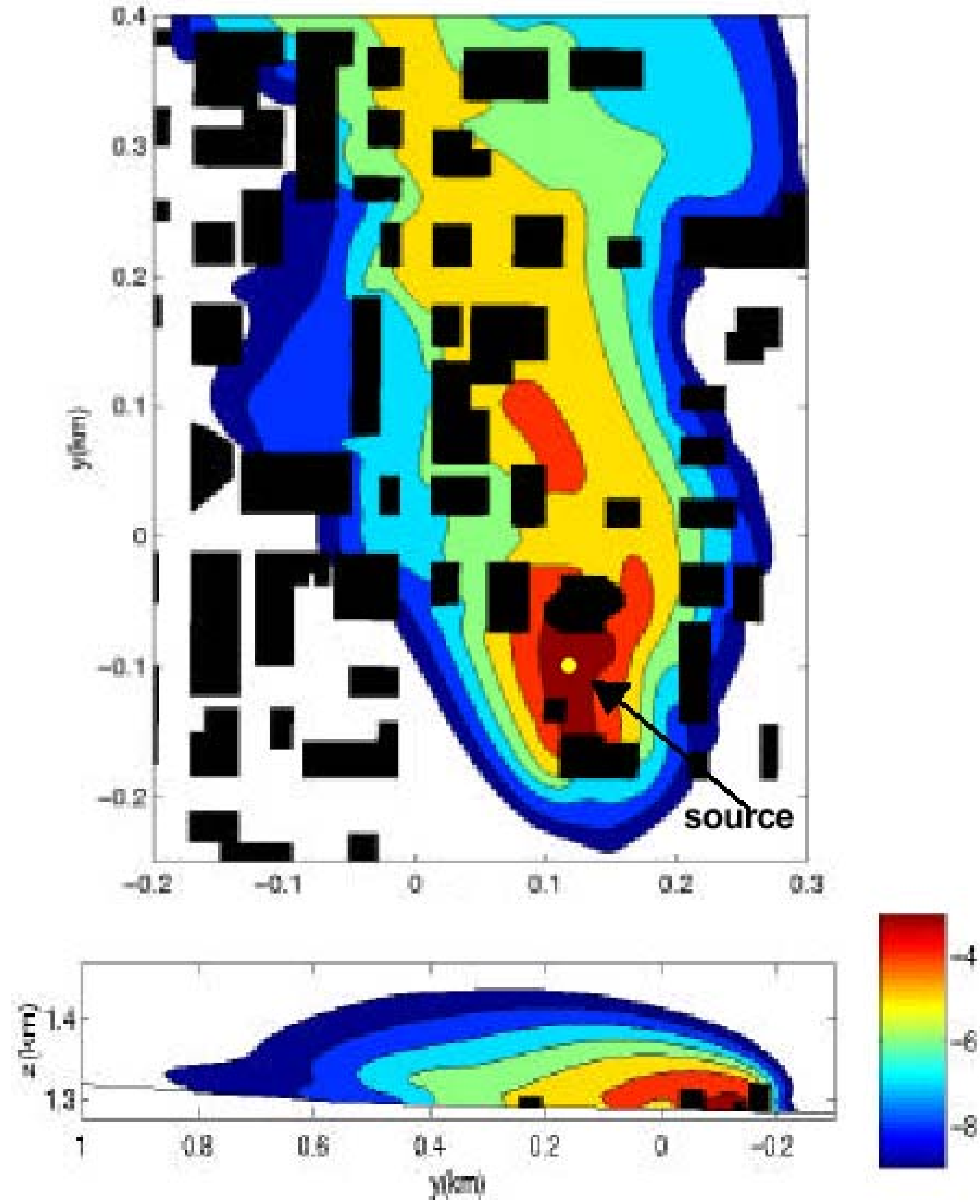

Figure 3. FEM3MP simulated patterns for a tracer gas release in Salt Lake City (source: Bob Lee, LLNL).

The mathematical basis of HPAC is statistical in nature. In simplistic terms, the program determines a probabilistic plume based on a statistical distribution, wind data, atmospheric stability, and source characterization. A brief mathematical description as described in Warner and Larson (2001) is:

> HPAC uses the Second-Order Closure Integrated Puff (SCIPUFF) model and an associated wind field model. SCIPUFF is a Lagrangian model for atmospheric dispersion that uses the Gaussian puff numerical method – an

> arbitrary time-dependent concentration field is represented by a superposition of three-dimensional Gaussian distributions. The downwind concentration is calculated from a turbulent diffusion parameterization based on second-order closure theory. This methodology provides a link between measurable wind-flow field velocity statistics and predicted dispersion rates. The second-order feature allows concentration variance to be estimated (in addition to mean concentration), and this uncertainty estimate can be used as the basis for probabilistic description of the dispersion prediction.

HPAC's predictions have been compared to those of NARAC (LLNL's Real-Time operational model) by comparing model predictions to measurements taken during the 1956 Prairie Grass field trials. Results from this comparison are detailed in the IDA Paper P-3554 (Warner & Bradley, January 2001). To compare the output of the two models, a two-dimensional graph is created for each field sample (termed the Measure of Effectiveness graph, or MOE graph). Each graph shows an area of predicted hazard, and an area of measured hazard. These two areas converge and typically create three regions: a region of overlap where model predictions match observations, a region of false positive, and a region of false negative. A perfect model has 100 percent overlap, and a poor model has 0 percent overlap. For all samples HPAC showed an overall overlap of 80 percent, 85 percent in the two axis of the graph, compared to NARAC which had a 94 percent, 62 percent overlap.

A study comparing quantitative differences between HPAC and a CFD model was not identified. Bob Lee, a researcher for LLNL who is involved with the development of FEM3MP, stated that CFD has shown significant accuracy improvements over the predictions of HPAC and NARAC. The reason is primarily due to CFD's ability to resolve details of the flow field, such as areas of recirculation and vortex shedding, which both result in very non-Gaussian concentration distributions. Users of the real-time operational models feel the increased accuracy of CFD models is not worth the extra computational time required. The extra computational time is estimated to be several orders of magnitude greater for a CFD analysis such as FEM3MP.

3.3 Discussion of External Dispersion Modeling

Both models have strong positive attributes, and similar shortcomings. Key observations include the following:

- FEM3MP is able to resolve transient flow details for large urban regions. Such details include non-Gaussian concentration gradients due to building aerodynamics including recirculation zones on rooftops, behind buildings, at the corner of buildings, etc. HPAC does not calculate the concentration gradients due to building aerodynamic effects.

- HPAC is fast and user friendly (based on the comments of HPAC support technicians). The use of FEM3MP is limited by the availability of researchers, computer resources, and computational time.
- FEM3MP is said to be more accurate by researchers involved in the development of the program. However, this statement has not been thoroughly documented with validation studies.
- HPAC is the model of choice for U.S. Military operations. This is due to its speed to obtain solution, and output that includes probabilities of the predictions. FEM3MP does not have probabilistic output; its accuracy must be judged by the user, based on the input assumptions.
- Both models are similarly affected by the assumptions of the meteorological conditions including the oncoming wind profile, atmospheric stability, and turbulent diffusion.

The two programs are quite different, and serve different purposes. HPAC is well suited for its mission of real-time predictions—it is fast and gives an idea of accuracy of results. On the other hand, FEM3MP is better suited for analytical studies. Solutions take much more time, but specific details of the flow field are revealed allowing design decisions to be made that may reduce an impact to a building due to a contaminant release. The accuracy of either program is difficult to validate. Past validation studies have primarily focused on qualitative comparisons, where the shape and direction of the plume is compared with observed plume shape and direction, rather than actual comparisons of measured and observed concentrations.

4 Review of Internal Dispersion Models

The two programs selected for a detailed review in modeling contamination movement within buildings are FLOVENT, a CFD program tailored for the built environment, and CONTAM, a multizone program commonly used in IAQ studies. FLOVENT is an excellent representation of a typical CFD program, and CONTAM is one of two multizone programs being used by industry. Both of these programs are available to the general public and a pool of experienced users, although small, does exist. FLOVENT is available for a cost (approximately $25,000 per year, which is similar for all CFD programs), while CONTAM is available free from the NIST website. Technical support is available for both programs.

4.1 CONTAM Overview

CONTAM is a multizone airflow and contaminant modeling software package developed by NIST. Its publicized capabilities include the following:

- It calculates airflow driven by infiltration, exfiltration, fans, wind pressures acting on the exterior of the building, and buoyancy effects induced by the indoor and outdoor air temperature difference.
- It calculates the movement of airborne contaminants. Considers the effects of airflow, chemical and radio-chemical transformation, adsorption and desorption to building materials, filtration, and deposition to building surfaces. Contaminants are generated by a variety of source mechanisms.
- It calculates personal exposure and provides assessment of risk to human health.
- It may be used to assess the adequacy of ventilation rates in a building, to determine the variation in ventilation rates over time and the distribution of ventilation air within a building, and to estimate the impact of envelope air tightening efforts on infiltration rates.
- It may be used to determine the indoor air quality performance of a building before construction, and to investigate the impacts of various design decisions related to ventilation system design and building material selection.

Numerous analytical mathematical relationships are used to calculate airflow and contaminant movement between the zones. Each mathematical relationship is based on simplifying assumptions.

The model uses the following assumptions:

- *Well-Mixed Zones*. Each zone is a single node. The air has uniform (well-mixed) conditions throughout including temperature, pressure, and contaminant concentrations.
- *Mass Conservation*. The mass of air within each zone is conserved by the model.
- *Airflow*. Airflow through the various small openings and cracks is modeled using either a power-law or quadratic relationship between airflow and pressure difference across the flow path. The program has a library of various coefficients from several sources. For example, the American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) source lists more than 100 different coefficients for different types of building components. Airflow through large openings is based on a separate model that allows for two-way flow, rather than the power-law or quadratic relationships, which are one-way flow relationships. Flow through ducts is based on Bernoulli's equation and various loss coefficients and friction factors. Fans may be included, and their performance may be based on the fan curves.
- *Thermal Effects*. Heat transfer is not included. However, to account for airflow between zones due to temperature variations, the zone temperature may be set. Zone temperatures can either be constant or can be allowed to change during transient simulations according to user-defined temperature schedules.
- *Contamination Source and Sink Models*. CONTAM provides several different elements for contaminant generation/removal processes. These models include the Constant Coefficient Model, Pressure Driven Model, Cutoff Concentration Model, Decaying Source Model, Boundary Layer Diffusion Controlled Model, and Burst Source Model.

4.2 FLOVENT Overview

FLOVENT uses CFD techniques to predict airflow, heat transfer, and contamination movement three-dimensionally within rooms and buildings. The effects of air density, viscosity, and turbulence are numerically represented through the fundamental equations of fluid flow. The result is a highly detailed and accurate picture of the air distribution, heat-transfer, and contaminant distribution in the modeled space. FLOVENT's advertised capabilities are:

- It provides full three-dimensional solutions to "Navier-Stokes" fluid flow and heat transfer equations.
- It uses the robust LVEL K-Epsilon Turbulence Model.

- It calculates steady-state or transient fluid behavior for laminar or turbulent flow conditions.
- It calculates natural, forced, or mixed-convection systems.
- It solves problems involving heat transfer within the air, within solid materials, or in both simultaneously (i.e., conjugate heat transfer).
- It allows for heat transfer by convection (within the air), conduction (within air or solid materials), and radiation (between surfaces of solid items).
- Trace contamination migration is calculated 3-dimensionaly. Contaminants must be in the gas phase, and density variations may be accounted for with the ideal gas law. Particles less than 10 microns are typically modeled as a gas phase contaminant meaning gravity effects are not included.
- It is possible to model five gas phase concentrations (e.g., humidity, chemical contamination, etc.) with various filtering mechanisms.
- It includes three-dimensional visualization and animation to facilitate communications and understanding of results.
- It provides built-in models, including fans, square diffusers, swirl diffusers, heat exchangers, and baffle plates, for more detailed modeling.
- It provides built-in calculation of industry-recognized IAQ measurements (i.e., Comfort temperature, Percent Mean Vote (PMV), Percent People Dissatisfied (PPD), Draft Temperature, and Local Mean Age of Air (LMA).
- It is capable of intelligent integration with solid modeling CAD systems, using file formats such as SAT, IGES and STL. The commonality between these file formats is that the geometry is described three dimensionally in an ASCI file format. AutoCAD is able to create a SAT, and STL a drawing file, and IGES is the geometry file for the solid modeling program Pro-E.
- It uses rectilinear grid for stable and fast computation times. Grid is automatically generated as the model is being created, and refined by user before simulation.

The mathematical basis of FLOVENT, and for CFD programs in general, is to solve the governing partial differential equations for fluid flow and heat transfer, with the addition of a suitable turbulence model. As stated previously, these equations cannot be solved analytically. Therefore the CFD approach is to transform the differential equations into a set of discrete algebraic equations and then solve the algebraic equations by an iterative procedure. The numerical methods behind the solution to these equations are well-established and can be studied in detail in most Fluid Mechanics textbooks (Patankar 1980).

For all CFD models, it is necessary to create a solution grid or mesh. The grid is composed of small discrete volumes that collectively make up the entire volume of the model. FLOVENT uses a rectilinear grid that is automatically created as the model is being built. As objects are placed within the solution volume grid lines are created from the boundaries of the object. The end result after all the model geometry is input is a coarse grid. At this point the user adds additional grid to achieve the resolution desired. (Other CFD programs, such as Fluent, have similar automatic grid generation capabilities. In addition to rectilinear grid Fluent also has the ability to create grid of different shapes to conform to curved shapes. Using a grid shape other than rectilinear results in an extra partial differential equation and thus increases solution time.) FLOVENT does not accept grid generated by a generic grid generation program.

For the representation of turbulence within the fluid, it is necessary to estimate or evaluate values of turbulent viscosity (and turbulent conductivity in the case of thermal analysis) with a turbulence model. To completely model turbulent flow with the fundamental equations (i.e., not use a turbulence model), it would be necessary to use a time step and physical dimension (cell size) small enough to capture all turbulent fluctuations at the smallest scales. Even with today's computing power, this is an impossible task for practical problems. Therefore, to overcome these limitations, variables are split into a mean and fluctuating component. These are then substituted back into the instantaneous equations, producing what is known as time averaged equations. The additional terms are referred to as the Reynolds stresses in the momentum equations, or Reynolds flux in the case of the thermal equation. The introduction of these additional terms into the fundamental equations results in an open set of equations (more unknowns than equations), and thus some form of closure is required to model these stresses. The closure equations required are known as turbulence models (often as a Reynolds-averaged-Navier-Stokes [RANS] turbulence model).

Many turbulence models have been developed, ranging from simple zero-equation models to the much more complex Reynolds stress transport equations. FLOVENT uses what is referred to as an LVEL K-Epsilon turbulence model. The LVEL uses the distance from the nearest wall (L), the local velocity (VEL), kinetic energy of turbulence (K), and its rate of dissipation (Epsilon). FLOVENT developers state "that this model has been tried and tested for a whole range of engineering applications. It is simple, but more importantly, it is stable. Only two extra differential equations are introduced and the convergence process is less prone to divergence than other, higher order turbulence models." Comparisons with experimental results are available for the following cases, "Bernard Convection in a Rectangular Cavity," "Fire Modeling Validation Report," "Laminar and Turbulent Flow and Heat Transfer between Parallel Surfaces," and "Natural Convection in a Closed Cavity." In all of these cases, FLOVENT predictions closely correlate with the experimental results.

4.3 Internal Dispersion Modeling

To further investigate these programs, a test model was created in each software package to compare CFD (FLOVENT) and multizone (CONTAM) models. Using a simple test model allows for the comparison of the fundamental assumptions required to build the model, the input time, the execution time, and results comparison.

The simple model consisted of the following assumptions common to both models:

- Single story office (100 m^2 plan area, 3 m high).
- Mix of open office space (75 m^2), private office (25 m^2).
- Common air handling unit (1,140 scfm total supply/ 240 scfm outside air).
- Ambient air – temperature 20 °C, no wind.
- Internal air – 20 °C all zones, thermally neutral with ambient air.
- Contamination was assumed to be carbon dioxide (CO_2), present as a trace contaminant. Ambient concentration was 350 parts per million (ppm), and internal generation was from 12 people, each generating 8.9e-6 kilograms per second (kg/s) for a total generation rate of 1.068e-4 kg/s of CO_2.
- Air was ducted to multiple supply registers (160 scfm x 2 private offices, 200 scfm x 2 + 140 x 3 for the open offices).
- Return air was brought back to the central air handler through three ceiling return grills located in the open office area, and then through a return air plenum located above the dropped ceiling.
- Office was positively pressurized, and thus there is no infiltration of ambient air.

In general, the total time for information gathering, and input, will vary depending on the user's experience. However, information gathering is thought to take a similar amount of time for either program. Typical information required to create a model might include building geometry specifics, mechanical air handling system operation, filtration, building leakage areas, zone temperatures, and characterization of contaminant and heat sources. If information gathering is approximately the same, then input times may be directly compared.

Input time for CONTAM was approximately 2 hours, while input time for FLOVENT was approximately 10 hours. Execution time (on a 4 Ghz computer) for CONTAM was less than 1 second, while execution time for FLOVENT on the same computer was approximately 3 hours. (Note the times quoted are based on an experienced user for both programs.)

Other Model Parameters included the following:

- CONTAM: 22 airflow leakage paths, six duct paths, two contaminant sources
- FLOVENT: 421,200 grid cells, average size 15cm x 15cm, smallest size 0.5 cm x 0.5 cm, LVEL K-E turbulence model.

Figures 4 through 10 show the input and output screens for both models. As expected, the CFD analysis gives a detailed picture of the airflow and contaminant movement throughout the model, whereas CONTAM only provides two reference points of contamination concentration. In this case the FLOVENT model identifies areas of high concentration that are not apparent in CONTAM. The extra information provided by the FLOVENT model requires a total time investment of approximately six times that necessary for the CONTAM model.

4.4 Comparison of FLOVENT and CONTAM Models

The model comparison indicated that both programs have advantages and disadvantages. Key observations included the following:

- The FLOVENT model clearly provides more detailed information. This additional information allows for characterization of concentration gradients in three dimensions within each zone. CONTAM zone level solutions are limited due to its "well-mixed" assumption.
- The CONTAM model has been tailored to account for various airflow paths (including leakage rates) through various building assemblies, and thus the program can link neighboring zones. FLOVENT can account for leakage, but the relationships are not readily accessible within the program. This results in additional time to create FLOVENT models, and in some cases, can complicate solution convergence.
- A clear advantage of CONTAM is its ability to simulate numerous transient effects that may affect contaminant migration, such as occupants coming and going, air handlers turning off and on, wind direction and magnitude changes, and varying contamination sources. Transient effects such as these are nearly impossible to account for in FLOVENT and other CFD packages, because of the computation time required.
- FLOVENT is superior in the presentation of results. The graphic three-dimensional images facilitate interpretation and understanding by the modeler, the project team, and decisionmakers. CONTAM output is largely numerical; additional time must be spent to interpret and present the results.
- CONTAM is capable of handling larger, more complicated buildings because of the reduced amount of the time required to set up and execute CONTAM models.

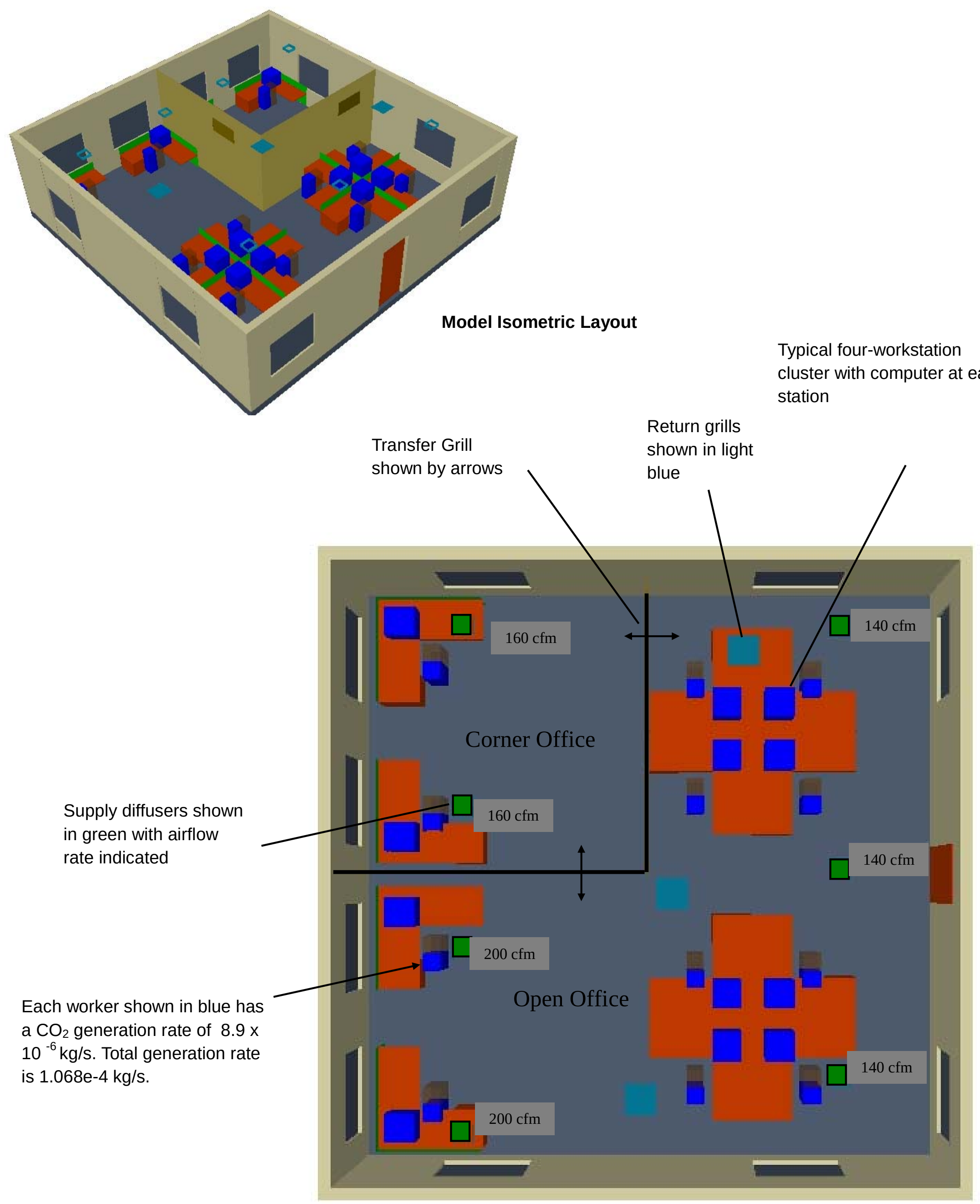

Figure 4. FLOVENT model plan layout.

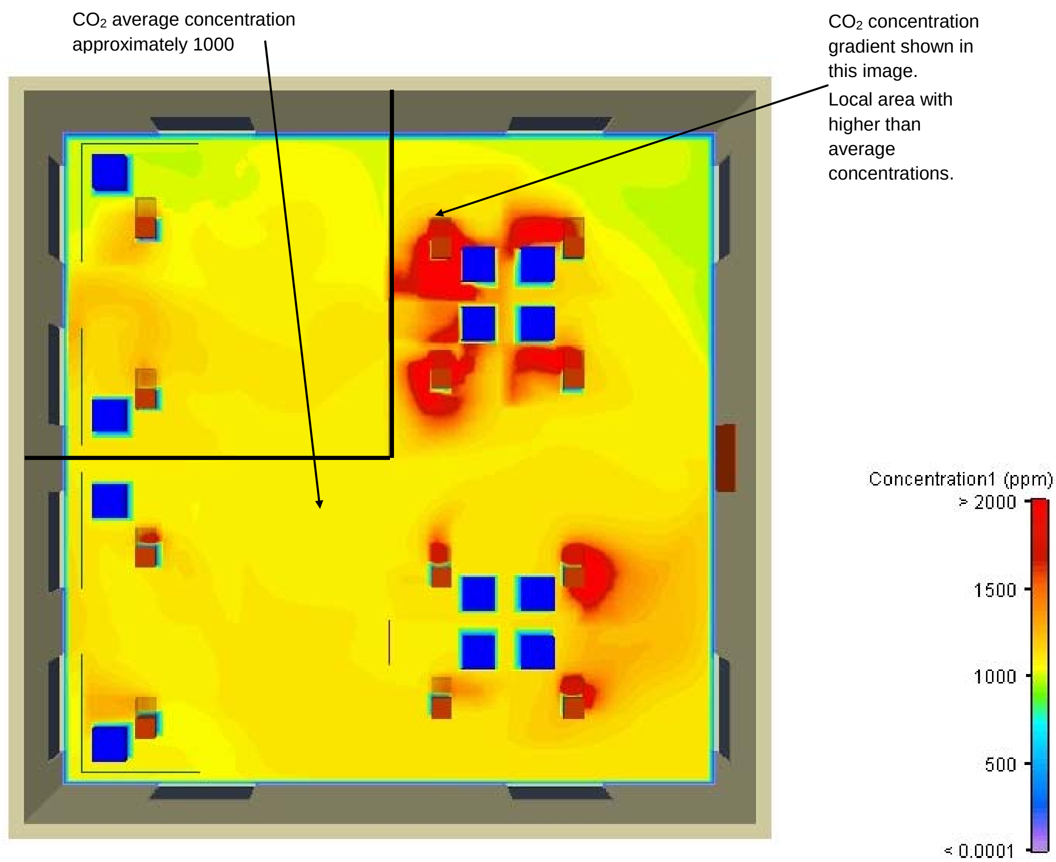

Figure 5. FLOVENT CO_2 concentration distribution.

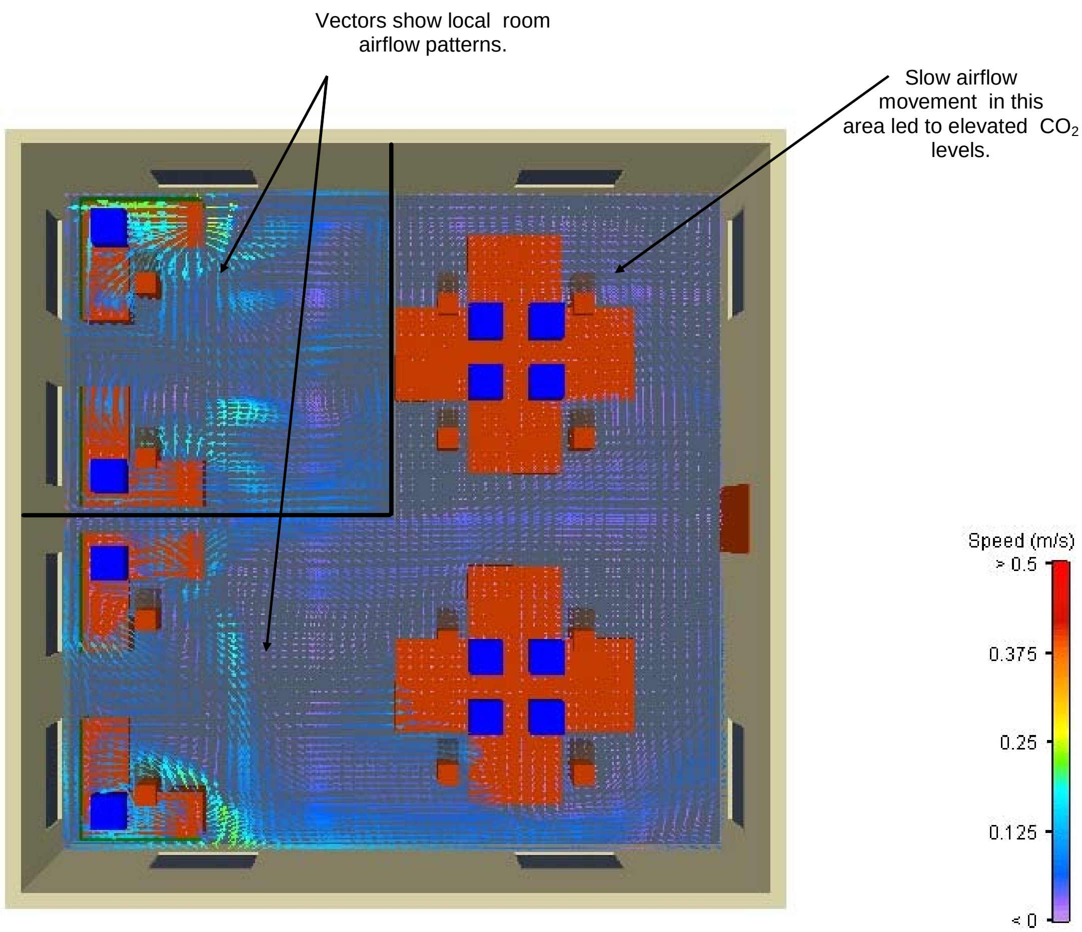

Figure 6. Vector section at 1m above floor.

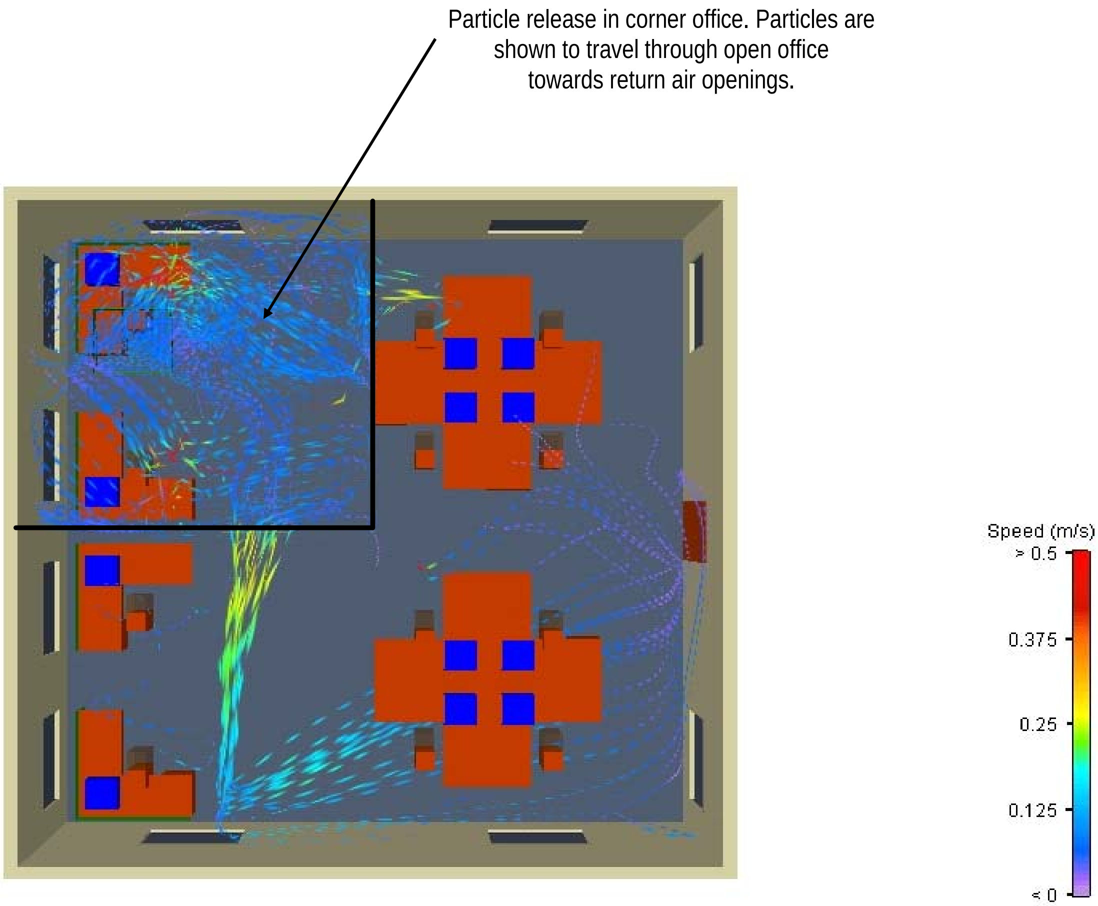

Figure 7. Particle tracking.

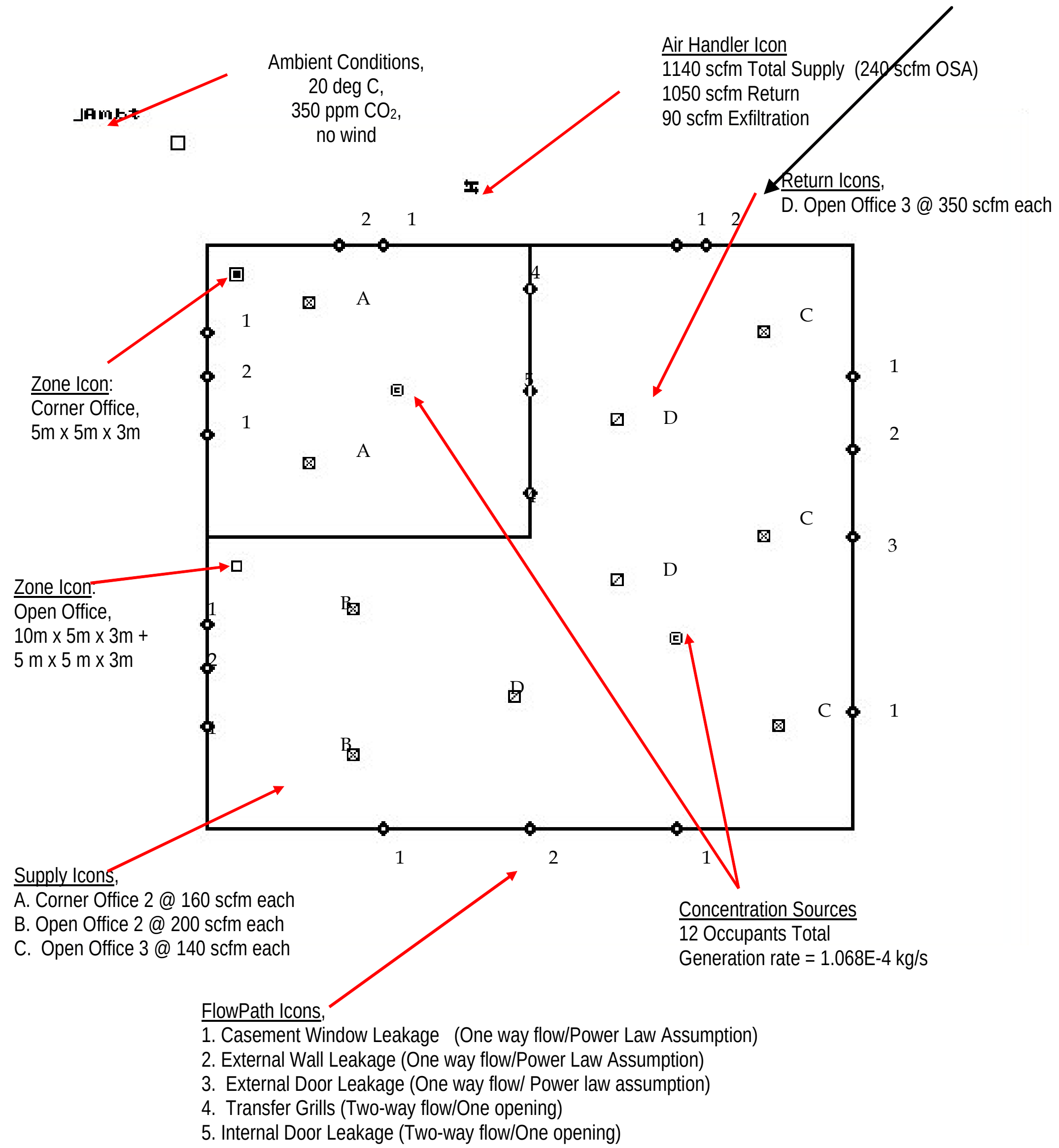

Figure 8. CONTAM input screen.

Colored lines indicate flow quantity and direction from each flow path. This diagram indicates a positively pressurized building with flow outwards from all zones.

CO₂ Conc in Open Space is 871 ppm

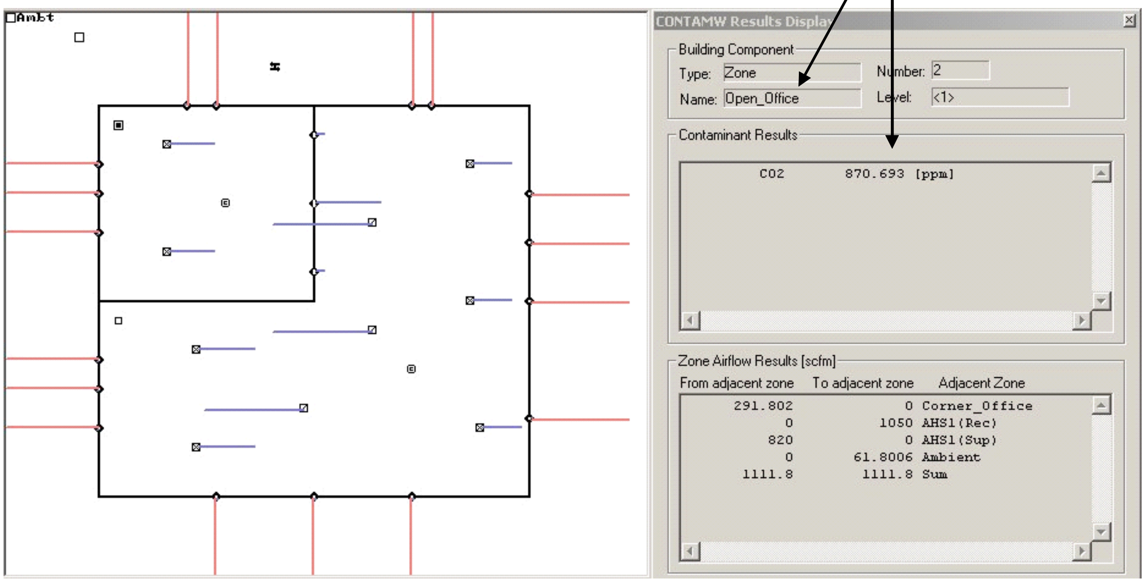

Figure 9. CONTAM output screen showing CO_2 in open space.

CO₂ concentration in Corner Office is 826 ppm

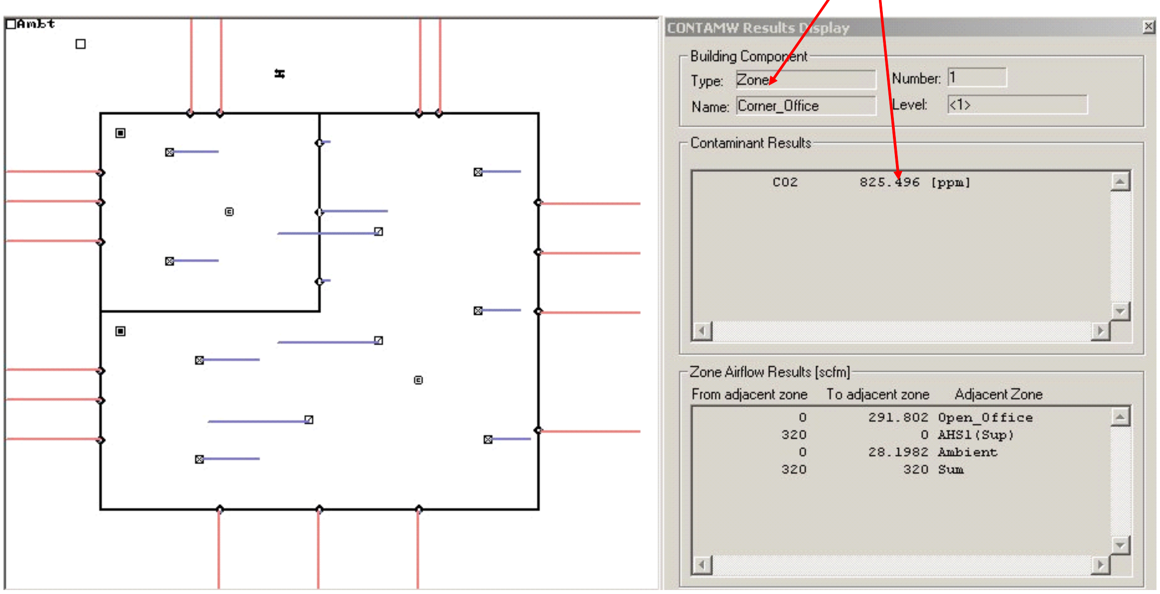

Figure 10. CONTAM output screen showing CO_2 in corner office.

The accuracy of these models depends primarily on two factors: the mathematical basis, and the simplification of the problem being modeled. In CONTAM, the most questionable simplifying assumption is using well-mixed zones. Multizone model users have noted that this is a crude assumption, and much research has been conducted on how to improve it. Using "zonal" models is one approach, in which the zones are subdivided into additional zones for greater resolution. However, even an extremely coarse CFD model using a standard KE turbulence model has been shown to predict airflow much more accurately than a zonal model (Mora et al. 2003).

Many of the other mathematical relationships that make up CONTAM are fairly basic in nature, meaning that an analytical solution is attainable and may be compared against experimental data. Complexity arises from of the sheer number of different ways to model the various components of a building system. For example, a single zone may have a window leakage relationship, a wall leakage relationship, floor leakage, duct leakage, two-way flow through a doorway, and contaminant sources and sinks. The validity of results with such a large number of assumptions is questionable. A CFD model used for a multizone analysis would be able to eliminate some of the assumptions by actually modeling the geometry (large openings for instance), but its use would also require similar assumption about envelope leakage.

To achieve accurate results, CFD modelers are primarily concerned with the simplifying assumptions that make up a model. An incorrect assumption may have a dramatic effect on results, often much greater than numerical error or differences in turbulence models. For instance, using an incorrect diffuser type, or specifying the wrong location for a return, will change the flow patterns within a zone to a larger extent than would changing the turbulence model.

However, turbulence modeling is the subject of much research. The uncertainty of modeling turbulence is apparent from the many turbulence models available. In most cases, the higher order turbulence models attempt to improve on the quantitative predictions for specific flow regimes; qualitative results remain similar between most turbulence models. This means that a CFD model user may use a simple turbulence model and still attain meaningful results. When using CFD for design purposes, this is an important point because often the model is used to identify elements that result in change, and not necessarily to predict variables exactly. A combination of CFD and Multizone Modeling would eliminate many of the current disadvantages of the standalone programs, resulting in a very useful program to further the understanding of CBR building protection design. Current research is under way to do this at LBNL (COMIS).

5 Summary, Conclusions, and Recommendations

5.1 Summary

This work has reviewed simulation software for prediction of dispersion of chem/bio agents in and around buildings. Four different numerical modeling technologies that may be used in protection of building against chem/bio threats were reviewed. The modeling technologies include CFD models, real-time operational models, regulatory models, and multizone models. Four selected software packages, two each for internal release and external release, were studied further in detail.

For modeling airflow and contamination movement within buildings (i.e., internal release) a typical CFD program (Flovent by Flomerics), and a multizone model (CONTAM by NIST) were selected for further review. Each software contributes in different ways to the overall understanding of contaminant migration through a building. Using one or the other may lead to incomplete conclusions depending on the question at hand. The CFD model provides fine details about the airflow and contamination movement within the individual zones of a building, whereas the multizone model assumes that each zone is well mixed and does not resolve airflow details.

The multizone model provides details about the air transfer between physically separated zones, and contaminant migration due to the numerous transient influences within a building. For instance, a multizone model may account for numerous transient effects that may affect contaminant migration, such as occupants coming and going, air handlers turning off and on, wind direction and magnitude changes, and varying contamination sources. On the other hand, the CFD model is limited to steady state conditions, or simple transient cases due to limitation in the computational resource, and generally does not consider physically separated zones.

The mathematical basis behind both models is fairly robust. This leads to the simplifying assumptions as being the most important factor influencing the accuracy of results. For cases with well-defined boundary conditions, both models correlate well with field observations. Current research is ongoing by LBNL to incorporate CFD within the multizone model COMIS. Another bold approach would be CFD simulation of a whole building without the multizone model as a tool for calculation of mass transfer between the zones. It is an interesting approach that takes advantage of the massive computational resources residing in DoD. Extensive computational resources and modeling requirements of realistic boundary conditions are expected to be outstanding challenges in this approach.

For modeling airflow and contamination movement external to buildings (i.e., external release), a high resolution CFD model (FEM3MP by LLNL), and real-time operational model (HAPC) were selected for further review. It was determined that the CFD model provided details about the flow field, which ultimately results in non-Gaussian plume distributions. This information may be used in design regarding decisions such as building orientation, shape, and air handler location. However, it is very time intensive to obtain these details. It is estimated that a FEM3MP analysis would take several orders of magnitude longer than a similar analysis using HPAC. HPAC has the advantages of being a low cost, fast, user-friendly option to predict general contaminant movement. It is well suited for the purpose of a fast prediction of the impacts of an emergency event, i.e., for the first-responders. However, its benefit to building design is questionable due to its inability to account for the aerodynamic effects of the urban environment. Like internal modeling, the accuracy of results for external airflow modeling is also highly dependent on the simplifying assumptions. The validation studies mainly concentrate on the comparison of qualitative details such as plume shape (presence or non-presence of a contaminant) and do not provide a direct comparison of measured concentrations.

5.2 Conclusions

The models reviewed in this report are the most advanced numerical tools available to predict contaminant migration in and around buildings. Each of the different modeling technologies will lead to useful results if applied to the appropriate problem with correct assumptions, i.e., indoor air quality application, regulatory pollution control, first-responder real-time application, or accurate calculation of contaminant concentration in a room. Thus, to achieve a useful result the model must be matched to the question at hand, and the critical assumptions must be well understood.

For the protection of building HVAC system against internal release of chem/bio agents inside a building, the following information is useful to protect people inside the building or for design of a chem/bio protection system as a part of the building system:

1. Quick detection of the contaminant and quick determination of a safe egression path.
2. The impact of HVAC system shutdown on the dispersion of released contaminants, i.e., dispersion due to transient pressure distribution inside a building and dispersion due to free convection.
3. Whether there is any better control of an HVAC system than the emergency shut down, e.g., de-pressurization of the source room and pressurization of the rest of the building.
4. If so, the simulation logic that should be built in the HVAC system and controller.
5. The impact of filtration and de-contamination systems on the HVAC design and operation.
6. Sensor location, detection level, and response time.
7. Real time specs for control of protection hardware (e.g., damper, actuator, emergency exhaust fan, etc.).
8. The exposure time for the occupants based on their location within the building, and the current building air handling system configuration.

The current CFD model (e.g., FEM3MP and Flovent), or the multizone model (e.g., CONTAM) may be able to address some of these issues. however, none of the software reviewed was adequate to address all these concerns accurately. Therefore, a suite of programs is necessary for proper modeling of airflow in and around buildings.

Probably the most important point, which is common to all of the models, is the consideration of the modeling assumptions. Poorly formed assumptions may lead to incorrect results even with the most mathematically sophisticated model. All of the various models reviewed have been validated against experimental results with good correlation. The validations are usually based on problems with well-defined boundary conditions. Inaccuracies in model predictions are typically generated as the problem complexity is increased and number of assumptions grows. Real life design problems are rarely simple, and numerous assumptions must be made. Making the right assumptions to arrive at the essence of a problem is the art of modeling, and is just as important if not more important, than the numerical accuracy of the model itself.

5.3 Recommendations

A combination of programs will be necessary to address all the design questions relating to CBR building protection. In the future, programs such as CFD and multizone modeling or CFD modeling of a whole building may combine to offer a single, consolidated solution, but at the present moment it is necessary to use the programs independently.

Models must be chosen for the problem at hand. Therefore, the models listed below are recommended in conjunction with the conditions given. For external modeling:

- FEM3MP should be used for detailed studies of external releases in large urban environments with complex airflow patterns. The project or study must have ample room in the design schedule, and a large modeling budget (>$100,000). This model should not be used in building designs with tight design schedules.
- HPAC should be used for studies of external release in large rural or urban environments when details of the airflow are not necessarily required.
- CFD (Airpak, Flovent, or similar) should be used to model external releases in small building clusters, or on a campus.

For internal modeling:

- CONTAM should be used for studies involving contamination movement throughout a whole building, taking into account transient effects. Because of the numerous conditions and assumptions possible, a detailed description must be made of the modeling approach.
- CFD (Airpak, Flovent, or similar) should be used to define the flow and contamination characteristics in large open spaces, and to specify HVAC system components such as supply register type and location. It should be used in cases where a three-dimensional contamination gradient is required.
- CFD whole-building simulation is not currently available; this capability needs further development to fill the gaps in the current multizone and CFD models. CFD models require substantial computational resources and will not be able to run in "real-time." CFD models, however, will be used as a valuable analytical tool that is required to generate realistic modeling information to be used in the real-time simulation tools for the first responders.

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Terms and Abbreviations

Term	Definition
Aerosol	Solid and liquid airborne particles, typically ranging in size from 0.001 to 100 microns
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc.
ERDC-CERL	U.S. Army Engineer Research and Development Center, Construction Engineering Research Laboratory
CFD	Computational Fluid Dynamics
cfm	Cubic feet per minute, a measure of volumetric rate
Chem/Bio	Chemical and Biological
CONTAM	A multizone airflow contaminant modeling software
fpm	feet per minute, a measure of velocity
FLOVENT	A CFD-based software for three dimensionally modeling airflow, heat transfer, and contaminant movement
GSA	General Services Administration
HPAC	Hazard Prediction and Assessment Capability
HVAC	Heating, Ventilating, and Air-Conditioning
IAQ	Indoor Air Quality
LES	Large Eddy Simulation turbulence model
Mass transfer zone	Adsorbent bed depth required to reduce the chemical vapor challenge to the breakthrough concentration
m^3/min	Cubic meters per minute, a measure of volumetric rate
NARAC	National Atmospheric Release Advisory Center
ppm	Parts per million
RANS	Reynolds-averaged-Navier-Stokes turbulence model
SOW	Statement Of Work
USACE	U.S. Army Corps of Engineers

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14. ABSTRACT

This project reviewed existing technologies that could protect the supply air systems of buildings from chemical/biological (chem/bio) contaminants. This research: (1) analyzed existing filtration technologies for building heating, ventilating, and air-conditioning (HVAC) systems, and (2) examined numerical models for predicting air flows in and around buildings during a release of chemical or biological agents. This report gives the results of the research into numerical models.

Researchers identified modeling products that would depict the results of a chem/bio release, and rated the models on resolution, cost, convenience, and accuracy. Four models were examined in depth, two for external and two for internal releases. The results provide a modeling approach that can be used to simulate the dispersion of contaminants inside buildings. Such a numerical simulation will help designers and managers evaluate possible ways to reduce occupant exposures to chem/bio contaminants.

15. SUBJECT TERMS

simulation modeling	HVAC	military installations
chem/bio agents	toxic chemicals	terrorism

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