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DEVELOPMENT OF HYBRID MODEL FOR ASSESSING CONCENTRATIONS OF TOXIC EFFLUENT AT AIR FORCE INSTALLATIONS

DR. R.L. PETERSEN, NORIAKI HOSOYA

CERMAK PETERKA PETERSEN, INC.
1415 BLUE SPRUCE DRIVE
FORT COLLINS CO 80524

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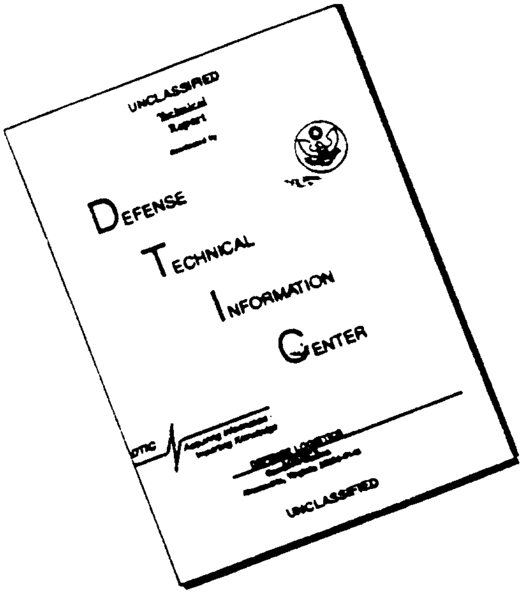

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R.L. Petersen, Ph.d., CCM, and Noriaki Hosoya

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Cermak Peterka Petersen, Inc.
1415 Blue Spruce Drive
Fort Collins CO 80524

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The main purpose of this evaluation was to develop a hybrid modeling approach to toxic vapor diffusion modeling in the vicinity of buildings or structures which influence plume behavior. The hybrid approach combines the use of physical (wind-tunnel) and computer modeling in order to improve the site-specific performance of gaussian puff and box-type hazard response models by accounting for pollutant trapping, redirection, and dispersion enhancement caused by the presence of structures. The documented project included reviewing the capability of wind-tunnel modeling to simulate nearfield dispersion, conducting wind-tunnel tests for a sample Air Force base environment, assessing limitations of the current AFTOX and SLAB models for treating dispersion in the vicinity of obstacles, development of a sample hybrid model, and suggesting a methodology for generalized application of hybrid modeling at any Air Force installation.

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PREFACE

This report was prepared by Cermak Peterka Peterson, Inc., 1415 Blue Spruce Drive, Fort Collins, Colorado 80524, under the Small Business Innovative Research (SBIR) Phase I program, Contract Number F08635-90-C-0392, for the Air Force Civil Engineering Support Agency, Civil Engineering Laboratory (AFCESA/RAVS), Tyndall Air Force Base, Florida 32403.

This report summarizes work done between May 1990 and February 1991. AFCESA/RAVS project officer was Major Michael Moss.

Because this is an SBIR report, it is being published in the same format in which it was submitted.

This report has been reviewed by the Public Affairs (PA) Office and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

Mike Moss
MICHAEL T. MOSS, Maj, USAF
Chief, Environmental Compliance R&D

Neil J. Lamb
NEIL J. LAMB, Col, USAF, BSC
Chief, Environics Division

Frank P. Gallagher III
FRANK P. GALLAGHER III, Colonel, USAF
Director, Air Force Civil Engineering
Laboratory

EXECUTIVE SUMMARY

A. Objective

The primary objective of this project was to assess the feasibility of improving the Air Force capability to manage potential air quality-related emergencies from releases at space or missile bases, or routine airbases. The scope of this effort would include dense and non-dense gas releases, and exposures to onbase and nearby communities.

The current models that are available to the Air Force are not compatible with the data needed to effectively implement the Air Force two-tier emergency response procedures that are used to manage high risk operations at selected bases. The major complication is that airbases differ from the idealized surfaces that serve as the basis for existing models. Structures at airbases modify ambient concentration fields, and provide alternative environments that need to be assessed to allow commanders to have a basis to make the critical decision to evacuate or shelter-in-place individuals at risk.

The specific technical objectives that formed the basis for the Phase I feasibility assessment of this problem are as follows:

1. To assess the relative significance of building effects versus overall modeling uncertainty.
2. To assess the feasibility of producing a practical model to account for building effects for non-dense and dense gas releases.
3. To ensure that model estimates developed through this project "failsafe", i.e. to minimize the potential to underestimate concentrations.

B. BACKGROUND

The U.S. Air Force routinely handles hazardous materials at space and missile bases, and to a lesser extent at typical airbases. These activities cannot be avoided because they are a necessary part of the Air Force mission, but there is a need to effectively manage environmental risks, risks that may arise from equipment failure, human error, or sabotage. The potential release of toxic vapors from these chemicals creates a health and safety threat to onbase personnel, and the general population in adjacent areas. The hazards can be associated with toxicity, flammability or explosivity. The Air Force has a good record of managing these risks. There is an incentive, however, to determine if the limitations of existing air quality models could be enhanced to improve emergency response capability for future operations. The vapor clouds can be released as dense or non-dense gas clouds. The focus of this report is on dense gas releases because of: (1) the potential for greater risks, and (2) the more limited research in this area.

Effective risk management relies heavily on the availability of sound technical information. Operations commanders need practical models to project potential impacts in a planning mode, and to respond to actual emergencies on a real-time basis. The Air Force has developed a two-tier emergency response procedure for selected bases, which is used to manage potential environmental emergencies. Current methods are available to estimate air quality impacts, but existing models do not consider the effect of structures on dispersion, nor indoor-outdoor differences in concentration (1,2,3,4,5,6). These are limitations that substantially reduce the effectiveness of existing models to meet the need for data to implement the Air Force emergency response procedures. Commanders need more realistic data to make informed decisions to evacuate or shelter-in-place affected on-base personnel, and the general population in the vicinity of a base.

C. SCOPE

The scope of the Phase I review included the following major tasks:

- Summarized recent accident history and potential accident scenarios at airbases, and the existing capability to respond to air quality emergencies.
- Evaluated the need to add building effects to an existing dispersion model.
- Presented a conceptual approach to include building influences on the ambient concentration field.
- Described how an existing dispersion model, SLAB, was selected as the basic model to be adapted for this study. Recommendations are shown for strengthening SLAB to meet the "failsafe" objective of this project.
- Recommended techniques to estimate indoor concentrations as a function of building type / service openings, meteorological conditions, and duration of release.
- Evaluated the feasibility of a visible interactive override option.
- A flowchart of major model features was developed as a guide to Phase II development.

- A full-scale field program option was summarized, which could be used in the future to test key "failsafe" features of the ambient and indoor model components.

D. METHODOLOGY

The following summarizes the methods used for the Phase I feasibility assessment:

Selection of Dispersion Model - We needed to select a preferred dispersion model that could be adapted to meet the needs of this project. The review was limited to models in the public domain. The SLAB, DEGADIS, ADAM and AFTOX models were considered, with the review focused on the following considerations:

1. Optimal model would be suitable for dense and non-dense gas releases.
2. Sought model with good documentation.
3. Smooth transitions from dense to non-dense gas characteristics was sought..
4. Readily adaptable to model modifications needed for project.

Failsafe Dispersion Model Review - For this project, the term "failsafe" is defined as follows . . "minimizing the potential to underestimate predicted concentration because of uncertainties in the model, while maintaining reasonable size hazard corridors. The intent is to balance the need to safely manage risk while avoiding impractical conservatism that unnecessarily disrupts mission-related activities, such as refueling operations, space launches, weapon testing, and so forth. Each component of the selected dispersion model, SLAB, was evaluated to identify limitations that would need to be adapted to meet the objective of meeting airbase modeling needs. The failsafe analysis focused on treatments that could underestimate concentrations because of site-specific factors and treatments that could systematically overestimate risks because of excessive conservatism.

Indoor Air Quality Modeling - Two additional models are needed to estimate indoor air quality as a function of ambient concentrations and building characteristics: (1) an infiltration model, and (2) a model to estimate indoor air quality. We reviewed infiltration models ranging from data intensive models to empirical models that can be used based on limited infiltration measurements. As part of this review, we also summarized available measured infiltration data, including non-residential (office buildings), residential, and aircraft hangars. Three indoor air quality models were reviewed to determine which model could be best adapted for this project: CONTAM, INDOOR, and MCCEM. These models are all in the public domain. The review focused on identifying the model that best represents the higher end of the state-of-the-art, and is best structured to serve as a submodule of this modeling system.

Development of Software for Modeling System - The approach was to design a system that would advance the state-of-the-art of emergency response management by having the following features:

- Failsafe model development.
- Ambient and indoor concentration estimates.
- Building effects.
- Egress analysis.
- Expert system features.
- means of tracking implementation of response actions, e.g. status of evacuation/sheltering, power status, etc.

E. TEST DESCRIPTION

The evaluation of alternative dispersion models, infiltration models, and indoor air quality models was based on review of available documents and some sensitivity testing. The failsafe review of SLAB was done by evaluating references of the model and extensive testing of the model aimed at isolating individual model components. This included executing SLAB for wide ranges of input conditions, and inserting WRITE statements into the code to display intermediate computations.

F. RESULTS

Figure 21 of the report (see Page 82) summarizes the modeling system. SLAB was selected as the preferred dispersion model, and CONTAM was selected as the most appropriate indoor air quality model for this study. Our findings also showed that limited field measurements, in conjunction with empirical modeling approaches, would best support the infiltration component of the study. The most significant findings can be listed as follows:

- The entrainment term in SLAB, which specifies that rate of cloud growth, was found to be overly sensitive to surface roughness, which would be an important issue for airbases. We identified a refinement to minimize the limitations to overcome this limitation. The emission term was identified as a potential area where the potential to unnecessarily extend the size of hazard corridors could be reduced by incorporating an emission modeling term into the model. A range of other, more minor issues, were identified that in a composite sense could adversely affect the failsafe goals of this project. Recommendations were provided to refine each term.

- The Air Force approach of using Short-Term Public Exposure Guidance Levels (SPEGLs), adjusted to 30-minute exposures, for all durations of emergency exposure may result in excessive hazard corridors for pollutants that have time dependent exposures. In some cases, with exposure greater than 30-minutes, the current approach may not afford adequate protection to health.

- A modeling system could be developed that would meet the needs for data at all bases, including bases that are covered by the two-tiered hazard corridor approach. A centralized management tool is needed, of which air quality modeling would serve as a supportive component, but not the end product. The goal of the system should be to provide expert system features to guide decisions, rather than to simply display concentration data. While there is no substitute for intelligent decisions made by an onscene commander, there is a benefit in terms of efficiency of actions and adherence to pre-established, preferred response procedures to recommend optimal response procedures based on model output.

CONCLUSIONS

The results of Phase I indicate that it would be feasible to develop an emergency modeling system that would effectively implement emergency response procedures, which currently are not met through existing modeling procedures. The development of the system proposed through the Phase I research would represent a major improvement in the state-of-the-art of emergency response modeling, which would produce benefits to other military applications (e.g. defense against chemical warfare against civilian or military targets), and improving industrial emergency response preparedness.

RECOMMENDATIONS

The next logical step in model development would be to develop a prototype model, and install the model at a base that handles a high volume of hazardous materials, such as Cape Canaveral. This would demonstrate the practicality of the system to Air Force and other interested agencies / industries that may participate in future funding of model development. As part of this outreach, a training workshop should be conducted at Cape Canaveral to train Air Force personnel, and other interested participants, and to obtain feedback on improving the system. After the prototype is tailored to best meet Air Force needs, the modeling system could then be installed at other bases selected by the Air Force. Detailed installation procedures could be used for high priority bases, such as Vandenburg and Edwards, with a more streamlined procedure for more routine installations. A centralized response system could be considered for non-priority bases, and as a back-up for priority base capabilities. As a subsequent effort, the Air Force could consider additional co-funded research to further enhance model development, such as a full-scale field test at a base undergoing decommissioning to demonstrate ambient concentrations, infiltration and indoor air quality.

Table of Contents

LIST OF FIGURES

LIST OF TABLES

GLOSSARY OF TERMS

ACH - Air changes per hour.

ADAM (Air Force Dispersion Assessment Model) - Dense gas dispersion model developed by the U.S. Environmental Protection Agency.

AFTOX (Air Force Toxic Chemical Dispersion Model)- Passive gas puff dispersion model developed by the U.S. Air Force.

Centerline Concentration - The maximum concentration in the center of a plume or cloud.

Code - Computer Program.

CONTAM - Indoor air quality model developed by the National Institute for Standards and Technology.

Dense Gas - A chemical cloud that is denser than ambient air because of high molecular weight, aerosol loading, and/or cold temperatures relative to the ambient air.

Dispersion Model - A computer program that uses meteorological data and source characteristics to estimate air pollutant concentrations.

Displacement Length - A term used in turbulence theory to account for the modification to the logarithmic wind profile by densely packed obstacles, such as a forest canopy or crops.

Entrainment - Vertical or horizontal entrainment refers to the mixing of ambient air into a pollutant cloud or plume.

Exfiltration - Outflow of air from a building interior to the ambient air.

F_B - Fraction of pollutant filtered by a building envelope and air cleaning equipment associated with an HVAC system.

Failsafe - The goal of minimizing the potential of a modeling system to underestimate concentrations.

Gravity Spreading - Increase in horizontal dimension of a cloud caused by slumping of a dense gas.

Far-Field - Distances relatively far from the point of release (e.g. > 1,000 m).

Hypergolic Fuels - Liquid fuels that ignite spontaneously upon mixing together.

IDLH - Concentration that is immediately dangerous (level) for health, based on 30-minute exposures.

INDOOR - Indoor air quality model developed by the U.S. Environmental Protection Agency.

Infiltration - Influx of ambient air into a building.

1/L (Scaling Length) - This term is approximately the inverse of the height where buoyant energy production equals wind shear energy production. Scaling length is used to indicate the stability of the atmosphere. If 1/L is zero, stability is neutral. For unstable conditions, 1/L is negative, and for stable conditions it is positive. In the ambient air, 1/L is independent of height in the surface layer.

MCCEM - Indoor air quality model developed by the U.S. Environmental Protection Agency.

Meander (Plume Meander) - The increase in cloud width caused by the wider range of turbulence scales that affect cloud horizontal spread as averaging time increases.

Mid-Field - For the purposes of this study, mid-field refers to distances in the range of 100 to 1000 m.

Mixing Height - The distance from the surface to the height where vertical growth is restricted.

Monin-Obukhov Scaling Theory - A technique to parametize the effects of surface roughness and atmospheric stability on profiles of wind speed, ambient temperature, and other parameters.

Near-Field - Distances relatively close to the source, e.g. distances < 100 m.

Obstacle - In this report, obstacle refers to buildings or other structures that are present at airbases.

One-Dimensional Model - A model where concentration is a function of downwind distance or time. Concentrations are not directly computed as a function of three-dimensional location relative to the center of the cloud.

PCBs - Polychlorinated biphenyls.

Service Opening Status - Status of windows, doors, and hangar doors in the open or closed position.

Shelter-In-Place - A decision made by an operations commander to order individuals to remain in structures within Tier I or Tier II hazard corridors because evacuation would be expected to produce higher exposures and risks.

SLAB - A dense gas dispersion model developed by Lawrence Livermore National Laboratory.

SPEGL (Short-Term Public Exposure Guidance Level) - A concentration threshold set to avoid irreversible health impairment if escape occurs within a 30 minute period.

Stability - Stability indicates the type and degree of turbulent mixing in the atmosphere. Neutral stability (moderate mixing) is dominated by mechanical turbulence. Stable conditions (suppressed mixing) results in mechanical turbulence being damped by the stable stratification. Unstable conditions (vigorous mixing) are mainly produced by buoyancy-induced turbulence, i.e. convective turbulence.

Surface Roughness - A term used to help characterize the influence of a surface on mechanical turbulence. Values range from approximately 0.01 cm for a calm water surface to 200-300 cm for the central business district of a major metropolitan area. Technically, surface roughness is the height at which the logarithmic wind profile goes to zero.

Tier I / High Hazard Corridor - In certain Air Force emergency response procedures, Tier I corridors are defined as one-half the concentration that is the immediately dangerous level for health (IDLH), plus a 50 percent safety margin.

Tier II / Low Hazard Corridor - Tier II corridors are defined similar to Tier I, but based on Short-Term Public Exposure Guidance Levels (SPEGLs).

v - Air exchange rate for a building.

Section I

INTRODUCTION

The U.S. Air Force routinely handles hazardous materials at space and missile bases, and to a lesser extent at typical airbases. These activities cannot be avoided because they are a necessary part of the Air Force mission, but there is a need to effectively manage environmental risks, risks that may arise from equipment failure, human error, or sabotage. The potential release of toxic vapors from these chemicals creates a health and safety threat to onbase personnel, and the general population in adjacent areas. The hazards can be associated with toxicity, flammability or explosivity. The Air Force has a good record of managing these risks. There is an incentive, however, to determine if the limitations of existing air quality models could be enhanced to improve emergency response capability for future operations. The vapor clouds can be released as dense or non-dense gas clouds. The focus of this report is on dense gas releases because of: (1) the potential for greater risks, and (2) the more limited research in this area.

Effective risk management relies heavily on the availability of sound technical information. Operations commanders need practical models to project potential impacts in a planning mode, and to respond to actual emergencies on a real-time basis. The Air Force has developed a two-tier emergency response procedure for selected bases, which is used to manage potential environmental emergencies. Current methods are available to estimate air quality impacts, but existing models do not consider the effect of structures on dispersion, nor indoor-outdoor differences in concentration (1,2,3,4,5,6). These are limitations that substantially reduce the effectiveness of existing models to meet the need for data to implement the Air Force emergency response procedures. Commanders need more realistic data to make informed decisions to evacuate or shelter-in-place affected on-base personnel, and the general population in the vicinity of a base.

There are three major objectives that guided this project:

1. To assess the relative significance of building effects versus overall modeling uncertainty.
2. To assess the feasibility of producing a practical model to account for building effects for non-dense and dense gas releases.

3. To ensure that model estimates developed through this project "failsafe", i.e. to minimize the potential to underestimate concentrations.

The U.S Air Force has supported previous research directed towards improving modeling tools for dense gas release scenarios. The following are the most relevant recent Air Force funded research in this area.

- SLAB (1,2)
- ADAM (5)
- Field studies (7)

Refer to Section II.C for descriptions of the models.

Model development for dense gas releases has focused on improving the general state-of-the-art. These efforts have set a foundation on which to develop modeling techniques needed to implement the Air Force emergency response procedures, procedures that need to be applicable to realistic airbase settings. Several important questions need to be resolved, however, before a model could be developed to directly meet Air Force emergency response data needs:

- How do typical airbase structures alter the basic assumptions of turbulence theory used in existing models?
- How do typical airbase structures modify the ambient concentration field?
- How do indoor concentrations differ from ambient concentrations as a function of structure type / service opening status, meteorological conditions, and duration of release.

This report explores these issues, and provides recommendations that could lead to prototype model development in Phase II, and subsequent full-scale confirmation.

The remainder of the report is organized as follows:

- <u>Section II</u> - Summarizes recent accident history and potential accident scenarios at airbases, and the existing capability to respond to air quality emergencies.
- <u>Section III</u> - Evaluates the need to add building effects to an existing dispersion model.
- <u>Section IV</u> - Presents a conceptual approach to include

building influences on the ambient concentration field.

- <u>Section V</u> - Describes how an existing dispersion model, SLAB, was selected as the basic model to be adapted for this study. Recommendations are shown for strengthening SLAB to meet the "failsafe" objective of this project.
- <u>Section VI</u> - Presents recommended techniques to estimate indoor concentrations as a function of building type / service openings, meteorological conditions, and duration of release.
- <u>Section VII</u> - The feasibility of a visible interactive override option is described.
- <u>Section VIII</u> - A flowchart of major model features is presented as a guide to Phase II development.
- <u>Section IX</u> - A full-scale field program option is presented, which could be used to test key "failsafe" features of the ambient and indoor model components.

If the objectives of this project are met, several major benefits could be realized. The focus of model development would be to meet the specific needs of Air Force emergency response procedures, not simply to develop a general purpose air quality model. An effective modeling system would need to meet a wide range of Air Force needs, including those of space and missile bases and typical airbases. The design would need to consider, however, the different levels of available data, and allow for suitable default data for bases that have less serious potential incidents. But, the model features would have general application for other military services, agencies and industry because the influence of structures on dense and passive gas ambient concentrations will be considered in realistic settings. Also, outdoor/indoor concentration estimates could be provided to support practical decisions to shelter-in-place or evacuate affected individuals, decisions that now need to be made by commanders and emergency response coordinators, without adequate guidance.

Model design will need to strike the proper balance between the need for confidence, i.e. to minimize the potential to underestimate risk (not best fit), and the need for reasonable size hazard zones. A best fit model would likely underestimate risks half the time, but what is needed is the outer envelope of expected concentrations. This approach is more consistent with the safety objectives of managing an air quality emergency. It was developed from the philosophy that an emergency response coordinator is more concerned with safety, and avoiding unnecessary delays in launch, fueling and weapon test operations, than the elegance of minimizing model bias.

Section II

CURRENT STATUS

The first step of model development is to clearly identify the specific needs for information. No model is optimal for all scenarios, therefore it is important to identify a primary focus. Three steps were taken to ensure that model development would be consistent with the Air Force need for data. First, air quality incidents that occurred at airbases during the past three years were reviewed and summarized, and potential worst-case Air Force accident scenarios were developed. Second, the current emergency response procedures were reviewed to determine the critical needs for data. Third, the availability and quality of input data to serve the emergency response models were evaluated. Each of these issues is addressed in this section.

A. AIR POLLUTION INCIDENTS

including hypergolic fuels, jet fuel, solvents, and inorganic gases (e.g. chlorine). Hypergolic fuels likely pose the most severe accident scenarios. The most recent three years of Air Force Pollution Incident Reports, the period of January 1988 through July 1990, were reviewed to determine the most common problems. Table 1 summarizes the results of this review. It is not clear that all incidents are reported as Pollution Incident Reports, but it would seem likely that all major incidents would be documented. Fifty-eight air quality related incidents were reported during this period. Of the 58 incidents, 26 were jet fuel spills, which is not surprising considering the large volume of jet fuels handled by the Air Force. Ten of the incidents involved PCB spills, which likely had a minor impact on air quality. The 12 releases of chlorine/solvents likely represent the most toxic materials released during this period. Releases internal to building are out of the scope of the present effort, but are a source term that could be added to the indoor component. Of the 58 releases reviewed, at least 8 were released indoors, where confined volumes could produce substantially elevated concentrations.

What can be concluded from the recent Air Force history? Perhaps the most important observation is that there were no reports of serious injuries or deaths attributed to air quality impacts at any airbase during this period. Storage tank failures

TABLE 1. SPILL DATA.

	Median Gallons	Maximum Gallons	# Releases
Jet Fuel	750	86,000	26
Hydrazine	NA	25	2
PCBs	5	27	10
Solvents	55	500	8
Chlorine	45 lbs	75 lbs	4
Misc.	NA	16,800	8

and operator errors during fuel transfers were the most common cause of emissions. Air Force experience is not unlike industry, where EPA has shown that a large majority of air quality accidental releases are from the storage of chemicals (8).

The recent history of actual incidents obviously is not an indication of the potential for severe accidents. A significant potential appears to exist for serious air pollution incidents because of the large size of storage tanks that contain hazardous materials. For example, a 160,000 gallon methylene chloride tank had a partial loss at Eglin airbase in 1989. A 1,000,000 gallon jet fuel tank had a partial loss at Homestead airbase in 1990. What would be the risks from toxicity, flammability or explosion hazard of a catastrophic tank failure? The record shows that, based on recent history, that the risks from hypergolic fuels clearly are not the only potential serious hazard at airbases.

No major dense gas releases were reported during this period, but the most significant potential accident would appear to involve the hypergolic fuels used at Cape Canaveral, Vandenberg, and Edwards airbases. While such accidents may be less likely than for other chemicals, there are potentially more serious health consequences for base personnel, and the offsite public. Section III presents an accident scenario involving hypergolic fuels at

Cape Canaveral. High ambient impacts were shown relative to Tier I and II guideline levels.

The review of the actual and potential air quality incidents at airbases points to the need for comprehensive modeling capability, tailored to airbase conditions that can effectively address both hypergolic fuel scenarios and the more routine accident scenarios for airbases.

B. EMERGENCY RESPONSE PROCEDURES AT AIRBASES

The degree of planning for potential emergency responses appears to have been developed to best meet the specific mission of an airbase. Typical bases have less need for sophisticated response capabilities, and therefore, appear to have less detailed emergency response plans in place. On the other hand, bases that handle large quantities of acutely hazardous chemicals require, and appear to have, more involved emergency response procedures. The most critical data needs for emergency response planning are at bases that use hypergolic fuels. This will be the focus of this section.

Certain Air Force emergency response procedures for hypergolic fuels define two-tier toxic corridors:

1. Tier I / High Hazard Corridor

A Tier I (high hazard corridor) is defined as one-half the concentration that is "immediately dangerous to life or health" (IDLH), which is adjusted to a 30-minute exposure, plus a 50 percent safety margin. Health effects experienced at concentrations below these thresholds should be reversible. Access within Tier I corridors is limited to mission-essential personnel. Personnel present in this zone have: (1) pre-assigned escape routes, (2) escape air or access to self-contained buildings, and (3) direct contact with the operations commander.

2. Tier II / Low Hazard Corridor

Tier II (low hazard corridors) are defined based on Short Term Public Exposure Guidance Levels (SPEGL), which are adjusted to 30 minute exposures. SPEGL's are established by the National Academy of Sciences to specify concentrations that are acceptable for unpredicted, single, short-term emergency exposures of the general public. SPEGL's are set to take into account a wide range of sensitivity of the general public, including children, individuals with dehabilitating diseases, and pregnant women.

There is some risk in the Tier II corridor, but it is less than Tier I. Procedures call for initially assigning Tier II areas based on worst case spill scenarios, such as complete loss of fuel during refueling operations, and then to recompute the low hazard corridor by identifying areas above the SPEGL for lesser spills. This approach is consistent with the need for quick guidance to initialize priority response actions, followed by refinement as the event unfolds. Response actions would be similar to Tier I (shelter-in-place or evacuate). In Tier II, the decision to evacuate or shelter-in-place would be more difficult because individuals would be more exposed to ambient influences because they would be unlikely to have self-contained air or be able to seek shelter in a self-contained structure.

The Tier I and II emergency response procedures appear to represent an effective risk management plan. The weakest link in the system, however, appears to be the lack of firm, scientific data to guide the critical decision to shelter-in-place or evacuate. What is the basis to decide whether affected personnel and the general public should be sheltered-in-place or evacuated? And if sheltered, when should personnel be evacuated after cloud passage?

The overall responsibility to implement the two-tier approach is delegated to the operations commander. This individual needs to make critical decisions within minutes of release, but the shelter or evacuate decision is difficult because indoor air quality is a function of building type, service opening status, meteorological conditions, and duration of release. Such decisions cannot be made effectively without adequate technical support. But, currently there is no systematic way to guide operations commander to make these critical decisions. While there is considerable uncertainty in such assessments, the operations commander should have the benefit of practical guidance that considers the state-of-the-art in ambient and indoor air quality modeling. More specifically, a modeling capability is needed that is conservative for the ambient concentration field, but minimizes bias between the ambient and indoor microenvironments. Such an approach is essential to provide the basis for a balanced decision to evacuate or shelter-in-place. This appears to be a significant limitation of the current Air Force emergency response procedures.

Estimating ambient and indoor concentrations, though, is only part of the information needed to support evacuation or shelter-in-place decisions. There also is an obvious need to consider integrated doses during egress from affected structures. If a modeling system could summarize the best available information on ambient and indoor concentrations, and could compare doses between egress evacuation routes and the shelter-in-place option, there could be an adequate basis to implement the Air Force emergency response procedures. Ingress-egress dose methodologies have long been used for nuclear energy contingency plans, and similar exposure techniques are needed to effectively implement the Air Force emergency response procedures. There is a need to consider assumed egress paths, speed of travel through indoor and ambient microenvironments, and estimate an integrated dose to show total exposures for shelter-in-place versus evacuation alternatives.

There appears to be one other weakness in the emergency response procedures that should be addressed. The Tier I and II hazard corridors are defined, and decisions to evacuate or shelter-in-place appear to be based on toxicity. In some cases, however, buildings in the near-field could be subject to explosivity or flammability hazards, which could affect the decision to evacuate or shelter-in-place. Guidance is needed to systematically support operations commanders need for information by considering maximum instantaneous core cloud concentrations relative to the lower limit for flammability or explosion. This feature is especially important considering the historical nature of air quality emergencies, i.e. injuries are usually related to toxicity, while deaths are generally caused by fire or explosions (8).

C. CURRENTLY AVAILABLE DISPERSION MODELS

A fundamental decision was made at the beginning of this project to adapt an existing model to meet the needs of this project, rather than to develop a new model "from scratch". This approach is cost-effective, and best builds on past Air Force funded work. The goal was to first identify a dispersion model that could best represent the ambient concentration field, without structures. Then the existing components were reviewed to assess the need to strengthen specific components, as necessary, to meet the "failsafe" objectives of this project. After these steps are completed, a conservative treatment of building alterations to the ambient concentration field, and an indoor component could be added to the strengthened model.

The scope of this study was limited to the review of public domain dispersion models. Only one-dimensional models were considered because the extended time required to execute three-dimensional models is inconsistent with the need for real-time data. While three-dimensional models likely are impractical for real-time emergency response, there could be a place for three-dimensional modeling and wind tunnel analysis to help parametize building influences on the ambient concentration field. Section IV(B) provides greater detail on the potential use of three-dimensional models for this project. The remainder of this section is devoted to one-dimensional models, which could serve as the operational model.

The following alternative models were reviewed:

SLAB - SLAB is a one-dimensional model that was developed by Lawrence Livermore National Laboratory. The program solves a set of coupled differential equations to estimate cloud height and widths as a function of downwind distance (continuous release mode) or travel time (puff mode). Volume average concentrations are, therefore, computed as a function of distance or time. SLAB is quasi three-dimensional because after the solution of the coupled differential equations, horizontal and vertical distributions of concentration are assumed. On this basis, concentrations can be estimated as a function of position relative to the centerline of the cloud. SLAB was designed to avoid separate solutions for the dense and non-dense gas phases, which promotes smooth transitions. The model can be run for four release types: (1) evaporating pool, (2) horizontal jet, (3) vertical jet or stack, or (4) instantaneous or short duration evaporating pool. SLAB can account for phase changes of pollutants between liquid and vapor states, and water liquid and vapor states. It cannot, however, consider pollutant reactions that can affect species and the buoyancy term in the model. SLAB considers the enhanced wind direction meander along the horizontal axis as a function of averaging time. Emission rates are input by the user, and cannot be computed within the code as a function of chemical properties, ambient and surface temperature, surface roughness, and meteorological parameters.

DEGADIS - Similar to SLAB, DEGADIS is a one-dimensional dense gas model with quasi three-dimensional features. This model can be run in a spill or vertical jet mode, considering instantaneous or continuous release. One of the most significant differences between DEGADIS and SLAB is that DEGADIS uses different equations for the dense and passive gas stages. This introduces the potential for model artifacts at the transition points. Similar to SLAB, DEGADIS can address phase changes for the pollutant and water, but also does not model reactions. Wind direction meander is modeled as a function of averaging time and Pasquill Gifford stability class. The emission term in DEGADIS also is simplified, and is not computed as a function of pollutant, surface and meteorological conditions. A review of the documentation for DEGADIS indicated that the modification of the existing code would be more difficult than for SLAB.

ADAM - At the time of this writing ADAM is still under development. This model also is a one-dimensional dense gas model with quasi three-dimensional features. The transitions between the dense gas and passive gas stages appear to be similar to DEGADIS. There are two enhanced features in ADAM, however, that are not available in other models. ADAM can model the effect of reactions on species changes and cloud buoyancy, and also can compute emission rates as a function of chemical, surface and meteorological conditions. As described in Section V(F), the reactivity feature is not considered essential for this study. The source term feature of ADAM, however, could strengthen the proposed modeling system, and should be reassessed in Phase II. Refer to Section V(E) for further details. The overall conclusion based on this review was that ADAM appeared to have more refined chemistry and source terms than SLAB, while SLAB appeared to have more desirable physical treatments. In balance, the structure of SLAB appears to be better suited for adaptation to this study.

AFTOX - AFTOX is an emergency response, puff model developed by the Air Force. AFTOX considers surface roughness influences on dispersion, and calculates dispersion coefficients based on continuous, rather than discrete stability classes. It was not reviewed in detail for this study because it lacked the essential feature of being able to model both dense and passive gas dispersion.

Table 2 summarizes the key features of these models.

TABLE 2. KEY FEATURES OF REVIEWED MODELS

"*" = contains feature

FEATURE	SLAB	DEGADIS	ADAM	AFTOX
Dense Gas Treatment	*	*	*	
Passive Gas Treatment	*	*	*	*
Quasi-Three Dimensional	*	*	*	NA
Reactions			*	
Phase Changes	*	*	*	
Smooth Transitions	*			NA
Readily Adaptable Code	*			
Emission Algorithm			*	
Building Downwash				
Indoor Concentrations				

"NA" = not applicable

SLAB was selected as the preferred model to adapt to this study because it best meets the desired model features for this study. The key features that resulted in the selection of SLAB are as follows:

- Most suitable for dense gas and non-dense gas scenarios.
- Relatively smooth transitions from dense to passive cloud.
- Code structure adaptable to modifications to be needed.

There were three desired features that are not met by SLAB: (1) building downwash influences, (2) indoor component, and (3) reactivity term. The remaining sections of this report indicate how the first two features would be added to SLAB. How important is the reactivity term? The initial conclusion is that it is not essential to add reactivity at this time. Refer to Section V.F for further information on reactivity.

D. AVAILABLE INPUT DATA TO SUPPORT RESPONSE ACTIONS

There are two major categories of data that are needed as input to a modeling system: (1) source characteristics, and (2) meteorological conditions. The focus of this section is on meteorological data. The storage and transfer of fuels and solvents is likely to be well documented. The maximum release will be available based on storage vessel capacities. When installing the modeling system at an airbase, the locations of potential release points would be identified and updated as necessary. Furthermore, the presence of nearby structures, which would be needed to account for building effects and any visual checkpoints, could be coded by wind direction when installing the modeling system for a specific airbase. These inputs are readily available, and simply would need to be accurately entered into the modeling system. Meteorological input data, on the other hand, appear to be the weaker link.

Meteorological data is critical to the successful application of any dispersion model, but especially for an emergency response model because it:

- Defines the direction of flow, and therefore, the hazard zones.
- Defines the speed of travel, and critical times for response actions.
- Characterizes spreading rates, which are critical to estimates of concentration.
- Temperature and relative humidity help define the buoyancy terms in the model.

There are some important questions to consider. What is the present coverage of meteorological parameters at airbases? How adequate are the specifications for the meteorological monitoring hardware? How suitable is the quality control of the meteorological monitoring systems? How adequate is the data recording system that will provide input to the real-time emergency response modeling system? These questions are critical to model development. Modeling is a combination of good quality input data and sound physical model treatments. A "failsafe" modeling system is highly dependent on the adequacy of input data. Data inputs cannot be ignored when designing the modeling strategy, if the objectives of the study are to be met. A sophisticated model with poor quality meteorological data is misleading, and worse yet, can lead to a false sense of security.

In this section, three key issues are presented, which involve the interface between the meteorological monitoring system and the emergency response modeling system: (1) parameter coverage / accuracy, (2) quality control, and (3) data recording medium.

1. Parameter Coverage / Accuracy

A typical airbase measures wind speed, wind direction, ambient temperature, and dew point temperature generally at a monitoring height of approximately 4-5 m. The phase-in of hot-wire anemometers at airbases (GMQ-20 upgrade), should provide suitable wind speed data to support an emergency response modeling system. The temperature and dewpoint temperature monitoring instrumentation are also in the process of upgrade to the FMQ-8 system, and appear to be adequate hardware relative to the sensitivity of the dispersion models to these parameters. Performance standards are shown in Table 3 for the upgraded systems:

TABLE 3. SPECIFICATIONS FOR METEOROLOGICAL PARAMETERS

Parameter	Instrument Accuracy
Wind Speed	+/- 1 knot
Wind Direction	+/- 3 degrees
Temperature	+/- 1F
Dewpoint Temperature	+/- 2F

A potential "failsafe" problem arises from the range in dispersion characteristics that can occur within a Pasquill Gifford stability class (9,10). For airbases that handle large quantities of acutely hazardous chemicals, there would be a clear benefit to augmenting the planned coverage to include matched delta temperature sensors (such as a 20-2 m separation). The delta temperature data, which are relatively easy to measure, would support the computation of bulk Richardson number. The theoretical relationship between gradient Richardson number and bulk Richardson number is well established (11). The gradient Richardson number could then be related to the Monin-Obukhov scaling length, which is used in SLAB to estimate entrainment rates. This upgrade is highly recommended for airbases that handle relatively large volumes of hazardous chemicals. Cape Canaveral, Edwards, and Vandenberg airbases already have delta temperature sensors (16-2 m) in place that could be used for this purpose. Similar systems also could be installed to enhance the confidence in the modeling system at selected bases that handle relatively large volumes of hazardous chemicals. Refer to Section V(G) for a recommended modification for relative humidity monitoring at high priority airbases.

2. Quality Control

There likely would be a benefit in terms of model performance that would result from an improvement in the quality control / quality assurance of the meteorological monitoring systems at Air Force bases[1]. Consistent calibration procedures, improved oversight and improved preventive maintenance all are important factors to support the effective use of the proposed emergency modeling system. Maintaining an effective meteorological monitoring system is an ongoing process that needs the following steps to adequately support the Air Force need for data to support emergency response modeling, and likely routine airbase operations:

- Sound and well documented siting criteria.
- Weekly data review by meteorologists.
- Timely repair of equipment malfunctions, with a goal of 90 percent or higher data recovery.
- Quarterly system calibration.
- Independent annual audit.

Ongoing and effective oversight of the meteorological monitoring system could minimize modeling errors that could result from unrepresentative meteorological data, such as:

- Errors in direction of hazard corridor.

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[1] Based on memoranda: from Captain Davenport to Captain Moss July 1990, and Captain Davenport to Captain Key, 27 October 1987.

- Inaccurate plume growth rates.
- Inaccurate speed of travel for pollutant cloud.

Some model uncertainty is inherent, and can best be addressed by conservatively representing terms through the "failsafe" modeling approach. Meteorological uncertainty, however, is an area where model uncertainty can, and should be, reduced, as feasible.

3. Data Recording System

The Air Force is phasing-in digitized meteorological systems[2], which constitutes a significant development for emergency response management. Digitized data will be updated every 5 seconds, with running 10-minute average σ_θ also updated every 5 seconds. For an emergency response system, the voltage readouts from the data logger channels should be directly input to the emergency response modeling system.

Automated meteorological data entry has important benefits to an emergency response modeling system, including the minimization of human error in data input, and enhanced response speed. The advantages of automation, however, include the potential problem of "blind" entry of inaccurate meteorological data into an emergency response modeling system, without suitable review. The responsible use of automated meteorological data requires: (1) a high level of quality control for the meteorological monitoring program, and (2) a user override option to allow preview of current meteorological data prior to model computations. These steps would help ensure that unreasonable meteorological data are not used as the basis for inappropriate response actions.

One of the most attractive features of automatic meteorological data entry is that a dedicated personal computer(s) could be used to continuously update Tier I and Tier II hazard corridors for all priority accident scenarios at a base. The update frequency would be a function of the number of priority scenarios and model run time. It would not be unreasonable to maintain 15-minute update frequencies on a continuous basis. If an accident occurs, the operator would only need to highlight the accident scenario on the opening menu and the system could be dedicated to continuous display of the applicable worst case scenario. This would allow for immediate response actions initially, while in the background more accurate release data could be used to scale-back the Tier I and Tier II hazard corridors to match less then worst case releases.

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[2] Personal correspondence between Captain Davenport and Captain Moss, July 1990.

Section III

EVALUATION OF THE NEED FOR ENHANCED TREATMENT OF BUILDING AFFECTS

There are two major reasons why the treatment of building effects could be important for the implementation of the Air Force emergency response procedures: (1) alteration of the ambient concentration field by building influences, and (2) differences between ambient and indoor environments. If consideration of the either, or both, of these factors affects the decision to evacuate or shelter-in-place affected individuals, there would be a need to incorporate building treatments into an operational emergency response model.

The influence of structures on the ambient concentration field is addressed in Section IV, which shows based on limited wind tunnel testing that buildings can significantly modify the concentration field for near-field receptors. In Section III, the second factor, i.e. the differences between ambient and indoor concentrations, is emphasized, however, because it appears that of the two factors, that the indoor issue is more significant for the decision to evacuate or shelter-in-place.

A. ACCIDENT SCENARIOS

Hypothetical accident scenarios were developed for Cape Canaveral, Patrick and Tyndall airbases. These scenarios were used to help describe the need to consider building effects in the emergency response modeling system:

1. <u>Cape Canaveral</u>

The assumed accident was a 280 gallon spill of N_2O_4 at the hypergolic fuels storage area. It was assumed that the emissions were released within a five-minute period. There are numerous buildings approximately 3300 to 5000 m north-northeast of the hypergolic fuel storage area. The closest distance of 3300 m was assumed for this example.

2. <u>Patrick</u>

There is a major storage area for chlorine at Building 323. Forty-two cylinders, each with 150 pounds of chlorine, are stored at this location.[3] In this example, it was assumed that one cylinder released its' contents within five minutes. There are five dormitories to the east of Building 323, with downwind distances ranging from approximately 15 to 135 m. The closest dormitory (15 m downwind distance) was used for this example.

3. Tyndall

There are six, one-ton chlorine cylinders stored at the sewage/water treatment plant at this airbase. The one-ton cylinders are delivered by trucks carrying multiple cylinders. This scenario involves a hypothetical truck accident where a single, one-ton cylinder empties near Building 546 during a five minute period. Buildings would be affected in the range of 15 - 300 m downwind. For this example, a downwind distance of 200 m was assumed.

B. MODELING APPROACH

Two models were needed to assess ambient and indoor concentrations. The current version of SLAB (2 October 1990) was used to estimate ambient concentrations for the distances where the buildings were located. These model runs were for five-minute releases. The indoor model consisted of a spreadsheet application of Equation 25 (Section IV), where indoor removal and indoor emission rates were set to zero for simplicity. Specific data were not available in Phase I to estimate specific infiltration rates for the affected buildings. For these examples, therefore, four categories of air exchange rates per hour (ACH) were modeled, i.e. low, medium, high, and windows open. The following air exchange rates were extracted from Table 7 (non-residential buildings):

Low = 0.03 ACH
Medium = 1.12 ACH
High = 4.20 ACH
Open = 10.0 ACH

C. RESULTS

Figures 1 through 3 present the comparisons of ambient and indoor concentrations for ACH values ranging from low to open window status. These figures highlight the importance of considering the differences between ambient and indoor

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[3] Personal communication with Captain Davoney, Patrick airbase, 28 December 1990.

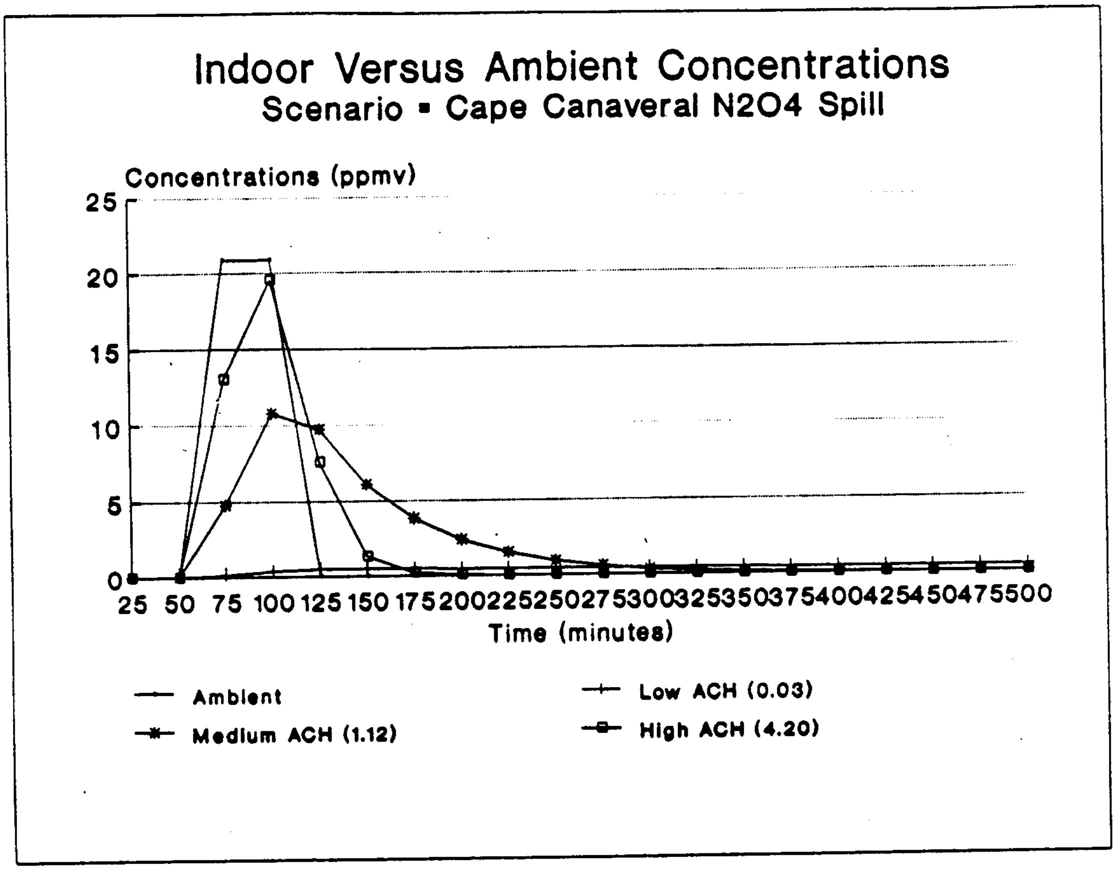


Figure 1. Comparison of Ambient and Indoor Concentrations for Cape Canaveral Accident Scenario.

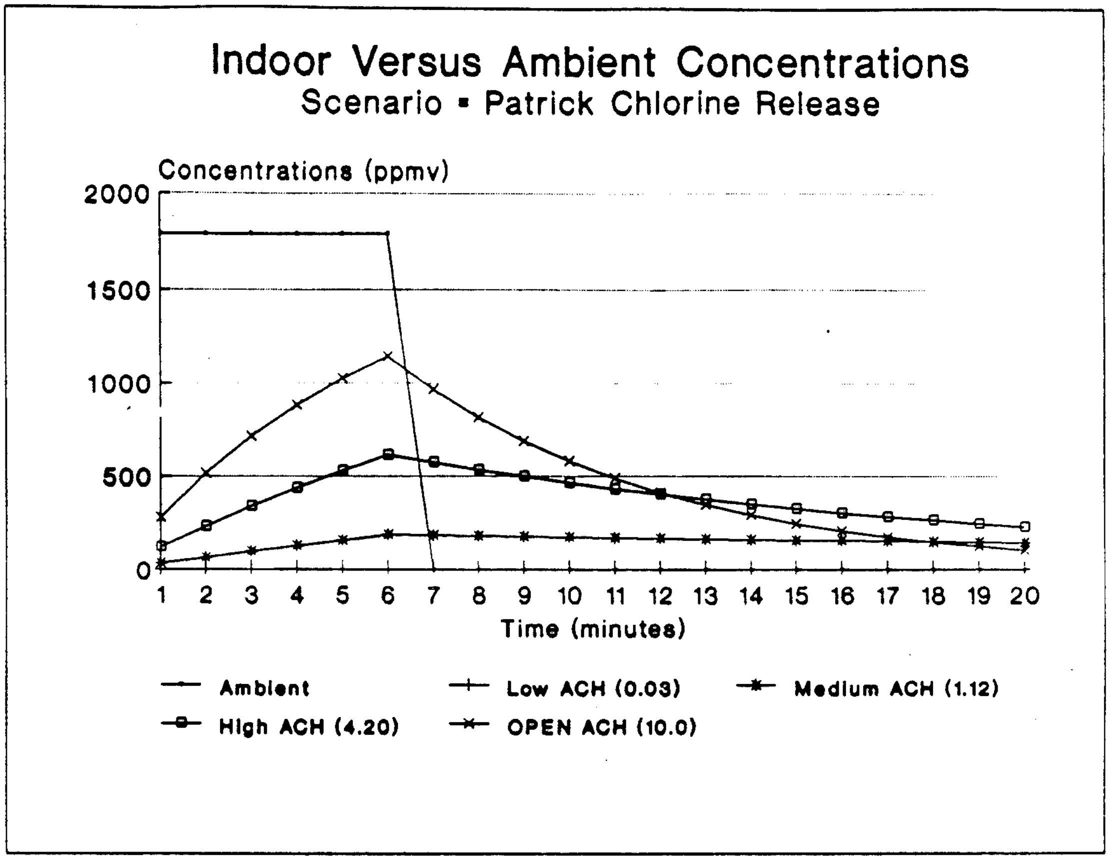


Figure 2. Comparison of Ambient and Indoor Concentrations for Patrick Accident Scenario.

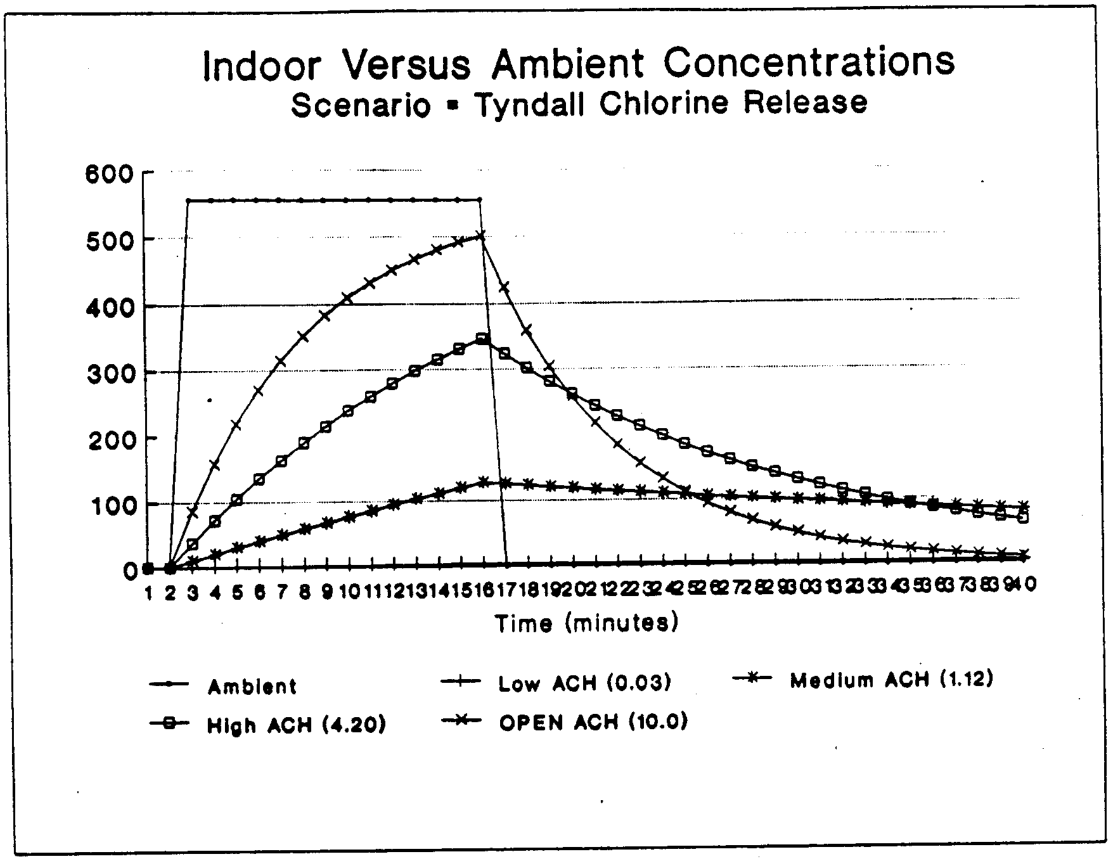


Figure 3. Comparison of Ambient and Indoor Concentrations for Tyndall Accident Scenario.

concentrations. The results show that buildings with high ACH or open windows can provide marginal improvement compared with exposure to the ambient air. Buildings with low ACH, on the other hand, can show orders of magnitude lower concentrations than the ambient air. These figures also highlight the benefit of evacuation after cloud passage. Particularly for tight buildings with low ACH, indoor contamination levels can persist for hours after cloud passage. These examples were based on five-minute releases. As release times and the duration of cloud passage increase, buildings offer less protection.

D. CONCLUSIONS REGARDING THE NEED TO CONSIDER BUILDING EFFECTS

These examples indicate that consideration of indoor concentrations is essential to implement the Air Force emergency response procedures, where an operations commander needs to choose between evacuation or shelter-in-place of affected onbase and offbase individuals. It appears that quantitative guidance is needed that considers ambient concentrations, infiltration rates as a function of building and service opening status, and release time. Additionally, to effectively guide evacuation decisions relative to the shelter-in-place option, an effective emergency response modeling system would also need to consider egress routes in order to compute expected doses for evacuation relative to the shelter-in-place alternative.

Section IV

CONCEPTUAL APPROACH TO MODIFY AMBIENT CONCENTRATION FIELD TO ACCOUNT FOR BUILDING INFLUENCES

There are two complications introduced by structures at an airbase: (1) greater limitations of the turbulence theory used in SLAB for rough surfaces , and (2) structural-induced modifications to the ambient concentrations field. Each complication needs to be considered during model design.

A. SURFACE ROUGHNESS COMPLICATION

The dense gas model SLAB, which was selected for adaptation for this study, estimates concentration as a function of surface roughness (1,2). Surface roughness affects entrainment (rate of cloud growth), and affects the wind speed term in the model. Overall, surface roughness is a sensitive term in SLAB. Figure 4 demonstrates this sensitivity based on setting SLAB sample problem #1 (methane release) to surface roughness of 0.0002 and 0.5 m.

The influence of turbulence on cloud growth rates can be parameterized by turbulence scaling theory. Knowledge of surface roughness and a scaling length term (1/L), which can be estimated from readily measured bulk Richardson numbers, allows for detailed estimates of profiles of wind speed, stability, and turbulence parameters needed for SLAB, and other models. While this is a useful method to parametize atmospheric turbulence, it has limitations.

Ideally, turbulence theory could estimate profiles down to the height where wind speed drops to zero, i.e. the surface roughness height. Surface roughness varies from 0.01 cm for a calm water surface to approximately 25-50 cm at an airbase and many industrial complexes. Most research that was used to support the development of dense gas models was conducted at flat desert or overwater field test sites, where surface roughness has been reported to be as low as 0.02 cm (7,12).

The difference between the surface, and the surface plus 0.02 cm, can be easily neglected, and turbulence theory should perform well throughout the surface layer. For roughness heights of 25-50 cm, however, the issue cannot be as easily dismissed, especially since dense gas plumes are generally characterized by low heights in the near-field. This factor, however, is not likely to adversely affect the use of SLAB to estimate hazard zones because by the outer limits of Tier I, and especially the Tier II zones, the top of the cloud would be well above the surface roughness

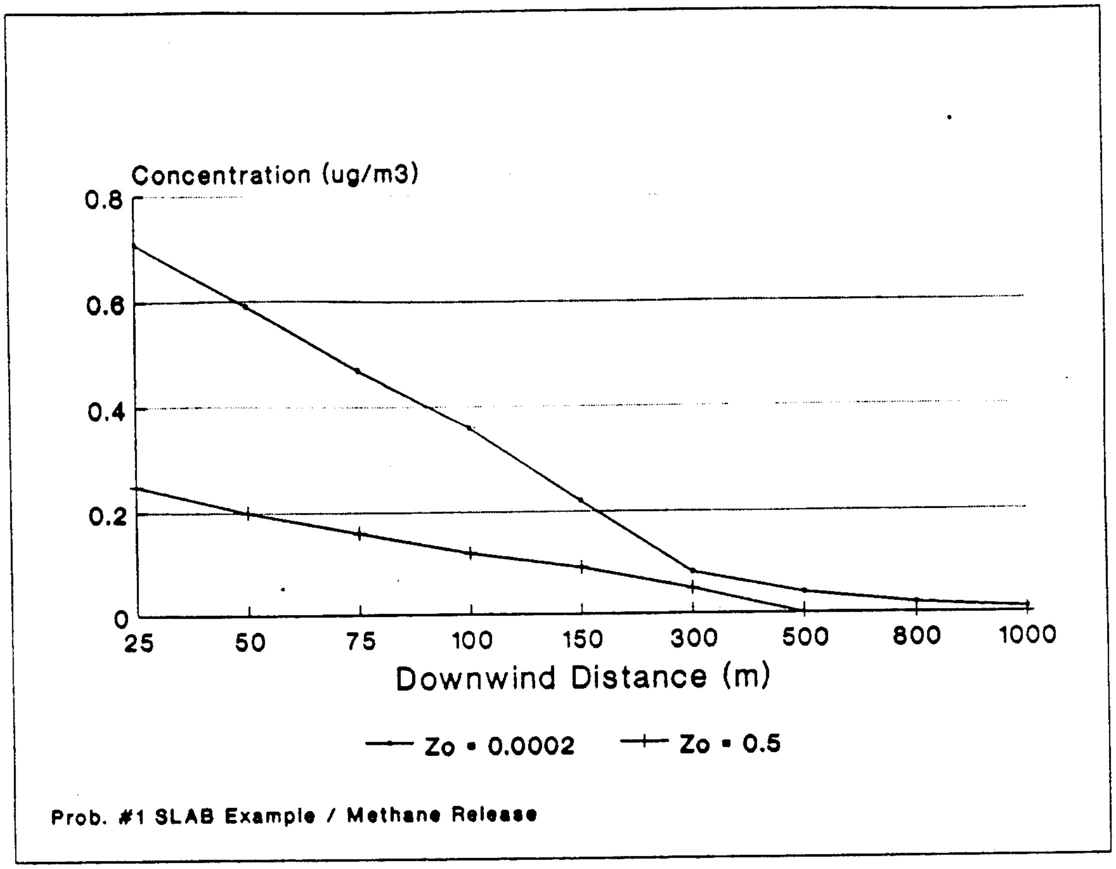


Figure 4. Sensitivity of SLAB to Surface Roughness.

height.

A potentially more troublesome complication involves the displacement height. If the ground is covered by tall roughness elements such as a forest canopy, crops, or even densely packed houses, the turbulence reacts as though the surface is near the height of the obstructions. Turbulence theory still applies, but heights need to be measured relative to the typical obstruction height times a factor on the order of 0.70 to 0.80, the product of which is defined as the displacement height (11).

Even though airbases have substantially larger surface roughness values than open settings, the displacement term does not strictly apply because there is much open space. If a displacement term were needed for an airbase, it likely would be much less than 70-80 percent of the typical obstruction height. Furthermore, the application of turbulence theory down to the surface, should result in a conservative treatment of low-level entrainment within the model because wake effects of obstacles would enhance entrainment in this region relative to the model treatment. Conservative treatment of entrainment within the model would lead to overestimates in the near-field concentrations, which is consistent with the failsafe approach.

In summary, the surface roughness complication to turbulence scaling theory is not expected to introduce major difficulties for the modeling approach. No modifications to the modeling approach appear to be needed to respond to these complications. The more difficult problem appears to be the alteration of the ambient concentration field caused by wake effects at downwind obstructions, which is described in the next subsection.

B. BUILDING-INDUCED ALTERATION TO AMBIENT CONCENTRATION FIELD

Building wake effects have been studied in greater detail for passive gas releases (13,14,15)) relative to the very limited study of building wake effects for dense gas clouds. Emphasis in this section has, therefore, been directed toward the dense gas releases. A similar approach would be used to adjust passive gas clouds.

A recent wind tunnel study conducted by Rowan, Williams, Davies & Irwin (RWDI) has shown that at least for low wind speeds, the presence of obstacles significantly influences dense cloud behavior (16). Through a series of test scenarios, the following was observed:

<u>Single Downwind Obstacle</u> (50 m downwind) - In the lee of the obstacle, concentrations were approximately four times lower than the no obstacle case.

<u>Single Upwind Obstacle</u> (29 m upwind) - Extremely high concentrations were reported in the lee of the obstacle (55 percent of release concentration). A low pressure zone apparently caused rapid transport toward the downwind face of the obstacle (16). RWDI reported concentrations 50 m downwind of the release to be a factor of two higher than the no-obstacle case. This scenario is an example where a model that did not consider building wake influences could show zero concentrations, while actual concentrations could be worst case.

<u>Uniform Array of Downwind Obstacles</u> - These tests showed preferred transport parallel to the obstacle array. Within the first 50 m of

travel, the uniform array of obstacles showed concentrations more than two times higher than the no-obstacle case. By 100 m downwind, there was little difference between the obstacle and no-obstacle cases. By 200 m, however, the presence of the obstacles resulted in significant reductions in peak concentrations. These findings were attributed to decreased entrainment in the near-field, with increased entrainment in the mid-field and far-field, which was attributed to the obstacles (16).

What can be inferred from the limited available data? The near-field potential to increase concentration is a failsafe issue that could potentially affect the decision to evacuate or shelter-in-place. The mid-field reduction in concentration may allow for reducing concentrations in this zone, which could result in less restrictive Tier I corridors, without sacrificing the safety features of the model. The RWDI research, however, showed that such reductions are a function of wind speed. Care would need to be taken to ensure that concentrations were not scaled back too much in this zone to account for enhanced dispersion from obstacles during high wind speed conditions. Far-field wake influences should be minor, i.e. Tier II boundaries are unlikely to be substantially affected.

There appear to be two major alternatives to include building wake modification to the ambient concentration field: (1) modifying the entrainment terms in the model, or (2) using a simplified scaling procedure to adjust near field and mid-field concentrations to conservatively represent the differences between the obstacle and no obstacle cases.

An approach has been proposed to empirically account for the modification of entrainment by obstacle influence (16). An exponential term could be used to show the modification to dense gas entrainment as a function of the areal coverage of obstacles (16). Entrainment is complicated by wide plumes with less potential for modification of horizontal relative to vertical entrainment, which may not be effectively addressed with a one-dimensional model. This approach (16) also may be too site specific for a general-purpose emergency response modeling system. The simplicity and conservatism of the scaling technique appears to be the more practical approach, considering the major limitations in the state-of-the-art. Final judgement will be reserved until Phase II, after ongoing research by RWDI is completed.

RWDI is currently engaged in a study for the Canadian Air Force that involves wind tunnel testing of dense gas releases at an airfield, which is likely to have structures that are similar to those at typical U.S. airbases. These results should be reviewed in Phase II, including an evaluation of how these results best could be extrapolated to non-neutral stability conditions.

Section V

STRENGTHENING THE SLAB MODEL

Dispersion models often are biased to overestimate or underestimate concentration. There is inherent uncertainty that limits the accuracy in model application. Often, the bias is not systematically high or low, but variable from application to application. For most models, there are so many components interacting that the direction and magnitude of model bias can be a function of meteorological conditions, surface features, pollutant, and mode of release. For example, the EPA Industrial Source Complex (ISC) model, the most widely used passive gas dispersion model in the U.S., appears to be biased as a function of urban or rural conditions, and also as a function of height of release above groundlevel (17). For such reasons, models are never fully validated, and limited testing is unlikely to adequately match an application at hand to allow model users to confidently indicate the direction of model bias.

The preceding uncertainties may be acceptable for regulatory programs, but pose major problems for emergency response. The management of an air quality emergency, or any safety related issue, requires confidence. If an analyst cannot be confident of accuracy, it is essential to strive to be confident that risks are not underestimated. This fundamental approach is not unlike the treatment of other safety issues, such as bridge construction, aircraft design or managing the risks from nuclear power. Bridges are not designed to just barely withstand the heaviest allowed load without collapsing, but a reasonable safety margin is used to safely manage uncertainty. The same concept should apply to emergency response modeling, where emergency response coordinators can be personally responsible for the health and safety of many individuals. Operations commanders need confidence that there are not major errors in applied modeling systems that underestimate concentrations for undefined circumstances. In this sense, the objectives of operational models are much different than those of research. Confidence is more important than accuracy when managing emergency response actions.

An effective way to evaluate a model for potential bias is to review the major components separately, rather than evaluation of the final model output. This concept was applied previously (18), which identified a major error in the plume rise algorithm in the Oak Ridge National Laboratory Atmospheric Transport Model (ATM), and a subtle error in the smoothing term of the widely used EPA ISCLT and LONGZ dispersion models. The plume rise error was only a major problem for sources with high buoyancy releases; if tested for other scenarios, the ATM model could perform well, even though the model could grossly underestimate concentrations for high buoyancy releases. Similarly, the smoothing errors in the ISCLT and LONG models resulted in bias as a function of compass heading from source to receptor, which would unlikely have been detected without a component analysis. Such limitations in an emergency response model could produce good model performance sometimes, perhaps when tested, but contain serious flaws for other applications.

For this study, the following major components of SLAB were reviewed to ensure that any bias to underestimate concentration could be minimized:

- o Entrainment
- o Assumed Distributions
- o Plume Meander
- o Wind Speed Profile
- o Source Term
- o Reactivity
- o Relative Humidity Term

The results of these reviews are presented in the following subsections.

A. ENTRAINMENT

A pollutant cloud grows by entraining ambient air. SLAB computes entrainment along the vertical and horizontal axes. The rate of entrainment is a function of cloud density relative to the ambient air, surface roughness, and turbulent scaling length (1/L) (1,2). An evaluation of SLAB revealed a high sensitivity to surface roughness. While it would be expected that a rougher surface would produce greater entrainment, SLAB appears to have the potential to overestimate the rate of entrainment for flow over a moderately rough surface, such as a typical airfield.

From low surface roughness scenarios, e.g. 0.02 cm, which apply to surface conditions when SLAB was evaluated (7), to typical airbase roughness lengths of 25-50 cm, differences in entrainment were found to be more than expected. Figure 5 demonstrates this sensitivity based on SLAB example problem #1, surface roughness values of 0.02 and 50 cm, and WRITE statements added to SLAB's entrainment subroutine. The sensitivity of SLAB to surface roughness was much greater than that observed with some preliminary model runs made with ADAM. ADAM generally showed only 10-40 percent lower concentrations when surface roughness was increased from 0.01 cm to 30 cm, which is more consistent with the expected sensitivity to surface roughness.

In fact, for a heavy gas such as chlorine and a surface roughness greater than 10 cm, SLAB produces an error message - - an error that is resolved by using a lower surface roughness value.

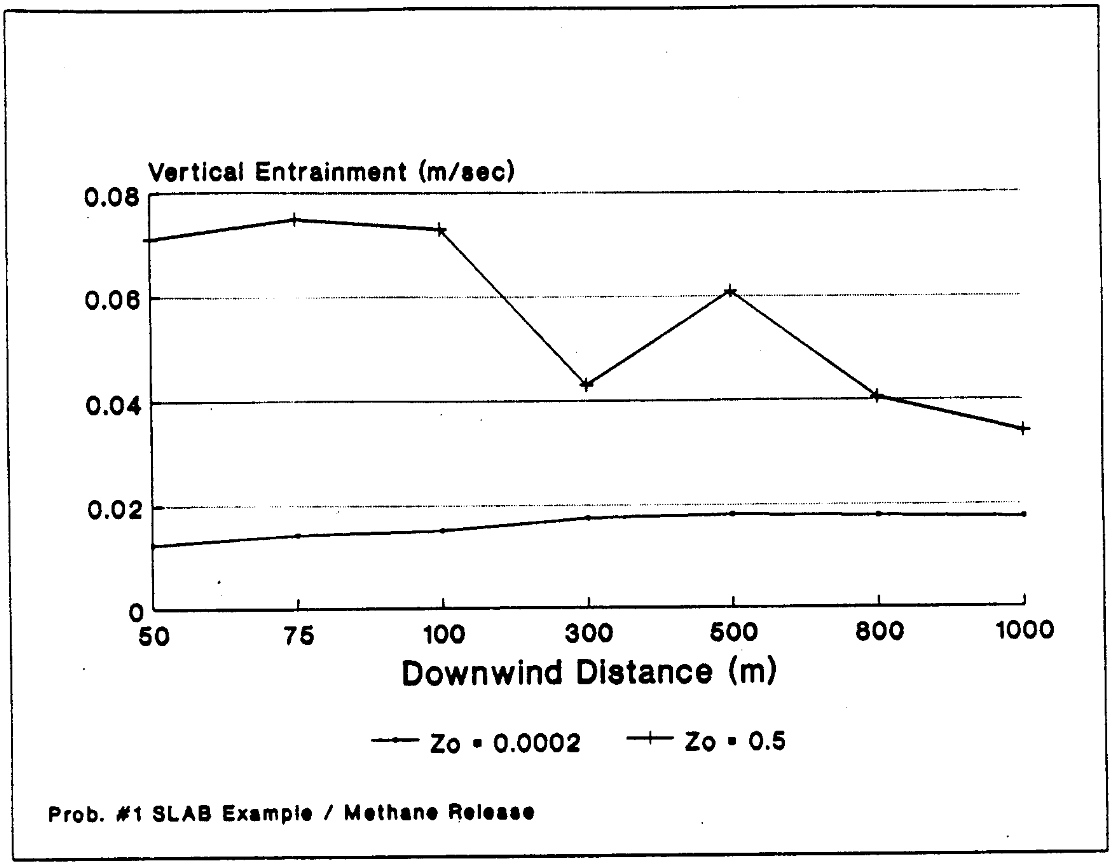
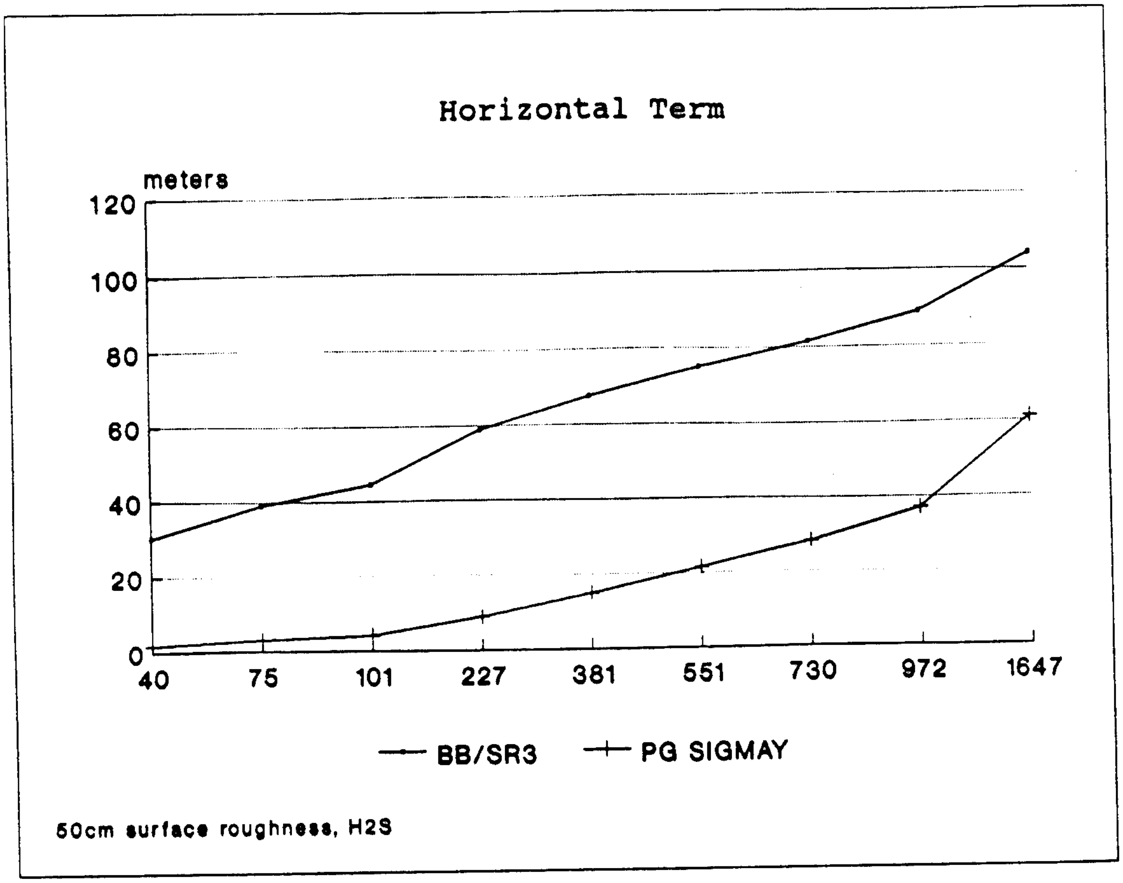


Figure 5. Sensitivity of the SLAB Entrainment Term to Surface Roughness.

Based on these observations, it appears that the roughness term needs to be revised before SLAB could be adapted for typical airbase applications.

Figures 6 and 7 compare sigma y and sigma z for a dense gas release using surface roughness values of 1 and 50 cm. These figures are based on a hydrogen sulfide release and 1/L set to 0.02. Figures 6 and 7 show the effects of entrainment on cloud growth. Pasquill Gifford dispersion coefficients are also provided as a point of reference.

Sigma values in SLAB are computed as follows (1):



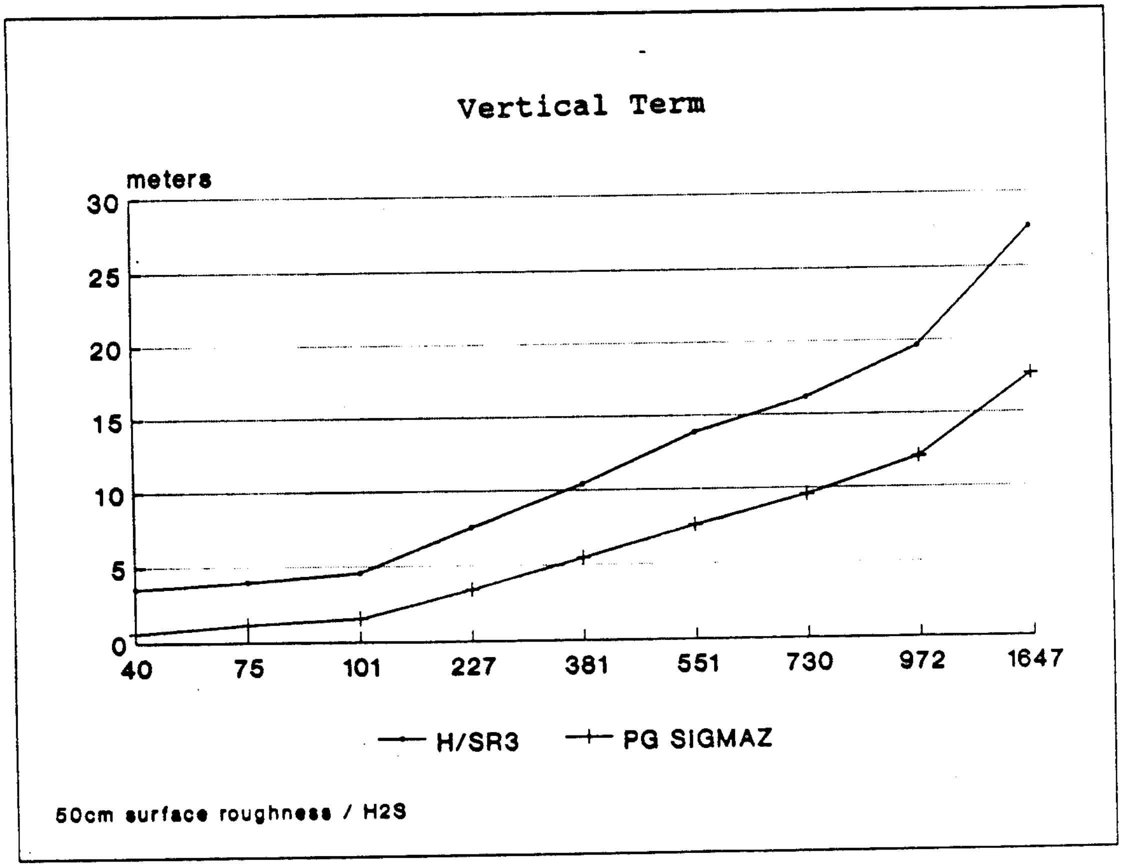
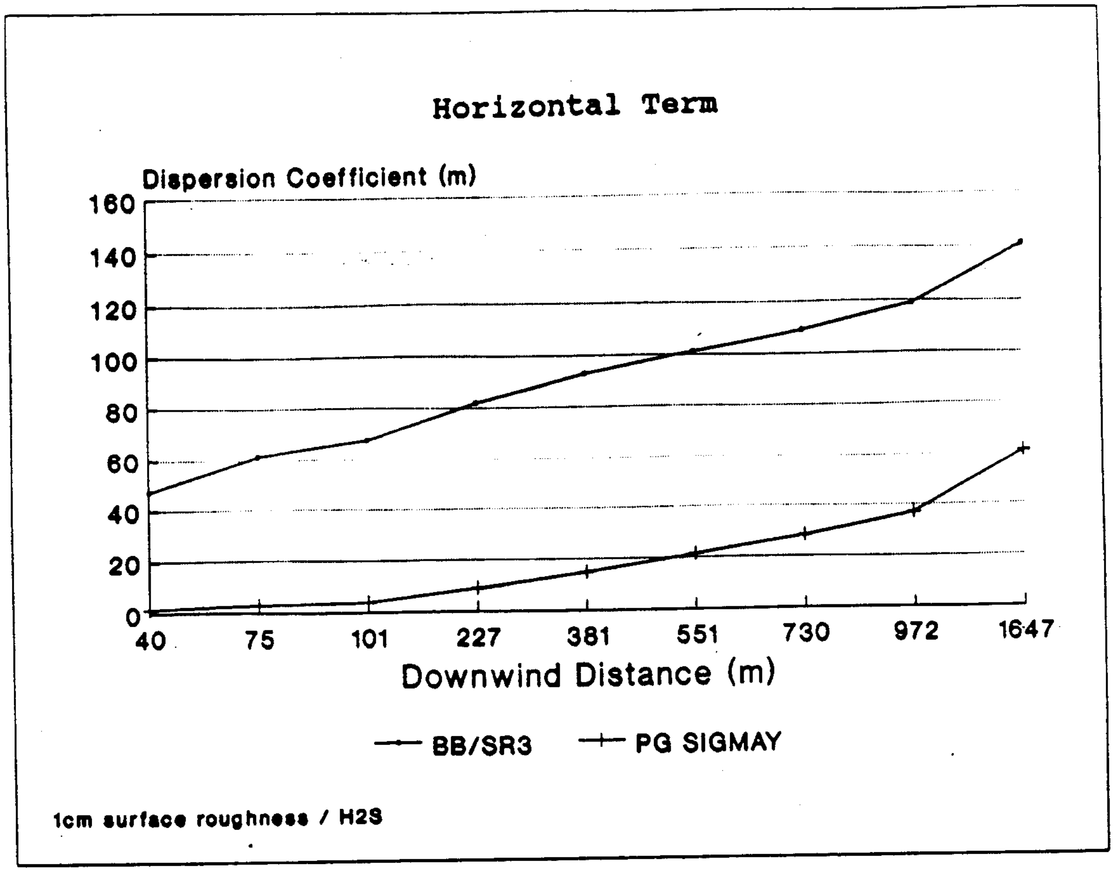


Figure 6. Horizontal and Vertical Dispersion Coefficients: Comparing SLAB Estimates With Pasquill Gifford Coefficients: 50 cm Surface Roughness.



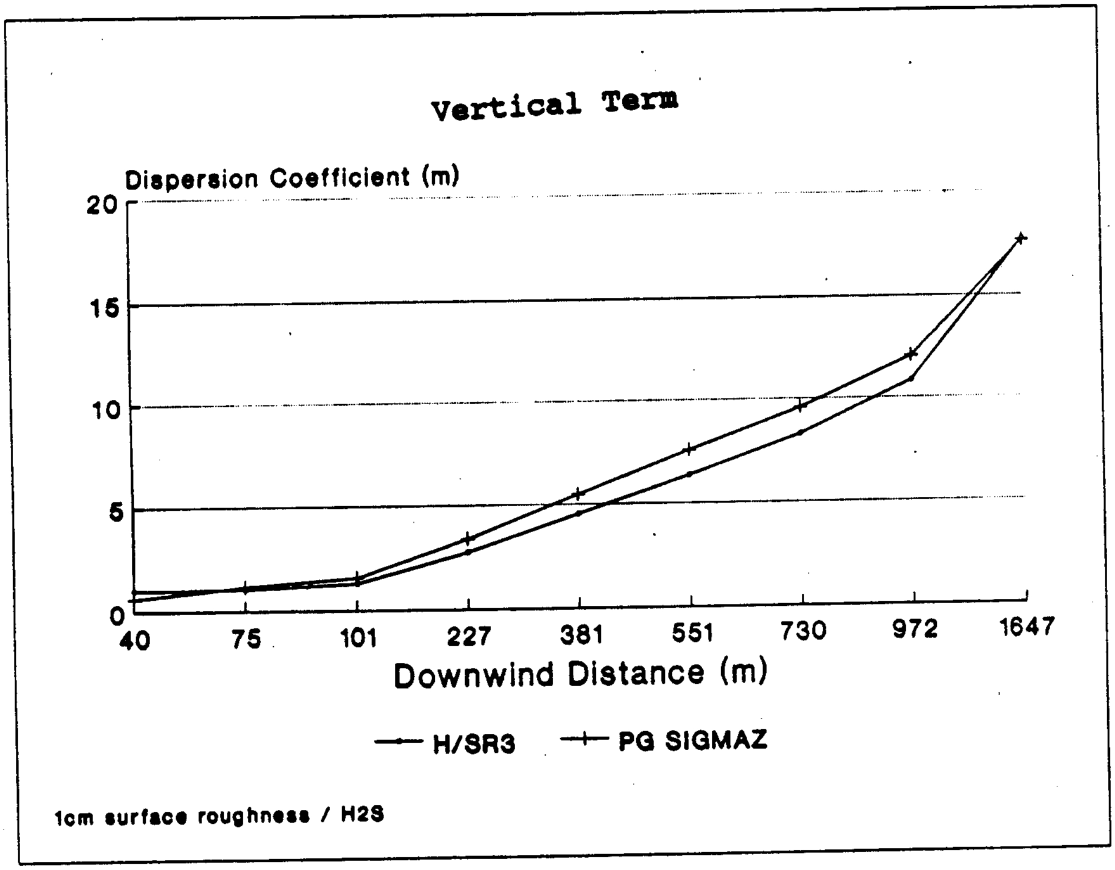


Figure 7. Horizontal and Vertical Dispersion Coefficients: Comparing SLAB Estimates With Pasquill Gifford Coefficients: 1 cm Surface Roughness.

$$\sigma_y = b/\sqrt{3} \qquad (1)$$
$$\sigma_z = h/\sqrt{3} \qquad (2)$$

where:

b= cloud half width
h = cloud height

The observed sensitivity of cloud growth rates to surface roughness cannot be explained by the enhanced mechanical mixing (19). The difference of 1-50 m in surface roughness would only produce a minor change in 1/L (19). Furthermore, comparison with Pasquill Gifford dispersion coefficients shows cloud growth rates in SLAB that appear to be inconsistent with those of standard passive cloud treatments. Additional testing of the model for a dense chlorine cloud also showed vertical dispersion rates that were too high relative to the Pasquill Gifford treatment. The shape of the SLAB cloud needs to be reevaluated in Phase II. The characterization of both horizontal and vertical dimensions of a cloud are important for this study because if the vertical extent of the cloud is incorrect, the potential would exist to make an incorrect choice between the shelter-in-place or evacuate alternatives for buildings with rooftop HVAC systems, i.e. is the HVAC system drawing clean or contaminated air?

Other researchers have used low surface roughness values to better match measured concentrations (20,21), possibly responding to the same observation of oversensitivity to surface roughness. An initial review of the entrainment subroutine in SLAB was done to help identify the cause of the apparent overestimate of cloud growth rates. The following steps were taken during this review:

- Reviewed Fortran code.
- Reviewed literature used as basis for entrainment calculations.
- Inserted write statements in entrainment subroutine in SLAB to fully display all intermediate terms.

The following presents the observations of this review, with a focus on vertical entrainment.

Vertical entrainment is estimated in SLAB as follows (1,2):

$$W_e = \frac{(1.5)\,(k)\,(u_*)}{\Phi_m} \qquad (3)$$

Where:

W_e = entrainment velocity in the vertical axis (m/sec)
k = 0.41 (von Karman's constant)
u_* = friction velocity of the cloud (m/sec)
Φ_m = Monin-Obukhov profile function (dimensionless)

The Φ_m function is defined as follows for stable and unstable conditions in SLAB (1,2):

Stable conditions:

$$\Phi_m = 1 + 5z/L \qquad (4)$$

Unstable conditions:

$$\Phi_m = (1-16z/L)^{-0.50} \qquad (5)$$

The scaling length 1/L used in Equations 4 and 5 is estimated from the Richardson number (Ri). Ri is computed in SLAB as a function of contributions from the ambient air and the cloud properties, based on research shown in References 22 and 23, as follows:

$$Ri = \frac{(u_{*_a})^2 (Ri_a) + (g)\,(0.025)\,\frac{(\rho-\rho_a)}{\rho}\,(h)}{u_*^2} \qquad (6)$$

Where:

ρ = cloud density
ρ_a = air density
h = cloud height
g = gravitational acceleration

The current version of SLAB divides Ri by h to estimate 1/L.

SLAB promotes smooth transitions because the approach to estimate cloud growth does not require arbitrary switching from one set of equations to another as the cloud transitions from a dense to passive cloud. This approach is appealing, especially since the modeling system could be used for passive or dense clouds. There are questions, however, that need to be addressed in Phase II. There are potential refinements needed, which appear to be most evident as downwind distance increases and the cloud becomes more passive. For research purposes, this may not be a major problem, but for implementing the Tier I and Tier II Air Force emergency response procedures, both the dense and passive stages of dense gas releases could be important. In fact, for all but transportation scenarios, hypergolic fuel accidents would need to emphasize far-field distances because of the isolation of these activities. The modeling system, therefore, will need to be effective at all distance scales. The issues of concern are summarized as follows:

1. Conversion From Ri to z/L

SLAB inherently assumes that Ri equals the z/L term for all stability conditions. The code divides Ri by cloud height (h) to estimate 1/L. This approach is consistent with turbulence research, but only for unstable conditions (11). The current approach, however, appears to be inconsistent with more standard practice for the more critical, stable conditions (11).

The following relationship between Ri and 1/L is generally used (11):

$$Ri=\frac{z}{L} \qquad if\ Ri \le 0 \qquad (7)$$

$$Ri = \frac{(z/L)}{[1+5(z/L)]} \qquad if\ Ri>0 \qquad (8)$$

The relationship between Ri and z/L for stable conditions applies to Ri less than or equal to approximately 0.20. In the near-field region of dense gas cloud transport, entrainment could be overestimated since the critical Richardson number could be exceeded or approached. Minimum vertical growth would be expected until surface heating reduced the degree of stability. Early cloud growth for dense clouds should be reassessed to confirm that the SLAB treatment does not overestimate near-field entrainment on this basis.

The 1/L value for ambient air is defined as a constant within the surface layer (11). Within SLAB, the 1/L term is variable because it includes cloud effects, but as downwind distance increases and cloud effects become negligible, 1/L should approach the ambient value. Figure 8 presents an example where 1/L in SLAB is compared with ambient 1/L. In the near-field, 1/L in SLAB is higher than 1/L ambient, as expected, because the dense cloud is stable relative to the ambient air. As shown, however, SLAB computes 1/L that is substantially lower (less stable) than the ambient air in the mid-field and far-field, which, in part, appears an artifact of the Ri to 1/L conversion.

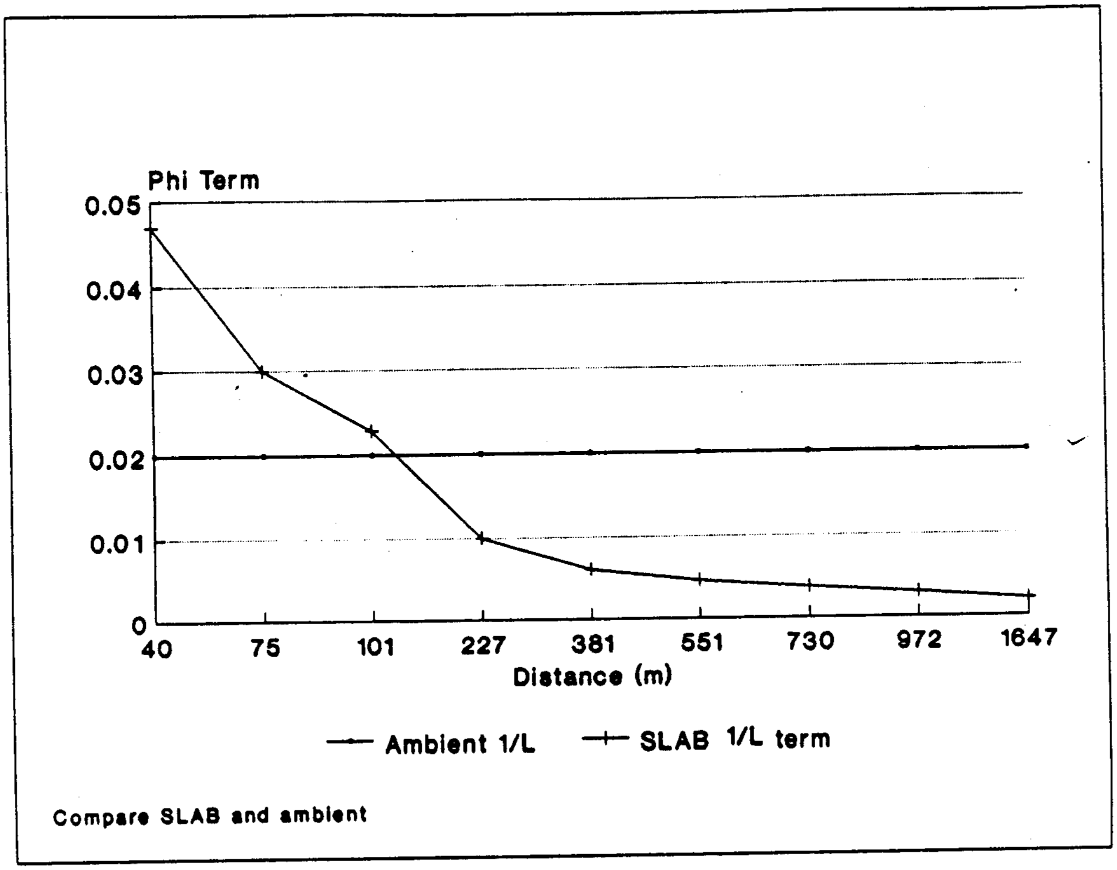


Figure 8. Comparison of SLAB Scaling Lengths With Ambient Scaling Length.

If the hypothesis were correct that the Ri to 1/L conversion introduces bias to the entrainment treatment in SLAB, SLAB would have been expected to substantially underestimate 1/L in the near field, but should have converged with the ambient 1/L as the cloud contribution to 1/L becomes negligible because the ambient contribution to 1/L is directly entered into SLAB, while the cloud contribution is converted from Ri. The SLAB estimates of 1/L, however, do not converge with the expected ambient values, as is shown in Figure 8.

The explanation may be that a scaling factor, which is used in SLAB to adjust the ambient contribution to 1/L, may compensate, in part, for the bias in SLAB to underestimate stability (1/L) in the near-field, but substantial underestimates of 1/L appear to be introduced in the far-field. The scaling factor in the code is computed as follows:

$$\left(\frac{1}{L_{amb}}\right)_{final} = \left(\frac{1}{L_{amb}}\right)_{computed} \frac{\left(1+\frac{hr}{zl}\right)}{\left(1+\frac{h}{zl}\right)} \qquad (9)$$

Where:

hr = the higher of the wind speed monitoring height or 3 m
h = cloud height
zl = stability parameter that is computed as follows (by assuming hr=3 in this example):

Stability Class	zl
1	11.0
2	5.0
3	2.2
4	1.0
5	1.8
6	2.6

As h grows relative to hr, the ambient contribution to 1/L is, therefore, further reduced. Note that the stability class term shown above is computed within SLAB as a function of user input 1/L and surface roughness, based on Reference 19.

It appears that for close-in distances, where the cloud characteristics significantly contribute to 1/L, the Ri to z/L conversion used in SLAB would act to underestimate cloud stability. This would lead to overestimating entrainment, especially in the near-field, where the zl adjustment term does not substantially compensate for the apparent bias in the Ri to z/L conversion. In the far-field, the SLAB Ri to z/L conversion problem would not be significant because the current code appears to only need refinement for the cloud contribution to 1/L. Without the zl adjustment, the 1/L term would have converged with the ambient value in the far-field. The zl adjustment factor, however, increases in importance with downwind distance, and the adjusted 1/L values appear to act to overestimate entrainment in the far field, based on Figure 8 and Equations 3 and 4.

There appear to be two other scaling factors, in addition to the zl adjustment, that act to reduce entrainment in the far field, which also should be reassessed:

<u>Wind Speed Scaling Factor</u> - The vertical entrainment rate is multiplied times the ratio of the wind speed at 4 m over the wind speed at the mid-point of the cloud. As the cloud height increases, the wind speed adjustment factor progressively reduces the entrainment rate. This factor appears to have been added to provide a better match with passive sigmas, because wind speed varies with height in SLAB, while Gaussian modeling holds wind speed constant as plume height increases. Wind speed could affect dispersion modeling through the transport term (pollutant injection speed into the atmosphere) and, conceivably, through it's influence on dispersion coefficients. The wind speed change with height, however, should not affect the injection rate. Furthermore, the Pasquill Gifford dispersion coefficients should empirically show the effect on sigmas of increase in wind speed on vertical growth. Based on these considerations, it is not clear that the wind speed scaling factor would be needed after the Ri to z/L conversion is refined.

<u>Mixing Height Scaling Factor</u> - Entrainment is multiplied times one minus the ratio of cloud height divided by mixing height. This term prevents vertical mixing through an elevated surface inversion layer, which is a necessary model condition. It appears, however, that this term could be refined for times when the top of the cloud is below the top of the mixed layer, and possibly during stable conditions. Further review would be recommended for Phase II.

In summary, it is not clear that these scaling factors should be retained after the conversion from Ri to z/L is refined. More research is needed in Phase II. Then it would be possible to reassess the need to adjust entrainment rates to account for wind speed scaling and mixing height restrictions. What can be concluded now? There appears to be the potential to underestimate entrainment in the far-field on the basis of the scaling factors, and thereby, adversely affect the delineation of Tier I and II hazard corridors. In the near-field, on the other hand, there appears to be a potential to overestimate entrainment, and thereby underestimate maximum risks. It appears that the overestimate of entrainment could be mitigated in part by setting the surface roughness term to a value lower than that representative of site conditions, which decreases the friction velocity and increases Φ_m during stable conditions, both of which act to decreases entrainment. This appears to have been done in References 20 and 21. The goal for Phase II, however, would be to resolve all fundamental limitations for airbase applications, such as those shown for entrainment, before developing additional code to address modifications to the ambient field and indoor concentrations.

2. Φ_m Term for Unstable Conditions

The Monin-Obukhov profile functions are defined in the literature as follows (11):

$$\phi_m = \left[1-16\left(\frac{z}{L}\right)\right]^{-.25} \qquad (10)$$

$$\phi_h = \left[1-16\left(\frac{z}{L}\right)\right]^{-.50} \qquad (11)$$

Where:

Φ_m = momentum profile function
Φ_h = heat (or other scalar) profile function

It is not apparent that the Φ_h function, which was used in SLAB to represent Φ_m, best represents the entrainment term. Figure 9 shows the difference between these two functions. As shown, the two functions diverge as downwind distance increases, which would appear to overestimate entrainment in SLAB, and thereby, act to underestimate concentrations during unstable conditions. The profile function for unstable conditions should be reevaluated, including the effects any scaling factors used during unstable conditions, to ensure that this component of the model adequately meets the failsafe objectives of model development.

Aside from scaling factors used in SLAB, the Ri to z/L conversion and unstable profile function would be most significant when atmospheric stability deviated significantly from neutral conditions. During neutral conditions, model performance would not

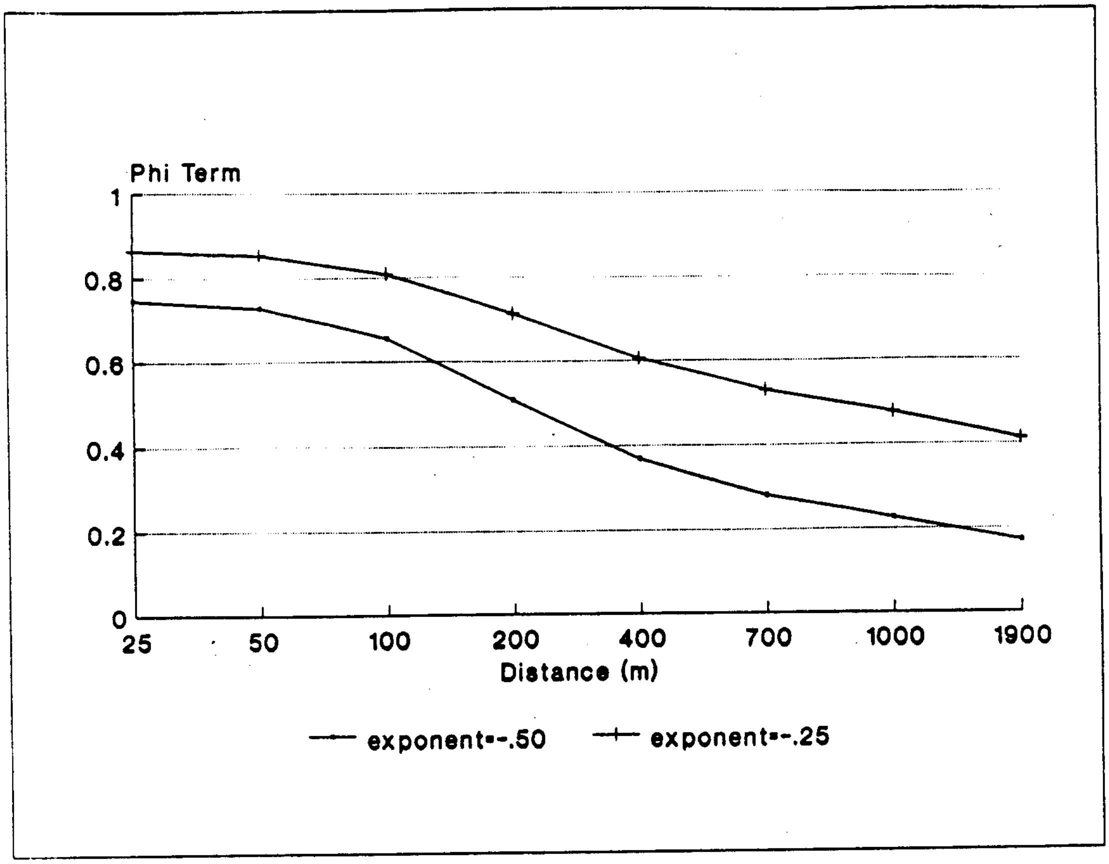


Figure 9. Monin-Obukhov Profile Function For Unstable Conditions Based on Exponents of -0.50 and -0.25.

be affected because z/L would equal zero and Φ_m would be unity. Most of the Burro and Coyote Series testing of the SLAB model were reported as neutral, slightly unstable or slightly stable (7 of 11 tests). Only Burro 8 was a stable test (7). It is possible that model performance could have been significantly different if SLAB were to be tested during non-neutral conditions, and over a rough surface.

3. Upper Limit of Monin-Obukhov Scaling Theory

The entrainment features of SLAB are based on the Monin-Obukhov scaling theory. Scaling theory is applicable within a lower and upper limit, relative to the ground surface. The lower limit was addressed in Section IV.A, but the upper limit could be a potential problem for entrainment. Scaling theory applies within the surface layer (e.g. 10 percent of the mixed layer), where u_* can be treated as constant. During the daytime, the surface layer can be 100 m or more, however during nighttime, stable conditions, the surface layer can be tens of meters (11).

SLAB reduces entrainment as the cloud grows relative to the depth of the mixed layer, but does it adequately consider the applicability of Monin-Obukhov theory in the surface layer? During the strengthening of SLAB in Phase II, the mixing height adjustment factor should be reassessed to ensure that u_* is not overestimated by extrapolating scaling theory above the surface layer.

B. ASSUMED DISTRIBUTIONS

SLAB is a one-dimensional model that simplifies computations by assuming uniform concentrations horizontally and vertically throughout a "slab", or crosswind cross-section of the cloud. The solution of the coupled set of differential equations used in SLAB only varies concentration as a function of downwind distance. Model users, however, are generally concerned with maximum (centerline) concentrations, and the variability in concentration as a function of distance horizontally and vertically from the centerline. SLAB <u>assumes</u> distributions along the horizontal and vertical axes to meet this need. Are these assumptions sufficiently conservative considering the degree of uncertainty?

SLAB assumes the following to characterize the distributions of concentration:

- A Gaussian shape
- $\sigma_y = BB/\sqrt{3}$ (12)
- $\sigma_z = h/\sqrt{3}$ (13)

Where BB = half width (m)
h = cloud height (m)
σ_y = horizontal dispersion coefficient (m)
σ_z = vertical dispersion coefficient (m)

How well do the SLAB distributions compare with standard Gaussian treatments of initial sigma values, such as the virtual point source technique, where there also is a need to match known plume dimensions? The most commonly applied passive dispersion model is the EPA Industrial Source Complex Model (ISC). This model uses the following assumed distributions to match a known volume source, based on the use of the virtual point source technique (15):

o $\sigma_y = BB/2.15$ (14)

o $\sigma_z = h/2.15$ (15)

The SLAB treatment, which divides cloud dimensions by $\sqrt{3}$ (or 1.73), therefore, assumes a more uniform distribution along the horizontal and vertical axes.

The assumed distributions in SLAB could potentially result in underestimating concentrations based on the preceding review. Centerline concentrations may be conservative in the near-field, at least for cold, dense clouds, which have been found to be relatively well mixed because of the convective effects produced by surface heating (12,13). There are two concerns, however, for the development of a failsafe model:

1. If the concentrations within the cloud were more uniform than the assumed distribution, there would be a potential in the near-field to underestimate concentrations towards the horizontal extremes of the cloud, and overestimate centerline concentrations.

2. There is a potential to underestimate centerline concentrations in the far field. While relatively uniform concentrations could occur in the near-field, distributions likely would develop in the far-field after convective influences diminish. At that point, the assumed distributions in SLAB would be more uniformly mixed than typical Gaussian treatments, and would, therefore, not converge with passive treatments. The difference in assumed distributions results in approximately 25 percent larger sigmas for both axes, which could combine to underestimate centerline concentration by a factor of approximately 50 percent, relative to a standard Gaussian treatment.

The preceding concerns should be addressed in Phase II. Modifications to SLAB could be made through the entrainment and/or distribution terms, if deemed necessary, to increase the conservatism in the treatment of cloud dimensions.

C. PLUME MEANDER

Plume meander along the horizontal axis has been shown to increase as averaging time increases (24). Longer averaging times subject the plume to a wider distribution of eddies, which act to widen the horizontal extent of the plume. SLAB uses a modification of the Slade approach (24) to account for enhanced horizontal meander. How well does SLAB represent plume meander for passive and dense gas dispersion over a wide variety of terrain conditions? There are two issues, which were reviewed in Phase I:

1. Is the Slade function universal for passive plumes?

2. How well does the SLAB approach represent a dense gas?

1. Slade Function As a Universal Function.

The Slade function was developed from measured standard deviation of horizontal wind direction data (σ_θ) collected at the smooth clipped grass surface of O'Neill Nebraska (surface roughness was roughly 1 cm (25)). Structural or terrain influences at an airbase introduce the potential to channel flow. Under these conditions, it is possible that the Slade meander function could reduce concentrations too much as averaging time increases. Note that the influence of structures to increase the entrainment rate, a separate issue, will be treated empirically based on wind tunnel data (refer to Section IV.B.

Wide-angle, dense clouds that are created by gravity spreading are not sensitive to the SLAB meander term. This point is shown in Figure 10. The potential exists to increase cloud width by too large a factor for dense or passive gas releases, however the model was shown in Figure 10 to be relatively insensitive to this term. In this figure, and Figure 11 that follows, the 30-minute average concentrations were factored to account for duration, as follows: (30-minute concentrations times 1800 seconds / duration (sec)).

It would be difficult to find a definitive basis to increase the conservatism of this term in the far-field. Since a 30 minute averaging period is a critical averaging time for Air Force emergency response procedures, meander should be reevaluated in Phase II to assess the potential need to arbitrarily reduce the SLAB meander term, e.g. by 50 percent to conservatively treat far-field meander in a failsafe model.

2. Slade Function to Represent Dense Gas Releases

A dense gas is likely to react more slowly to horizontal meander because of the greater inertia relative to a passive gas. Theoretically, the Slade treatment (24) could overestimate meander on this basis. While the Slade function is not directly applicable to a dense gas, this issue does not appear to be major. While a cloud is significantly denser than the ambient air, gravity spreading produces a wide-angle cloud, which results in the

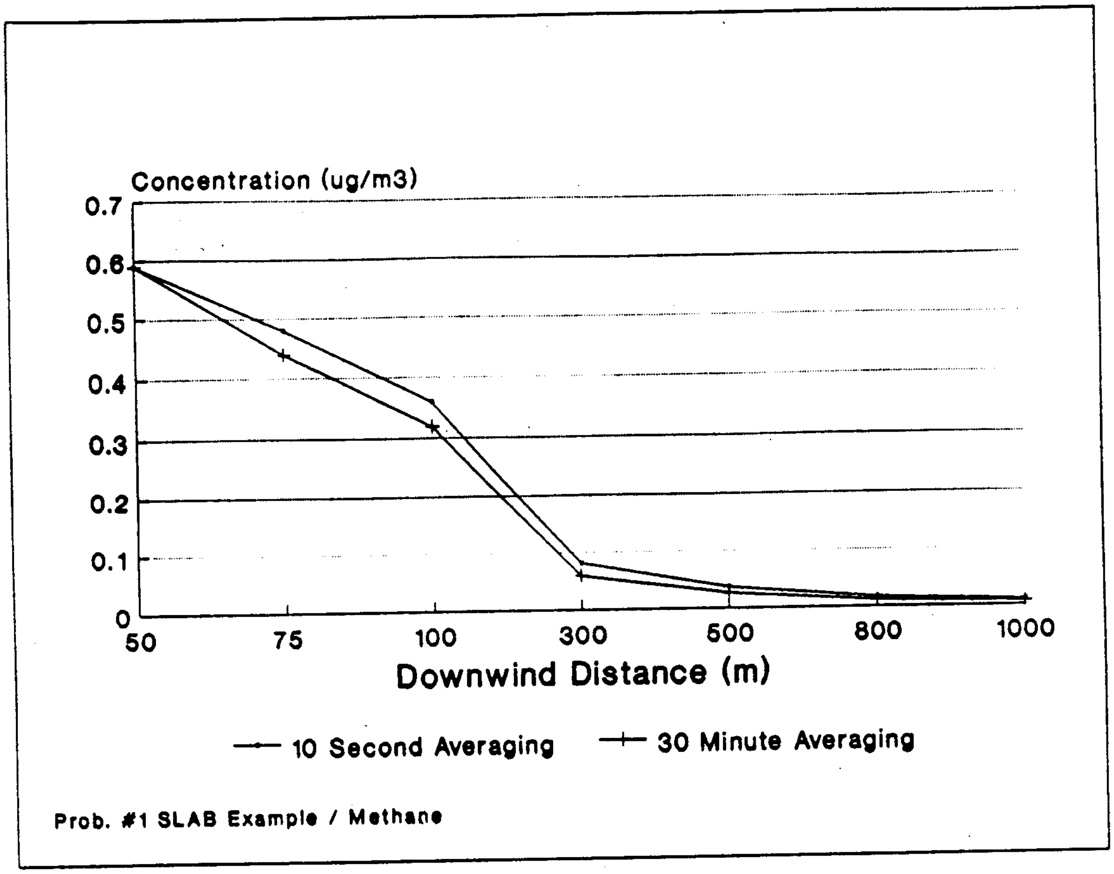


Figure 10. Sensitivity of the Wind Direction Meander Term in SLAB.

Gaussian weighting function in SLAB to be relatively insensitive to averaging time. As density difference and gravity spreading diminishes, the cloud would behave more like a passive cloud. It appears, based on Figure 10, that potentially up to a 15 percent overestimate could occur in the meander term in the first 100 m of travel. There appears to be a need to follow-up further on this point in Phase II.

Sensitivity testing was done to determine if high wind speeds could pose a potential problem because research showed narrow dense gas plumes during high wind speed periods. Figure 11 shows the significance of the meander term for a rather extreme, 20 m/sec wind speed. It was found that differences still were within approximately 10-15 percent of the 10 second averages.

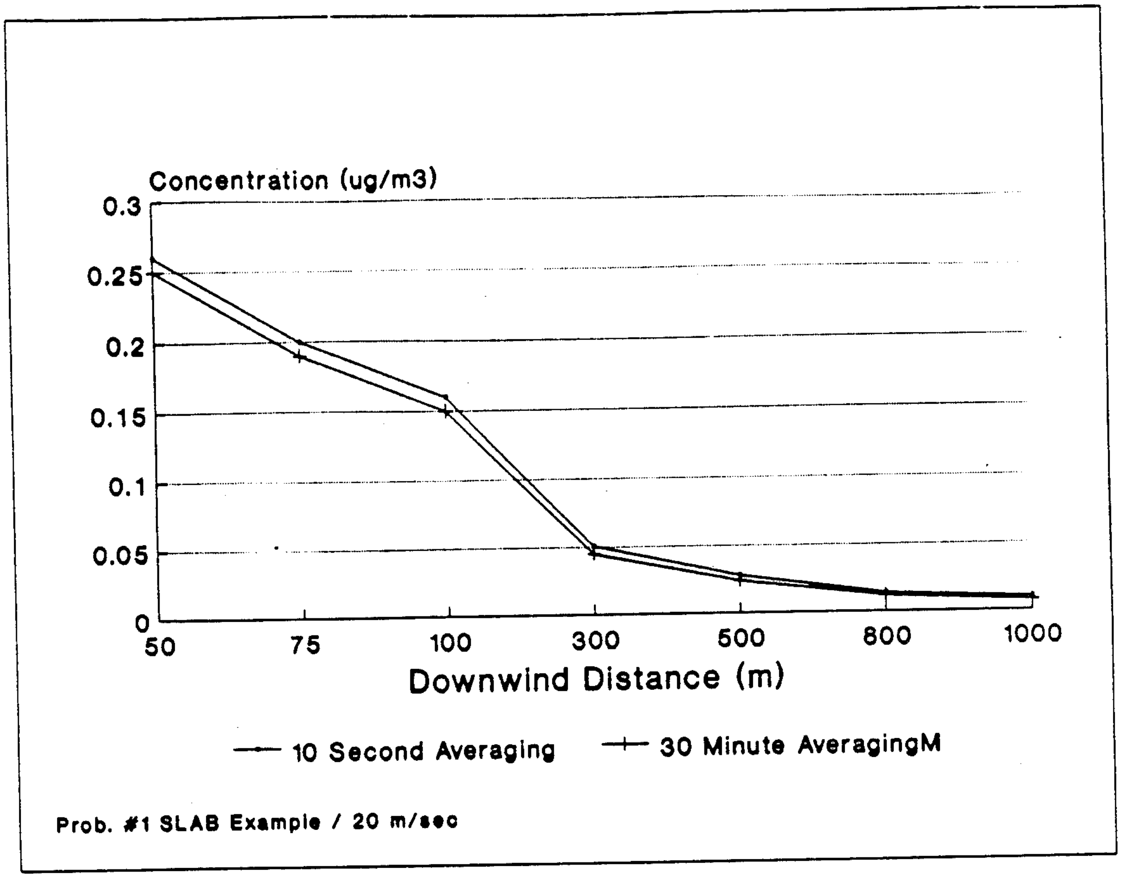


Figure 11. Sensitivity of the Wind Direction Meander Term in SLAB During High Wind Speed Conditions.

In summary, follow-up is recommended for Phase II. Since 30-minute averages are needed for the Air Force emergency response procedures, more confidence is needed that this term does not result in underestimating concentrations for some applications. It appears, however, that only minor differences in model output will result from refinements to the meander term.

A related question, which also needs further consideration, is the definition of acceptable concentrations as a function of averaging time. The Air Force emergency response procedures currently are based on 30-minute exposures. How well does this approach represent longer or shorter duration episodes. Ideally, it would be preferable to relax the threshold for short exposures and tighten the threshold for longer duration exposures. Perhaps consideration of acceptable ceiling concentrations and integrated dose would be a preferable approach for pollutants that are time dependent.

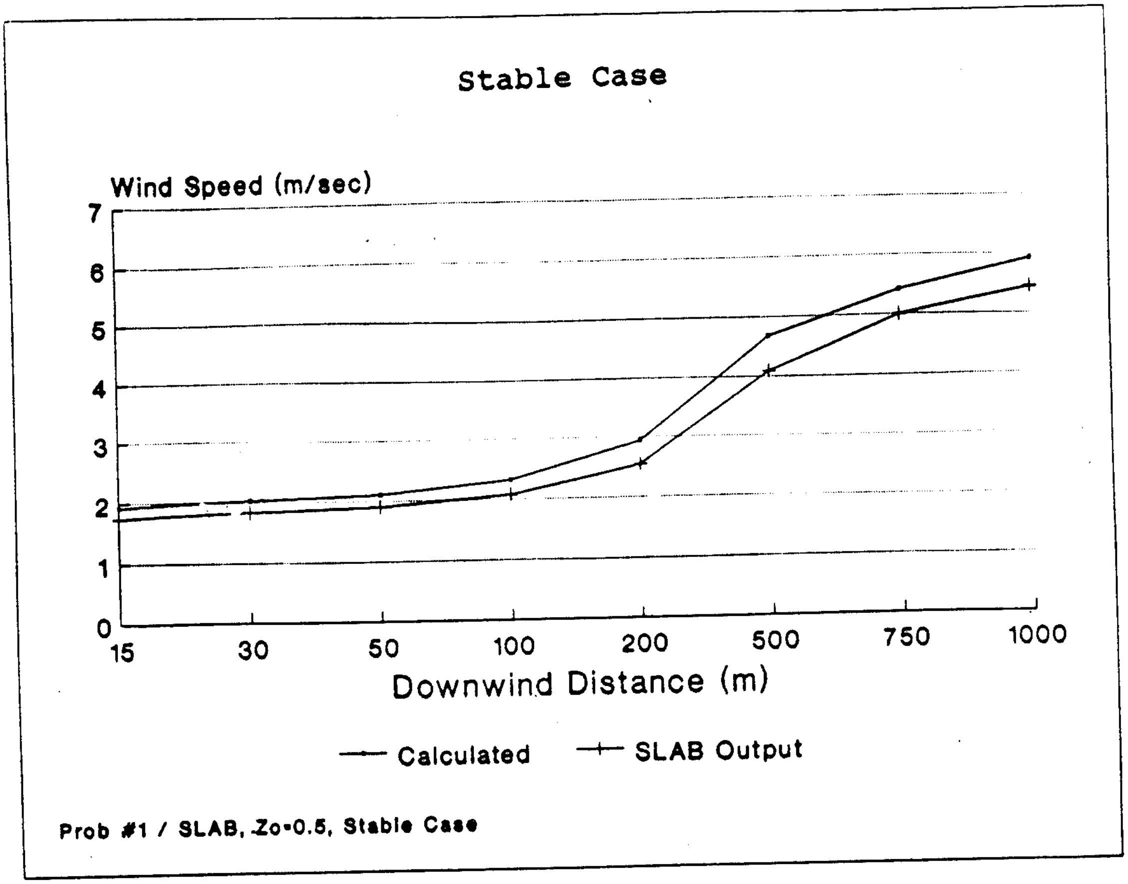
The Committee on Toxicology of the National Research Council takes the approach for time dependent pollutants of establishing an acceptable exposure for the shortest exposure of interest (26). In its simplest form, the product of concentration times time is treated as a constant in order to estimate acceptable concentrations for longer duration exposures (26). If applicable for the pollutant of interest, this approach could relax acceptable exposures for durations less than the current 30-minute SPEGL's and tighten acceptable exposures for longer duration episodes. In this manner, the acceptable health criteria could be made more consistent with the exposure modeling conducted within the emergency modeling system. In short, the uniform 30-minute SPEGL may be an unnecessary simplification for the emergency modeling system that could be developed in Phase II. This is a difficult problem, but an issue that should at least be reevaluated in Phase II to ensure that overly restrictive hazard corridors are not established for short-duration incidents, and unprotective corridors are not set for longer duration incidents.

D. WIND SPEED PROFILE

A review of the SLAB code indicated that Monin-Obukhov turbulent scaling theory was used to extrapolate wind speeds from instrument exposure height to cloud midpoint height. The procedure used in SLAB was reviewed, and SLAB output was compared with manual calculations based on Reference 11. Figure 12 shows the results. The two approaches compare reasonably well, however, 10-15 percent differences are shown. These treatments should be reevaluated in Phase II to refine the procedure, as necessary.

E. SOURCE TERM

The source release rate can be a complex term. For example, for a spill the evaporation rate can be a complicated function of ground surface temperature, ambient temperature, vapor pressure, wind speed and surface roughness. Applications of SLAB can simplify the source term for a spill by effectively assuming that the evaporation rate equals the spill rate. There is no function to compute an emission rate in SLAB. As the surface cools, however, the evaporation rate likely diminishes significantly (5).



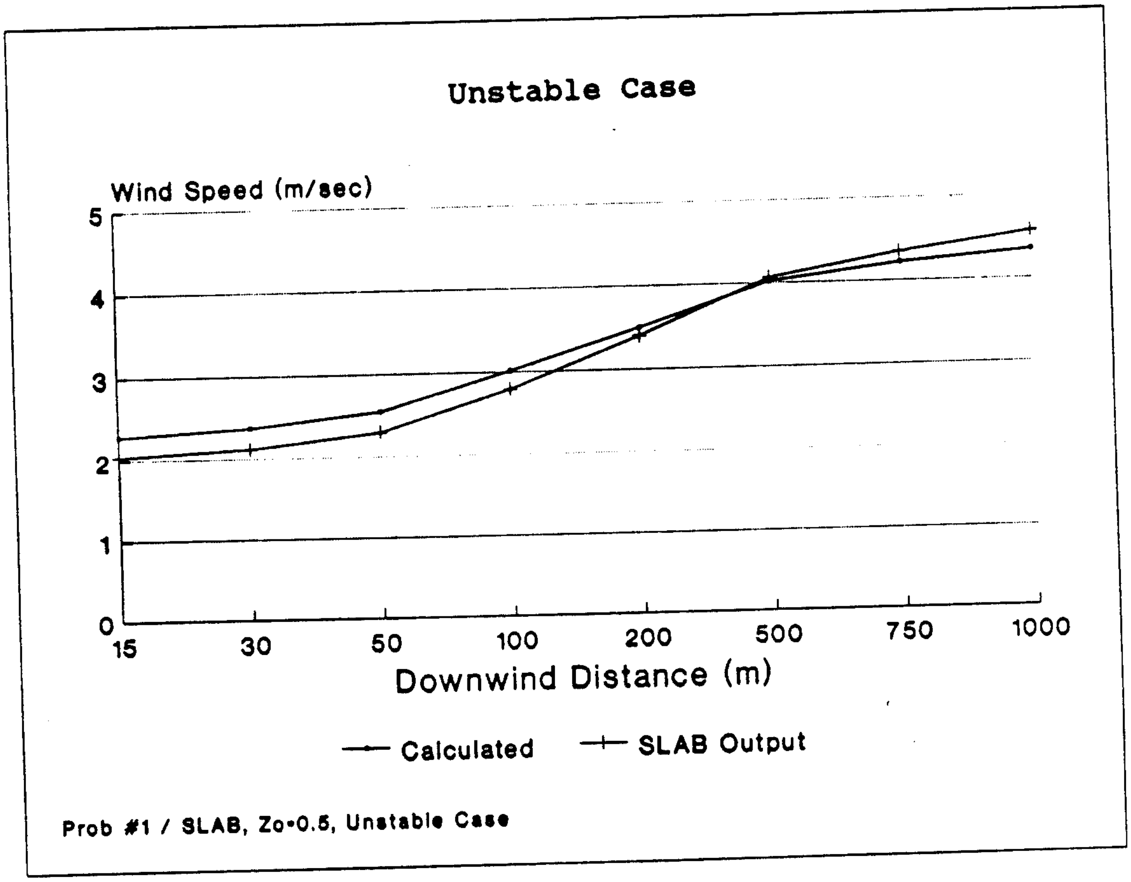


Figure 12. Calculated Wind Speed Profiles Versus SLAB Output.

The current version of SLAB can conservatively represent the emission rate, but the source term may be unnecessarily conservative for Air Force applications, especially since 30-minute averaging periods are critical. If average emission rates during a 30-minute period, for example, were substantially overestimated by SLAB, it is possible that Tier I and Tier II corridors would be too large, which could unnecessarily restrict Air Force operations. The decrease in the source term as a function of time may not be as significant for the field testing of SLAB (e.g. the Coyote and Burro series) (7). For these tests (7), overwater releases were used, where surface cooling likely would not be as significant as for a ground surface.

The goal of the failsafe approach is to minimize the potential to underestimate concentration without unnecessarily increasing the size of hazard corridors. It is necessary to minimize the potential to underestimate concentrations and risks for applications that may be particularly sensitive to some model components. It is equally important, however, to avoid overly conservative assumptions. This is an important point for further review in Phase II. Two actions are recommended:

1. Provide guidance to estimate the spill rate as a function of tank/pipe rupture size, and other relevant parameters.

2. Evaluate the feasibility of providing a model option to refine the source term, relative to the present conservative treatment. Consider the feasibility of incorporating a source term similar to that used in the ADAM model (5), or a fast-response parameterization that adequately accounts for the most sensitive factors in the source term. Phase II should consider all ongoing work by the Air Force on emission rate modeling.

F. REACTIVITY

SLAB considers phase changes of pollutants and water vapor, but the current code does not consider reactions. For Air Force applications, reactivity is potentially important for a pollutant such as N_2O_4, which dissociates rapidly in the atmosphere to form NO_2. In the case of N_2O_4, the differences in toxicity between parent and daughter compounds may not be important because it could be assumed that all of the N_2O_4 reacts to form two moles of NO_2. Of potentially greater concern would be the endothermic reaction of the N_2O_4 to NO_2 conversion, which could affect the buoyancy term in the model. By testing the sensitivity of relative humidity, a term that affects buoyancy, it was found for heavy molecular weight compounds, such as N_2O_4, that SLAB was relatively insensitive to buoyancy effects. The effect of reactivity on the buoyancy term, therefore, does not appear to be a major issue for model applications involving heavy molecular weight pollutants. Another issue that should at least be considered in Phase II is the scenario of liquid fluorine transportation accidents. This pollutant reacts with water to form hydrogen fluoride, which is somewhat less toxic than the primary release.

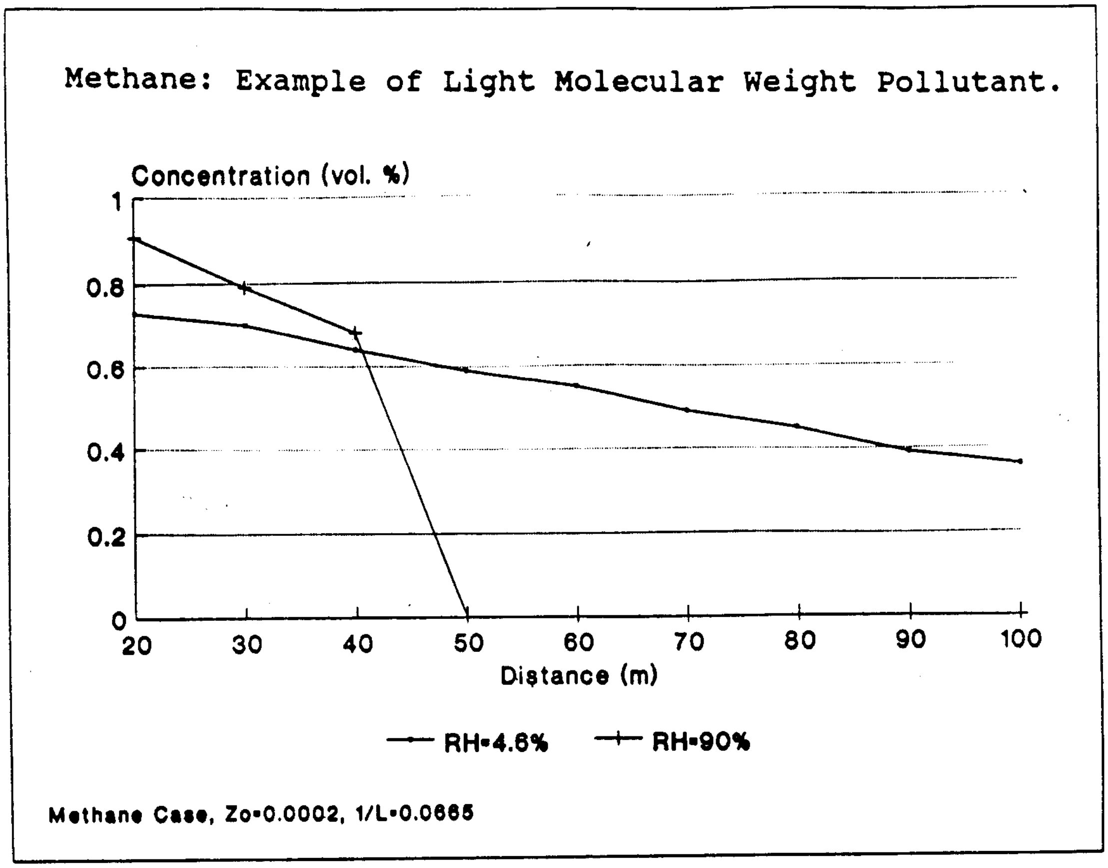
In Phase II, it would be recommended that the modeling system be adapted to at least correct the stoichiometry (e.g. 2 moles of NO_2 per mole of N_2O_4) but not to specifically consider reactivity at this time. Reactivity may warrant further review in Phase II if the final pollutant list for model development includes pollutants where buoyancy changes during reaction would significantly alter model output, e.g. for pollutants with molecular weights less than ambient air (molecular weight 28). Another reason to specifically include reactivity would be if parent and daughter compounds had substantially different toxicity. If necessary, the treatment in ADAM, or alternative treatments under current development, would be considered for adaptation to the modeling system.

G. RELATIVE HUMIDITY

Relative humidity is input to SLAB because the latent heat released during the phase changes of water vapor to liquid droplets within the cloud can be an important contribution to cloud buoyancy. The extremely cold temperatures of some dense clouds can cause condensation of the water vapor within the cloud, with the latent heat associated with the phase change then warming the cloud. As the cloud is transported downwind, it entrains air, and is warmed by surface heating. The cloud temperature eventually approaches ambient temperature, and condensed water can then revert to the vapor state, which in turn cools the cloud.

The sensitivity of SLAB to relative humidity was evaluated. For pollutants that are lighter than air when warmed to ambient temperature, it was found that the added buoyancy of high humidity greatly affected concentrations in the far-field. The cloud would "lift off" the ground within the modeling domain after it warmed to ambient temperature. Heavy molecular weight pollutants that are denser than air when warmed to ambient temperature, on the other hand, were not sensitive to relative humidity. Figure 13 shows examples of the sensitivity to relative humidity of methane (light molecular weight pollutant) and N_2O_4 (heavy molecular weight pollutant).

These comparisons show that the accuracy of relative humidity data input to SLAB can be important for light molecular weight pollutants. Methane and ammonia are examples of potentially affected pollutants. Light molecular weight pollutants may not be top priority pollutants for Air Force applications, but it is important to ensure that the emergency response modeling system has failsafe features for all pollutants that could be addressed. If joint agency / industry efforts could occur in Phase II, or


Methane: Example of Light Molecular Weight Pollutant.

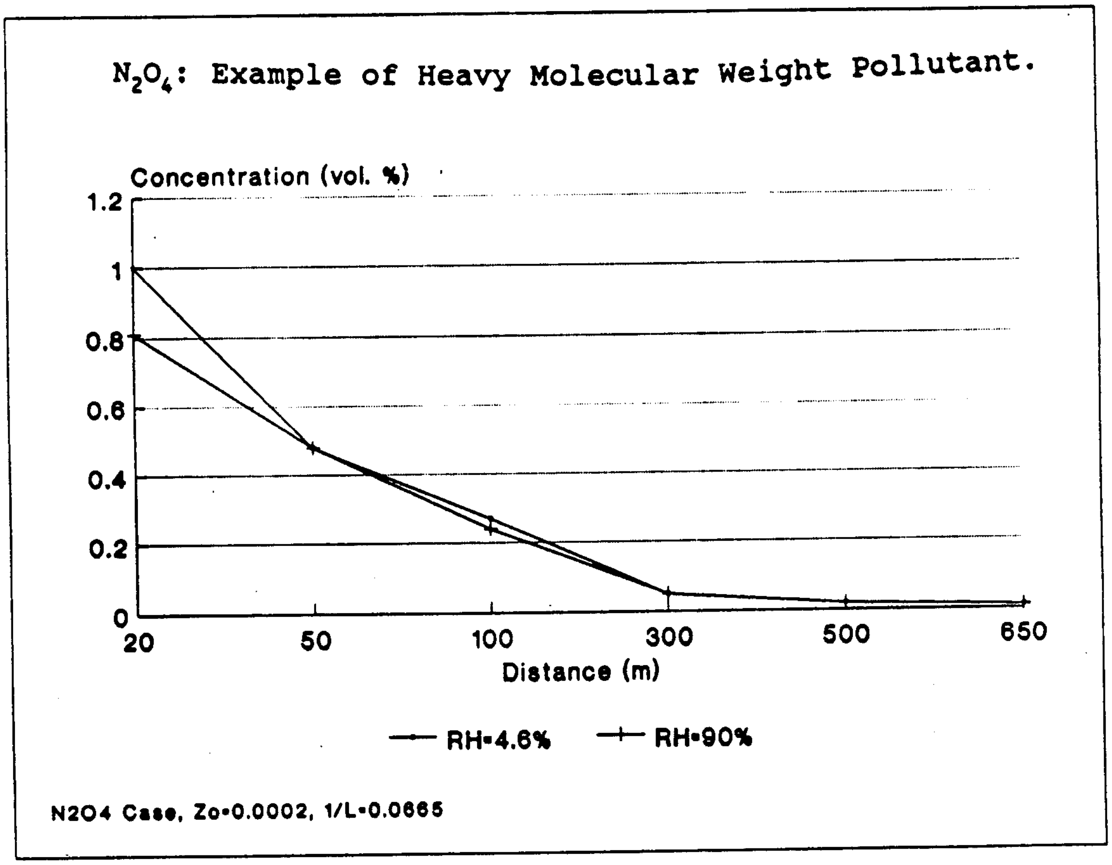

N_2O_4: Example of Heavy Molecular Weight Pollutant.

Figure 13. Sensitivity of SLAB to Relative Humidity.

beyond, this issue may deserve further review, even if Air Force priority pollutant lists do not include light molecular weight compounds.

For light molecular weight compounds there are two major concerns: (1) instrument accuracy, and (2) profiles of relative humidity:

1. Instrument Accuracy

Typically, humidity is one of the more difficult meteorological parameters to measure on an automated basis. Wet and dry bulb temperature measurements are generally reliable, but are not readily adaptable to automated monitoring. Dew point temperature is often measured in an automated meteorological monitoring system, but can be prone to sensor malfunction because of the complexity of the cooling cycles of the instrument and other factors. For bases that handle light weight pollutants, including concerns involving spills of jet fuels, quality assurance of parameters used to estimate relative humidity should be carefully reviewed if SLAB would be used to support emergency response actions.

2. Profiles of Relative Humidity

Vertical gradients in relative humidity can be pronounced during stable conditions, i.e. when worst-case dispersion conditions occur (27). Vertical gradients in ambient relative humidity can be a significant function of cloud height, but SLAB treats this term as a constant in the thermodynamics subroutine.

There does not appear to be an overall benefit to increase the complexity of the model to treat relative humidity as variable with height because: (1) there generally would be insufficient data to characterize the vertical gradient in relative humidity, and (2) there is an incentive to keep the model fast-response, and therefore, not to add unnecessary complexity. Especially since the relative humidity term is held constant as a simplification in the thermodynamics, it would require substantial model modification to treat relative humidity as a variable. The objective would be to seek a simple solution to ensure that the vertical profile of relative humidity does not produce a failsafe problem.

The most obvious solution to this potential problem would be to avoid monitoring relative humidity at low-level exposure heights. The current monitoring height for most Air Force monitoring stations is 2-4 m, which may be too low to conservatively represent relative humidity during stable conditions. The cloud could be treated as more humid than actual ambient conditions. For airbases where light molecular weight scenarios are of importance, it would be recommended that a monitoring height of 10 m be used, which would conservatively represent relative humidity during these sensitive stable conditions.

In summary, there are numerous features of SLAB that need to be reevaluated in Phase II to ensure that the failsafe objectives of this project are met. This step must be satisfactorily completed before proceeding to modify the code to include building wake effects and to include an indoor air quality component. Actual changes to the code would be made in coordination with staff of Lawrence Livermore National Laboratory (LLNL), the developers of SLAB, to ensure that the efficiency of the model structure is retained. Also, any refinements to SLAB that are proposed to better meet the objectives of this project will be submitted to the Phase II review committee to seek consensus prior to making any code changes.

Section VI

INDOOR AIR QUALITY MODELING

This section presents a review of modeling issues that need to be considered in developing the indoor air components of the emergency response modeling system. Section VI(A) introduces the mass-balance principles that form the basic framework for indoor air quality models. Underlying principles of air exchange and building leakage are further summarized in Section VI(B). Basic features of leading public-domain models for indoor air quality are summarized in Section VI(C), and considerations to be addressed for incorporating indoor air quality into the overall dispersion model are discussed in Section VI(D).

A. GENERAL MASS-BALANCE FRAMEWORK

The most widely accepted indoor air quality models are based on principles of mass conservation. That is, a mass balance is struck to keep track of material that enters and leaves the airspace in question. Within this conceptual framework, contaminant concentrations are increased by source release from within the defined volume and by transport from other airspaces including outdoors. Similarly, contaminant concentrations are decreased by transport exiting the airspace and, for reactive species, by removal to chemical/physical sinks within the airspace or conversion to other species or forms. The main elements of the mass balance are illustrated in Figure 14.

Relationships are most often specified through a differential equation where contaminant gain (transported input plus sources) and contaminant loss (transported output plus sinks) interact as follows:

$$dM/dt = Vdc/dt = G - LM, \text{ or} \qquad (16)$$

$$dC/dt = G/V - LC \qquad (17)$$

where:

V = volume of the airspace
t = time
M = total contaminant mass in the airspace
C = air concentration of the contaminant (mass per unit volume)
G = rate of contaminant gain (mass per unit time)
L = fractional loss per unit time.

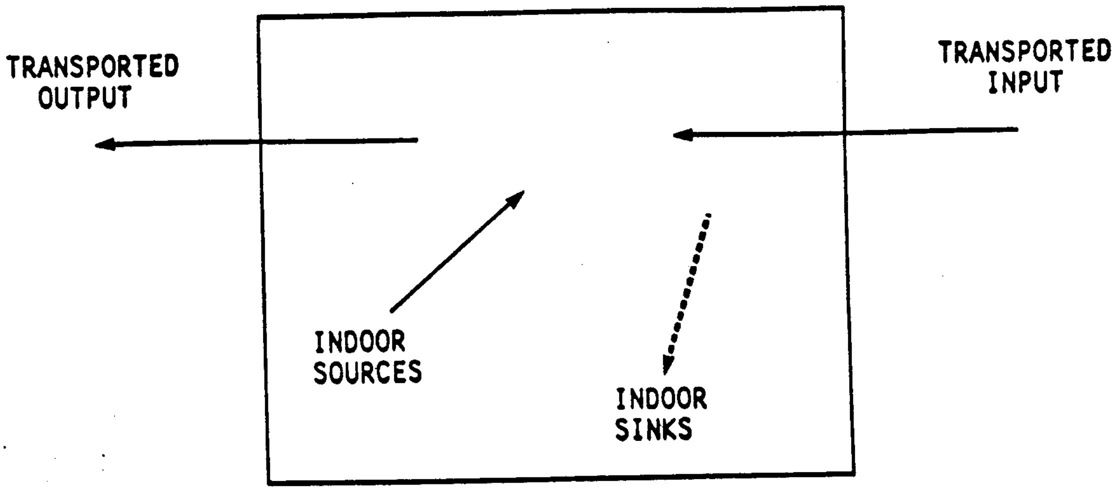


Figure 14. Basic Mass-Balance Relationships.

Under the assumption that mechanisms for loss and gain remain constant for a time interval t_0 to t, the preceding equation may be integrated analytically to give:

$$C_t=C_o e^{-L\Delta t}+\frac{G}{(VxL)}(1-e^{-L\Delta t}) \qquad (18)$$

where C_0 and C_t are, respectively, the initial and final concentrations, and Δt is the elapsed time from t_0 to t.

Algorithms drawn from this basic mass-balance description form the principal framework for simulating contaminant behavior in indoor settings. A National Academy of Sciences report (28) cites Reference 29 as among the first to apply the mass-balance approach. Several years later, Turk (30) applied the mass balance to several different cases and presented a detailed analysis of transient and steady-state behavior. A range of example applications of the mass-balance description is presented in Reference 31.

Single equation mass-balance models have been tailored to examine contaminants in chamber experiments (32,33) as well as in full-scale buildings (34,35). In applying the mass balance to real situations, the generalized mechanisms of contaminant gain and loss must be expanded to acknowledge specific sources, transport, and sinks.

The rate of contaminant gain, G, is related to source emissions and contaminant transport. In the simplest case, involving only an indoor and an outdoor airspace,

$$G = S + Q\ C_{out} \qquad (19)$$

where:

S = emission rate of the source (mass per unit time)
Q = volume flow rate from outdoors (volume per unit time)
C_{out} = ambient concentration (mass per unit volume).

The mass rate of contaminant loss from the airspace of interest is proportional to the concentration as well as the intensity of the loss mechanisms. The fractional loss rate, L, includes transport as well as chemical/physical sinks:

$$L=\frac{Q}{V}+K \qquad (20)$$

where:

Q = volume flow rate exiting the airspace (volume per unit time)
K = removal rate for chemical and physical sinks (per unit time).

The removal rate, K, accounts for contaminant removal other than transport, and is sometimes called simply the decay term. Depending on the contaminant of interest, mechanisms may include radioactive decay, various chemical reaction pathways, reversible / irreversible sinks, or removal by filtration. K is usually treated as a contaminant- and situation-specific first-order rate constant with units of inverse time (i.e., h^{-1}).

As a corollary to the contaminant mass balance, a transport balance must be maintained. The amount of air entering the airspace must be compensated by an equal amount exiting. The air exchange rate, ν, has intrinsic units of inverse time (e.g., h^{-1}). Air exchange is generally stated in air changes per hour (ACH) and is a useful concept for tracking the transport balance and simplifying notation:

$$\frac{Q}{V}=\nu \qquad (21)$$

Thus,

$$\frac{G}{V}=\frac{S}{V}+\nu C_{out} \qquad (22)$$

$$L=\nu+K$$

The general mass balance can be stated more fully as:

$$\frac{dC}{dt}=\frac{S}{V}+\nu C_{out}-(\nu+K)\,C \qquad (24)$$

or,

$$C_t=C_o e^{-(\nu+K)\Delta t}+\frac{(\frac{S}{V}+\nu C_{out})}{(\nu+K)}(1-e^{-(\nu+K)\Delta t}) \qquad (25)$$

As outdoor air enters the building, a certain fraction of the contaminant (FB) may be intercepted by the building envelope and air cleaning equipment, resulting in a filtration or scrubbing effect. When this concept is incorporated into models, the outdoor infiltration term becomes $\nu(1-F_B)C_{out}$.

Equation 25 operates through the assumption of perfect mixing. That is, emissions are assumed to be rapidly dispersed throughout the geometric volume defined by walls, floors, and ceilings, and the air exchange process is assumed to be equally effective everywhere in the airspace. Where air circulation patterns limit dispersal and mixing, the concepts of effective volume and mixing factor can be applied separately or together to treat these conditions (31).

The effective volume cV defines the volume that is actually involved with pollutant dispersal. The value of c is unity when the entire volume is involved (as when a fan encourages complete mixing).

Similarly, to relate imperfect mixing to the air exchange process, the mixing factor can be introduced. As with effective volume, the mixing factor (generally denoted by m) modifies the air exchange rate to give the effective air exchange rate, $m\nu$. In classical terms, the mixing factor is the ratio of actual residence time (corrected for decay processes) to that derived from the air exchange rate (36). It can also be expressed as the ratio of the concentration in the exit stream to the indoor concentration when mechanical ventilation systems are at work. The value of the mixing factor is a function of position with respect to air movement patterns, and can exceed unity under strongly stratified conditions.

The mass balance model is frequently called the single-chamber model. In this description, pollutant transport is dominated by air exchange with the outdoors and is useful for modeling single rooms and buildings that are well mixed. When a building must be treated as a network of interconnected volumes, separate mass balances are struck for each indoor volume and a system of simultaneous equations results (37,38).

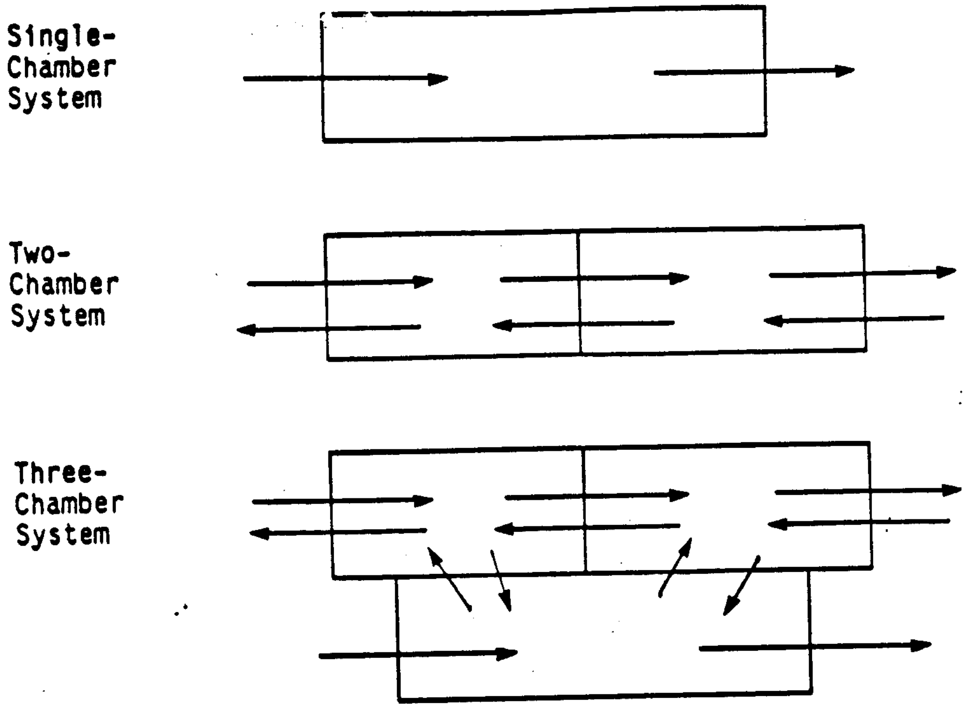
In a single-chamber system, only the infiltration / exfiltration airflow requires specification. For multiple-chamber systems, however, each chamber requires specification of interchamber airflows as well as infiltration/exfiltration. As shown in Figure 15, a two-chamber system is characterized by six airflows, and a three-chamber system is characterized by twelve airflows. Generalizing, a system composed of N interconnected chambers requires (N + 1) • N airflows to be specified.

With the added complexity, notation is augmented to clearly identify features (Figure 16). For the "ith" compartment of the system, Equation 25 becomes:

$$\frac{dCi}{dt} = \frac{S_i}{V_i} + Q_{oi}C_{out} + \sum_{i \bullet j}^{n} \frac{Q_{ji}C_j}{V_j} - \left(\frac{Q_{io}}{V_i} + \sum_{i \bullet j}^{n} Q_{ij} + K_i \right) C_i \qquad (26)$$

where:

Q_{oi} = volume flow rate from outdoors
Q_{ji} = volume flow rate from the "jth" chamber to the "ith" chamber
Q_{ij} = volume flow rate from the "ith" chamber to the "jth" chamber.



N Chamber System Requires (N + 1) • N Airflows

Figure 15. Airflows for Multiple-Chamber Modeling.

B. AIR EXCHANGE

1. Theoretical Framework

The major factors responsible for the infiltration of air into a structure are well understood from a theoretical perspective. The relationships underlying mathematical models of air infiltration have been reviewed by the Air Infiltration and Ventilation Centre (AIVC) (39), established by the International Energy Agency. The summary that follows is based in large part on the AIVC review.

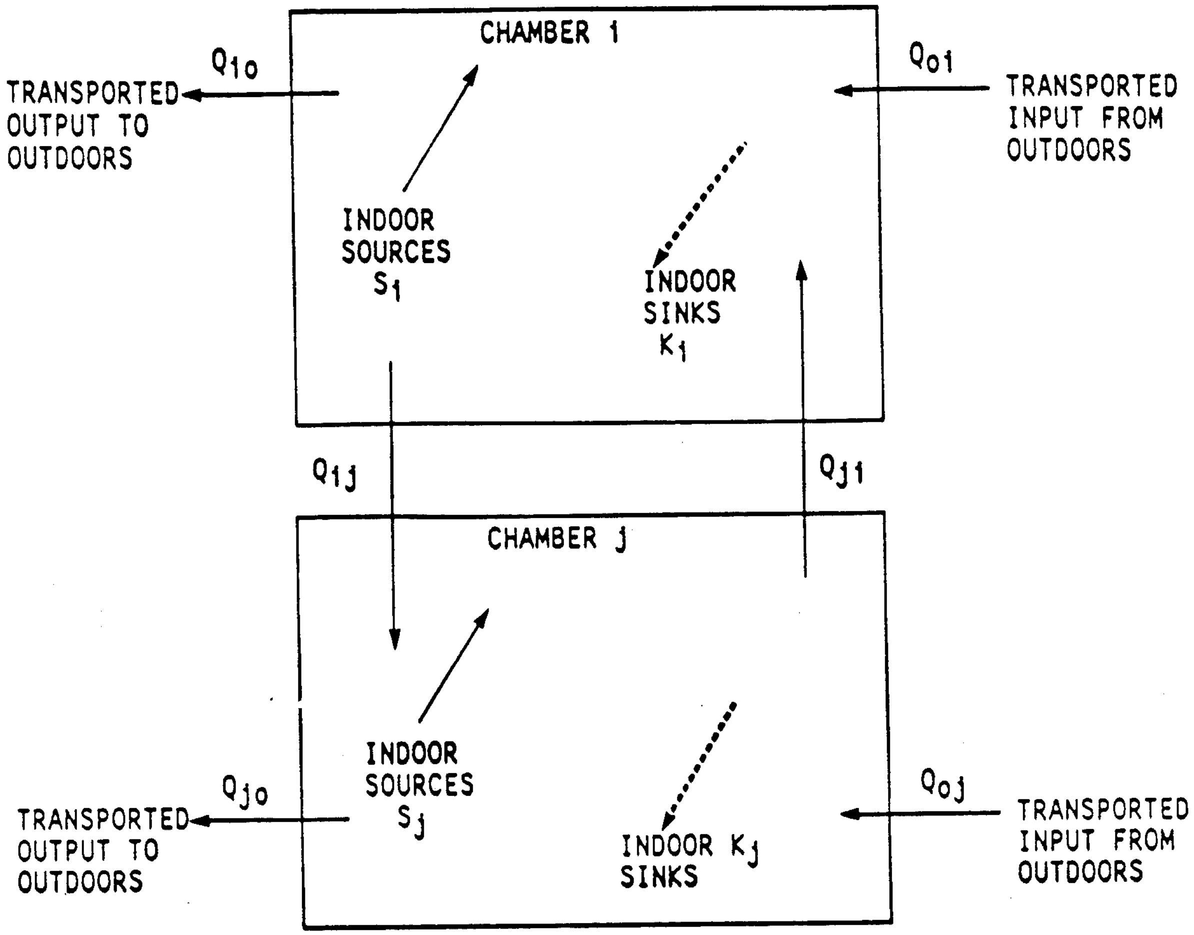


Figure 16. Basic Mass-Balance Relationships for Multi-chamber Approach.

The flow of air through openings in a building can be expressed by the equation:

$$Q=k(\Delta P)^{n} \qquad (27)$$

where:

k = a flow coefficient (m^3/sec at 1 pascal)
n = a flow exponent
ΔP = is the pressure difference across the opening (pascals)

Q = the flow rate through the opening (m^3/sec).

The flow coefficient is related to the size and geometry of the opening, along with the flow rate. The flow parameters for a building can be determined from leakage tests on individual components, from published values such as those provided by Reference 40, or from leakage characteristics determined by pressurization tests for the entire building.

The pressure differences that drive the air infiltration process are caused by the action of wind and stack effects. The wind effect is given by:

$$P_w = \left(\frac{\rho}{2}\right) C_p v^2 \qquad (28)$$

where:

P_w = pressure on the exterior of the building (pascals)
ρ = air density (kg/m3)
C_p = pressure coefficient
v = wind speed (m/s).

The pressure coefficient is a function of location on the building exterior, building shape, and the surrounding terrain. Most information on such coefficients is from wind tunnel tests on scale models of isolated buildings or simple arrangements of buildings. AIVC recently announced the availability of CPBANK, a data base of wind pressure coefficients for prevalent building shapes accumulated through years of wind tunnel testing (41).

The stack effect arises as a result of differences in temperature between a building's interior and exterior. These differences produce an imbalance in the pressures exerted by the internal and external air masses, thereby creating a vertical pressure gradient. When delta T (indoor-outdoor temperature) is positive (i.e., warmer indoors), air tends to enter through openings in the lower part of the building and escape through openings at higher levels. The flow direction is reversed when delta T is negative. The level at which the transition from inflow to outflow occurs is called the neutral height. The pressure difference resulting from stack action between two vertically displaced openings is given by:

$$P_s = \rho_o h \left(\frac{1}{T_o} - \frac{1}{T_i}\right) \qquad (29)$$

where:

ρ_o = the air density at 1/2 (T_o + T_i) and ambient pressure
h = the vertical distance between openings (m)
T_o and T_i = outdoor and indoor temperatures, respectively (K).

2. Air Infiltration Models

Mathematical models of air infiltration based on the above relationships range from single-cell or single-chamber approaches to multi-cell methods. Where appropriate, the actions of mechanical ventilation systems are readily incorporated. The single-cell approach assumes the building to be at a single internal pressure, whereas the multi-cell methods partition the interior into individual rooms or sections. Single-cell models can be used to predict whole-building air exchange rates and are therefore useful for energy calculations. However, they do not consider air movement within a building. Although multi-cell approaches provide much useful information, they require substantial data to describe the internal flow network and can involve complex computations. Only in limited situations, such as multiple story buildings that are relatively close to potential release areas, would multi-cell analysis be necessary for this emergency modeling system.

A variety of mathematical models for air infiltration exist; a number of these models have been reviewed and compared, for example, in reference 42. The latest model, COMIS (Conjunction of Multizone Infiltration Specialists), is a modular model produced through a multinational team approach (43). Available models share a similar theoretical basis in that they all address the indoor-outdoor pressure difference during the infiltration process, which is maintained by the action of wind and stack effects. In general, these models take the form of a flow network whereby nodes representing regions of different pressure are interconnected by leakage paths. Models generally differ in the level of detail such as the number of nodes they treat or the specifics of leakage paths (e.g., individual components such as cracks around doors or windows versus a combination of components such as entire sections of a building). Such models, however, may not be readily adapted to the emergency modeling system because the inputs required (e.g., leakage areas, crack lengths) cannot be easily gathered by the typical user.

A more practical approach for the emergency modeling system would be to estimate air infiltration rates through the use of empirical models. Such models typically rely on collection of infiltration measurements under a variety of weather conditions; the relationship between infiltration, windspeed, and temperature difference is estimated through techniques such as regression analysis and is typically stated in the following form:

$$ACH = a + b|T_i - T_o| + cU^n \qquad (30)$$

where:

ACH = infiltration rate, h^{-1}
$|T_i - T_o|$ = absolute value of the indoor-outdoor temperature difference (C)
U = windspeed, m/s
n = exponent with a value typically between 1 and 2
a, b and c = parameters to be estimated.

Relatively good predictive accuracy can usually be obtained for individual buildings through this type of empirical approach, and seasonal or annual average infiltration rates can be calculated using average temperature and windspeed compiled from local meteorological data. The preferred approach to estimate infiltration rates for this project would be to select on the order of 10 "model" structures, which would form a data base to estimate infiltration for other similar buildings at the base. At least 2-3 field programs would be done for a range of meteorological conditions to establish appropriate coefficients. This approach would be effective, and not expensive. If 3-4 priority airbases were evaluated on this basis, the data base could be generalized for the structures at lower priority airbases.

In the future, further review may be warranted to evaluate the potential differences in infiltration and exfiltration rates for dense and non-dense gas clouds. This potentially is a Tier I (near-field) issue. The infiltration of dense gas clouds could be faster that passive infiltration, and the lower floor and basements could "fill" until the pollutants are warmed to ambient temperature and are transported in the manner of a passive gas. The differences between passive and dense gas air exchange rates likely are a function of service opening status. This issue could be evaluated by GEOMET, based on theoretical grounds, and possibly comparative infiltration experiments. Differences between the movement of dense and passive gases into structures could be important for the decision to shelter-in-place or evacuate affected buildings.

3. Air Exchange Data

Air leakage in buildings has been a subject of active research for over 40 years. Extensive field measurements, however, were not contemplated until the energy crises of the 1970s strengthened the economic incentives to reduce air leakage. Since then, research issues have also embraced indoor air quality and maintenance of human comfort, broadening the objectives for measurements in all types of buildings. This section briefly summarizes the range of observed air exchange rates.

Residential buildings have received the most attention. In the early 1980s, researchers at the Brookhaven National Laboratory (BNL) disclosed a convenient technique for measuring air exchange and internal airflows using diffusion-based release and sampling of perfluorocarbon tracers (PFTs) (44). Since then, the PFT technology has been used in over 100 separate research projects with BNL serving as the analytical laboratory. Resulting data from over 4,000 residences was recently assembled into a data base by BNL, Versar, and GEOMET (45). Summary analysis of the data indicates that air exchange rates in residential buildings range over a full order of magnitude, from 0.14 ACH for fairly tight homes to 1.9 ACH for fairly leaky homes. The median air infiltration rate is at 0.43 ACH. These observations are consistent with the range suggested in standard references (40).

Although interest is growing, relatively few air exchange measurements have been conducted in non-residential buildings. Grot and Persily (46) studied eight newly constructed office buildings, observing a range similar to those found in residences (Table 4). More recently, Turk et al. (47) studied 38 non-residential buildings in the Pacific Northwest, reporting a range of 0.3 to 4.2 ACH with an average of 1.5 ACH (Figure 17).

Very few measurements of air exchange have been taken in large open buildings such as aircraft hangars. Ashley and Lagus (48) carried out tracer gas measurements, however, at Air Force and Naval facilities located in California, Maine, North Dakota and Virginia. Measured air exchange rates (Table 5) are comparable to those shown in Reference 47 for large offices and other non-residential buildings. The data in Table 5 were collected with hangar doors closed. The high ACH for Minot, North Dakota is attributed to an open hangar door during testing, and should be considered an outlier. As shown through this example, service opening status at the time of cloud approach is important for implementing Air Force emergency response procedures, as it greatly affects decisions to evacuate or shelter-in-place.

Air exchange rate data are normally collected with operable doors and windows closed so that measurements reflect air leakage (or, in the case of larger buildings, air leakage plus mechanical ventilation). Relatively few experiments have been reported concerning natural ventilation. Reference 49 reports the effects of various patterns of window openings in a British home. They found that under moderate winds (9 mph), air exchange rates would triple when either windward or leeward windows were opened; opening all windows provided an eightfold increase. In the study of aircraft hangars cited above, Ashley and Lagus (48) found that opening a single panel of the main doors on the downwind end of one hanger offered only marginal effect (0.75 ACH versus a previous

TABLE 4. MONTHLY AVERAGE VENTILATION RATES (Source: Reference 46)

Month	Anchorage[b]	Ann Arbor[c]	Columbia	Fayetteville[d]
January	0.46	0.47	0.64	0.32
February	0.46	0.47	1.09	0.32
March	0.46	0.47	1.09	0.35
April	0.75	1.96	1.10	0.35
May	1.10	1.94	0.69	0.65
June	1.22	0.94	0.68	0.36
July	1.22	0.50	0.68	0.36
August	1.22	0.50	0.68	0.36
September	1.22	1.94	0.68	0.36
October	0.75	1.96	1.10	0.35
November	0.46	0.86	1.09	0.35
December	0.46	0.47	0.64	0.32

Month	Huron	Norfolk	Pittsfield[e]	Springfield[e]
January	0.26	0.70	0.40	1.00
February	0.26	0.70	0.40	1.00
March	0.32	1.05	0.38	0.95
April	0.14	1.00	0.67	0.76
May	0.52	0.75	1.25	0.62
June	0.53	0.58	0.50	0.59
July	0.16	0.58	0.50	0.59
August	0.53	0.58	1.19	0.59
September	0.52	0.75	1.25	0.62
October	0.13	1.00	0.67	0.76
November	0.32	1.05	0.84	0.96
December	0.26	0.70	0.40	1.00

[a] All the ventilation rates are in units of exchanges per hour.

[b] Based on outside temperatures from Homer, AK.

[c] Based on an average of outside temperatures from Flint and Detroit, MI.

[d] Based on outside temperatures from Ft. Smith, AR.

[e] Based on outside temperatures from Hartford, CT.

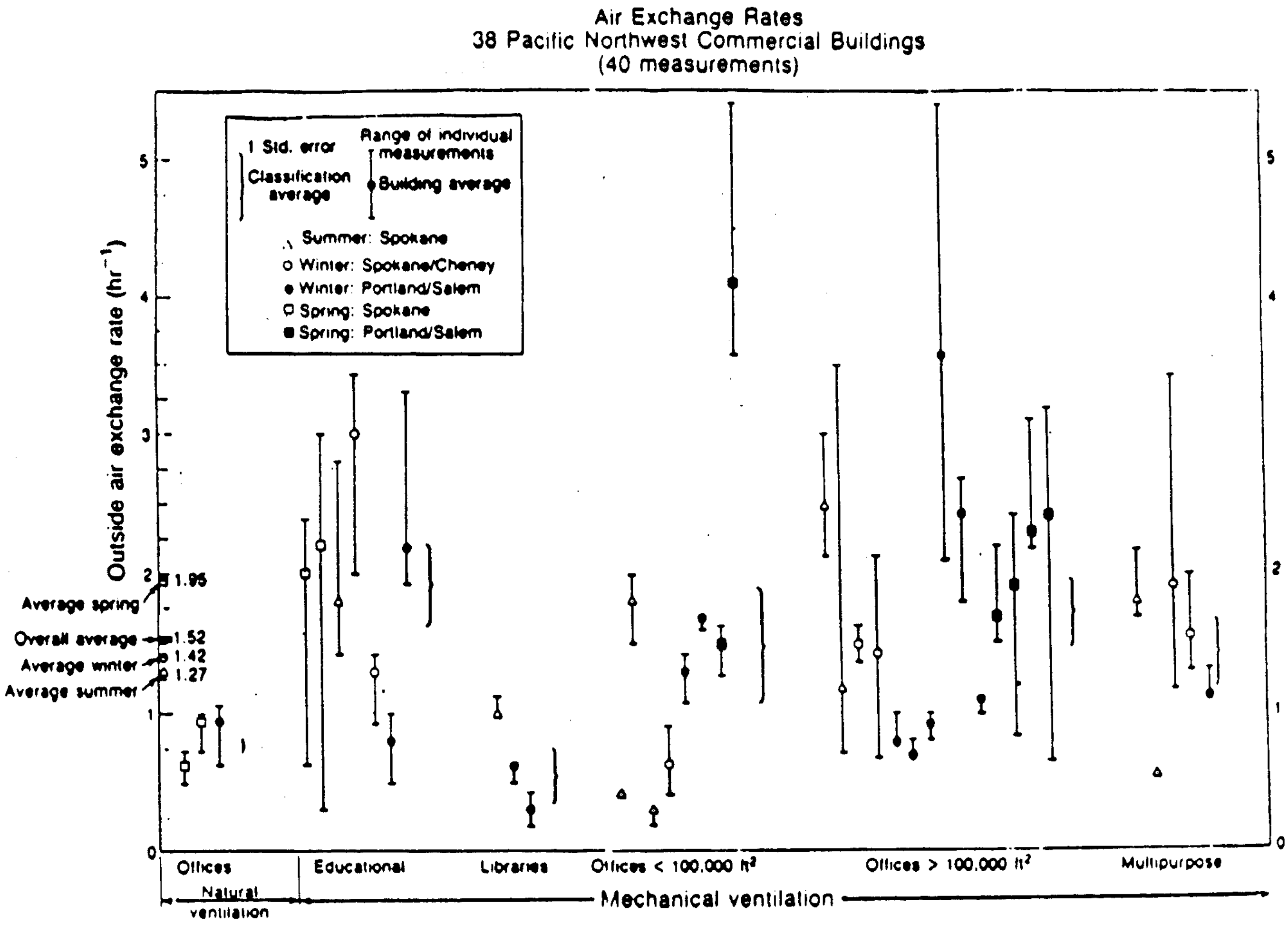


Figure 17. Ventilation Rates Classified By Building Type (Source: Reference 47)

closed-hanger observation of 0.6 ACH). Opening one section at each end of the hangar, however, increased the air exchange rate tenfold (6.3 ACH).

C. INDOOR AIR QUALITY SOFTWARE MODELS

Indoor air quality models usually are developed to meet specific purposes, and therefore, reflect the technical objectives, user sophistication, and reporting requirements related to the originating needs. Converting such models to alternative purposes often requires either a reworking of the original implementation or a compromise of the new use.

Given the relative simplicity of the mass-balance framework, it is not surprising that indoor air quality models have proliferated in the desktop or personal computing environment. Although software code has been developed for implementation in the minicomputer environment (see, for example, Reference 35), the availability of standard programming languages and compilers readily supports upwardly and downwardly compatible translations.

For this project, we are interested in public domain models that could be adapted to the needs of the emergency response modeling system without invading proprietary rights. From previous work (50), it is apparent that there are at least three models that meet this requirement, while representing the higher end of the state-of-the-art:

> CONTAM--developed by researchers at the National Institute of Standards and Technology (formerly the National Bureau of Standards) with support from the U.S. Environmental Protection Agency and the U.S. Department of Energy (51,52,53).
>
> INDOOR--developed by researchers at the Indoor Air Branch of the U.S. Environmental Protection Agency's Office of Research and Development (54).
>
> MCCEM--developed by GEOMET researchers for the U.S. Environmental Protection Agency's Office of Toxic Substances (55,56).

Table 6 summarizes the key features of these models.

1. CONTAM

The CONTAM indoor air quality model was developed by

TABLE 5. MEASURED AIR EXCHANGE RATES IN AIRCRAFT HANGARS (Adapted From Reference 48)

Facility	Volume (m^3)	Air Exchange (ACH)
Norfolk, VA	96,220 66,222	1.3 0.7
Minot, ND	28,158	2.3
McClellan AFB, CA	24,621	0.6
Brunswick, ME	2,410	0.8

*Adapted from Ashley and Lagus (1986).

researchers at the Building Environment Division of the National Institute of Standards and Technology (NIST) to simulate pollutant movement and concentration variation in buildings. The developmental effort has been supported under interagency agreement with the U.S. Environmental Protection Agency, with additional support from the U.S. Department of Energy. Model formulations and testing are described in two major reports (52,53). Ongoing refinements were recently summarized (57).

This model is capable of treating multiple contaminants, sources, and zones. Relevant features of CONTAM 87 include the following.

Airflows - In the terminology of the model, directional airflow from one chamber to another is called a flow element. Flow elements may be specified as either simple flow (consistent with instantaneous and complete mixing) or convection-diffusion flow (to treat imperfect mixing). The magnitude of the flow elements may be varied over time. Time histories composed of discrete time intervals are defined by specifying an initial and final time and a system of flow elements for each interval. This option provides the capability of modeling time-variant airflows such as would occur with heating, ventilation, and air conditioning (HVAC) systems. Each flow element may be assigned a filter efficiency for each chemical being modeled. This feature is useful if a chemical is likely to be partially removed by filters in the air handling system, which could be a precautionary measure for structures that

TABLE 6. SUMMARY OF FEATURES OF INDOOR AIR QUALITY MODELS.

Features	CONTAM	INDOOR	MCCEM
User interface	Command processor	Menu	Menu
Zones/spaces	Multiple	Multiple	Multiple
Contaminants	Multiple	Single	Single
Sources			
Multiple	Multiple	Multiple	Multiple
Initialized indoor levels	Yes	Yes	Yes
Outdoor levels	Yes	Yes	Yes
Release mechanisms			
Simple emission factors	Yes	Yes	Yes
Pre-formatted emission function	No	Yes	No
User-specified emission function	Yes	No	Yes
Sink effects			
First order decomposition	Yes	No	Yes
Deposition velocity	Indirect	Yes	No
Re-emission	Indirect	Yes	No
Infiltration	Time schedule	Constant	Constant
Interzonal transport	Time schedule	Constant	Constant
Exposure	No	No	Yes

are not self-contained and could be in relatively high impact areas in the event of an accident at a base.

Emissions - Species-specific contaminant generation rates can be assigned to each chamber, however, indoor sources are not within the scope of this project. More importantly, the user can specify outdoor concentrations to any desired level of detail through the time-scheduling framework.

Sink Effects - Chemical and physical transformations and sinks are handled by defining one or more sets of contaminant-specific rate terms, and then assigning specific sets of rate terms to specific chambers. This approach allows straightforward treatment of special circumstances (e.g., a catalytic process unique to one chamber) as well as generalized processes (e.g., first-order decay). The sinks for nitrogen tetroxide, which disassociates to form NO_2 should be studied in greater detail in Phase II. Indoor sinks for NO_2 could have a major effect on decisions to evacuate or shelter-in-place. There is a considerable data base on NO_2 sinks, however, the rates of loss likely are quite variable among building types. Residential structures, for example, could have a substantially different sink for NO_2 than aircraft hangars. An effective modeling system, would need to consider available data on NO_2 sinks to best guide evacuation or shelter-in-place decisions. As for many complex issues that will need to be considered, the goal is to use the best available data to guide response actions. In many cases, data is sparse and uncertain, but could provide better guidance than the default case of totally neglecting complex and important terms. For NO_2, first order decay rates likely can be estimated for the modeling system. Other pollutants of primary interests will also need to be reviewed in comparison with available data on indoor sinks.

Numerical Solutions - Finite difference methods are employed to solve the mass-balance equations. Binary files are created for storage of flow element data, kinetics element data, and time history-related data to ease the memory burden.

2. INDOOR

INDOOR was developed by researchers at the U.S. Environmental Protection Agency to allow rapid analysis of pollutant migration in a building under specified airflow conditions. Model formulations, results of early testing, and the user's manual are contained in a recent report (54). The model is written in Microsoft QuickBASIC for the IBM-PC, XT, AT and compatibles.

The program features a menu-driven user interface to transfer control among menus, data entry, and executable functions. Design principles follow a user-friendly pattern, prompting data entry through a series of menus and formatted screens that represent data entry forms. Relevant features of INDOOR include the following:

Airflows - The model accommodates a nominal maximum of 10 rooms, and allows detailed specification of HVAC air circulation rate, makeup air fraction, and fraction of time on. Specification of room-specific airflows is aided by a set of interlocking data entry forms that update the flow balance as each entry is made. The model allows the HVAC and rooms to contain a filter with user-specified removal efficiency. Airflows may be specified as two cases for a given run to convey an alternating pattern that is repeated each hour to mimic operation of air handling systems. The model randomly switches between these two states so that the simulated HVAC system is on for the fraction of time specified by the user.

Emissions - Generalized source terms for the model can be incorporated as emission factors, however, this option is not likely to be used in the emergency response modeling system.

Sink Effects - The model accepts user-defined sink terms for each pollutant. Input values correspond to a deposition velocity (m/h) and are combined with the interior flat surface areas of each room (walls, ceiling, floor) automatically read in from the room definition panel to define first-order removal rates (h^{-1}). Re-emission from the sink is also user-defined in terms of a rate constant and a critical concentration threshold.

Numerical Solutions - Finite difference methods are employed to solve the mass-balance equations. The time step to increment the difference solutions is user-definable (5 seconds is the default value); the program automatically monitors for numerical instability, adjusting the time step downwards in response to instability or upwards (increasing speed of execution) if results meet tolerance. Individual simulations are limited to treating one pollutant at a time, which is consistent with the emergency response modeling system.

3. MCCEM

The Multi-Chamber Consumer Exposure Model (MCCEM) was developed by GEOMET for the U.S. Environmental Protection Agency, Office of Toxic Substances, Exposure Evaluation Division. Model formulations and the user's manual are contained in recent reports (55,56). The model is written in Microsoft® QuickBASIC for the IBM-PC, XT, AT and strictly compatible microcomputers. Because of the structure and complexity of the program, it is likely that MCCEM would require extensive modifications to execute on other hardware systems.

MCCEM is of modular construction. The main program provides user-interactive features, and uses control logic to execute the different modules at appropriate times. The user input module contains a sequence of input screens to facilitate user-entered values and selection of default settings for model execution. Relevant features of MCCEM include the following.

Airflows - Interzonal airflows and infiltration/exfiltration rates are user-selected from cases stored in data files. Cases may be selected by geographic area and season. Version 2.0 of MCCEM accommodates a maximum of four indoor zones.

Emissions - Source terms can be represented by user-entered values that correspond to grams per hour. A spreadsheet format allows detailed specification of outdoor concentration profiles (the default setting assigns a value of zero for each time step). Indoor concentrations are homogeneously initialized using the outdoor concentration value assigned to the very first time step.

Sink Effects - The model accepts a user-defined term to describe pollutant removal processes. The sink term is stated in terms of a first-order decay constant; the default value is zero.

Numerical Solutions - Direct solutions to mass-balance equations are used to speed model execution. The user may specify model execution in short-term mode (up to 168 hours at 1- to 60-minute reporting increments) or in long-term mode (up to 365 days at 1- to 24-hour reporting increments). Summary statistics (mean, standard deviation, maximum, and percentage of reported values at or above a user-specified level) are also calculated during the course of model execution. To develop a range of estimates, MCCEM also allows the user to perform a Monte Carlo simulation on several input parameters for zone-specific concentrations or exposure. A sensitivity option permits the user to selectively change parameters (indoor volume, air infiltration rate, emission rate, decay rate, and ambient air concentrations) using parameter-specific multipliers that range from 0.001 to 1000 (default value is 1.000).

4. Conclusions / Model Selection

Each of these models has a demonstrated performance record for calculating indoor air concentrations with acceptable accuracy. A recently completed GEOMET study (50) challenged the three models to simulate a variety of indoor air quality scenarios that were supported by experimental data. When armed with appropriate inputs, model results agreed well with the experimental data, and model-to-model differences were trivial.

The principal differences across the models arise primarily in the ways that operational details are invoked. Table 6 summarizes the leading features of each model. Early considerations for the overall dispersion model would favor incorporation of CONTAM because the command processor / user interface is readily worked into the background of larger programs. Reference 57, for example, successfully incorporated CONTAM into a complex indoor air model used to simulate ventilation systems and indoor pollutant behavior.

The indoor air quality code that could be used in the emergency modeling system would not assume complete mixing between floors unless floors were interconnected through a common HVAC system. If there were no HVAC connection, the ground-level infiltration would be assumed limited to the affected floor. If HVAC controls were to be added help protect potential high impact areas, the model could consider these benefits. Careful consideration would be needed, however, of the degree of control as a function of natural infiltration. This factor could be especially important if the building was not overpressurized.

D. MODEL DEVELOPMENT ISSUES

Currently, air infiltration modeling and indoor air quality modeling are separate, but linkable, processes. That is, models exist to define air exchange rates as a function of meteorological conditions, building leakage configuration, and mechanical systems operation, and models exist to define indoor contaminant levels as a function of outdoor concentrations, air exchange, indoor sources, and contaminant properties. No single model currently exists, however, to fully integrate all processes into one grand indoor air quality simulation routine. The proposed emergency response modeling system could fulfill this need.

By examining the range of observed air exchange data, characteristic values could be established to best meet the needs of the emergency modeling system. Figure 18, for example, illustrates the time series of modeled indoor concentrations associated with a 30-minute cloud-passage episode for a building whose air exchange rate is 1 ACH. The indoor concentration profile is characterized by two trends: (1) ingrowth during the period when the cloud is present, followed by (2) dilution as indoor levels recede after the cloud passage. During the ingrowth period, the rate of increase indoors is controlled by the air exchange rate, and the maximum level is determined by the duration of the cloud passage. Mathematically, the maximum indoor level (C_{max}) can be expressed as a function of the cloud concentration (C_{out}), air exchange (ν), and cloud duration (T_p):

$$C_{max}=C_{out}(1-e^{-\nu T_p}) \qquad (31)$$

As shown in Figure 19, C_{max} reaches approximately 50 percent of the cloud concentration when νT_p reaches a value of 0.7; if νT_p reaches a value of approximately 2.3, we can expect C_{max} to reach about 90 percent of the cloud concentration. If air exchange rates are relatively small and cloud durations are brief, the indoor environment affords some protection. The protection level,

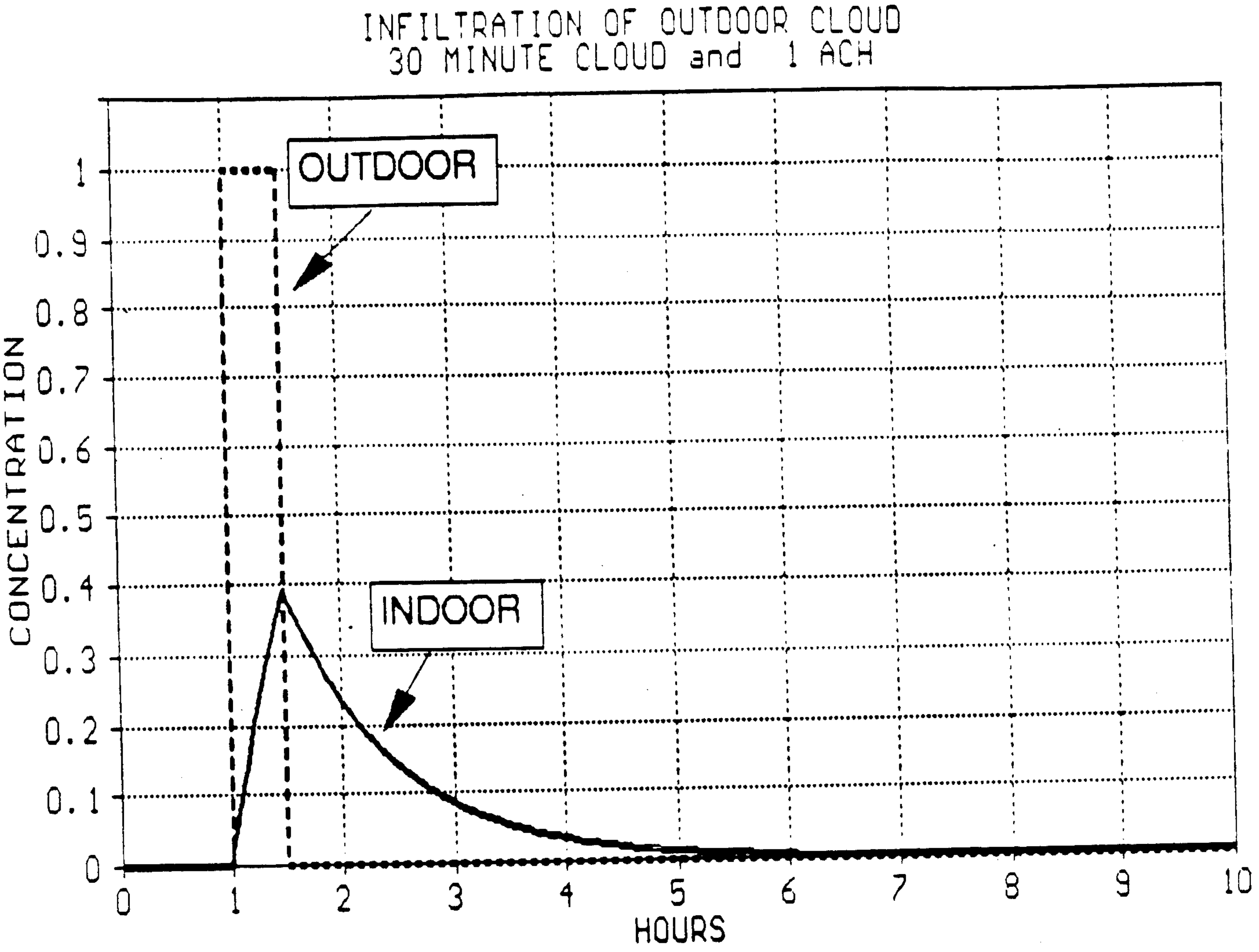


Figure 18. Example Time Series From Single-Chamber Mass-Balance Model.

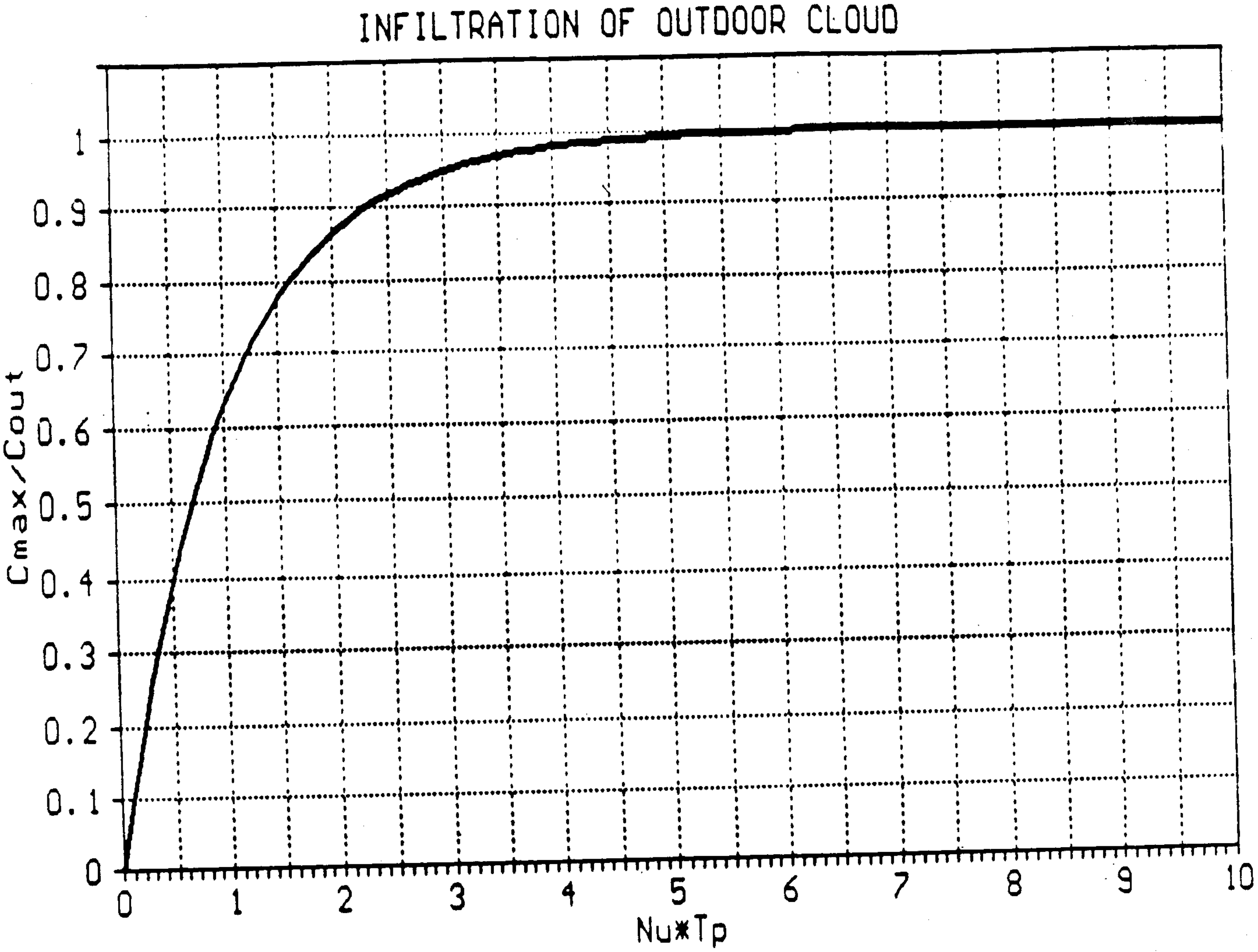


Figure 19. Indoor Maximum Concentration Versus Air Exchange (N_u) and Cloud Passage Times (T_p).

however, is limited to reducing peak indoor concentrations. Even though indoor concentrations are lower, they prevail for a longer time, such that the integral under the indoor concentration profile approaches the integral under the outdoor profile, if individuals were to remain indoors after cloud passage. The importance of peak relative to average exposures varies with the chemical of interest. Dose is important for some pollutants, while peak concentration is more critical for others. On this basis, the protection afforded by sheltering-in-place is a function of the characteristics of the pollutant.

The dilution effects of air exchange follow an exponential trend. Diluting peak indoor concentrations by 90 percent requires approximately 2.3 air changes. As shown in Figure 20, this could require nearly half a day in extremely tight structures but can be accomplished fairly rapidly at higher air exchange rates. From this graph, it is clear that recognizing occurrences of relatively low air exchange (e.g., $v < 1$ ACH) is especially important following cloud passage.

Table 7 summarizes the range of measured air exchange rates described in this section along with the calculated 90-percent response time (i.e., the time necessary to achieve ingrowth or dilution by 90 percent). This response-time parameter is important because it defines the critical time width for both the ingrowth and dilution periods. Thus, for the lowest air exchange rate in the table, 0.14 ACH, the cloud needs to remain at the building for about 16 hours for indoor levels to approach the cloud concentration, and another 16 hours must elapse after the cloud moves on before indoor levels recede to 10 percent of the peak indoor value. The composite values listed at the bottom of the table were synthesized by averaging across the building categories. These provide generalized values for buildings of unknown air exchange.

During the ingrowth period, if the building air exchange rate greatly exceeds the 3 ACH assigned to the worst-case scenario (as could occur in a hangar with all doors opened), negative consequences are minimized because indoor levels cannot exceed the cloud concentrations. Cloud passage would need to be fairly brief (less than 20 minutes) to underestimate indoor levels by more than a factor of two. On the other hand, if the actual air exchange rate during the ingrowth period is very small compared to the worst-case scenario, then indoor concentrations would be overpredicted during this period. In the case of an energy efficient office building (approximately 0.3 ACH), the indoor maximum from a one-hour cloud passage would be overestimated by approximately a factor of four.

For buildings that are not specifically tested for infiltration during model installation, or for non-priority bases, it could be possible to assign buildings to one of three tightness

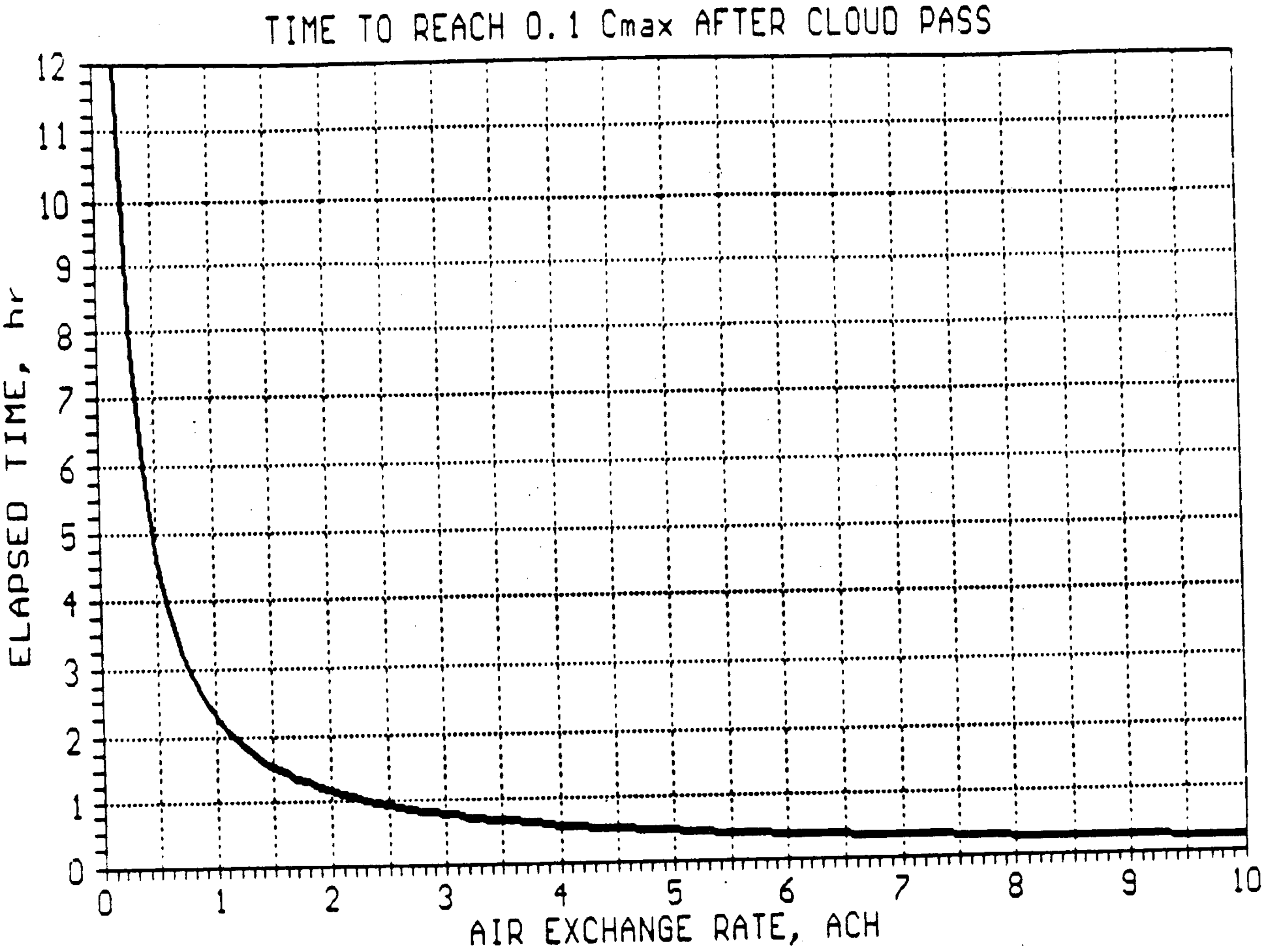


Figure 20. Time Required to Dilute Indoor Concentrations By 90 Percent.

TABLE 7. SUMMARY OF AIR EXCHANGE RATES FOR VARIOUS TYPES OF BUILDINGS.

Building Category		Air Exchange Rate	Time to Achieve 90 Percent Change
Residential	Low	0.14	16.4
	Median	0.52	4.6
	High	1.90	1.2
Non-Residential	Low	0.03	7.7
	Median	1.12	2.1
	High	4.20	0.6
Aircraft Hangars	Low	0.60	3.8
	Median	1.17	2.1
	High	2.30	1.0
Composite	Low	0.3	7.7
	Median	1.0	2.3
	High	3.0	0.8

categories (e.g., low, medium, and high) and to assign the composite rates in Table 8 (0.3, 1.0, and 3.0 ACH) to these categories for modeling purposes. Such an approach could provide reasonable accuracy in some situations, but could potentially produce errors of unknown direction and magnitude in other situations (e.g., building assigned to tightest class assuming windows closed, whereas windows are actually open when an emergency occurs). At a high priority base that is conducting a fuel transfer operation on stand-by basis, service opening in sensitive areas can be controlled, but in uncontrolled, offbase areas, there would be greater uncertainty in this term. It is important to make the best estimates of service opening status to choose between the evacuation or shelter-in-place options for Tiers I and II. Default window and door status could be established as a function of ambient temperature, time of day, and day of week (refer to Section VIII).

The above discussion provides an initial basis for adding an indoor air quality component to the emergency modeling system, but subsequent steps could consider refinements to enhance the realism in the model output. For example, the validity of the single-chamber model is dependent on the adequacy of the assumption of a well-mixed interior volume. However, many high-rise buildings and multiple-use buildings are purposefully designed to segregate the interior into largely independent zones. Hospitals, for example, generally segregate special-care wards, operating theaters, and laboratories. For buildings tall enough to extend above the cloud, vertical separation of air handling systems would also warrant more detailed attention in the model to avoid introducing bias between ambient and indoor environments.

The CONTAM software represents probably the best means to incorporate multiple-chamber modeling into the overall dispersion model. The command processor is ideally suited to receiving dispersion predictions and delivering indoor air predictions. The specificity and breadth of input data, however, grows with model complexity, requiring varying degrees of attention on a building-by-building basis.

Much of the information necessary for more complex indoor air quality modeling can be acquired from the architectural / engineering plans for buildings (e.g., HVAC flow capacity, and definition of indoor zones). Some critical information, however, can only be acquired by field measurements. For example, inadvertent air movement between indoor zones through stairwells, elevator shafts, or service chases is best quantified through tracer-gas studies. Indeed, a full-scale field trial to simulate cloud passage impacts would provide invaluable data. During installation of the emergency modeling system at high priority bases, these data could be acquired and interpreted.

Section VII

VISIBLE INTERACTIVE CHECKPOINTS

Dense gas dispersion and transport is more complex than passive gas treatment. The modeling analysis needs to consider thermodynamics, gravity spread, transportation and dispersion as a function of mass of emission, and phase changes for pollutant and water vapor in the cloud. Considering the additional complexity relative to passive gas modeling, there is greater potential for error. But, there also is a potential benefit to dense cloud modeling - - a benefit that often is not available for passive cloud analysis, i.e. dense clouds are often visible.

A visible plume provides the potential opportunity for a real-time, mid-course correction. It is important for a failsafe philosophy to consider all available information that could shed light on whether or not the modeling system is conservative. Follow-up in Phase II would be recommended to further assess the feasibility of a conservative override option. Clearly, the relationship between a visible plume and other cloud characteristics is complex, and needs careful review before developing a conservative override option. There is a substantial possibility that this option may not be feasible. There would be a substantial benefit, however, to ensure that model output is not grossly underestimating risk, which appears to warrant further, limited review.

An intensely cold, dense cloud often is clearly visible because of the condensation of water vapor within the cloud. The cloud will remain visible until entrainment and surface heating warm the cloud above the dewpoint of the cloud. While visible, there is the potential to assess the conservatism and general adequacy of several key terms of the model, including cloud growth rates, speed of travel, and direction of travel.

A. CLOUD GROWTH RATES

A pollutant cloud grows by entraining ambient air and by gravity spreading. Often, pollutants will be well mixed within a cloud because of the convection produced by surface heating. Ongoing entrainment as a function of downwind distance will develop distributions of concentration and other cloud-influenced parameters (such as humidity), which would show cloud influences weighted toward the center of a cloud, and the approach of ambient conditions at the fringes. In terms of entrainment, the primary goal of the override option would be to avoid the scenario where the plume is more concentrated than model estimates because of inaccuracies in the entrainment or gravity spreading terms.

Visual checkpoints offer the potential to compare observed to predicted cloud growth rates. Comparisons are complicated, however, because cloud width and height is likely to be greater than the visible plume (12,59). This effect appears to be caused by the greater influence of ambient conditions at the edges of the cloud, which could increase temperature above the dew point even though concentrations at that point within the cloud are significantly elevated in comparison with ambient concentrations. This issue needs careful review, especially since researchers (60) have shown that with rough surface elements that the gravity spreading was less than expected based on the HEGADAS model; in Phase II, the implications of these findings would need to be reviewed in terms of SLAB (strengthened version). This could be an important failsafe issue, especially if the modeling system overestimates gravity spread for rough surfaces. The Shell research (60) should be considered in any follow-up on the conservative visible override option. While it can be acknowledged that the visible plume should be smaller than the modeled plume, how much smaller should it be? When is additional conservatism needed to ensure the model output is failsafe in a real-time mode? Considering the potential benefits of a visual override feature, and the complexity of this issue, comments will be sought from British researchers, who have studied visual effects of dense clouds (12,59,60), during Phase II.

The following needs to be done to assess the feasibility of incorporating a conservative visual interactive override option into the modeling system:

1. Review raw data of past full-scale field tests that have documented visual records.

2. Run <u>strengthened</u> SLAB for each test.

3. Compare observed visual cloud growth data with model estimates of cloud heights, cloud widths, and model estimates of <u>visible</u> cloud dimensions.

4. Assess typical relationships between estimated and observed visual cloud dimensions, and estimated and observed concentrations, in the near-field, mid-field, and far-field. Emphasize Maplin Sands experiments (12,59) where visual estimates were based on computer enhanced techniques.

5. Evaluate wind tunnel testing data in a similar manner to the above.

6. Consider special case effects, such as aqueous aerosols formed

by water soluble clouds (such as ammonia), which also may need to be evaluated in terms of a conservative visual override option.

While implementing an override option would be challenging, there are encouraging developments from existing research. The Maplin Sands study (12,59) showed that visual dimensions were reasonably consistent with modeled data based on HEGADAS at approximately 100 m downwind. After distributions apparently were established, however, and the edges of the clouds apparently had much lower concentrations than the centerline, the visual dimensions were significantly less than the modeled cloud dimensions. It also is encouraging that the Maplin Sands tests could estimate visual lengths, which were only 25 percent longer than the modeled estimates (12,59). These tests, however, were not affected by large roughness lengths, which may further complicate the issue at airbases. After the entrainment term in SLAB is refined, it would be useful to determine if the excessive gravity spread noted in HEGADAS for rough surfaces (60) also occurs with SLAB.

If a conservative visual override option is found to be feasible, a procedure could be developed to scale back cloud dimensions to conservatively represent observed cloud behavior. <u>In no case would concentrations or hazard corridors be reduced based on the visual override option; this option would only be used as a "safety net" to further enhance the failsafe features of the modeling system</u>. For example, if horizontal dimensions were to be scaled back to ensure conservative centerline concentrations, the original hazard corridor widths would be retained to enhance the safety features of the modeling system.

It is likely that a different procedure would be needed to scale back cloud dimensions in the near-field, compared to mid-field and far-field locations. In the near-field it may be feasible to assume uniform concentrations within SLAB. Then, if cloud dimensions were observed to be significantly less than predicted dimensions in the near-field, a scale-back procedure could be applied to better match observed dimensions. In the mid-field and far-field, this approach may not be appropriate because the distribution of concentrations within the cloud may develop to the point that the preceding approach would be overly conservative. The feasibility will be assessed of using the pollutant concentrations (volume fraction) as the basis to infer the weighting of cloud versus ambient properties as a function of horizontal and vertical position relative to the cloud centerline. Estimates could then be made of the visible extent of the cloud by considering the likely distributions of water vapor mixing ratios and temperatures within the cloud. Estimating temperature as a function of position will need to consider the differences in heat capacity of air and the pollutant, when weighting temperature based on volume fraction pollutant concentrations.

B. SPEED OF TRAVEL

The speed of pollutant travel can be an important factor for evacuation decisions. Visual tracking of a cloud, as a confirmation of travel speed, would only be viable for an initially advancing cloud front. In the steady state, it would be difficult to find a point of reference within the cloud to track travel speed. The transfer operations of extremely hazardous chemicals are carefully planned at airbases, with emergency response capability generally on a stand-by basis. The advancing cloud could be observed if an accident occurred while personnel were on stand-by.

If observed travel times were found to differ significantly from model estimates, visual tracking could provide a basis to adjust critical response times, as necessary. As a conservative measure, response times would only be shortened by this procedure in order to enhance the safety of evacuation measures.

C. DIRECTION OF TRAVEL

If the direction of travel of the cloud is different than that estimated by the available meteorological data, or if the centerline meander range is wider than expected, it may be necessary to increase the width of a hazard corridor. This consideration could be especially important for an airbase, such as Cape Canaveral or Patrick, which are located near a land/water interface that could be subject to variable, localized wind flows. The visual override procedure would not remove areas from the modeled hazard corridors. Again, the goal of all elements of the visual tracking procedure, would only be to increase the conservatism of the modeling system based on observable effects. For wind direction, this could mean expanding the width of the hazard corridors to include the observed path (in addition to the original hazard corridors).

D. TRACKING PROCEDURE FOR VISUAL CHECKPOINT

All visual interactive checks would require user estimates of the size and travel speed of a cloud as a function of downwind distance or time. It would not be appropriate to rely on crude estimates of observed cloud dimensions. The recommended approach would be to set up an onscreen graphical display, showing horizontal and vertical planes for each potential trajectory, including major buildings and surface features. If a user selected the visual override option, they would be prompted to mark an onscreen graph to show the horizontal and vertical extent of the cloud at selected downwind distances. It would require additional installation time to set up the onscreen visual references, but could be worth the expense for bases that have the greatest potential for emergency release of acutely toxic pollutants.

Once the screen was marked at the checkpoints, all comparisons with modeled parameters could be automated by the software. An automated procedure would be less prone to error and faster than alternative approaches. Where the cloud growth (horizontally or vertically), path width, or travel speed significantly differed from the model output, the model estimate could be conservatively adjusted, as necessary, after the one-dimensional computations are completed.

Visual interactive software, such as proposed here, may have application for model uses for other military applications and civilian uses. This technique could be readily adapted for industrial applications. It may also be possible to develop a streamlined package that could be applied in battlefield applications for defense of a position against chemical or biological warfare agents. Such software could be integrated into more comprehensive computerized battlefield guidance systems that are currently under development. Computer mapping of hazard corridors could promote relocating troops to safer positions.

Section VIII

FLOWCHART OF MODEL DEVELOPMENT

This section summarizes how the analyses that were conducted in Phase I could be developed into an emergency response modeling system. The need for a system was established in Section III, and the feasibility of model development was shown in Sections IV through VI. In Phase I, we can show a conceptual approach in flowchart form. The flowchart could be refined in Phase II based on the additional analyses described in this report.

Figure 21 shows the major features of the modeling system, including the input module, the adjustment to the ambient concentrations to account for building influences, indoor air quality model code, total dose exposure module, evaluation of toxicity and flammability / explosivity hazards, the visual override feature, and the output displays. Model output features would heavily rely on state-of-the-art graphics to improve the clarity of the model displays, and to reduce the time to interpret and react to the results.

The emergency modeling system would have three major functions: (1) technical analysis, (2) decision support, and (3) graphical guidance displays / hardcopy documentation.

A. TECHNICAL ANALYSIS

Software design would include model development, and development of an input data module.

1. Model Development

Figure 22 summarizes the model features of SLAB that were identified in Phase I as requiring follow-up review in Phase II to strengthen SLAB. After these changes, SLAB could serve as an effective foundation to add the building features required to meet the objectives of this project. Other FORTRAN subroutines would join SLAB to form the modeling system to do the following:

- Conservatively adjusting the ambient concentration field to account for building affects.
- Infiltration model.
- Indoor air quality model.

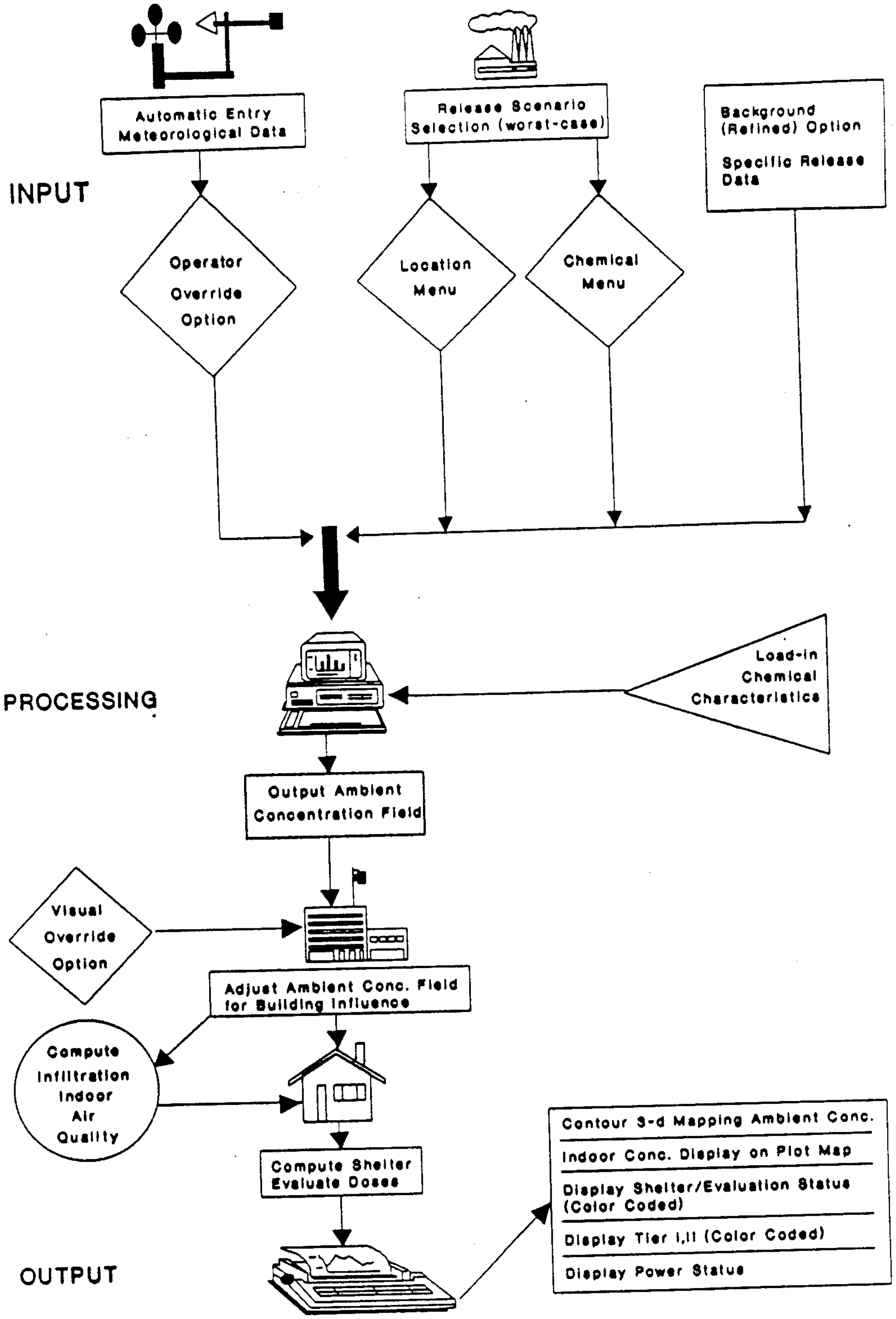


Figure 21. Flowchart of the Development of the Emergency Response Modeling System.

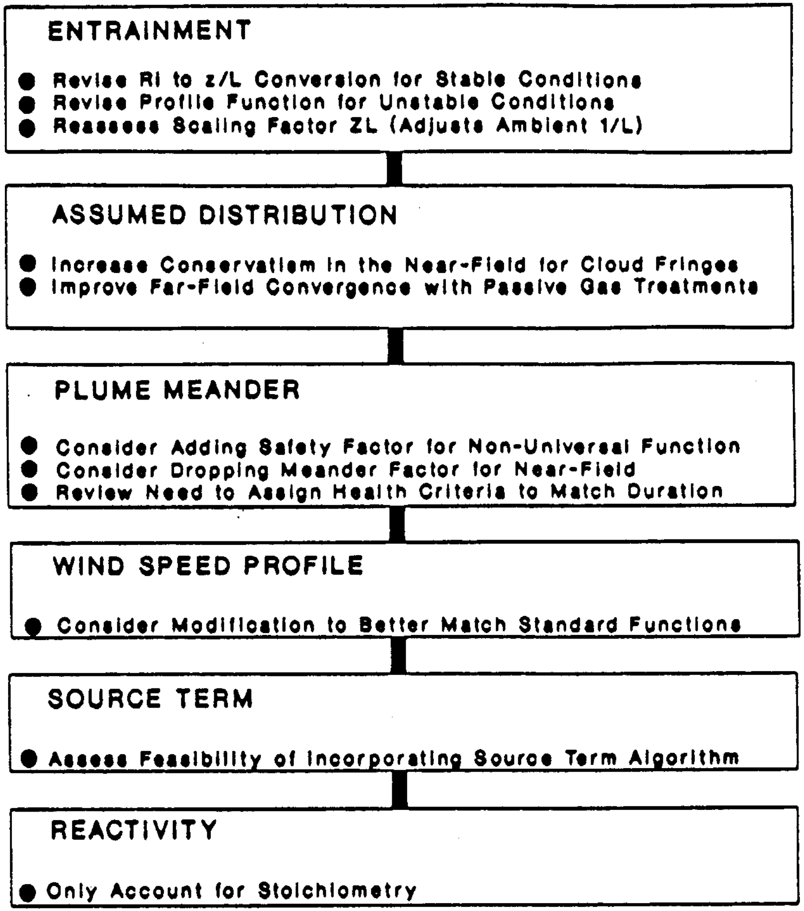


Figure 22. Summary of Follow-Up Review Required to Strengthen SLAB

- Dose estimates (ceiling and 30-minute) for shelter versus evacuation (egress analysis) option for each building

Once data entry is completed for either the manual or standby options, the system would create model input files by loading appropriate data to match the pollutant and buildings(s) characteristics for the application at hand. The model output would then be used to conduct the egress analysis. The egress calculations that would be used to guide the decision to select between the shelter-in-place or the evacuation options.

Egress calculations require knowledge of the indoor and outdoor environments through which individuals would pass when proceeding from their present location to the established evacuation area outside the influence of the pollutant cloud. These paths would be pre-set during installation of the model at a base, as follows:

- Function of wind direction flow quadrant.
- Would need to estimate: path of travel, mode of travel (by foot or vehicle), speed of travel for each segment to be analyzed.
- Execution will compute 30-minute doses and maximum ceiling concentrations for the shelter-in-place and evacuation options. Guidance from the Air Force Project Officer and review committee will be needed to establish a protocol to select between the shelter or evacuation options based on the 30 minute and ceiling comparisons.

2. Data Input Module

Success in real-time emergency response modeling is highly dependent on streamlined data entry. The key inputs would quickly be entered by interactive, menu-driven prompts, e.g. a grid map to locate the scenario, a pollutant menu, and a spill/release menu. Three types of data are needed:

1. Mandatory Inputs - Mandatory inputs would only be needed for essential parameters needed to define location, pollutant and mode of release.

2. Pre-set - but option to override. These data would be hardwired into the model, but there would be an option for user override, as appropriate. Examples would include meteorological data (hardwired into system) and service opening status for affected buildings. Override would simply require overwriting on-screen parameters.

3. No decision required - input data are pre-set at installation. Inputs would be hardwired, as appropriate, (e.g. surface roughness by release location and trajectory, chemical properties, building properties, e.g. HVAC data. There is no benefit to burdening a user with any input that could be effectively pre-set at installation.

Table 8 summarizes model inputs, and shows which inputs are preset, which are present as defaults with user override, and which require specific inputs for the refined model runs. (Mixing height would be estimated as a function of 1/L, but could be overriden at bases such as Cape Canaveral or Vandenberg, which have real-time mixing height data.

Table 8. INPUT DATA ENTRY

Input Data	Preset at Installation	Auto Load-in Met Data	User Input for Initial Run	User Input for Refined Run	Preset / Override Option
Wind Speed		*			
Wind Direction		*			
Amb. Temperature		*			
Pressure	*				
Delta Temperature		*			
Relative Humidity		*			
Mixing Height					*
Pollutant			*	*	
Scenario Location			*	*	
Total Emissions				*	
Duration Emissions				*	
Chemical Specs.	*				
Spill Data	*			*	
Surface Roughness	*				
Status / Serv. Op.	*				*
Infiltration Coef.					
Building Specs.	*				
Indoor Temperature					*
Air Exchange Data	*				

B. DECISION SUPPORT

A tool is needed that provides not only a basis for decisions, but also tracks the implementation of decisions and depicts other relevant factors, such as power status at all structures, location of emergency response personnel, etc.

There is no substitute for intelligent decisions made by an onsite operations commander that is responsible for managing an emergency. There is a benefit, however, in terms of efficiency of actions and adherence to pre-established, preferred response procedures, to guide operation commanders by incorporating into the emergency response modeling system the judgement and experience of emergency response experts within the Air Force and elsewhere. The goal is to provide consistency in approach, while retaining flexibility to respond to problem-specific factors.

Expert judgement could be coded into rule-based decision logic that could guide all model applications. In this sense, the emergency modeling system would have features of an expert system that uses both the technical data and the Air Force emergency response procedures (and rule-based decision logic) as inputs to define the preferred actions based on the type of emergency and the modeled concentrations. GEOMET staff experienced in rule based reasoning, could help guide this portion of the software development. A wide range of decision support could be provided within the framework of the emergency response modeling system, e.g:

- Preferred control procedures, e.g. how to select optimal measures to control spills or gaseous releases based on release characteristics and the severity of the predicted impacts.

- Should the decision to evacuate or shelter be more heavily weighted to 30-minute average concentrations or ceiling concentrations?

- How should the critical nature of some operations be factored into the decision to choose between the evacuation or shelter options? For example, personnel that are deemed essential to mission or emergency response actions might be sheltered at their work stations, even though less essential personnel that were subject to the same exposures would be evacuated.

- Preferred steps to alert media, and the chain of command?

Such procedural judgements are best made during installation and not on an "ad hoc" basis during the midst of a response action. Our goal would be to focus the thought process of the operations commander to decisions that need onsite judgments, and provide them with the benefit of procedural guidance that represents the Air Force management's preferred course of action for specific situations.

Priority is given in this project to allowing an active emergency response coordinator (preferably from Cape Canaveral, where the prototype would be installed) and other knowledgeable Air Force personnel to help develop the rule-based guidelines for emergency response management, which would be coded into the emergency response modeling system. This would greatly strengthen Air Force management of air quality-related emergencies. Decision-oriented output is an important factor to our approach. The review committee to be established for this project will provide the necessary multidisciplinary talents needed to develop a practical emergency modeling system that is designed to be a comprehensive and practical emergency response tool. It would be helpful to coordinate a meeting with Air Force emergency response experts during the first meeting of the review committee.

During model development, we would look to input from the emergency coordinator on the review committee to add other data that would help guide decisions and track progress during an emergency response action. For example, a file is needed that contains one record for each onbase building and offsite gridded areas that shows the following codes that would be used in the graphics displays to show current status:

Building # or Area Grid #	Evac/Shelter Code	Power Code

0 = evacuate

1 = Shelter

2 = Evacuation completed

0 = Shutdown power

1 = Power on

2 = Power shutdown completed

In this manner, the modeling system could guide a response and summarize current status of evacuation versus shelter-in-place actions. The system would be updated as conditions change, based on changes in meteorological conditions or release characteristics, but the status of each building would need to be consistently tracked throughout the response. For example, if a building were evacuated early in the response, this would be tracked throughout the response as an evacuated structure. Similarly, if a decision were made early in the response to shelter-in-place individuals within specific building(s), but wind conditions then resulted in a change of this decision, the color coding for this building could be updated and tracked through the completion of evacuation.

In the real-time mode, there is an immediate need for information to guide response action. A primary goal of this project would be to provide immediate guidance, with no wait time for computer execution. To achieve this objective, the approach would be to continuously maintain a ready state at high priority bases through two major alternatives to provide real-time data:

a. Continuous updating of meteorological data at a dedicated computer, which would continuously store current worst case impacts for all priority potential accident scenarios (e.g. tank rupture, transfer operation spill, etc.). In this way, all priority scenarios would have available displays on a continuous basis, which would be instantly available in the event of release. The user would just need to indicate which scenario to display on the computer screen. Updates could be provided on a real-time basis, limited only by the update frequency of the real-time connection with the meteorological monitoring system, and model execution time to simulate all priority scenarios. Such a system could be used at individual bases, and at a centralized, national response center.

b. For bases without access to real-time updating of meteorological data, the approach would be similar to the above, except that model output would be pre-run for a range of spill and meteorological conditions. Prompts would be used to identify the correct pre-run data set to conservatively represent current release conditions, and this output would be used for immediate guidance, while more refined runs would be made in the background.

With either approach for data entry, there would be an incentive to pre-set as many inputs (with operator override) as possible for the refined model runs that could be made in the background. Examples of inputs that could have preset defaults include the following:

- o Surface roughness could be coded as a function of wind direction and scenario location. These inputs could be established during the installation of the code, based on the Lettau technique that considers typical obstacle height, silhouette area, and average lot area (61).

- o Service openings (windows, hangar doors, etc.) could be defaulted as a function of ambient temperature, hour of the day, and day of the week. Such information would be base-specific and possibly building-specific offbase service opening status would need to be defaulted in a similar manner to produce unbiased estimates of indoor versus ambient air quality.

C. GRAPHICAL GUIDANCE DISPLAYS / HARDCOPY DOCUMENTATION

There is a primary and secondary goal for the output displays: (1) on-screen graphical displays are needed to support the management of an emergency response action, and (2) hardcopy data are needed to document the basis for the actions taken and to support post-response reviews aimed at improving Air Force emergency response actions. Both types of output are needed. Hardcopy documentation is straight-forward. Graphical displays are more critical and are emphasized in the following descriptions.

Color coded on-screen graphical displays would support emergency response management at the command center of the affected airbase, with an option for a hard-copy printout. A modem connection to a centralized Air Force, or joint services emergency response command center, could also be used in the future as a backup to local capabilities for onbase or transportation-related emergencies. The modeling system output would be updated, e.g. every five minutes or whenever major changes in meteorological or emissions characteristics occur.

The key features of the on-screen displays would include color codes for major features, which could be overlaid onto the base map shown on-screen, e.g.:

Tier I / Tier II Status
- Tier I boundary identified in black
- Tier II boundary identified in yellow

Building Status
- Blinking green = to be evacuated
- Solid green = evacuation was completed
- Solid red = shelter-in-place
- Blinking brown power box = power to be shut-down
- Solid brown power box = power was shut-down

Location of Emergency Response Personnel
- Location of emergency response personnel could be shown by symbols, if entered by the operations commander.

As feasible, the feature of providing Tier I and Tier II hazard zones on split screens would be used so that the scale not in current review could be displayed as an insert. If possible, an option would be provided where the insert boxes could be reversed, such that the Tier II map could be the primary map and Tier I shown in the insert. The power recommendations would be based on input from the modeling component (explosivity potential), consideration of the HVAC intake height versus cloud height, and consideration of essential electrical equipment, such as essential power generators, elevators, and essential computer systems.

D. UPDATING THE EMERGENCY RESPONSE MODELING SYSTEM

It is likely that if this model were to be developed that there would be ongoing refinements to the program and user's guide, changes that would evolve over time. The most efficient means of maintaining a current code and user's guide would be to maintain an online version of the current program and guidance. EPA maintains the SCRAM system, which is an online repository for updating EPA dispersion models. It is recommended that access to SCRAM, or an equivalent system, be explored if model development will proceed into Phase II.

Section IX

FULL-SCALE FIELD TEST OPTION

As described in this report, the currently available models are not well suited for a rough surface, such as an airbase, and do not provide sufficient guidance to aid Air Force emergency response decisions, such as to shelter-in-place or evacuate. The planned model development would provide model-based guidance to support such decisions, but model development could benefit by full-scale testing designed to confirm that the modeling system is reasonably conservative for a range of meteorological conditions, release scenarios, and averaging times.

One of the major challenges of full-scale field testing would be to find a suitable location. The goal would be to test the modeling system at an airbase with typical surface features. There would be two components that could be evaluated, both of which are virtually untested at this time: (1) transport and dispersion characteristics for dense gas flows past obstacles, and (2) the indoor component of ambient dense gas releases, including dense gas infiltration rates and indoor air quality.

Such testing would benefit a broad user community, including the Air Force, the other military services, federal agencies, and industrial users. There would be a potential for shared funding in Phase III.

The general test design can be sketched now. At the completion of model development in Phase II, the option for a full-scale field test could be refined. It is likely that the cost of full-scale field option would be several million dollars. The components of the test would include the following: facility selection, release gases, data collection procedures, and data interpretation.

A. FACILITY SELECTION

The goals of selecting a site for full-scale model testing would include the following:

o Avoid significant disruption of base operations.

o Select a base that contains typical structures (hangars, office structures, warehouses, etc.)

o Avoid locations with complex terrain issues.

The most likely options would be an Air National Guard training facility (e.g. Gulfport, Mississippi), or an Air Force base that is being deactivated. A short list of potential bases would need to be prepared that meet the above conditions. For these locations, it would be necessary to consider the availability of at least a 30-day window for field testing, in relation to favorable climatological conditions for available periods.

B. RELEASE GASES

The field program should focus on dense gas releases, since passive releases have been studied in much greater detail than dense gas releases. The characteristics of the release gases that could create the dense clouds for the field study would need to meet the following criteria:

1. Not life threatening, except for oxygen deficiency.
2. Nonflammable and nonexplosive (structure safety).
3. Noncorrosive (protect electrical equipment).

It appears that mixtures of liquid nitrogen and sulfur hexafloride, or liquid carbon dioxide and sulfur-hexafluride would meet the above criteria, and could be readily distinguished from background concentrations. A major concern that would need to be addressed in the field testing protocol would be the procedure to mix the weighting gas (e.g. N_2) and the tracer gas (sulfur hexafloride). The liquid nitrogen mixture would have the desirable feature of being dense only because of cold temperature of the release. As the cloud warms to ambient temperature, the cloud density would rapidly transition to a passive cloud because the molecular weight of nitrogen is approximately the same as the ambient air.

C. DATA COLLECTION PROCEDURES

The goal would be to release the dense gas upwind of desired trajectories, which would result in plume travel past selected "model" building structures. On the order of four downwind arcs would be selected as follows:

- 50 m downwind, (before buildings encountered).
- 100-150 m downwind (after buildings encountered, if possible).

- Approximately 500 m downwind (past model buildings(s))

- Approximately 1000 m downwind (well past the range of buildings to be tested).

Six to ten monitoring sites would be instrumented per arc (dependent on financial resources). Two to three monitoring heights would be instrumented per station (e.g. 1, 4, and 8 m above groundlevel). Additionally, at least 2-3 sampling locations would be instrumented inside all "model" structures. Concurrent infiltration research would be conducted for all instrumented buildings. At least three preferred trajectories would be sought to characterize each set of structure types. A range of meteorological conditions (stable, unstable, and neutral) would be sought for the tests.

D. DATA INTERPRETATION

The objective of data interpretation would be to improve the physical treatments of the modeling system to ensure that model operations are failsafe, but not overly conservative. The following would be done during data interpretation:

1. Use the Phase II modeling system to match conditions for each field test. The model would be run for each test period.

2. Evaluate what the measured data reveal about the strengths and weaknesses of model performance.

    - Look beyond just statistics, i.e. search for physical reasons for potential model modifications.

    - Avoid optimizing model to match test data set.

3. Ensure that the ambient concentration field adjustment procedure to account for obstacles is reasonably conservative.

4. Ensure that the indoor code adequately represents infiltration rates, and concentrations are reasonably conservative as a function of time.

Any changes to the modeling system that are proposed based on the interpretation of the full-scale field test would first be approved by the project review committee to ensure that changes will result in a general improvement in model performance, and not a model optimization for the field data set. Another role of the committee would be to ensure that model changes are fully documented, and code development could easily be traced by independent analysts. After physical treatments in the model are refined, the modeling system would be rerun to compare with the measured data set. Comparisons would include before and after model performance evaluations.

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