EVALUATION AND ENHANCEMENT OF COMPUTATIONAL TECHNIQUES IN INDOOR AIR QUALITY ANALYSIS

by

Tara Srinivas

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DEDICATED TO

MY FAMILY

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LIST OF ABBREVIATIONS

ACH - Air Changes Per Hour

ASHRAE - American Society for Heating, Refrigerating, and Air Conditioning Engineers

CFD - Computational Fluid Dynamics

HVAC - Heating, Ventilation and Air Conditioning

IAQ - Indoor Air Quality

LRN - Low Reynolds Number

OSHA - Occupational Safety and Health Administration

NIOSH - National Institute for Occupational Safety and Health

ABSTRACT

Computational techniques are an important tool of research for Indoor Air Quality (IAQ) analyses. The two approaches commonly adapted are the Multizone approach and Computational Fluid Dynamics (CFD) approach. Both of these approaches are invaluable in their contributions towards indoor air research.

The primary objective of this thesis was to design an effective technique for coupling the two models, multizone and CFD and implement this technique in a parametric study to determine the suitability of this approach in specific areas of indoor air research.

As a preliminary step to designing this powerful design tool, an in-depth study of the two models was conducted. Several critical areas of application were identified for the two models. PHOENICS performed better when the airflow characteristics were dependent on local influences such as location of flow obstacles, contaminant sources, etc. CONTAM was unable to identify such variations in the intrazonal structure. But CONTAM remains the dominant model in the coupled analysis due to its global approach of analyzing the indoor air quality. Hence the focus of this thesis is to enhance the predicting capabilities of CONTAM so that it is better suited to analyze the details of the indoor environment.

Finally, a technique was developed to enhance the simulating capabilities of the multizone model by incorporating critical data from the CFD model that improved the CONTAM predictions in specific areas of IAQ analysis where the local influences from zones dominate the flow characteristics of occupied spaces.

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1. INTRODUCTION

1.1 Indoor Air Quality

Most people spend more than ninety percent of their time in an artificial climate like offices, factories, public buildings, home, etc. (Turiel, 1985). Exposure to indoor air pollution has been recognized as a major contributor to human health risk by environmental professionals since levels of contaminants, especially volatile organic compounds are generally higher indoors than outdoors. The negative effects of poor indoor climate condition on the performance of the occupants are described in several investigations conducted by OSHA, NIOSH, and Health and Welfare Canada. This stresses the importance of maintaining a healthy and comfortable indoor climate in terms of thermal comfort and indoor air quality. In order to focus on the occupant instead of the room or the building requires knowledge about the indoor airflow patterns and contaminant distributions. In this thesis, the focus is on the improvement of indoor air modeling techniques and on the design and management techniques.

Since the energy crisis of the 1970's, the insulation of buildings has been improved to increase energy efficiency and lower energy costs. Most buildings such as offices etc. have no access to natural ventilation. With lower room loads, ventilation rates have been lowered to reduce energy costs. These architectural design and management techniques have become a trend in the buildings since the 1970s. Such a reduction in the air supply causes an increase of the concentration of indoor contaminants such as carbon dioxide and particulate, and sometimes generates a non-uniform distribution of air temperature. The effect of energy conservation techniques has become one of the leading causes for poor indoor air quality (IAQ) in buildings. This fact has been the subject of research in several studies such as Turiel (1983), Turiel (1985), and Bourbeau (1997). Such problems in buildings have often been one of the causes for "sick building syndrome". People working in such buildings have been known to experience sore eyes, or running or blocked nose, dry throat, lethargy, headaches, and sometimes asthma. In most cases the cause for sick building syndrome is inadequate ventilation (Turiel, 1983, Carpenter, 1996, and Bourbeau, 1997).

Despite the increasing interest in indoor air quality problems, only limited research has been conducted which integrates the analysis of contaminant sources, HVAC system operation and building characteristics. The interactions between HVAC systems and building characteristics are important as they relate to both causes of IAQ problems and their solution. Studies have shown that lowered ventilation rates may not be the only source of indoor air quality problems in buildings. A building is a very complex system that has several time-variant factors acting on it at the same time that contribute to indoor air quality problems.

Buildings are constructed and operated in many different ways. Unfortunately, this complexity makes understanding and predicting airflow and contaminant transport patterns a site-by-site evaluation process. The impact of an indoor air quality control system on contaminant levels in a building depends on the buildings characteristics, the design and performance of the IAQ control devices, the characteristics of the contaminants to be removed by the devices, the contaminant sources, the existence of any contaminant sinks within the building and the ambient conditions of weather and outdoor contaminant concentration. Most of the research has employed simplified approaches to studying the complex behavior of a building and its systems. Experimental studies have often focused on the performance of individual pieces of equipment without considering the interactions with the building, the HVAC system, and the ambient conditions. Given the complexity of buildings and the necessity for a site-specific solution makes experimental studies a far too expensive and non-feasible option in many cases. Computational techniques on the other hand are a far more attractive option, given the recent advances in computer technology and their speed of operation. This development has created significant potential for improving the monitoring and supervision of building systems in order to optimize operational performance while minimizing and solving problem areas ahead of time.

Computer modeling has become an important aspect of indoor air quality analysis since the technique provides flexibility, ease, and speed in determining problem areas while giving an insight into the design and implementation of optimal conditions. The techniques that have been used in computing airflow and contaminant transport in buildings are: multizone modeling technique and room airflow modeling technique.

Multizone airflow and contaminant transport modeling takes a macroscopic view of indoor air quality by evaluating how average contaminant concentrations in the different zones of a building as contaminants are transported through the building and its HVAC system. The multizone approach is implemented by constructing a network of elements describing the flow paths (HVAC ducts, doors, windows, cracks, etc.) between the zones of a building. The network nodes represent the zones that are modeled at a uniform pressure, temperature, and contaminant concentrations.

Detailed or room airflow modeling takes a microscopic view of indoor air quality by examining the detailed flow fields and contaminant concentration distributions within a room. Room airflow modeling applies the principles of conservation of momentum, mass, and energy through the use of a computational fluid dynamics (CFD) technique. Accurately modeling an entire building with a CFD program would involve an unmanageable amount of detail and would require massive amount of effort in computing and data entry. A whole building CFD model has never been attempted due to the uncertainty in the production of meaningful results due to such an effort.

1.2 Whole Building Approach (Multizone Modeling)

Infiltration and exfiltration of air through exterior envelopes and interzone airflow rates in buildings affect the whole building ventilation rates, outdoor airflow rates to individual rooms, concentration levels of airborne contaminants, and heating and cooling loads. Air movement and convective contaminant transport within multizone buildings are caused by pressure differences across openings in exterior walls and in partitions between individual zones. These pressure differences are caused by wind, thermal buoyancy and mechanical ventilation systems. For a building with known leakage characteristics and ventilation system airflows under given weather conditions and contaminant source strengths, multizone airflow and contaminant transport models can predict the airflow and contaminant transport rates from one zone to another, or to the outside, and the contaminant levels in each zone.

Multizone models use a network approach to obtain a set of nonlinear equations derived from a mass balance at each node and an iterative solution technique based on the

Newton-Raphson method to solve for the pressure at each node. These pressures are then used to calculate the steady-state airflow rates to and from each zone based on the given leakage values. Using these airflow rates, contaminant source strengths and information on other contaminant transport mechanisms, these programs can also calculate contaminant concentrations in each building zone. Multizone models fully account for the complexity of infiltration and ventilation airflows in multizone buildings. These models can be used to understand air movement in multi-story buildings, to predict interzonal airflow patterns and zonal contaminant concentration levels. The models are also capable of evaluating the performance of the building ventilation systems under different operating conditions. Modeling can also be useful to designers, builders, and code enforcement officials to predict whether the performance of a building will comply with fire, energy, and indoor air quality codes and standards.

Multizone airflow models require information on the building being modeled including physical dimensions of the building, airflow resistances of the airflow paths, the configuration of mechanical systems, ventilation system airflow rates, wind pressure coefficients on the building façade, and ambient weather data. Contaminant dispersal analysis requires additional information including contaminant source strengths, source removal rates from indoor sinks, and outdoor contaminant concentrations. As with the case with most computer simulation studies, there is generally limited information available on the required inputs. Hence the portrayal of the building is simplified to a major extent. It is generally impractical to include all building zones, leakage openings, ventilation system components, and façade details affecting wind pressure distribution when modeling airflow in multizone buildings. However, studies in the past have shown that valuable information can still be obtained based on the available information and less than complete idealization of the building. An idealization of a multizone building refers to its representation as a multizone airflow system in a manner that captures the important features of the building and the airflow phenomena being studied. The idealization of a multizone building depends on the building layout, the ventilation system configuration and the objective of the modeling effort. While multizone models offer the most comprehensive approach to studying the overall indoor airflow characteristics of a building, much work is required to improve the predicting capabilities so that errors in predictions can be minimized.

1.3 CFD approach (Room Airflow Modeling)

Airflow inside a room is complex. Studies have shown the importance of obtaining the detailed computation of airflow in a room in order to accurately predict occupant comfort. The supply and exhaust locations, room geometry, furnishings, as well as temperature gradients, determine a specific flow pattern in a room. Accurate predictions of velocity, temperature and concentration distributions in a room have thus become a very important criterion while designing the ventilation systems. The flow in most rooms is unsteady, three-dimensional and buoyant (Chen *et al.*, 1988) as many studies have indicated. There can be fully turbulent regions as well as regions with little or no turbulence. Because of this complexity, there is little information available about room airflow patterns to engineers. ASHRAE Fundamentals Handbook (1993) provides correlations that the engineer could use to predict the throw of the supply air. The throw is the distance an air stream travels from the supply opening before the velocity is reduced to a specified level. Outside this throw region however the engineer has to depend on "rules of thumb" and experience. The increase in cases relating to "sick building syndrome" (Turiel, 1983, Carpenter, 1996) and the growing awareness among the people regarding these problems are encouraging researchers and engineers to follow more accurate prediction techniques to solve problems ahead of time. Most rooms are unique and the approach of the "rules of thumb" can definitely not provide sufficient information about the flow patterns in a particular room and problems of air distribution associated with that room. The computer technology has certainly gained an edge over experimental indoor air quality studies due to the recent advances in the technology and its increased accuracy in predictions as proved by several studies.

Computational Fluid Dynamics (CFD) has become a fast developing area for the prediction of indoor airflow. There are numerous practical flow problems related to buildings that can be solved by numerical techniques. A successful numerical model would be an ideal tool to help a researcher understand the complex phenomena of flow problems and help in the creation of optimal design solutions. Success has already been achieved in the predictions of several complex areas in indoor air quality (IAQ) analysis such as detailed calculations of indoor air velocity, temperature and contaminant concentration distributions within a zone or a room, and in computing the hourly heat supply or heat extraction of a room (Chen *et al.*, 1988, Bauman *et al.*, 1992).

CFD models offer the advantage of understanding the detailed flow characteristics of a zone based on the design input data such as the inlet flow rate, contaminant source strengths, presence or absence of heat generating sources, and flow obstacles in a space. CFD models are powerful tools that provide the engineers an insight into the problem areas of a building, which can then be resolved by offering a solution just for that one zone instead of the whole building and thus reduce expensive alterations. Most of the studies in the past have used the CFD approach to analyze individual zones due to the complexities and the time involved in considering more complex problems. CFD models offers a window of opportunity into the complex world of indoor airflow research that still remains to be tapped to its maximum potential.

1.4 Combined Approach

The two models, Multizone and CFD, have remained reasonably reliable in their prediction of IAQ problems in buildings and their applications are always individualistically approached. The two models have typical applications in IAQ analysis of buildings with the multizone models being the more popularly adopted technique since it provides an overall picture based on several different aspects of the building such as outdoor air characteristics, HVAC data, etc. The demand for the use of the CFD approach in IAQ analyses increased with the increasing awareness of indoor air quality problems in buildings. The idea of a coupled approach of modeling with the two techniques is still a very new idea that requires further research, validation, and determination of implementation areas.

A realistic approach to modeling the indoor space would require the effective combining of the two models in order for the generated results to be meaningful. The multizone models are effective for calculating air and contaminant exchange between rooms of a building, the HVAC system and the outdoors. But in reality the temperature and contaminant concentrations vary in space based on several factors including the physical characteristics of the room, object placements, inlet-outlet locations, etc. The exchange of contaminant distribution then becomes a function of the local values near the flow paths, which are the points of interactions. Thus it may be critical to have both types of knowledge while designing effective ventilation systems as well as the indoor design of the space under consideration.

1.5 Thesis Objective

The objectives of this thesis are summarized below. The focus of this work has been on the evaluation of contaminant distributions based on indoor and outdoor characteristics of an office building using CONTAM and PHOENICS.

Preliminary work:

1. In-depth study of the theoretical background of the two programs, CONTAM (multizone) and PHOENICS (CFD)
2. Literature review of the status of research
3. Validation of CONTAM and PHOENICS against experimental studies

Advanced work:

4. Assessment of Simulation Capabilities: To assess the capabilities of the individual models through parametric studies that provides an in-depth look into the functionalities and applications of the models in complex indoor air quality analyses situations
5. Identification of Need for Improvement: To determine the shortcomings of the two models and identify prospective areas that provide opportunities for improvement of simulation capabilities

Research Contributions

6. PHOENICS Simulation: In this thesis work, the focus of the PHOENICS study will be on the assessment of complex indoor configurations using PHOENICS. Several critical design considerations such as location of flow obstacles, contaminant source locations and source strengths, and effect of heat sources will be studied in detail.

7. Comparative Analysis: To conduct a direct comparison of the two models by implementing them in a parametric study of IAQ analysis of an office space. This comparison will provide an insight into the strengths and weaknesses of each of the models in order to enable effective coupling.

8. Development of a Coupling Technique: To develop a suitable technique for the coupling of the two models where an actual exchange of data between the two models can be implemented. An efficient coupling will enhance the knowledge of the air movement in the whole building as affected by the outdoors as well as the local influence within occupied spaces of the building.

2. BACKGROUND

2.1 Introduction

As a preliminary step to developing effective simulation techniques for the indoor environment, a detailed literature review was conducted to study the progress in research to date on the applications of the two modeling techniques, multizone and CFD. Research works that have identified deficiencies in the two approaches and those that have suggested or implemented possible variations or improvements to the current state-of-the-art technology have been described in this chapter.

2.2 Recent work

2.2.1 Multizone Models

One of the objectives of the literature search for this study was to identify suitable studies to be used for the validation of CONTAM. Some of the major contribution towards the research for multizone models in indoor air quality analysis has been from the BFRL (Building Fire Research Laboratory) publications. This organization has several experimental and well-documented numerical studies to its credit in the area of indoor air quality research in office, residential, school, and apartment buildings (Persily, 1994, Persily *et al.*, 1994, Persily, 1995, Walton, 1995, and Emmerich, 1998). Most of the validation studies selected for this work have been obtained from the numerical and experimental work published by the researchers from BFRL organization.

Haghighat *et al.* (1989) and Feustel and Sherman (1992) have discussed in detail the theory of multizone airflow models. The paper by Feustel and Sherman (1992). gives an overview of the existing multizone models and given a review of the studies that have used these models. Studies that have applied these models in different types of buildings are also available in the literature. Persily (1995), and Emmerich (2000) have evaluated the airflow characteristics in residential buildings. Emmerich (2000) has evaluated the ability of mulitzone models in predicting the impact of residential IAQ control technologies. Simulated and measured results of air change rate, average particle concentrations were compared for a one-room test house. Persily (1994) and Carpenter (1996) have examined the airflow and contaminant concentrations in office buildings using multizone models.

The usefulness of these models in ascertaining energy management and indoor air quality control has been researched by Carpenter, 1996, and Ayari *et al.*, 2000. In the study by Carpenter (1996), CONTAM was used to evaluate the usefulness of CO_2- based demand controlled ventilation systems in maintaining indoor air quality and aiding in energy conservation in office buildings. It was found that such ventilation systems are not always successful in containment of contaminants in buildings. Ayari *et al.*, 2000 used a multizone model to determine the indoor air quality of an underground parking garage. In the study by Ayari *et al.* (2000), the unsuitability of just the multizone models in IAQ analysis was discussed and a CFD model was used to determine more detailed assessment of the indoor airflow characteristics of the underground parking garage.

2.2.2 CFD Models

The application of CFD in IAQ analysis has gained importance over the years. The technique has evolved and numerous results have indicated the widespread applicability of CFD for the simulation of indoor airflow patterns. Several publications have given us the proof for the success of this method in indoor air quality analysis such as Chen *et al.*(1988), Haghighat *et al.* (1989), Murakami and Kato (1989), Chen (1992), and Chen (1999). The range of airflow simulations, which originally comprised of laminar, one-and two-dimensional, steady, and isothermal situations, has been enlarged to include turbulent, three-dimensional, transient, and buoyancy affected flows. The literature search has revealed the importance of assessment and selection of the models that are to be employed to computer room airflows. Most of the simulation studies have employed the standard k- ε model with wall functions due to the ease in implementation. An assumption of this model is that room airflow is fully turbulent. Room airflows, however, have regions that are fully turbulent, as well as regions with little turbulence (Chen, 1992). The set of model equations in the standard k-ε model is suitable for high Reynolds number flows. For wall flow, where the local Reynolds number is very low, the equations are normally used in conjunction with empirical wall function formulas. The logarithmic wall function (Launder and Spalding, 1974) that is widely used today can still yield rather good results for fully developed, zero-pressure gradient boundary layers in the outer region. However, Hammond (1982) showed that the velocity profile for a plane wall jet is very different from that at the zero-pressure gradient in the outer region, and the logarithmic wall function is invalid there without any modifications (Chen, 1992). The boundary velocity profile of airflow in a room may be located somewhere between that of the zero-pressure gradient and that of the plane wall jet. Hence, the wall function can hardly present good results for the airflow near walls in a room (Chen *et al.*, 1988). Chen *et al.* (1988) also reported that airflows in rooms, natural or mixed convection, have an overall turbulence Reynolds number that are rather small.

His study argued that the high Reynolds number k-ε model of turbulence with the logarithmic functions may not be suitable for use both near the wall and far away from it. Therefore, it is necessary to apply an appropriate low-Reynolds number model of turbulence for computation of flows that have both fully turbulent regions as well as regions with little turbulence. In the recent years, many studies have successfully implemented LRN models to compute indoor airflows. Patel *et al.*, 1986, conducted a review of all the existing LRN models and discussed in detail the theory and the constants that are applicable to each of these models. Chen *et al.*, 1990, incorporated a LRN model to a commercial code and used the modified code to predict natural convection flow in cavities with Rayleigh numbers in the order of 10^{10}. The effect of buoyancy production terms in the k and ε equations has also been explored by this study. The study as in the case of a few other studies (Schulte 1996, Chen *et al.*,1990), have expressed the suitability of LRN turbulence models over the Standard k-ε models in indoor airflow computation. These studies have substantiated this aspect by comparing the results of their studies with experimental studies and found a close match in the data. The current study will be using a LRN turbulence model to assess airflow and contaminant movement in indoor spaces.

Several papers have researched into the effect of flow obstacles on air movement and contaminant distributions in rooms. Bauman *et al.* (1992) investigated a wide range of partition configurations and environmental parameters to study the comfort and ventilation conditions in workstations. Nielson (1998) investigated the influence of office furniture on the air movement in a room with mixing ventilation, and found that the furniture affected the air movement in the lower part of the room, but not in the upper part. Lee and Awbi (1998), have studied the effect of interior partitions on the air movement in a room with mixing ventilation. They found that the interior partitions could affect the airflow and contaminant movement in indoor spaces. This implied the existence of an optimal height for contaminant movement control between the supply and exhaust zones. Haghighat *et al.* (1989), in their study found that the airflow patterns in ventilated rooms are not simply affected by the location of the door, but the overall plan of the relative positions of the door, the air supply and exhaust.

Several studies were identified as suitable references for the validation of PHOENICS based on recommendation from other researchers, the detailed nature of measurements, and suitability of the type of flow considered and the applicability of the studies for the current study. The study by Cheesewright *et al.* (1986), and the study by Chen (1999) were the primary sources for validating the accuracy of PHOENICS in this thesis work.

2.3 Need for Coupling Techniques

The question is, will CFD technique or multizone technique alone provide an effective solution to analyzing building airflow and contaminant movement? With the current technology, the answer would be no. While multizone models provide an approach where the overall interaction at different levels can be applied to identify indoor air quality in buildings, they result in erroneous predictions due to the lack of knowledge of detailed space configurations of different zones as part of the input data. While the CFD technique has gained immense importance in solving air quality problems in individual spaces (Chen *et al.*,1988, Haghighat *et al.*, 1989, Baumann *et al.*, 1992, and

Chen,1992), it is very difficult to generate results on transient characteristics of a space or steady-state characteristics of a whole building. Thus a definite need has been identified for a more comprehensive technique to solve indoor air quality problems in buildings.

The current trend has been to couple multizone models with building energy analysis programs such as DOE-2, and ENERPLUS. Many papers by Schneider (1990), Tuomaaca (1995), Carpenter (1996), and Chen (2000) have researched into the potential benefits of such an integrated efforts. While this coupling technique has received attention from researchers and several publications discuss the details and advantages of this technique, very limited published literature was found on the advantages of coupling multizone with CFD models. Multizone models remain the major instrument for computing the airflow characteristics in buildings since they provide the results based on the outdoor as well as the indoor characteristics of a building. Recently the awareness of increasing indoor air quality problems in buildings made the CFD techniques invaluable in research on air quality in buildings. But the CFD technique is very involved and requires several hours of computational time to solve complex indoor air spaces. While in theory, the airflow pattern for the whole building can be solved using this technique in practice the computational effort would be far too high. Even to portray a single space with consideration to heat sources, contaminating sources, locations of flow obstacles and such details would add an incredible increase to the amount of input data as well as computational time. Thus, research involving the two techniques such that the advantages of the two methods have been used in order to enhance the prediction capabilities of computer models and help achieve realistic results is essential.

A study by Carpenter (1996) used the multizone model, CONTAM to evaluate the indoor air quality in an office building. Formaldehyde and carbon monoxide were the two contaminants in question. It was found that CONTAM was very effective in identifying indoor air quality problems related to transient characteristics of contaminant generation over a 24-hour period. One of the major problems identified in this study was also a noted shortcoming of multizone models. It was found that the meeting room in the office building showed very high levels of carbon monoxide as compared to the other spaces. This study suggested the importance of knowing the detailed flow and contaminant source characteristics of individual spaces as being a crucial segment in determining the overall indoor air quality of a building. A study by Ayari *et al.* (2000) applied the two models in order to get a better picture of the indoor air quality of an underground parking garage. In this study it was found that the use of multizone model alone did not provide a detailed picture of the airflow characteristics of the garage.

Schaelin *et al.* (1993) have addressed this issue at a basic level. In their study, they described a technique to conduct such a coupled analysis and also discussed the importance of identifying crucial areas for such applications. A recent study by Musser (2001) conducted a more detailed analysis of this approach. While in this study also the actual data exchange between the two models did not occur, the advantages of using these models in specific situations was discussed in detail. In this study, four possible combinations of analyses were examined. Both the rooms were analyzed with CFD, with multizone and also two scenarios where in the more critical zone was evaluated with CFD. It was found that the use of the combined approach provided more accurate solutions than the individual model predictions.

2.4 Algorithm for the thesis work

The algorithm used in this thesis work involves interaction between the two models, CONTAM and PHOENICS at various levels. The primary goal was to improve the predicting capabilities of the multizone model, CONTAM by applying the knowledge of detailed analysis from PHOENICS.

In the first approach, the exchange occurs at only one level where the suitability of a certain design consideration for the multizone model is further corroborated by the CFD analysis with changes made to the original consideration when the design value was found to create IAQ problems as identified by the CFD model.

In the second approach, a more interactive exchange environment has been applied where the data from the CFD model has been used to vary the input data for CONTAM in order to improve its predictions. The resulting improvements in the predictions have been discussed in detail by offering comparisons between the coupled approach and multizone approach alone.

A more detailed description of the algorithm has been provided in Chapter 6 of this thesis work.

3. THEORY

3.1 Introduction

This chapter discusses the theory for the two models, CONTAM and PHOENICS that will be used in the thesis work, CONTAM, the multizone model and PHOENICS, the CFD model. Both models have received good recommendations from studies that have used them in the past. Before applying the programs for the thesis study, it is important to have a good understanding of the theories upon which the programs are based. An overview of the mathematical models for the two programs, have been discussed in the following sections.

3.2 CONTAM, Multizone Model

3.2.1 Nomenclature for CONTAM

{B} - is a column vector

C - is the removal rate

{C} - correction vector

F - non-flow processes

G - is the contaminant generation rate

[J] - is the square Jacobian matrix

$k_{\alpha\beta}$ - is the kinetic reaction coefficient in zone i between species α and β,

m - mass of air in zones (kg)

P - zone pressure (Pa)

R - gas constant for air (J/kg.K)

R - is a removal coefficient,

S - source strength

T - zone temperature (°C)

t - time (s)

V - zone volume (m^3)

w - airflow rate between zones (kg/s)

Greek Symbols

η - is the filter efficiency in the path from zone to zone

α - contaminant species

β - contaminant species

ρ - density (kg/m^3)

δ - partial differences of properties

Subscripts

i - zone i

j - zone j

α - contaminant species

β - contaminant species

3.2.2 Theory of CONTAM

The fundamental assumption in CONTAM as is in other multizone models is that the building can be modeled by some number of zones of well-mixed air. Such programs stand as a compromise of accuracy, complexity, and speed between a single-zone model and a Computational Fluid Dynamics model of the entire building. The theory presented below is based on the collation of information from Walton (1984), Feustel *et al.* (1992), and Walton (1995).

The air flow rate from zone j to zone i, $w_{j,i}$ (kg/s), is some function of the pressure drop along the flow path, $P_j - P_i$:

$$w_{j,i} = f\,(P_j - P_i) \qquad (1)$$

The mass of air, m_j (kg), in zone i is given by,

$$m_i = \rho_i\, V_i = P_i\, V_i \,/\, R\, T_i \qquad (2)$$

where,

P_i = zone pressure (Pa),

T_i = zone temperature (K),

V_i = zone volume (m^3), and

R = 287.055 (J / kg.K) (gas constant for air)

For a transient solution the principle of conservation of mass states that:

$$\delta\, m_i \,/\, \delta\, t = \rho_i \,.\, \delta\, V_i \,/\, \delta\, t + V_i \,.\, \delta\, \rho_i \,/\, \delta t = \Sigma_j\, w_{j,i} + F_i \qquad (3)$$

where

m_i = mass of air in zone i,

$w_{j,i}$ = airflow rate (kg/s) between zones j and zone i,

F_i = non-flow processes that could add or remove significant quantities of air from the zones. Such non-flow processes are not considered in CONTAM and flows are evaluated by assuming quasi-steady conditions leading to:

$$\Sigma_j w_{j,i} = 0 \tag{4}$$

The steady-state airflow analysis for multiple zones requires the simultaneous solution of equation (4) for all zones. Since the function in equation (1) may be and usually is, nonlinear, a method is needed for the solution of simultaneous nonlinear algebraic equations. The Newton-Raphson method solves the nonlinear problem by an iteration of the solutions of linear equations. In this method, a new estimate of the vector of all zone pressures, $\{P\}^*$, is computed from the current estimate of pressures, $\{P\}$, by,

$$\{P\}^* = \{P\} - \{C\} \tag{5}$$

where the correction vector, $\{C\}$, is computed by the matrix relationship

$$[J]\ \{C\} = \{B\} \tag{6}$$

where $\{B\}$ is a column vector with each element given by

$$B_i = \Sigma_j \, w_{j,i} \qquad (7)$$

and [J] is the square Jacobian matrix whose elements are given by

$$J_{i,j} = \Sigma \, \delta \, w_{j,i} / \, \delta P_j \qquad (8)$$

The CONTAM program contains subroutines for each airflow element which computes mass flow rates and the partial derivative values for a given pressure difference input.

Equation (6) represents a set of linear equations which must be set up and solved for each iteration until a convergent solution of the set of zone pressures is achieved. In its full form [J] requires computer memory for N^2 values, and a standard Gauss elimination solution has execution time proportional to N^3. The skyline solution process is applied in CONTAM program. This method can be used to solve equations with symmetric and non-symmetric matrices. It stores no zero values above the highest non-zero element in the columns above the diagonal and no zero values to the left of the first non-zero value in each row below the diagonal.

Analysis of the element models will show that

$$|J_{i,j}| = \Sigma_{j \neq i} \, |J_{i,j}| \qquad (9)$$

This condition allows a solution without pivoting, although scaling may be useful. CONTAM allows zones with either known or unknown pressures. The constant pressure zones are included in the system of equations and equation (6) is processed so as to not change those zone pressures. This gives flexibility in defining the airflow network while maintaining the symmetry of equations. In CONTAM, the ambient air is treated as a constant pressure zone. The ambient zone pressure is set to zero causing the computed zone pressures to be values relative to the true ambient pressure and helping to maintain numerical significance in calculating pressure differences.

Mathematical Theory – Contaminant Dispersal

A zone is a region of uniform air temperature and contaminant concentration which may correspond to a single room, a portion of a room, or several well-coupled rooms. The mass of contaminant α in zone i is

$$m_{\alpha,i} = m_i \, C_{\alpha,i} \qquad (10)$$

where m_i is the mass of air in zone i and $C_{\alpha,i}$ is the concentration mass fraction of α. CONTAM performs trace analysis only. The contaminant concentration must be low enough so as not to significantly change the density of the air-contaminant mixture.

Conservation of contaminant mass for each species produces the following basic equation for contaminant dispersal in the building:

$$d\, m_{\alpha,i} / dt = -R_{\alpha,i} C_{\alpha,i} - \Sigma_j \, w_{i,j} C_{\alpha,i} + \Sigma_j \, w_{j,i} (1 - \eta_{\alpha,j,i}) C_{\alpha,j} + m_i \Sigma_\beta \, k_{\alpha\beta} C_{\beta,i} + G_{\alpha,i} \qquad (11)$$

where

$C_{\alpha,i}$ is the removal rate ,

$R_{\alpha,i}$ is a removal coefficient,

$k_{\alpha\beta}$ is the kinetic reaction coefficient in zone i between species α and β,

$\eta_{\alpha,j,i}$ is the filter efficiency in the path from zone j to zone i,

$G_{\alpha,i}$ is the contaminant generation rate, and

$w_{i,j}$ is the rate of air flow from zone i to zone j

This differential equation is approximated by an implicit difference equation. There is one such equation for every contaminant in every zone. These equations must be solved simultaneously for all zones and contaminants.

CONTAM allows the user to define the generation, $G_{\alpha,i}$ and removal, $R_{\alpha i}$ coefficients for some simple cases. The general source/sink model uses the following equation:

$$S_\alpha = G_\alpha - R_\alpha . C_\alpha \qquad (12)$$

where S_α is called the contaminant α "source strength". CONTAM maintains the same equation ordering for the contaminant equations as is used for airflows except that for each zone there is an equation for each contaminant species. These simultaneous equations are solved by the non-symmetric skyline method.

3.3 PHOENICS, CFD Model

3.3.1 Nomenclature for PHOENICS

A_μ, A_t, A_{c1} – turbulence model constants where $A_\mu = 0.0165$, $A_t = 20.5$, and $A_{c1} = 0.05$

C - concentration

C_1, C_2 - model coefficients for equation (2.12)

$C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\varepsilon 3}$ - model constants for equation (2.16)

c_p - specific heat (J/kgK)

D - diffusion coefficient of concentration

f_1, f_2 - damping functions

g - gravitational acceleration (m/s^2)

G_k - buoyancy production term

H - room height (m), enthalpy

H^+ - dimensionless temperature

H_w - wall temperature (°C)

k - kinetic turbulent energy (J/kg)

l - length (m)

l_{mix} - mixing length (m)

Nu - Nusselt number

p - pressure (Pa)

P_k - shear production term

Pr - Prandtl number

q''_w - wall heat flux (W/m^2)

Re - Reynolds number

Ra - Rayleigh number

S - source term

T - temperature (°C)

t - time (s)

U - main stream velocity (m/s)

u - velocity component in x direction (m/s)

u' - mean velocity component (m/s)

u^+ - dimensionless velocity

u_T - friction velocity ($\sqrt{\tau_w / \rho}$)

v - velocity component in y direction (m/s)

V - supply velocity (m/s)

w - velocity component in z direction (m/s)

x,y,z - Cartesian coordinates (m)

y - distance from the wall (m)

y^+ - dimensionless distance from the wall

Greek Symbols

d - differences of properties

δ - partial differences of properties

δji - Kronecker delta

ε - kinetic turbulent energy dissipation (W/kg)

Γ - diffusion coefficient (kg/m.s)

κ - von Karman's constant (= 0.4187)

ρ - density (kg/m^3

μ - kinematic viscosity (m^2/s)

μ_t - turbulent or eddy viscosity (m^2/s)

σ - turbulent Pr number

σ_k - turbulent energy diffusion coefficient (= 1.0)

σ_ε - turbulent energy dissipation diffusion coefficient (= 1.3)

τ - shear stress (N/m^2)

τ_w - wall shear stress (N/m^2)

Subscripts

C - concentration of pollutant

H - enthalpy

k - turbulent energy

t - turbulent

u_i, u_j - index notation of velocity component

x_i, x_j - index notation of coordinate axis

ε - dissipation

w - wall

Superscripts

+ - dimensionless

' - averaging components of instantaneous value

" - flux per unit volume

3.3.2 Theory of PHOENICS

3.3.2.1 Governing equations and turbulence modeling

A flow field can be described by the conservation of mass, momentum, energy (dry air) and contaminant species. Given the boundary conditions, the resulting flow pattern is determined by solving the combined Navier-Stokes and energy or any other scalar equations (2.1 to 2.4, Kays and Crawford, 1993).

Conservation of mass:

$$\frac{\delta \rho}{\delta t} + \frac{\delta}{\delta x_i}(\rho u_i) = 0 \qquad (13)$$

Conservation of momentum:

$$\frac{\delta}{\delta t}(\rho u_i) + \frac{\delta}{\delta x_j}(\rho u_i u_j) = \frac{-\delta p}{\delta x_i} + \frac{\delta}{\delta x_j}[\mu (\delta u_i / \delta x_j + \delta u_j / \delta x_i)] + \rho g_i \qquad (14)$$

Conservation of energy:

$$\frac{\delta}{\delta t}(\rho H) + \frac{\delta}{\delta x_i}(\rho u_i H) = \frac{\delta}{\delta x_i}[k / c_p * \delta H / \delta x_i] + S_H \qquad (15)$$

Conservation of contaminant species:

$$\frac{\delta}{\delta t}(\rho C) + \frac{\delta}{\delta x_j}(\rho u_j C) = \frac{\delta}{\delta x_j}(\rho D * \delta C / \delta x_j) + S_c \qquad (16)$$

where the final term on the right side of the equation 14 is the buoyancy term. In equation 15, k is the thermal conductivity of air and S_H is the source term that maybe caused by chemical reaction. In equation 16, D is the diffusion coefficient of concentration and S_c is a source term generated from chemical reaction in equation 16. In equations 13 to 16, u_i is the velocity component (u,v,w), p is the pressure. The time is indicated with t, x_i is the coordinate axis (x,y,z), μ is the kinematic viscosity, ρ is the density and g_i is the gravitational acceleration.

In order to simulate flow fields three dimensionally, at a sufficient fine mesh and time step to capture all the essential spatial and time scales, a large amount of computing time is required. Therefore, turbulence models for the mean turbulent flow have been developed that calculate the statistical characteristics of the turbulent motion by averaging the flow equations over a time scale much larger than that of the turbulent motion. This approach assumes that for many engineering flow problems knowledge of the high frequency fluctuating motion of the turbulent flow often is superfluous. The calculation of the average turbulent flow pattern is possible on a relative coarse mesh and, for steady state flow problems, at steady state. As a result computing time is brief compared to Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES).

For the turbulence models, mean conservation equations are derived by introducing the Reynolds decomposition for the instantaneous variables in equations 13 and 15 and time averaging the equations. The averaging process results in new unknown terms, $-\rho u_i' \, u_j'$ and $-\rho u_i' H'$, the Reynolds terms. The first term is the eddy shear stress which is called the Reynolds stress (τ_{ij}). The latter can be considered as a diffusion term for the enthalpy or any other scalar quantity under consideration.

The determination of the Reynolds terms requires extra equations to solve the problem. This represents the closure problem. The correlation of the Reynolds terms to the mean flow field is resolved by turbulence models. Most turbulence models are based on the concept proposed by Boussinesq approximation that assumes that the turbulent stresses are proportional to the mean velocity gradients, analogous to the viscous stresses in laminar flows:

$$\tau_{ij} = -\rho u_i' u_j' = \mu_t [\delta u_i / \delta x_j + \delta u_j / \delta x_i] - 2/3\, \delta_{ij} \rho k \qquad (17)$$

$$-\rho u_i' H' = \Gamma_t\, \delta H / \delta x_i \qquad (18)$$

where μ_t is the turbulent or eddy viscosity, a property of flow, Γ_t the turbulent scalar diffusivity, δ_{ij} the Kronecker delta and k is the turbulent kinetic energy. The second term on the right hand side of equation 17, which can be considered as a dynamic pressure, will be ignored because it is small (Chen *et al.*,1988).

3.3.2.2 LRN Turbulence Model

Numerical simulation has been applied to ventilation flows for more than twenty years. Several papers have given a review of these models such as Patel *et al.*, (1986). The current status and potential capabilities and limitations of using CFD for analyzing indoor airflows have been discussed by Chen (1992). Among the existing turbulence models, research (Chen *et al.*, 1990) has indicated the LRN models as being better in their prediction capabilities of complex room airflow situations in comparison to the other models

The standard k-ε model formulation, as discussed earlier is suitable mainly for high Reynolds number flows. Room airflows however, are characterized by near wall regions and stagnant regions with very little turbulence. In both of these regions, the effect of viscous transport becomes dominant. Such regions are better accommodated by a low Reynolds number k-ε model. Recent research has mainly concentrated on developing such LRN formulations and validating the accuracy of these models in indoor airflow predictions. A review of the LRN models are given in Patel *et al.* (1986). Some of the older models include those of Lam-Bremhorst etc. while more recent models include Myong and Kasagi (1990), Nagana and Tagawa (1990), and Heindel *et al.* (1994). LRN models use damping functions in the eddy viscosity model (EVM) equation and the k and ε transport equations to calculate flows to the wall surfaces without wall functions. The k and ε transport equations for a LRN model are generally expressed as

$$\frac{\delta}{\delta t}(\rho k) + \frac{\delta}{\delta x_j}(\rho u_j k) = \frac{\delta}{\delta x_j}[(\mu + \mu_t / \sigma k)\, \delta k / \delta x_j] + \rho\,(P_k + G_k - \varepsilon) \qquad (19)$$

and

$$\frac{\delta}{\delta t}(\rho \varepsilon) + \frac{\delta}{\delta x_j}(\rho u_j \varepsilon) = \frac{\delta}{\delta x_j}[(\mu + \mu_t / \sigma_\varepsilon)\, \delta \varepsilon / \delta x_j] + \rho * 1/T\,(C_{\varepsilon 1} f_1 P_k + C_{\varepsilon 3} G_k - C_{\varepsilon 2} f_2 \varepsilon) \qquad (20)$$

where σ_k, σ_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, $C_{\varepsilon 3}$ are model constants and f_1 and f_2 are damping functions. The damping functions are generally dependant upon the local turbulent Reynolds number and are given by

$$Re_t = \rho k^2 / \mu \varepsilon \qquad (21)$$

and upon the dimensionless distance to the wall, y^+. The best models are carefully designed to reproduce the near wall behavior given by Direct Numerical Simulation (DNS) data (Kim and Moser, 1987).

The damping functions play a very important role in the convergence of the flow problem. Several researchers have come up with models having variations in the depiction of the damping functions.

The Lam-Bremhorst model (1981) depicts the damping functions in the following manner:

$$f\mu = (1 - e^{-A\mu Rk})^2 \, [1 + A_t / Re_t] \qquad (21)$$

$$f_1 = 1 + [A_{c1} / f_\mu]^3 \qquad (22)$$

$$f_2 = 1 - e^{-Ret_2} \qquad (23)$$

where the turbulence model constants are $A_\mu = 0.0165$, $A_t = 20.5$, and $A_{c1} = 0.05$, R_k and Re_t are turbulence Reynolds numbers.

The present study will use LRN turbulence model as proposed by Lam-Bremhorst in the computation of indoor airflow.

3.3.2.3 Numerical Methods

An analytic solution of the coupled, non-linear, partial differential equations for a three-dimensional, turbulent flow field is not possible. The use of numerical methods is inevitable and therefore the calculation of a flow problem requires the discretization of that flow field into space and time. Finite volume and finite element methods are used to obtain a numerical solution. In both methods the discretized equations represent the flow problem in each control volume or element. The finite volume method has been applied in the PHOENICS software to solve the flow problems.

Discretization

Discretization in space requires the flow field to be divided in small control volumes. Different types of control volumes and grid topologies are possible, hexahedral and tetrahedral control volumes and structured and unstructured grids.

Integration over the control volume in order to balance the conservation equations requires the calculation of the cell face values of the scalar variable ϕ so that the convective and diffusive fluxes can be determined. This requires an interpolation from the ϕ-value at the cell center to the cell face. Different interpolation schemes are available. The application of a specific scheme for a variable depends on the grid alignment to the flow field. Higher order schemes present a better accuracy as a first order scheme introduces numerical diffusion when the flow field is oblique to the grid alignment. Higher order schemes however show a less stable solution procedure.

Solver

Solving the equations on a structured grid allows the application of line-iterative methods as the line Gauss-Siedel method. The equations for a variable are solved directly along one line of control volumes applying the tri-diagonal matrix algorithm (Patankar, 1980). The calculation is continued with the next line applying the latest available boundary values. The solution process can be improved via block correction along a line of control volumes. The added correction satisfies the balance over the control volume block (Patankar, 1980). A further improvement can also be obtained by applying a multi-grid solver. Corrections are determined from a successively coarser grid which is constructed from a block of control volumes. These corrections are added to the fine grid solution during the iteration process (Hutchinson and Raithby, 1986: referred in Chen, 1992). For unstructured grids a line-iterative method cannot be applied. The Gauss-Siedel solution process is combined with the multi-grid technique. An algebraic scheme is used to determine the coarse level mesh.

An iterative approach is required to obtain the separate but coupled flow field variables, from an initial guessed flow field. The solution of the flow field is complicated by the pressure source term in the momentum equation. The pressure field cannot be determined from a separate equation. Patankar (1980) describes a procedure in which the pressure field is obtained via the continuity equation, the Semi-Implicity Method for Pressure-Linked Equations (SIMPLE). Given an initial pressure field, the momentum equations are solved. A pressure correction is obtained from the revised continuity equation and the velocity component values are corrected subsequently. After the calculation of the coupled flow field variables, as temperature and turbulent quantities, the corrected pressure is taken as the new pressure field and the procedure is repeated until a converged solution is obtained. All flow field variables are stored in the cell center of the control volume. A linear interpolation procedure is applied to obtain the pressure value at the face of the control volume, as is necessary for solving the momentum equation (Choi *et al.*, 1990). In this way an oscillatory pressure field is prevented without the application of a staggered grid. This approach is useful when boundary fitted coordinates are used for non-orthogonal boundaries of a flow problem. For large local gradients of the pressure, as with large buoyant forces, the discretization should be refined. Also a staggered grid approach may be re-introduced for the calculation of the face pressure. To prevent a similar oscillatory solution for the flow field when solving the continuity equation, a momentum-weighted averaging is applied for the velocity that is based on the convection and diffusion effects.

When the buoyancy force is of the same order of magnitude as the pressure gradient the convergence is poor because of the relative small contribution of the convective and viscous terms. This results from the sequential solving process of the SIMPLE-algorithm. A correction term can be incorporated in the revised continuity equation that accounts for the buoyancy force.

Convergence

Due to the non-linearity of the problem the solution process is controlled via relaxation factors. A relaxation factor controls the change of a variable as calculated after each iteration. The convergence is checked by several criteria: the mass and heat conservation should be balanced; the residuals of the discretized conservation equations must steadily decrease; and the change in field values between two iterations should be very small.

4.VALIDATION AND EVALUATION OF SIMULATING CAPABILITIES OF CONTAM AND PHOENICS

4.1 Introduction

Any computer model, before being applied in a specific study needs to be validated against results from experimental studies. This is essential to ensure confidence in the results that are obtained and for future applications. This chapter discusses the validation of the two models that will be used in this thesis study: multizone model, CONTAM and CFD model, PHOENICS. The validation was done to test the capabilities of the models in the commonly used application areas of each of the models. This chapter also discusses the results from a parametric study that was conducted with CONTAM to evaluate its simulating capabilities. Although the validation and parametric study of the CONTAM program was conducted on several types of buildings, the results presented here have been restricted to an office building (Persily, 1994) and parking garage (Ayari *et al.*, 2000) which bears more relevance to the thesis topic.

4.2 CONTAM

4.2.1 Validation of CONTAM

4.2.1.1 Steady State Simulations

The description of the office building and HVAC system discussed in this section are based on the details obtained from the experimental and simulation study conducted by Persily (1994), and Persily (1995) respectively. The office building used in the simulation study is based on an actual building located in Portland, Oregon that was the subject of a study of ventilation and indoor air quality (Persily, 1994). The office building is a seven-story, mechanically ventilated building with one story below grade and a two-story underground parking garage. Details of the building and the HVAC descriptions can be obtained in reference (Persily, 1994).

Results of steady state airflow and contaminant transport have been presented in this section. The office building used in this study was constructed in 1986 and 87 (Persily, 1994) and was designed to comply with the requirements of ASHRAE Std. 62-1981. According to this, the minimum outdoor air intake requirement was 2.5 L/s/person based on an occupancy rate of 7 people per 100sq.m and a ceiling height of 3.5 m including return plenum. This translates to about 0.18 ach (air changes per hour) as opposed to the current value of 10 L/s for office building (0.72 ach). Based on the design airflow capacity that has been specified, capacity of each minimum outdoor air intake fan being 2 m^3/s and the maximum design flow capacity being 47.2 m^3/s, the theoretical values of 0.16 and 3.8 ach are obtained for minimum and maximum outdoor air intakes. The values of ach are in compliance with the ASHRAE Std. 81 for minimum outdoor air intakes but for maximum outdoor air intake it is a little lower than the value specified.

Table 4.1: Comparison of minimum and maximum outdoor intake rates with values from experimental study and numerical study (Persily *et al.,* 1994.)

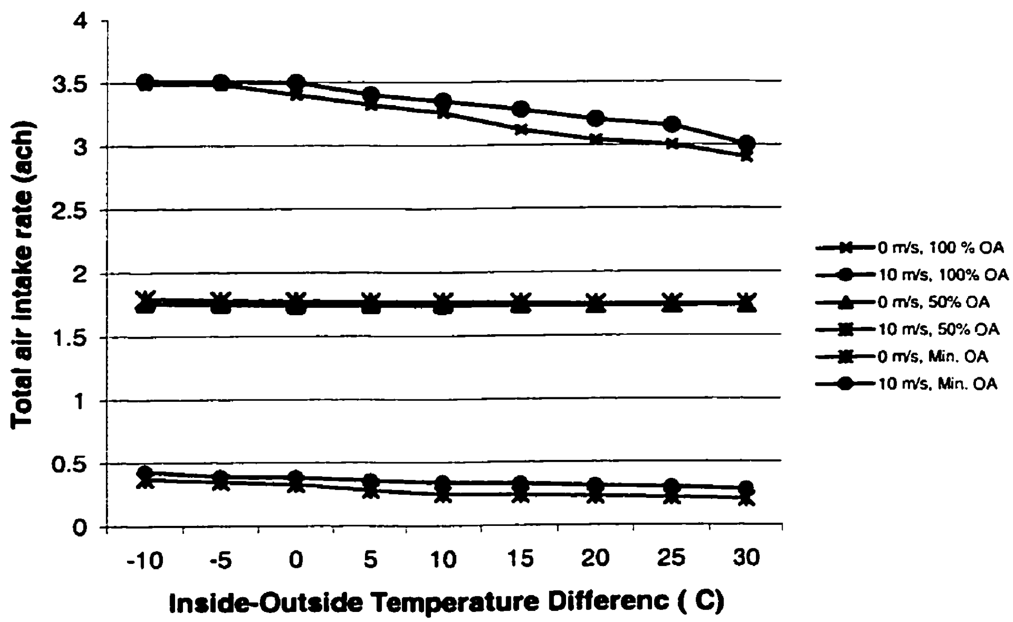
Data	Minimum Outdoor Air Intake (ach)	Maximum Outdoor Air Intake (ach)	% Difference	
			Min.	Max.
Theoretical Calculations	0.16 ach	3.8 ach	37.5% (Theoretical and current)	20% (Theoretical and current)
Experimental Study (Grot *et al.*, 1989)	0.2 ach	2.6 ach	25% (Persily *et al.*, and Grot *et al.*)	20% (Persily and *et al.*, and Grot *et al.*)
Simulation Study (Persily *et al.*, 1994)	0.15 ach	3.12 ach		
Simulation Study (current)	0.22 ach	3.04 ach	10% (Current and Grot *et al.*)	17% (Current and Grot *et al.*)

The results from this simulation study are compared further with the results from the simulation study of Persily *et al.* (1994). The building airflow rates were calculated at all three levels of outdoor air intake for the same values of wind speed and temperature differences as used in the study by Persily *et al.* (1994). to enable comparison and validation of results.

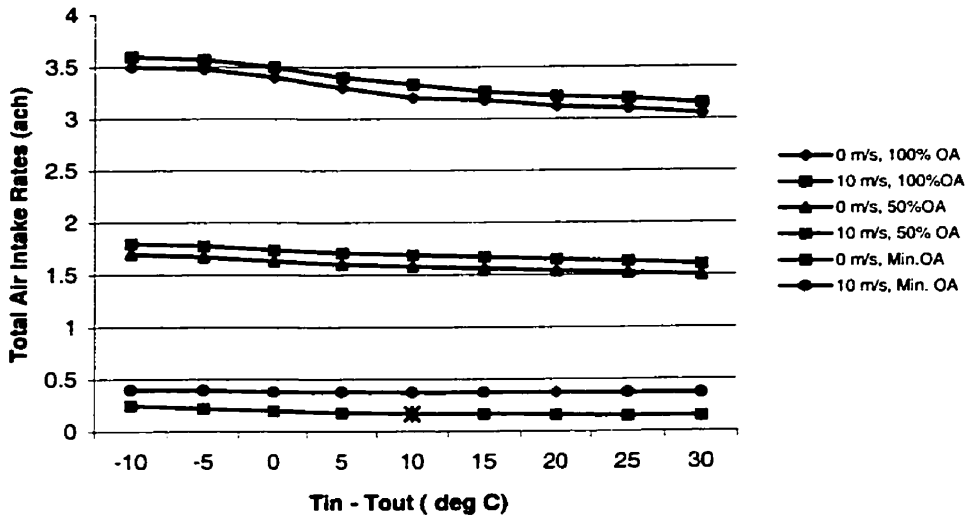
Figure 4.1(a) shows a plot of calculated total air intake rates as a function of the indoor-outdoor temperature difference. The total air intake rate is equal to the flow rate of outdoor air brought into the building by mechanical ventilation plus the infiltration rate through the building envelope. Although there is a slight reduction in the air change rate with the increase in temperature difference, the increase in wind speed does not affect the values significantly due to the dominance of mechanical ventilation.

Figure 4.1(b) is a graph of the values obtained in the simulation study conducted by Persily *et al.* (1994). The slight difference in values obtained by the two studies could be due to the difference in idealization of the office building as considered while conducting the simulations. The values are however close enough (based on values obtained in previous research) to validate the accuracy of the modeling and simulation technique applied by the current study.

Figure 4.1 Total air intake rates of office building



a) Current Study



b) Persily et al.(1994)

Predicted values of air change rates at three different levels of outdoor air intakes are compared with the results from Persily *et al.* (1994) for a no wind condition in Table 4.2. It is seen that there are significant differences in the values for 50% and minimum outdoor air intake conditions while that for 100% intake matches very closely.

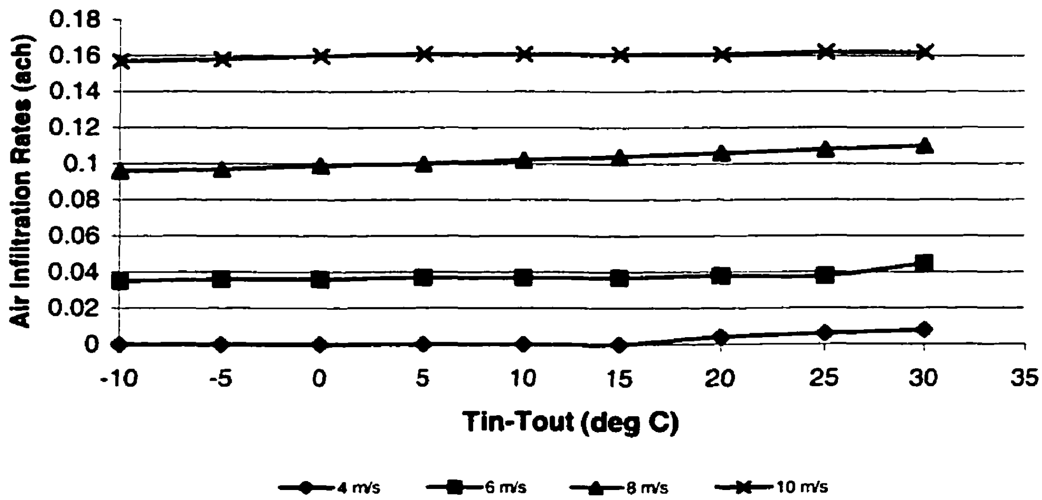
The predicted envelope infiltration rates of the whole building for the 100% intake case are plotted against the inside-outside temperature difference as shown in Figure 4.2. The dependence of infiltration rate on temperature differences is almost negligible due to the dominance of mechanical flows.

Table 4.2: Air change rates of the office building at three different outdoor air intakes at zero wind speed conditions

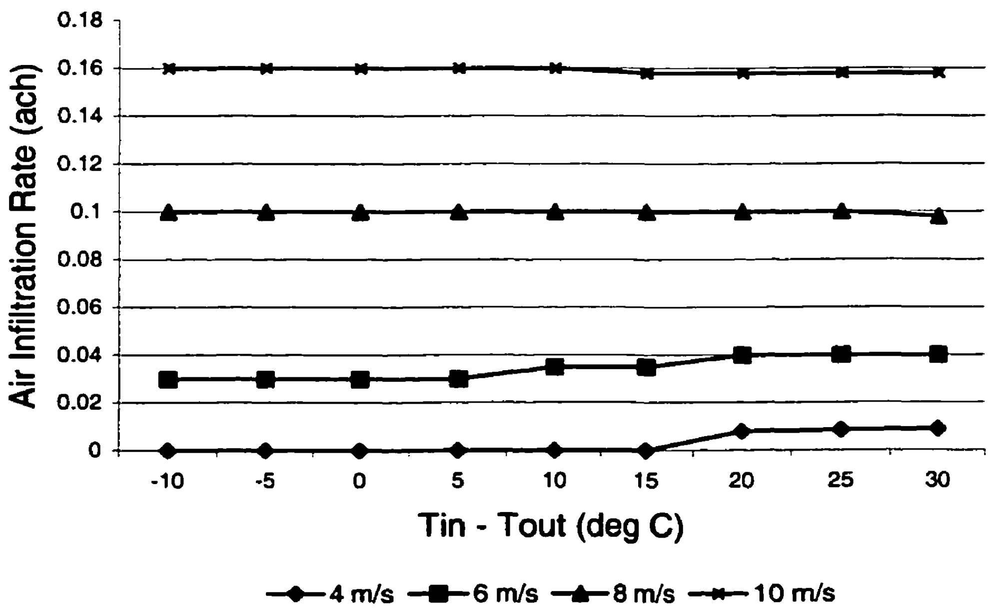
Temp Diff. In Deg. C	100% OA intake, 0 m/s			50 % OA intake, 0 m/s			Minimum OA intake, 0 m/s		
	This Study	Persily *et al.* 1994	% Diff.	This Study	Persily *et al.* 1994	% Diff.	This Study	Persily *et al.* 1994	% Diff
-10	3.49	3.5	0.3	1.76	1.7	3.5	0.3	0.25	20
-5	3.48	3.48	0	1.75	1.67	4.7	0.29	0.22	31
0	3.4	3.4	0	1.74	1.63	6.7	0.27	0.2	35
5	3.32	3.3	0.6	1.74	1.6	8.8	0.25	0.18	38
10	3.26	3.2	1.8	1.74	1.58	10	0.22	0.17	29
15	3.15	3.18	0.9	1.74	1.56	11.5	0.22	0.16	37.5
20	3.04	3.12	2.5	1.74	1.54	12.9	0.22	0.15	46
25	3	3.1	3.0	1.74	1.52	14.5	0.22	0.15	47
30	2.9	3.05	4.9	1.74	1.5	16	0.21	0.15	40

It is seen that for lower values of wind speed, there is almost no infiltration of air into the building. The building is apparently positively pressurized for lower levels of wind speed and thus prevents any infiltration from occurring. The values show only a slight increase for values of wind speed greater than 6 m/s.

Figures 4.2 Predicted Air Infiltration Rates for the Office Building for the fan-on condition (current study & study by Persily *et al.*, 1994 respectively)



a)



b)

The office building under consideration has also been evaluated for contaminant movement under varying conditions of temperature and wind speed. The study examines the radon transport in the building and compares the results with the simulation study of Persily *et al.*, 1994. A soil zone was introduced beneath the lowest level of the office building. The soil zone is connected to the outside by an airflow resistance equal to 0.0085 cm^2 / m^2 (Persily,1994). The simulation techniques adapted by Persily *et al.* (1994) is closely followed in order to enable comparison of results. The soil zone is also connected to the lowest level of the building by a minimal airflow resistance. The ambient concentration of radon was assumed to be 10 Bq/m^3. Steady-state indoor radon concentrations were calculated for each of the building zones on the basis of the airflow rates that are calculated for a given set of weather data and ventilation flow rates.

The following section presents the radon transport simulation in the office building. The results are presented for two different cases for the condition of minimum outdoor airflow intake. Tables 4.3 and 4.4 compare the results obtained with the results from the simulation study of Persily *et al.* (1994).

The study has considered a hypothetical situation for radon simulation in the office building. The radon simulation strategy is also crucial in obtaining realistic values. In the case of this study the radon was assumed to enter at a constant rate of 0.02 $Bq/s/m^2$ of the basement floor area. Table 4.3 presents the calculated concentrations of Radon for no wind condition as a function of the temperature difference. Radon entry rate is found to increase with the increase in temperature difference due to stack effect. The higher floors see the effect of radon entry only at temperature differences of 20 and 30 deg C.

Table 4.3: Radon Values in Bq/m^3, wind speed of 0 m/s, minimum outdoor air

	Results obtained : Current Study				Results obtained : Persily *et al.* (1994)				
Temp. Diff. Deg C	Bldg. ach	Level B1	7th Floor	Average Value	Bldg. ach	Level B1	7th Floor	Avg. Of Floors	% Diff.
-10	0.372	11.0	10.3	10.6	0.19	10.4	10.3	10.3	2.9
0	0.328	10	10	10	0.17	10.0	10	10	0
10	0.250	9.9	9.9	9.9	0.16	9.7	9.7	9.7	2.1
20	0.220	12	16.8	15	0.15	10.8	16.0	14.8	1.35
30	0.205	11	19	17	0.15	10.2	18.7	16.9	0.6

It is seen that for temperature differences of less than or equal to 10 deg C radon does not enter the building. For positive temperature differences, basement depressurization occurs which is typical in winter conditions and this results in increase of radon entry in the building. The values obtained in this study are a little higher, but not significantly so, compared to the values obtained by the simulation study of Persily *et al.* (1994). The contaminant concentrations are based on the calculated airflow rates and since the values of the airflow rates obtained by this study are higher the contaminant concentrations have also followed the trend.

Table 4.4: Radon Values in Bq/m^3, Tin – Tout = 30 deg C, minimum outdoor air

	Results obtained: Current Study				Results obtained : Persily *et al.* (1994).				
Wind Speed m/s	Bldg. ach	Level B1	7th Floor	Average Value	Bldg. ach	Level B1	7th Floor	Avg. Of all Floors	% Diff.
0	0.205	11	19	17	0.15	10.2	18.7	16.9	1.7
2	0.260	11	19	17	0.16	10.3	18.6	16.8	1.8
4	0.268	11.5	18.8	16.5	0.18	10.6	17.8	16.0	3.1
8	0.272	9.5	9.5	9.5	0.27	9.0	9.0	9.0	5.5
10	0.284	9.5	9.5	9.5	0.33	9.0	9.0	9.0	5.5

Table 4.4 presents the concentration of radon for varying wind speed conditions and at a constant temperature difference of 30°C. For lower wind speed conditions radon enters all floors of the building since the building would be negatively pressurized at this point. For higher wind speeds the building becomes positively pressurized and thus prevents the entry of radon into the building. The values obtained by the study match very closely with those obtained by Persily *et al.* (1994).

In both simulations, the level of Radon in the building is well under the value considered as critical by Health Canada (150 Bq/m^3 or 4 pCi/L).

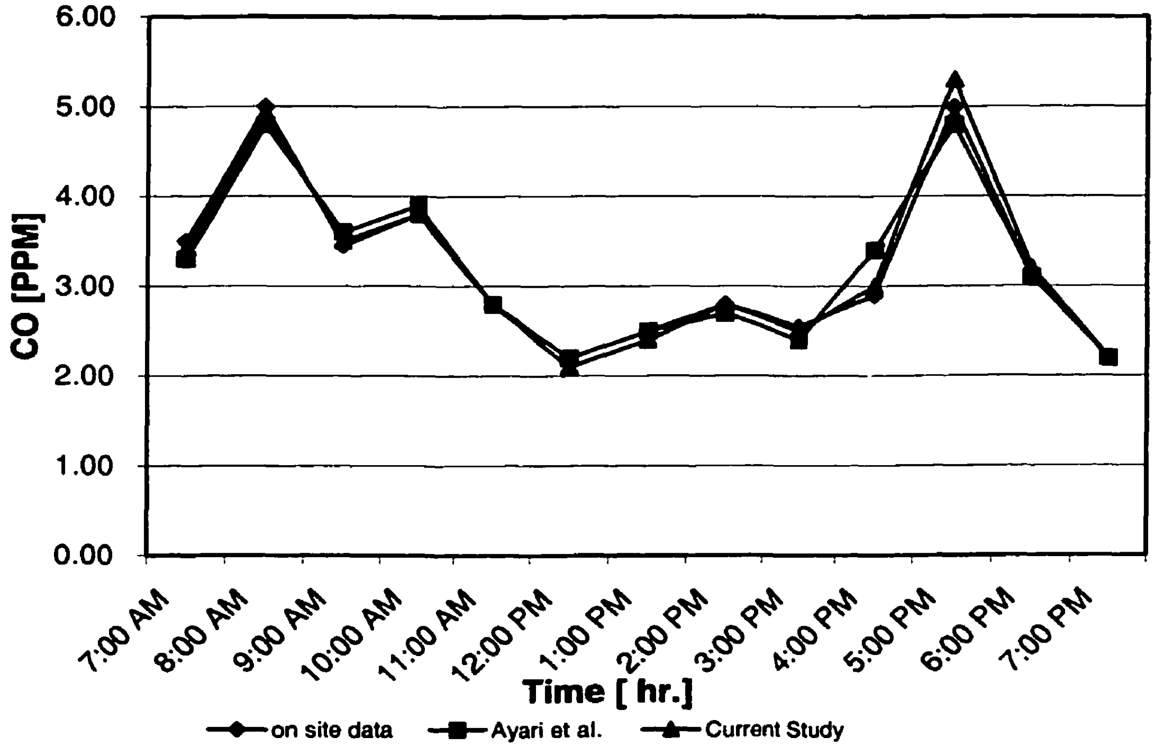
4.2.1.2 Transient State Simulations

Transient simulations were conducted to assess the build-up of carbon monoxide in the parking garage over a period of 24 hours. The simulation study considers a two level parking garage located in Denver, Colorado. This study was the subject of an experimental study where the carbon monoxide concentrations were measured for a 24-hour period (Ayari *et al.*, 2000). The parking garage has two identical levels of total floor area of 5570 m^2. The first level of the garage has 88 car parking capacity and the second floor can hold 105 vehicles.

Figure 4.3 shows the variation in carbon monoxide concentrations calculated using CONTAM over a 24-hour period. The graph shows the comparison of the results from this study to those obtained from field measurements and another simulation study (Ayari *et al.*, 2000). One of the objectives of the study by Ayari was to determine whether the specified ventilation rate for enclosed parking facilities as prescribed in ASHRAE Std. 62-1999 is really required to contain the concentrations of carbon monoxide under the required levels. The prescribed ventilation rate in ASHRAE standards is 7.5 $L/s/m^2$ of gross floor area independent of the vehicle types, number of moving vehicles and the travel time. The field study by Ayari measured an air change rate between 5-7 ach. This study predicted an air change rate of 5 ach. The objective was to determine whether this airflow rate was sufficient to maintain a good indoor air quality in the parking facility.

The graph shows the variations in the carbon monoxide concentration over the 8-hour period during the hours of operation of the facility. The facility did not have any specified energy conservation plan. The fans were on for the entire period of operation of the facility. From the figure it is seen that the values of CO concentration reaches a peak between 7 am and 9 am. This increased level is possibly due to the arrival pattern of the office workers in that building. The values reduce considerably during the slow periods of the day, reaching higher values again between 4 pm and 6 pm which coincides with the departure time of the occupants in the building. The values of CO concentration also rise in value during the lunch hour period. The results obtained using CONTAM are in close agreement with the values and the trend generated by the experimental study and the simulation study (Ayari *et al.*, 2000). The carbon monoxide average over the 8-hour period remains approximately around 3 ppm in both the studies. This is well under the prescribed 9 ppm for an eight-hour average (OSHA Standards, Health Canada)

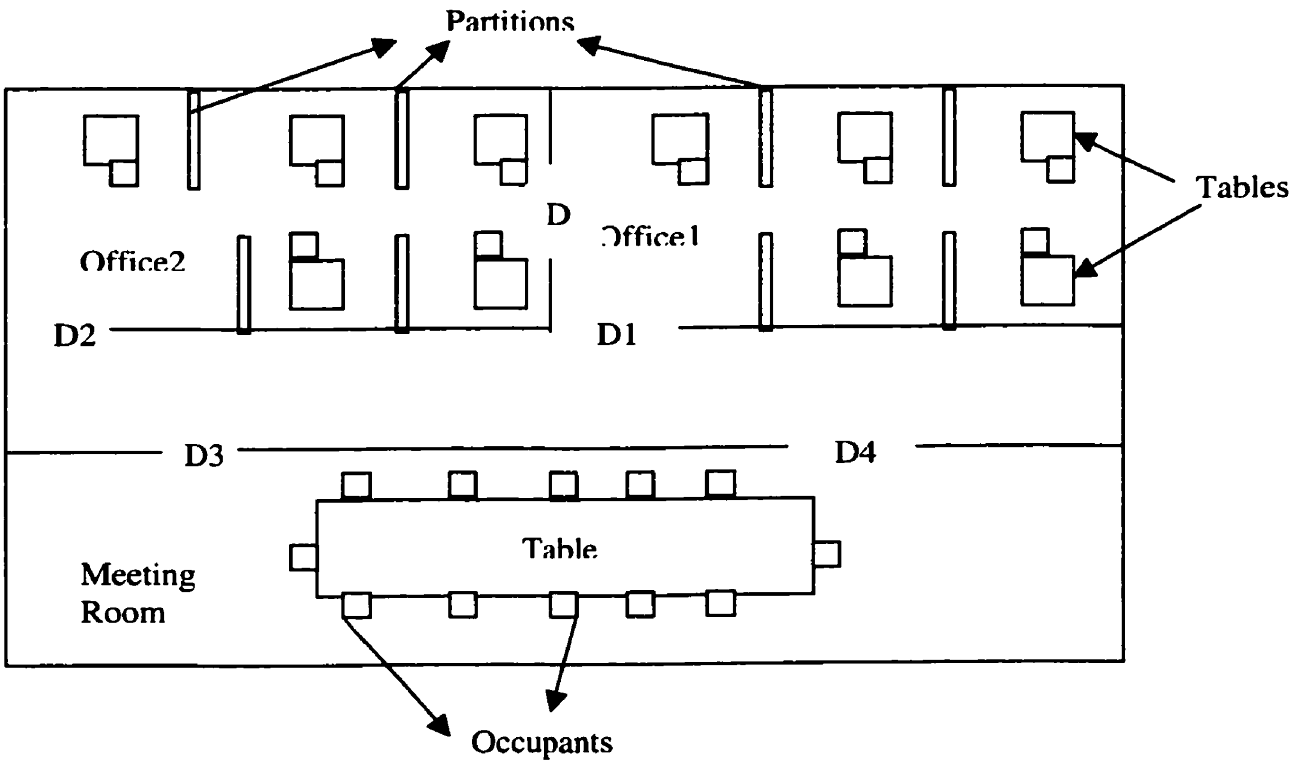
Figure 4.3 Carbon Monoxide Concentrations Over a 8-hour period



4.2.2 Parametric Study: CONTAM

The office layout shown in the Figure 4.4 contains two office spaces and a meeting room. A hallway separates the office spaces from the meeting room. A doorway is located between office 1 and office 2. The interior space configuration of office 1 and office 2 is based on the space design of configuration 4 from Chapter 4 (see Section 4.3.2.3) of this thesis work. The space design of the meeting room consists of a long table with chairs for the occupants as shown in figure.

Figure 4.4 Floor plan of the office space



In this section the adequacy of the inlet velocity into the office space is evaluated by changing the contaminant loads in the configuration above. The objective was to determine whether the designed flow rate maintains good indoor air quality in all the zones of the office under minimum, medium and maximum contaminant loads. In PHOENICS it is difficult to predict transient concentrations of contaminants. In this study, simulations with PHOENICS have been restricted to steady state ones. In CONTAM, the doorways leading in and out of each zone have been considered as a zone in order to determine the contaminant exchange at the point of interaction between the zones. Transient contaminant concentrations have been computed using CONTAM.

4.2.3 Input Data

Three different scenarios based on a typical office schedule have been considered. The arrival time or close to departure time when the contaminating sources are minimal, the peak load during mid-morning, afternoon periods and a specific case of heavily contaminated office space such as a meeting room and the overall interactions in different zones that could occur due to such an increase in the levels of contaminating sources.

The input data for the two programs have been listed in the Table 4.5. ASHRAE Std. 62 (1999) recommends 10 L/s/person as the design standard for ventilation systems for office spaces. This section will try to evaluate whether this is a good recommendation for the office in consideration. A better idea might be obtained with the coupled analysis, which will be studied in Chapter 6. For the specified office space the recommendation of 10 L/s translates to about 220 L/s per floor based on a maximum occupancy of 22 persons. While providing adequate airflow into a building is extremely beneficial from an indoor air quality perspective, it increases energy consumption and the environmental impacts associated with providing this energy (Persily *et al.*, 1994).

Table 4.5 Input Data for CONTAM and PHOENICS

Input Parameters	**Input Values**
1. Ventilation Flow Rate	0.22 m^3/s
2. CO_2 Source	15 L/h/person
3. Occupants	
a) Minimum Occupancy (Case I)	6 occupants (3 in office 1 and 3 in office 2)
b) Normal Occupancy (Case II)	10 occupants (5 in office 1 and 5 in office 2)
c) Maximum Occupancy (Case III)	22 occupants (5 in office 1, 5 in office 2, and 12 in meeting room)
4. Space Occupancy Schedule	
a) Office 1 and Office 2	8 am – 9 am ---- Minimum Occupancy 9 am – 10 am --- Normal Occupancy 10 am – 11 am --- Maximum Occupancy 11 am – 4 pm --- Normal Occupancy 4 pm – 6 pm --- Minimum Occupancy
b) Meeting Room	8 am – 10 am ---- Empty (No Occupants) 10 am – 11 am --- 12 Occupants 12 pm – 5 pm --- No Occupants

4.2.4 Simulation Results

Steady State

The airflow simulations remain the same in all three cases, since the air intake design remains the same during all three simulations.

Table 4.6 Airflow rate in kg/s

Zones	Airflow rate (kg/s)
Office 1 to Office 2 (through doorway), D	0.015
Office 1 to Corridor (through doorway), D1	0.018
Office 2 to Corridor (through doorway), D2	0.00985
Meeting room to Corridor (through doorway), D3	0.012
Meeting room to Corridor (through doorway), D4	0.015

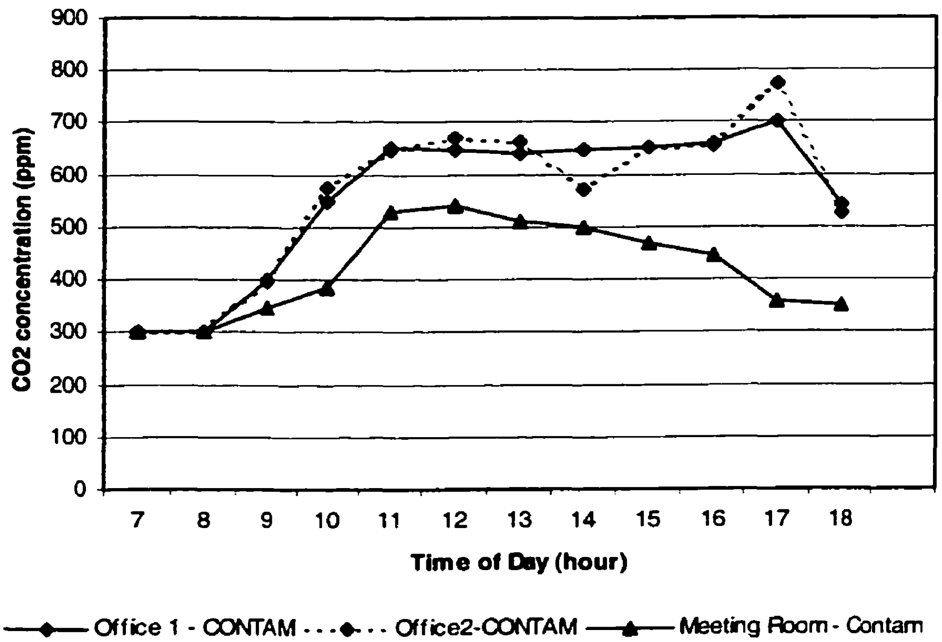
Given in Table 4.6 are the values of air velocities as computed by CONTAM at the doorways to various zones. The computed CO_2 concentrations in the zones are presented in Table 4.7.

Table 4.7 Carbon dioxide concentrations in ppm (steady state values)

Zones	CO_2 concentration (ppm) Case I (minimum occupancy)	CO_2 concentration (ppm) Case II (normal occupancy)	CO_2 concentration (ppm) CaseIII (maximum occupancy)
Office 1	649	695	702
Doorway between office 1 and 2, D	642	645	740
Office 2	672	702	709
Doorway between office 1 and corridor,D1	591	622	650
Doorway between office 2 and corridor, D2	562	593	660
Corridor	587	625	754
Doorway1 between corridor and meeting room, D3	545	560	701
Doorway2 between corridor and meeting room, D4	542	559	697
Meeting room	542	549	805

The simulation of CO_2 concentrations in various zones as computed by CONTAM is shown in the Table 6 for the three cases. It is seen that the average range as computed by CONTAM remains within the specified limit of 800 ppm for the first two cases. But the interaction of increased contaminant levels in the meeting room makes way for a slight increase in CO_2 levels in most of the zones. However the predictions made by CONTAM for the maximum occupancy conditions does not show a significant increase in the levels of CO_2.

Figure 4.5 CO_2 concentrations at minimum occupancy



Figures 4.5 to 4.7 show the 8-hour transient contaminant data at the three different occupancy levels of maximum, normal and minimum rates. It is seen that predicted levels as depicted in Table 4.6 for the three different cases coincide with the values approximately between 2 and 3 pm for the transient calculations shown in Figures 4.5, 4.6 and 4.7.

Figure 4.6 CO_2 concentrations for normal occupancy

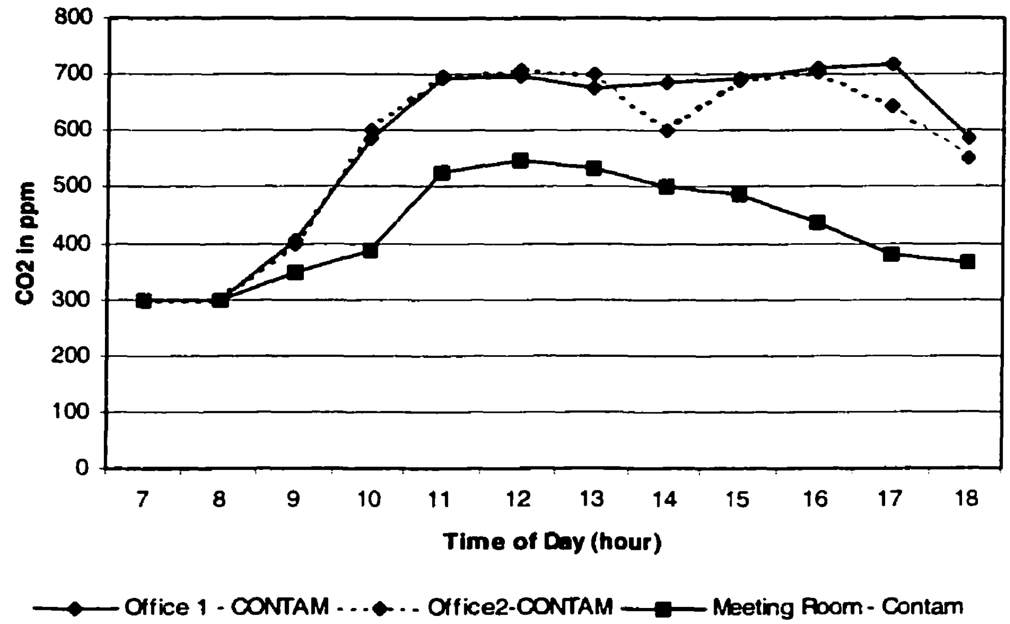
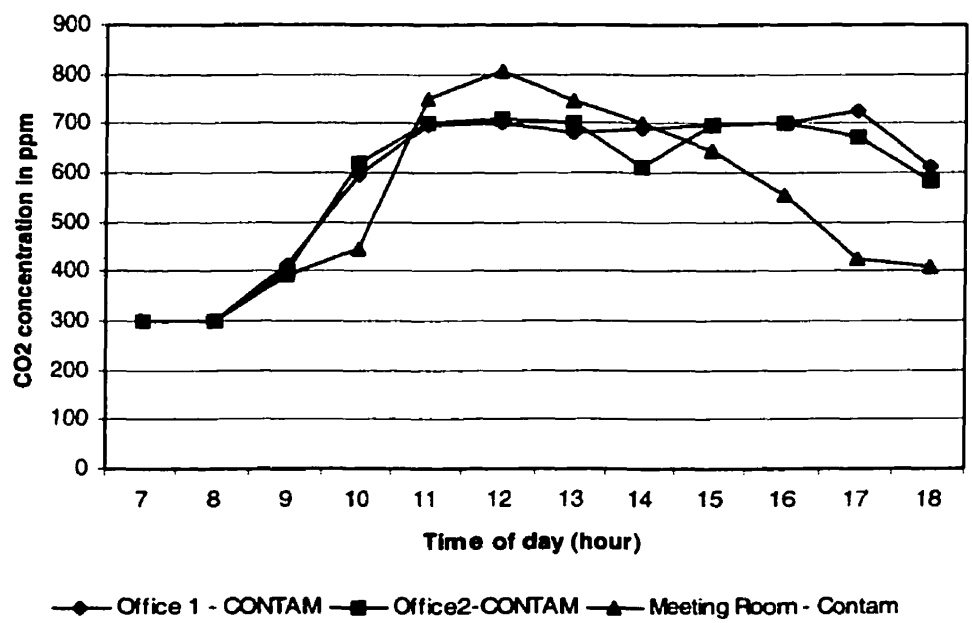


Figure 4.7 CO_2 concentrations for maximum occupancy



It is seen from the above results that CONTAM is able to simulate the trends in the occupancy variations at different times and the steady contaminant concentrations in zones quite accurately. At this point of the discussion, however it is not known whether the predicted values of contaminant levels are accurate. This will be further discussed in Chapter 5 where PHOENICS is also used to simulate this office building.

4.3 PHOENICS

4.3.1 Validation of PHOENICS

The PHOENICS model was validated against the experimental study of Chen, (1999). A small office was the subject of the experimental study. Details of the space configuration (shown in Figure 4.8) and the input details can be can be obtained from the study of Chen (1999).

Figure 4.8 Dimensions of the office

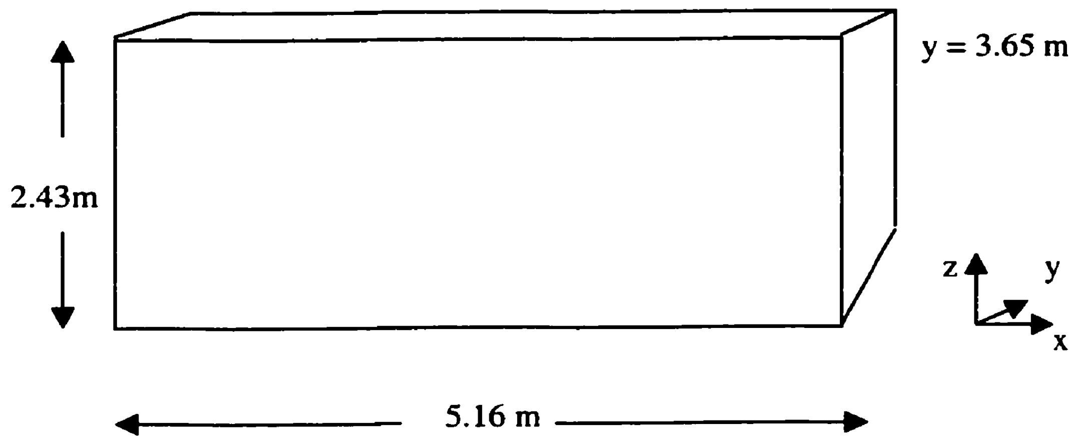


Figure 4.9 Velocity in the office at y = 1.83 m (predicted values)

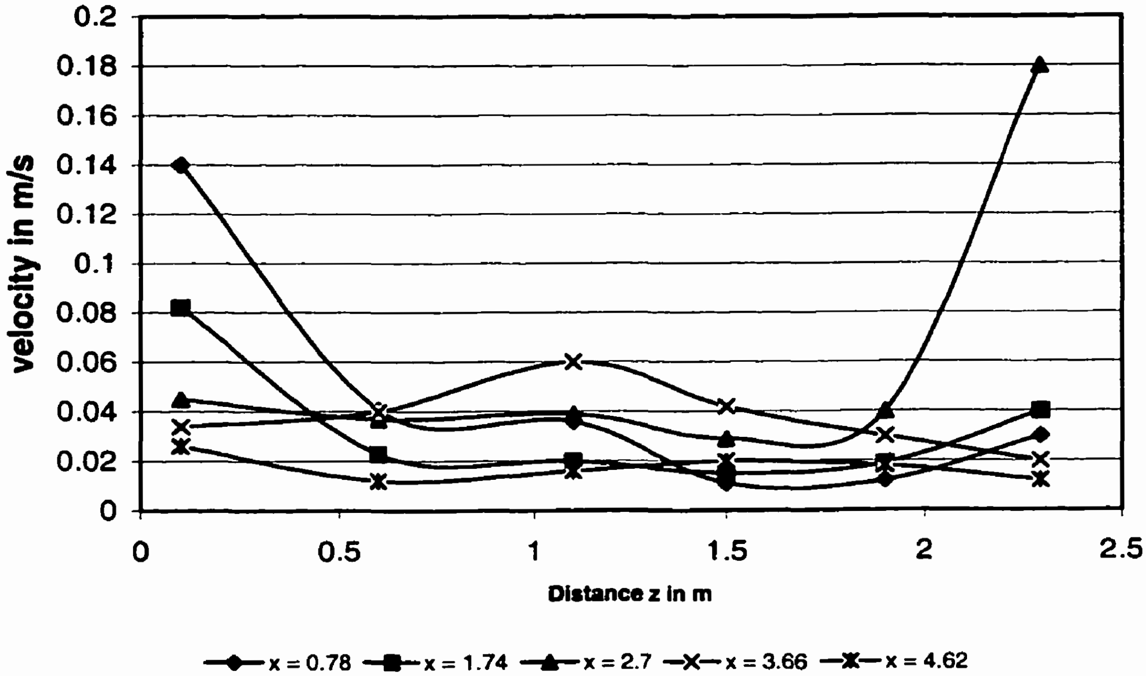
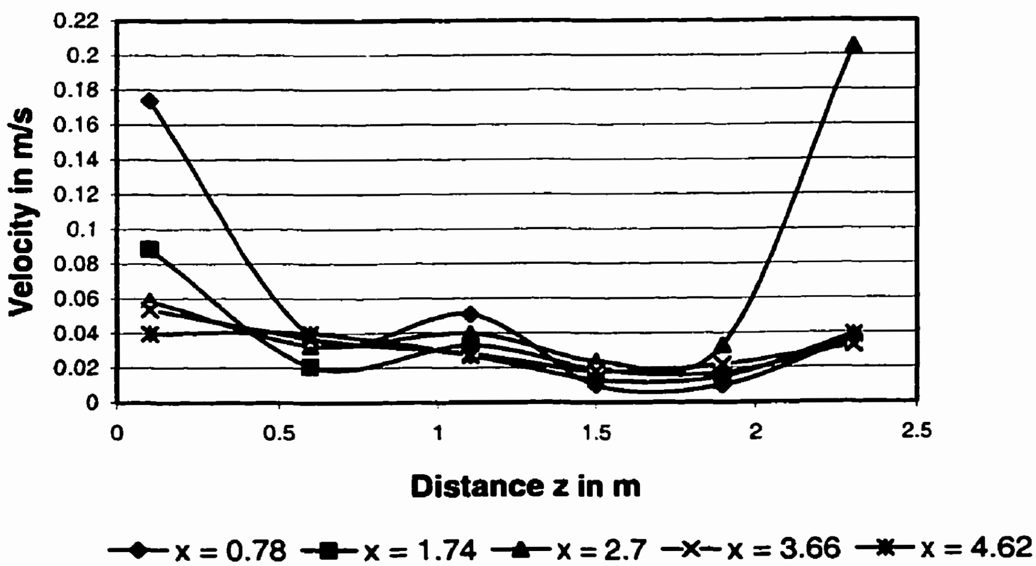


Figure 4.10 Velocity in the office at y = 1.83 m (experimental values, Chen 1999)



Figures 4.9 and 4.10 compare the air velocity values as predicted by this study against experimental values measured by Chen (1999). The computed values show a close match with the experimental values. In order to get a clearer picture of the comparison between the two studies, Tables 4.8 and 4.9 provides the comparison between measured and predicted values and the percentage error variation from the experimental values.

Table 4.8 shows the comparison of measured and computed values of air velocity at three different sections of the office. The percentage variations from the measured values have been calculated to analyze the accuracy of the LRN model used in the study. The computed values seem to show a marked variation at certain levels of the room where the predictions were significantly higher compared to the measured values. The predicted values generally showed higher air velocity levels in the vicinity of heat sources in comparison to the measured values. This trend was maintained even in the contaminant concentration predictions as will be shown at a later section in this chapter.

The measurements typically depend on the accuracy of the instruments and several other physical factors that could vary the accuracy of the results. At the same time the numerical predictions are often affected by the general simulation techniques adapted and the computer models used to generate the computations. The LRN model predicts the velocity variations in the room quite well and matches closely with the measured values.

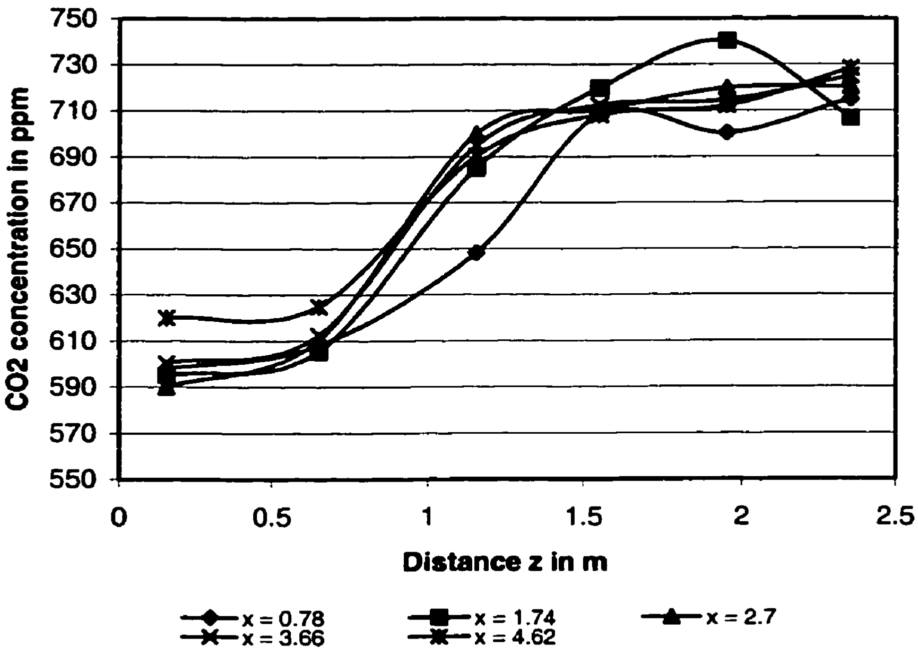
The concentration gradually increases as it moves upwards towards the ceiling. This concentration gradient is one of the expected advantages of the displacement ventilation systems wherein the concentration gradients increase gradually upwards leaving lower concentration levels in the occupied zones of the rooms. In the mixing ventilation systems, the concentration levels would vary in different parts of the rooms.

Table 4.8 Comparison of measured and predicted values of air velocity in m/s

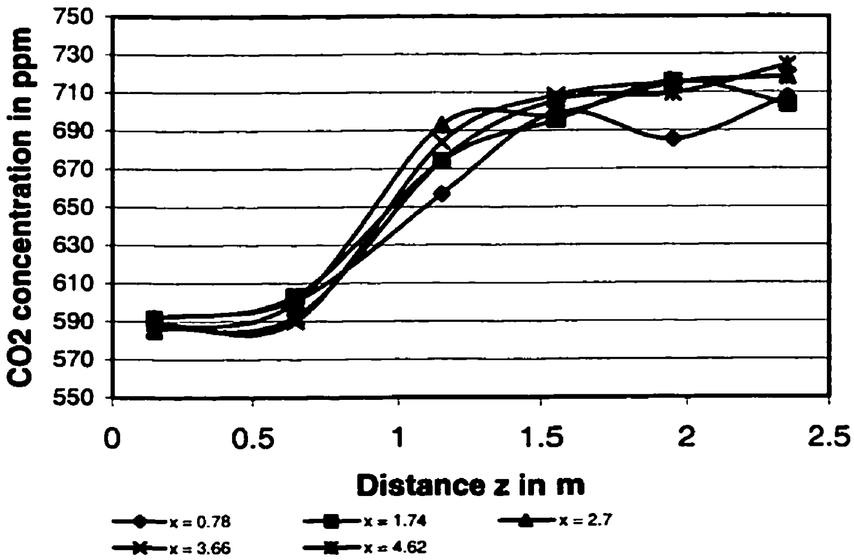
y = 1.83m									
	x = 0.78 m			x = 1.74 m			x = 2.7 m		
Z,m	Chen 1999	Present Study	% Diff.	Chen 1999	Present Studv	% Diff.	Chen 1999	Present Studv	% Diff.
0.1	0.174	0.14	19.5	0.089	0.082	7.87	0.059	0.045	23.7
0.6	0.039	0.041	5.12	0.021	0.023	9.52	0.033	0.037	12.1
1.1	0.051	0.036	29.4	0.033	0.02	33.3	0.04	0.039	2.5
1.5	0.01	0.011	10	0.019	0.015	21.0	0.024	0.029	20.8
1.9	0.01	0.012	20	0.017	0.019	11.76	0.033	0.04	21.2
2.3	0.037	0.03	18.9	0.034	0.04	17.6	0.205	0.18	12.1

Figure 4.11 shows the variations of CO_2 concentrations at two sections of the office. The predictions and experimental values match very closely as shown in the graphs. The contaminant levels have lower values near the floor and show a vertical increase in values nearing the ceiling of the rooms. The values also show a higher trend near the contaminant sources.

Figure 4.11 CO_2 concentrations at y = 1.83 m



a) Predicted contaminant concentrations



b) Experimental values (Chen 1999)

Again the predicted values match closely with the measured values. The accuracy of the predictions has been further clarified by presenting the direct comparison between the measurements and predictions in Table 4.9.

Table 4.9 Comparison of measured and predicted values of CO_2 in ppm at y = 1.83m

y = 1.83m										
x = 0.78 m				x = 2.7m			x = 4.62m			
0.15	592.25	598	0.97	585.28	590	0.8	586.66	620	5.68
0.65	601.2	608	1.13	600.11	610.5	1.7	592.56	625	5.47
1.15	656.77	648.2	1.3	693.07	700	0.99	674.36	690.4	2.37
1.55	699.29	708.3	1.3	698.6	710.3	1.67	705.99	708.3	0.33
1.95	685.46	700.4	2.18	714.85	719.9	0.7	709.46	712.2	0.38
2.35	707.84	715	1.01	718.3	720.4	0.29	724.4	728.3	0.54

The study is based on the office configuration described by Chen (1999) where the optimum size and location of partition have been determined by measuring the resulting air velocity and contaminant distributions in the occupied space.

Figure 4.12 is a comparison with the experimental values at different sections of the office. The predictions are in close agreement with the experimental values as seen in the graph.

Figure 4.12 Predicted and measured air velocity at y = 1.83m

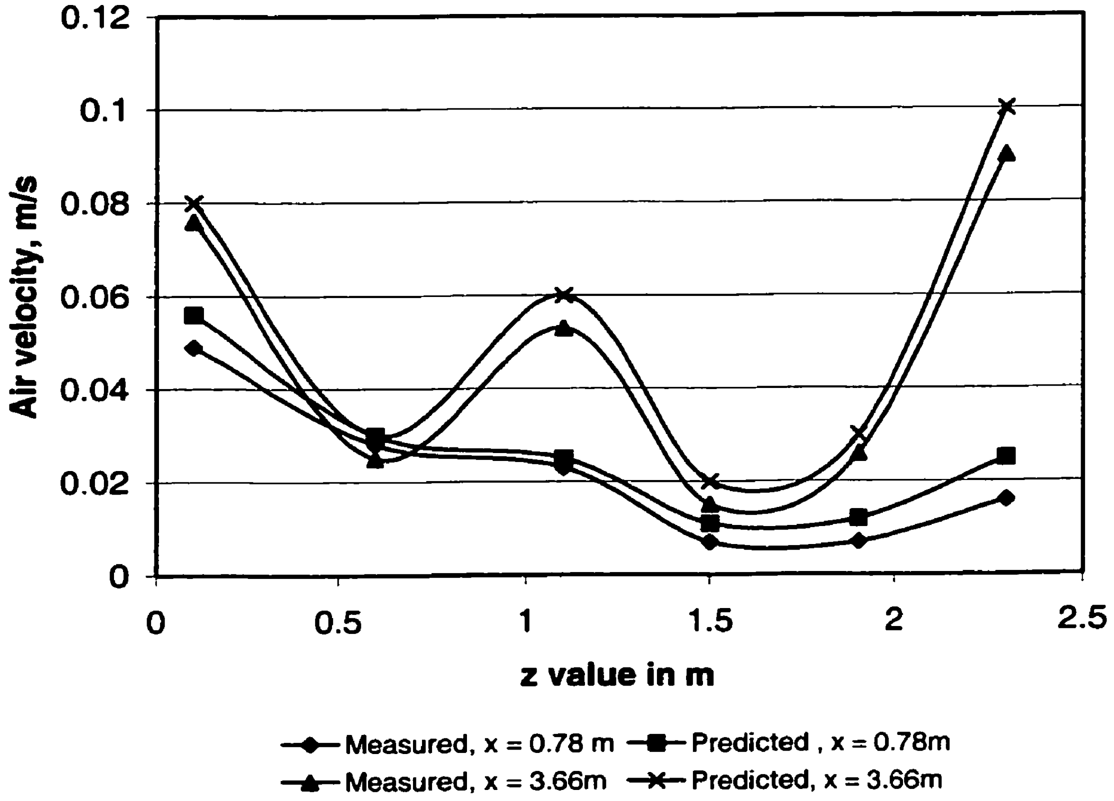


Figure 4.13 Contaminant concentrations y = 1.83, x = 3.66m

Figure 4.13 represents the contaminant distribution shown in a specific section of the room for the base case. The contaminant levels remain at lower values near the breathing zone of the occupants on both sides of the partition. The values gradually increase towards the ceiling of the office. The values do show an accumulated increase on one side of the partition.

Figure 4.14 Predicted and measured contaminant concentrations at y = 1.83m

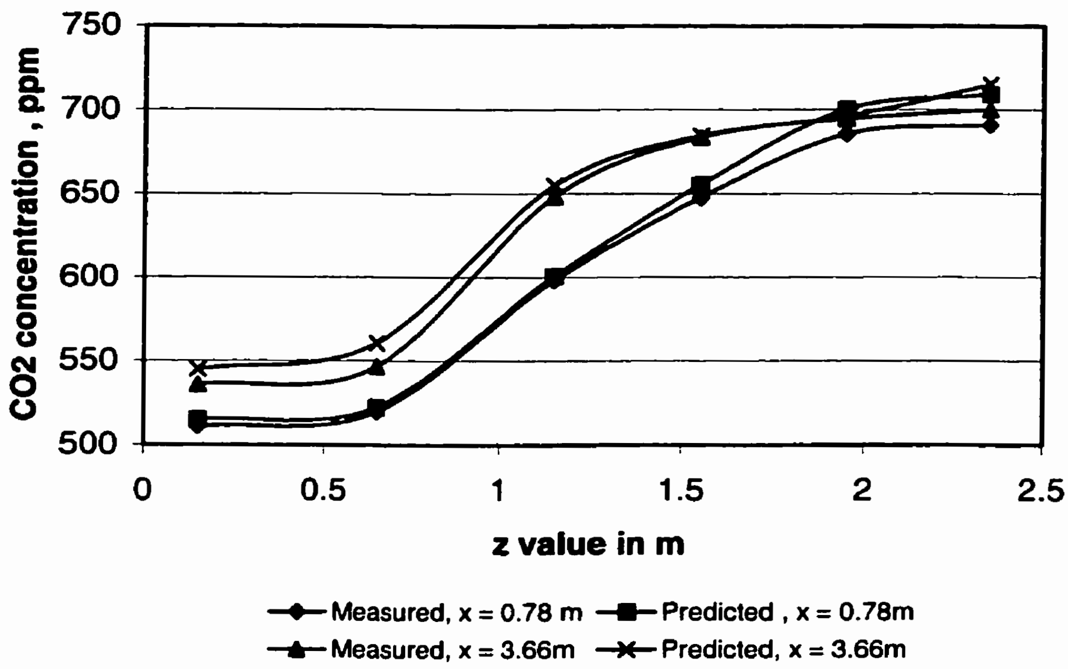


Figure 4.14 is a graph that compares the values of measured and predicted values of CO_2 concentration in the office. The predicted values are in close agreement with the experimental values.

This partition configuration works well for the office space since it maintains adequate airflow on both sides of the partition while maintaining the levels of contaminant fairly low in the occupant level. The values show a gradual increase towards the ceiling level.

5. PHOENICS: PARAMETRIC STUDY

5.1 Introduction

In this chapter, PHOENICS parametric study has been discussed in greater detail since this segment of the work is a contribution of this thesis study towards research. The geometry and space configuration of the indoor space (office) is more complex than those considered in previous research. Several critical indoor space considerations have been studied in detail in this chapter.

Chen's (Chen 1999) case that was described in Chapter 4, Section 4.2.1, is considered as the base case and the starting point for the following parametric study. Having tested and validated the base case with a more complex indoor space design, such as the existence of partitions or flow obstacles in the office, various alternative design options are tested to determine the possibility of optimizing design. The design considered in this simulation study is still quite basic and does not include complexities found in realistic situations.

5.2 Partition Configuration

Case II No flow obstacles

In this case the room is devoid of any furniture or occupants as flow obstacles. The contaminant source is still located in the office. Figures 5.1 and 5.2 show the air velocity and contaminant concentration contours for case II.

Figure 5.1 Air velocity contours for case II

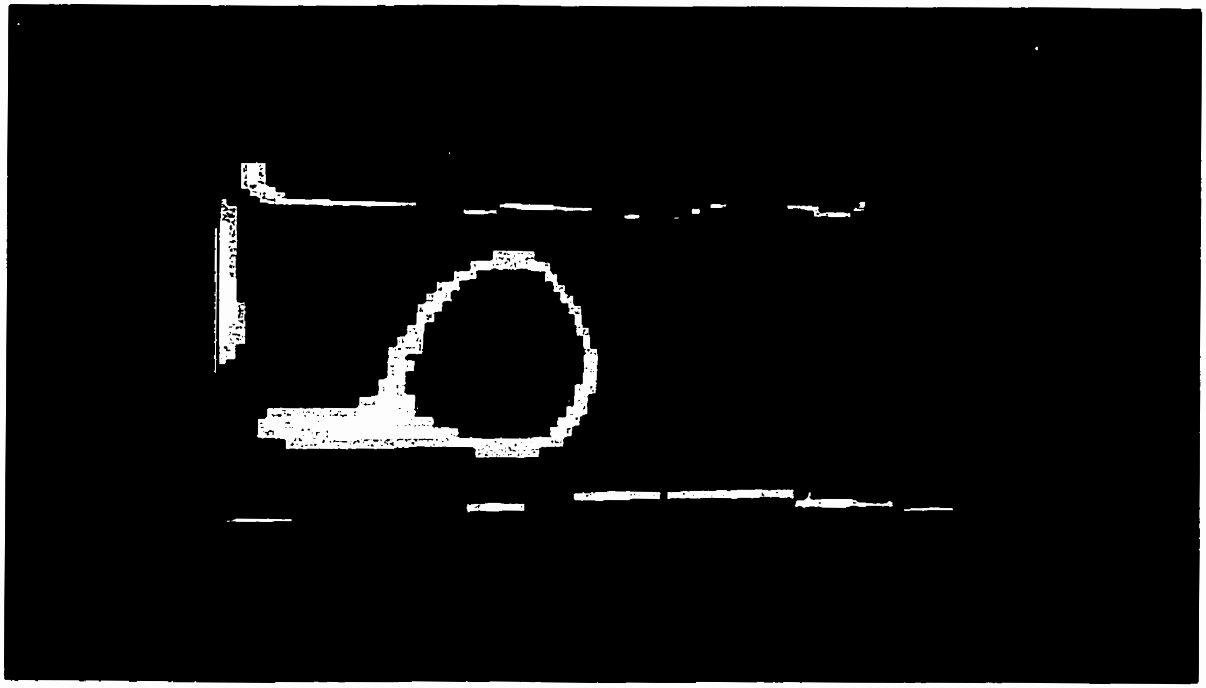
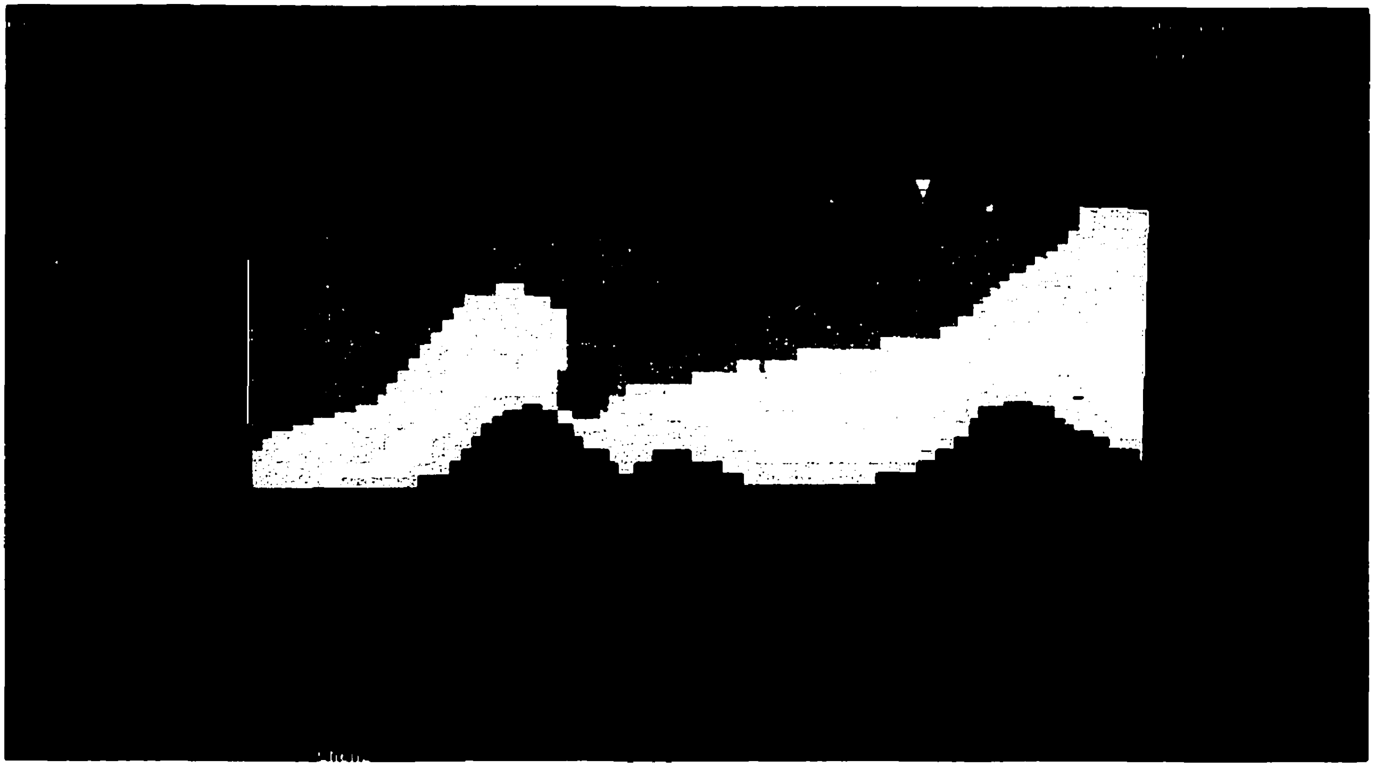


Figure 5.2 Contaminant distributions for Case II

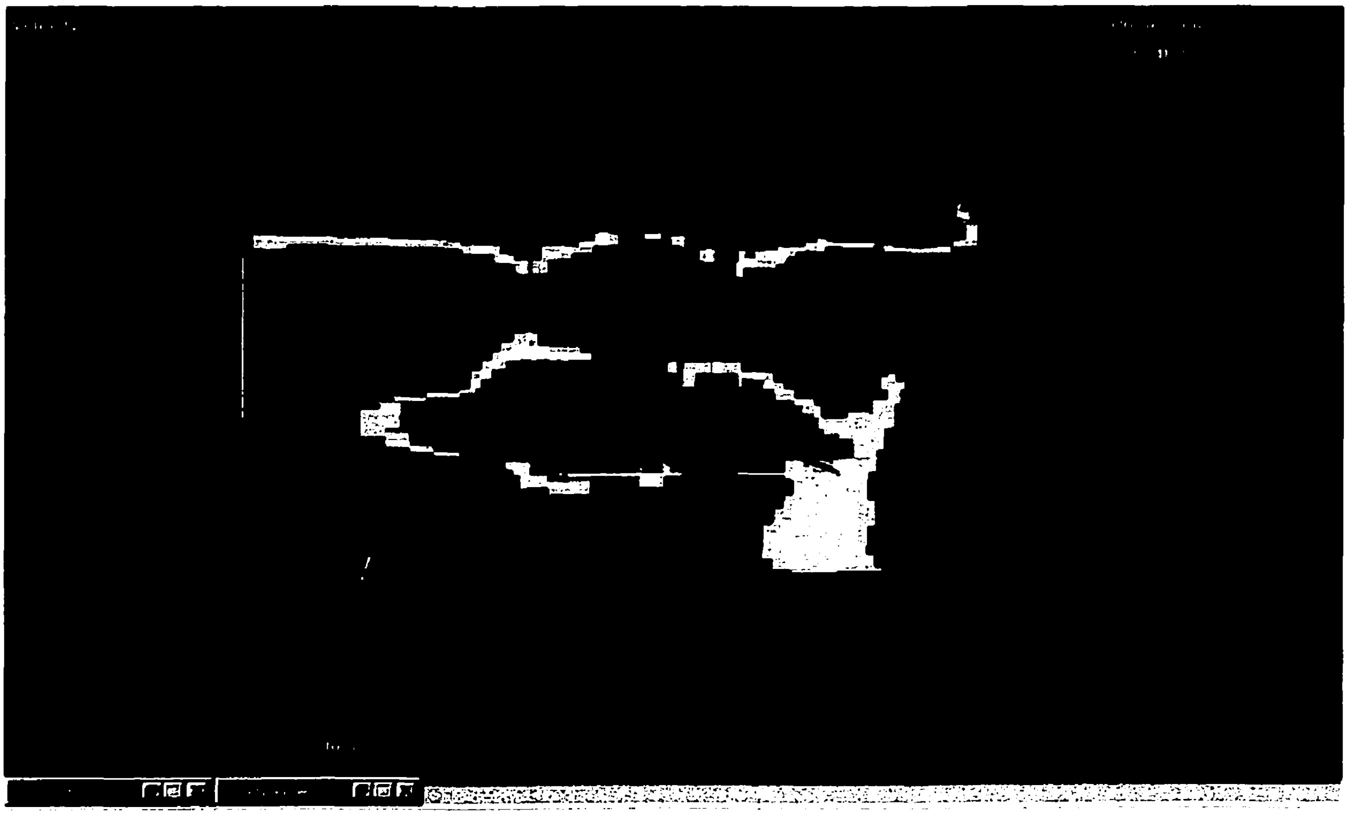


As depicted in the figures above, the lack of flow obstacles and heat sources in the office results in better air movement and lower contaminant levels in the room. The contaminant contours show a significant reduction in the levels in the occupied spaces as well as the levels near the exhaust. The values only reach a maximum of about 640 ppm near the ceiling. A small increase occurs near the contaminant source.

Case III No partition

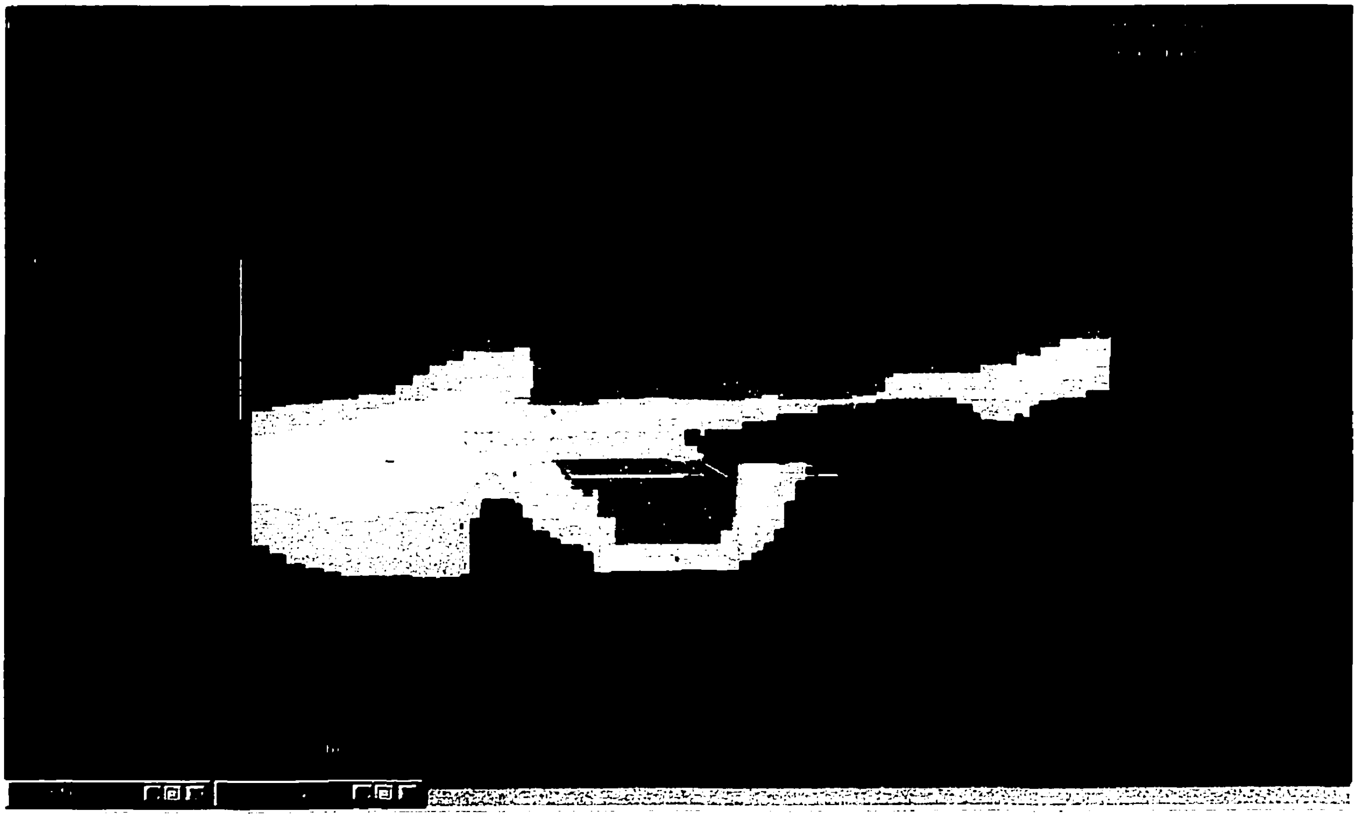
The case set-up remains similar to the base case except for the non-existence of the partition. This will help determine the influence of flow obstacles such as partitions on the overall air quality levels in an occupied space.

Figure 5.3 Air velocity contours for case III



It is seen that the air velocity levels are higher when compared to the case with partitions (base case). It would follow that the contaminant levels would also be lower in the occupied levels of the room as shown in Figure 5.4 when compared to case with partitions. The contaminant levels are higher when compared to the case with no flow obstacles or heat sources in the room (case II). The levels of contaminant near the ceiling reach close to 720 ppm. At the occupant's breathing zone the levels remain between 550 – 645 ppm.

Figure 5.4 Contaminant concentrations for case III



Case IV Increase in partition height (width same as in base case)

The partition height or in general size have been found to have an impact on the air quality in office spaces (Haghighat *et al.*, 1989). In this study the height and the width of the partition have been varied while keeping one of the parameters as that of the base case to determine their individual influence. Figures 5.5 and 5.6 show the air velocity and contaminant concentration distributions for an increase in the partition height.

Figure 5.5 Air velocity contours for case IV

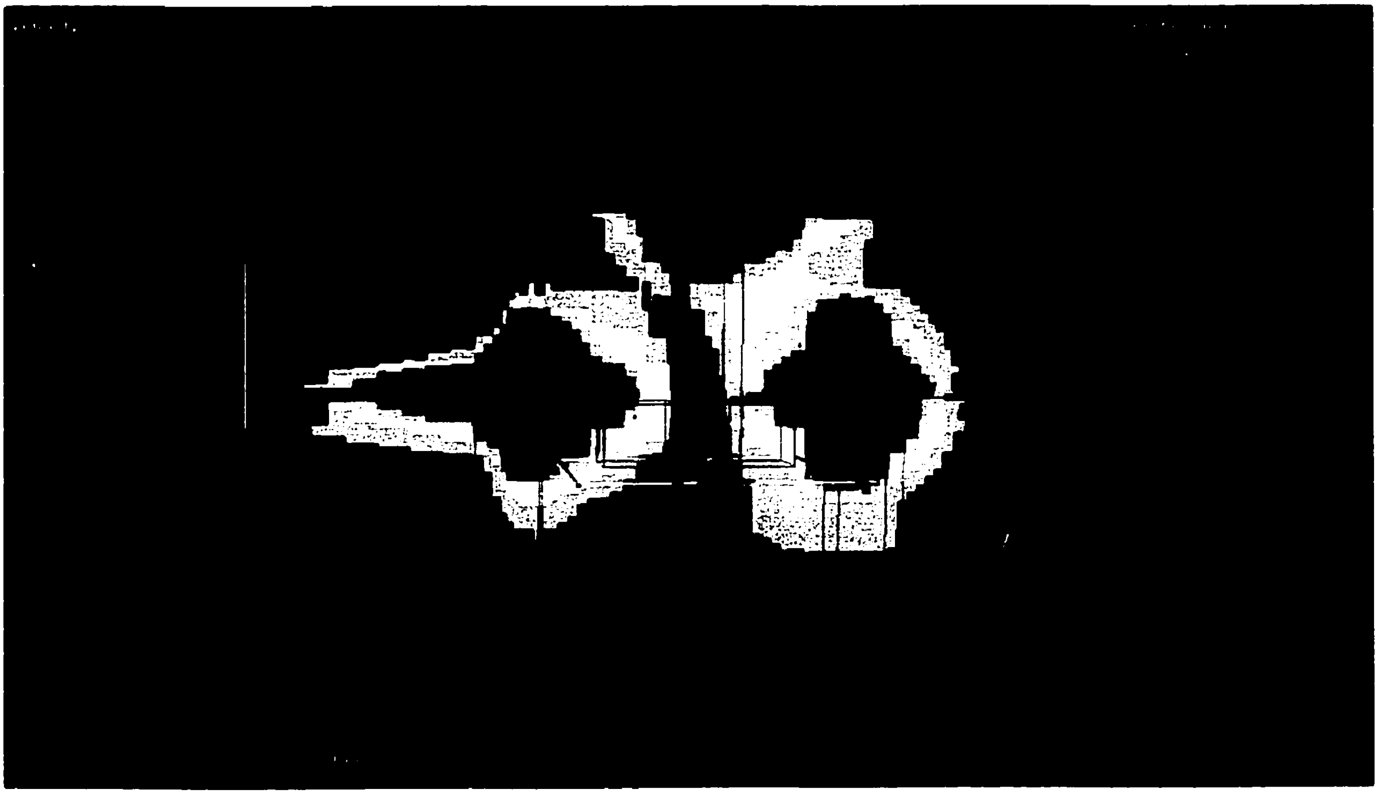
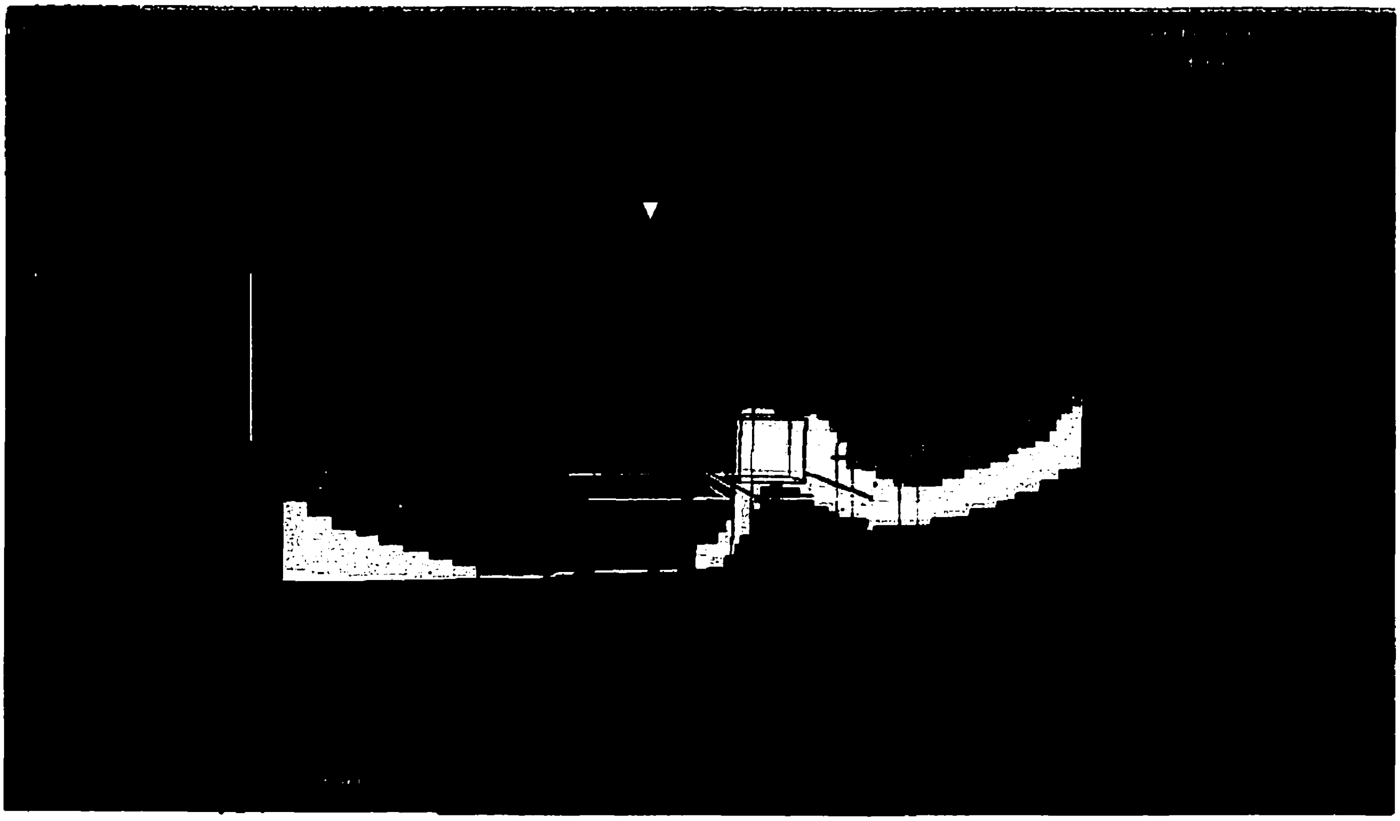


Figure 5.6 Contaminant contours for case IV



The predicted results again show a better air circulation on one side of the partition. The air velocity is higher on the right side of the partition while the left side has relatively lower air movement. The contaminants reach very high levels on the stagnant side reaching close to an average of 730 ppm from floor to ceiling height near the occupants.

Case V Increase in the partition width

In this case the partition width has been increased from 1.84 m (base case) to a value of 2.65m. The predictions of air velocity and contaminant movement are shown in Figures 5.7 and 5.8.

Figure 5.7 Air velocity contours for case V

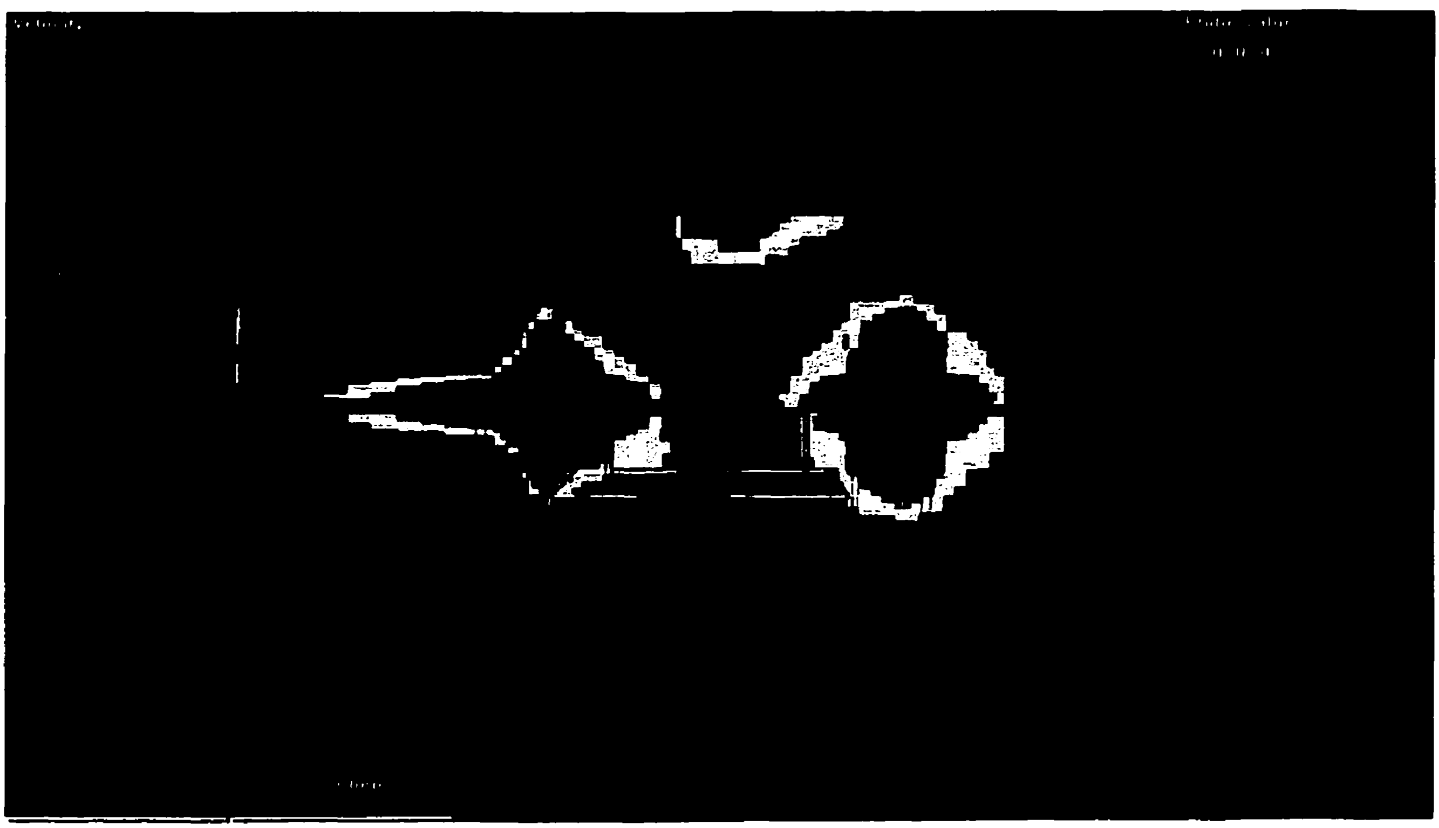
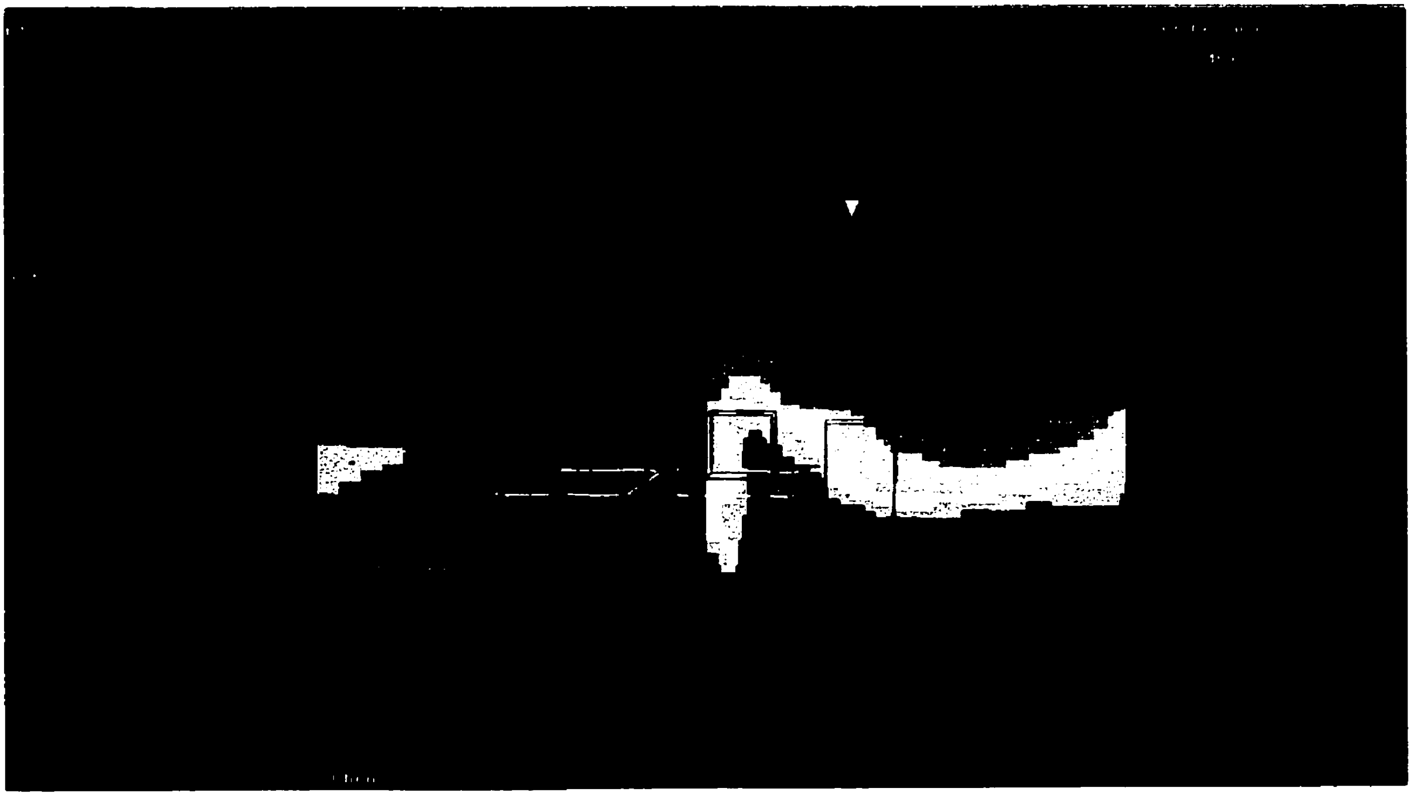


Figure 5.8 Contaminant distributions for case V



Figures 5.7 and 5.8 indicate an increased air velocity on one side of the partition when compared to the other sides. This results in elevated levels of contaminant on one side of the partition at the occupant level. The contaminant levels on this side of the partition are quite high right from the floor level.

Discussion of Results

Table 5.1 shows a summary of the results as obtained in the 5 cases.

Table 5.1 Summary of the parametric study, influence of partition on air quality

Partition configuration	Air velocity	Contaminant movement
Case I (Chen, 1999)	Good air circulation on both sides of the partition	Low values on both sides of the partition at the occupant level.
Case II (No flow obstacles, no heat sources)	Good air movement in all parts of the room. Values lower than with the presence of heat sources.	Low levels of contaminants at breathing levels in the room. Low values even near the exhaust (ceiling)
Case III (No partitions)	Good air movement in the office space. Values higher near the heat sources.	Good containment of contaminant near the occupant level.
Case IV (Increase in partition height)	Low velocity on one side of the partition	Increased contaminant levels towards the left of the partition.
Case V (Increase in partition width)	Air stagnation on one side of the partition.	Increased pollutant levels on one side. Levels remain high right from the floor level.

The summary indicates the existence of an optimal partition configuration that enhances air circulation and lower CO_2 levels in the office space. The study also proved that the absence of flow obstacles do increase the air quality in the room. The presence of heat sources was seen to increase air velocity. The study has demonstrated that it is worth giving careful consideration to partition designs in order to maintain lower contaminant levels in occupied spaces (case IV and case V).

5.3 Location of inlet/outlet and contaminant sources

The location of contaminant source and inlet and outlets has been examined in this section of the study. The same office configuration (Chen, 1999) is used for this study. The major difference in this study is that the evaluations have been made in an empty room with the office being divided into two zones with a door right in the middle of the two zones. The inlet velocity is taken as 2 m/s. The study follows the analogy applied by Haghighat *et al.* (1989). Two different configurations have been evaluated.

Case I Exhaust and contaminant in zone B

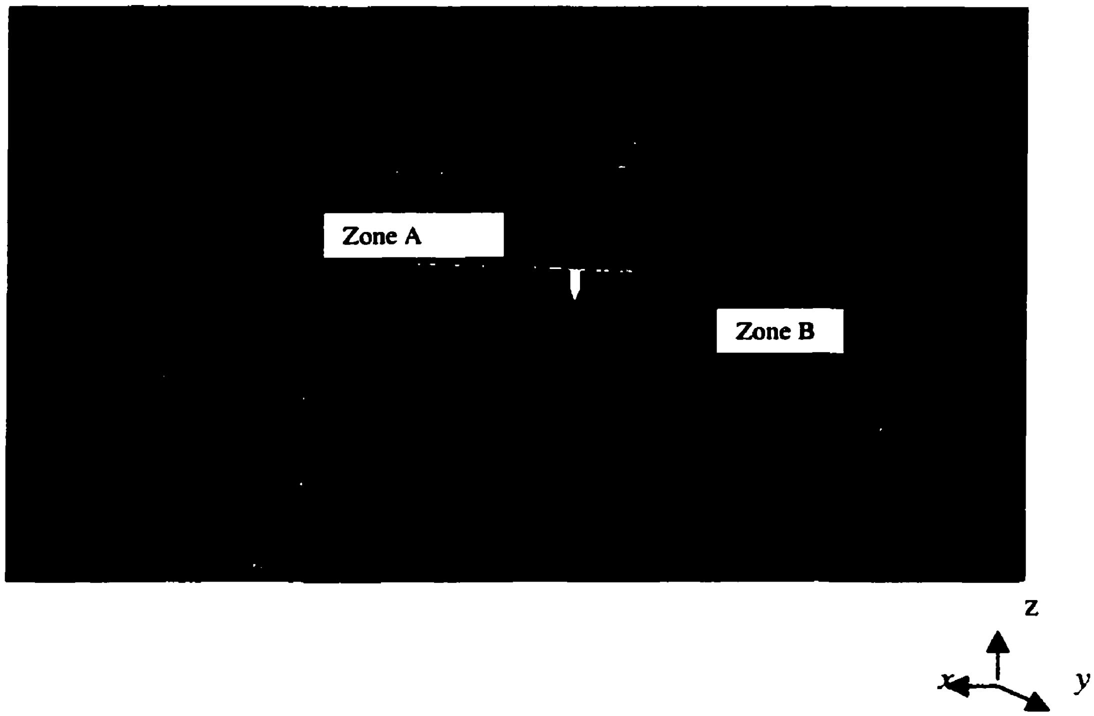
Case II Contaminant in zone A

Case III Contaminant and a flow obstacle in zone A

Case IV Contaminant and heat source in zone A

Case V Variation of the inlet location, contaminant source in zone A

Figure 5.9 Office configuration

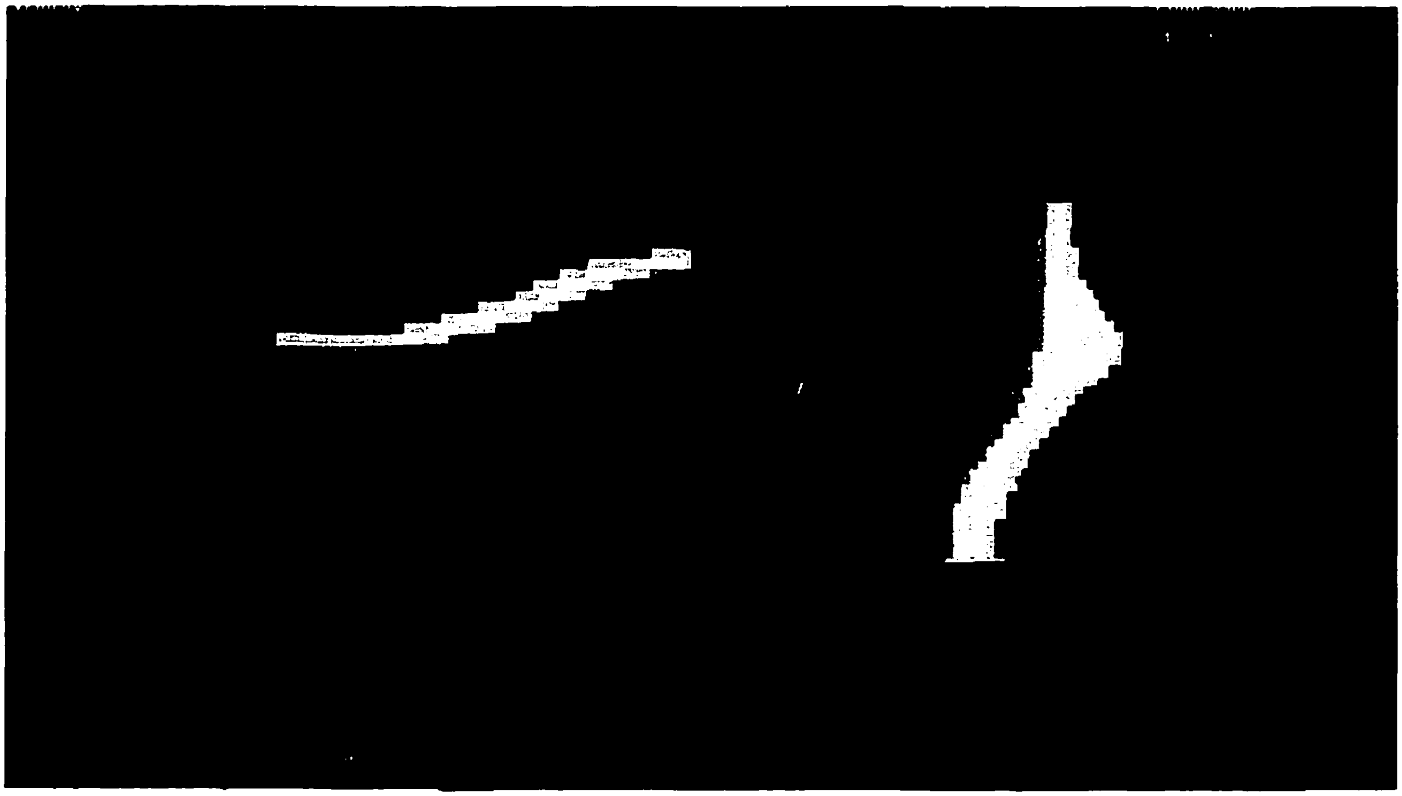


5.3.1 Case I Exhaust and contaminant source in zone B

In this case the contaminant source is placed in zone B. The exhaust is also located in zone B. The results of the airflow simulations for this case is as presented below:

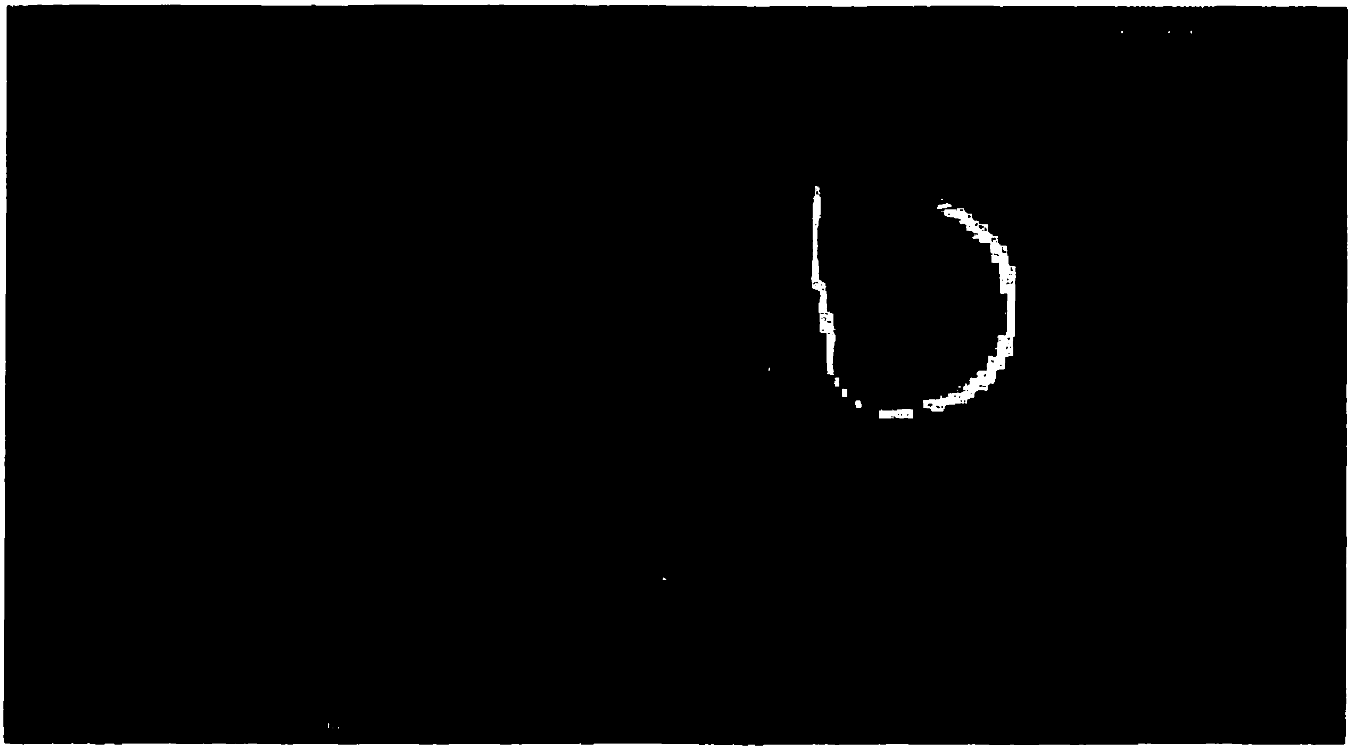
Figure 5.10 shows that the air movement in both the zones are good resulting in reasonably satisfactory air circulation in both the zones. The resulting contaminant distribution shown in Figure 5.11 indicates that the contaminant in the zone with the exhaust remains in zone B.

Figure 5.10 Air velocity vectors for case I



It is seen that even in zone B the concentration of the contaminant remains well contained. The contaminant spread occurs only close to the source and has zero value in the rest of the zone. Zone A remains free of any contaminant infiltrations.

Figure 5.11 Contaminant concentration contours for case I



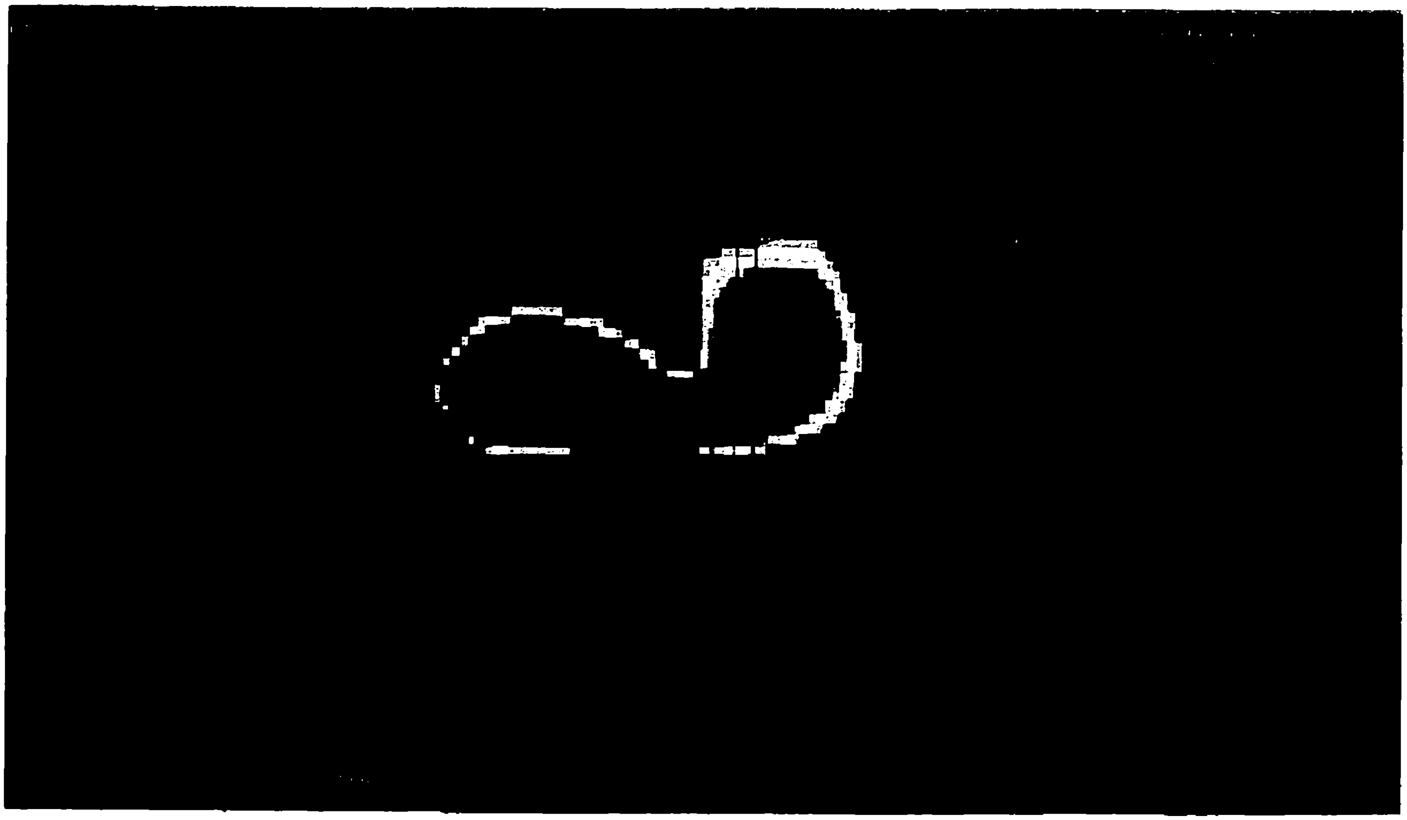
5.3.2 Case II Contaminant in zone A and exhaust location in zone B

In this case the contaminant source is now located in zone A where the diffuser is also located. The exhaust opening is placed in the ceiling in zone B. The resulting air velocity and contaminant distributions are presented in Figures 5.12 and 5.13.

Figure 5.12 Air velocity contours for case II

When the contaminant is located in zone A and the exhaust in zone B, both zones are affected by the presence of the contaminant. The levels of the contaminant are quite high at the occupant level. But the air velocity contours show good air circulation in both zones indicating that the location of the obstacle in a zone different from the contaminant source location could be the major cause for the increased levels of contaminants in the zones.

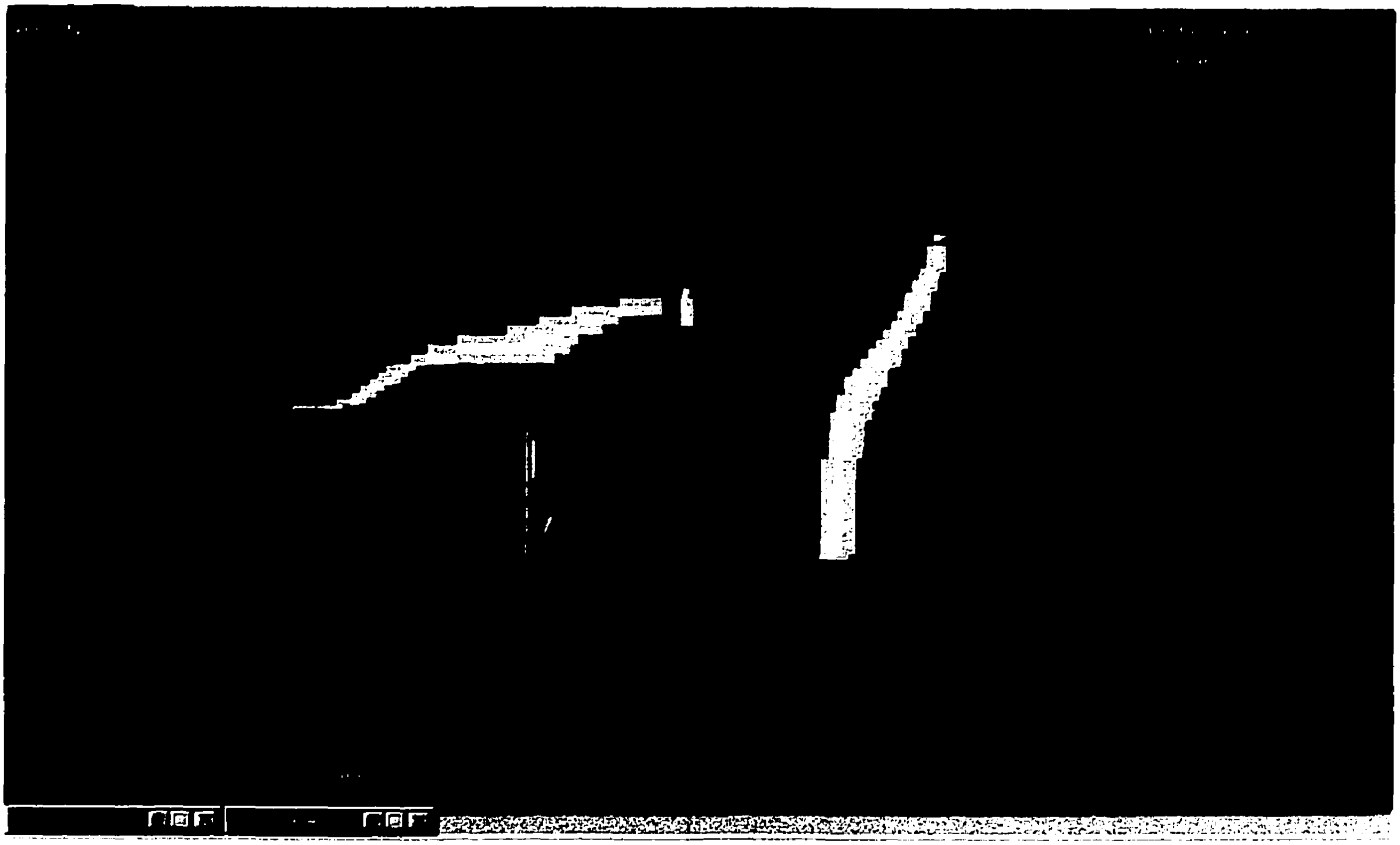
Figure 5.13 Contaminant concentrations for case II



5.3.3 Case III Contaminant source and a flow obstacle in zone A

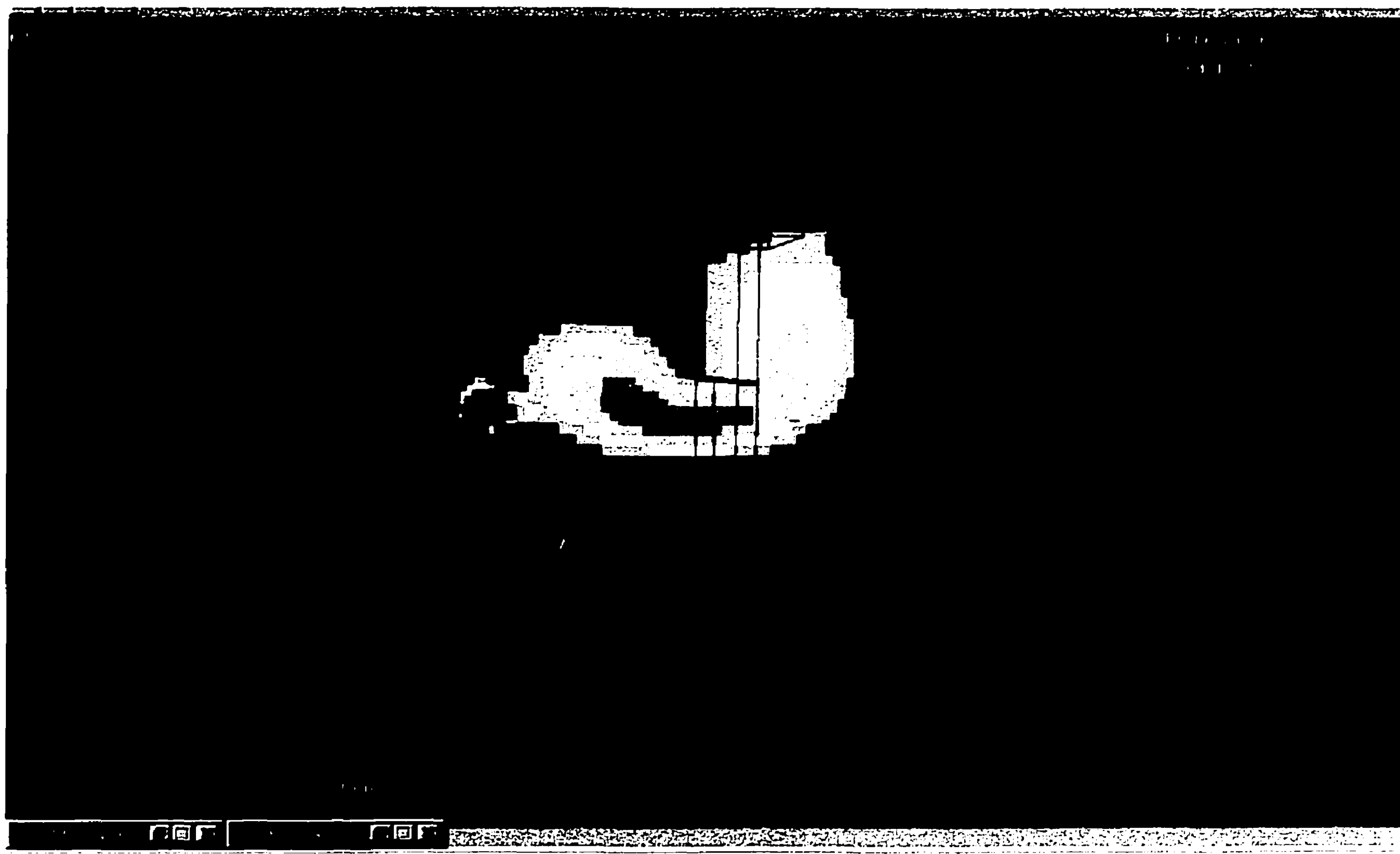
A flow obstacle, a chair is located in zone A. The assessment of the influence of such flow obstacles on the air movement the resulting contaminant distribution has been the purpose of this exercise. Figures 5.14 and 5.15 show the air velocity and contaminant distributions in the office space.

Figure 5.14 Air velocity contours for case III



Although the location of a flow obstacle in the zone should be expected to hinder the air circulation in both the zones, in this case the obstacle placement does not seem to cause a deterioration of the air velocity. Figure 5.15 actually shows that the concentration of contaminant, though present in both the zones is much less compared to the levels present in the previous case. This again indicates the presence of a beneficial or optimal obstacle location that could enhance air movement or at least not affect air distribution or increase contaminant concentrations in occupied spaces. This evidence highlights the importance of design considerations that could optimize the space and energy usage.

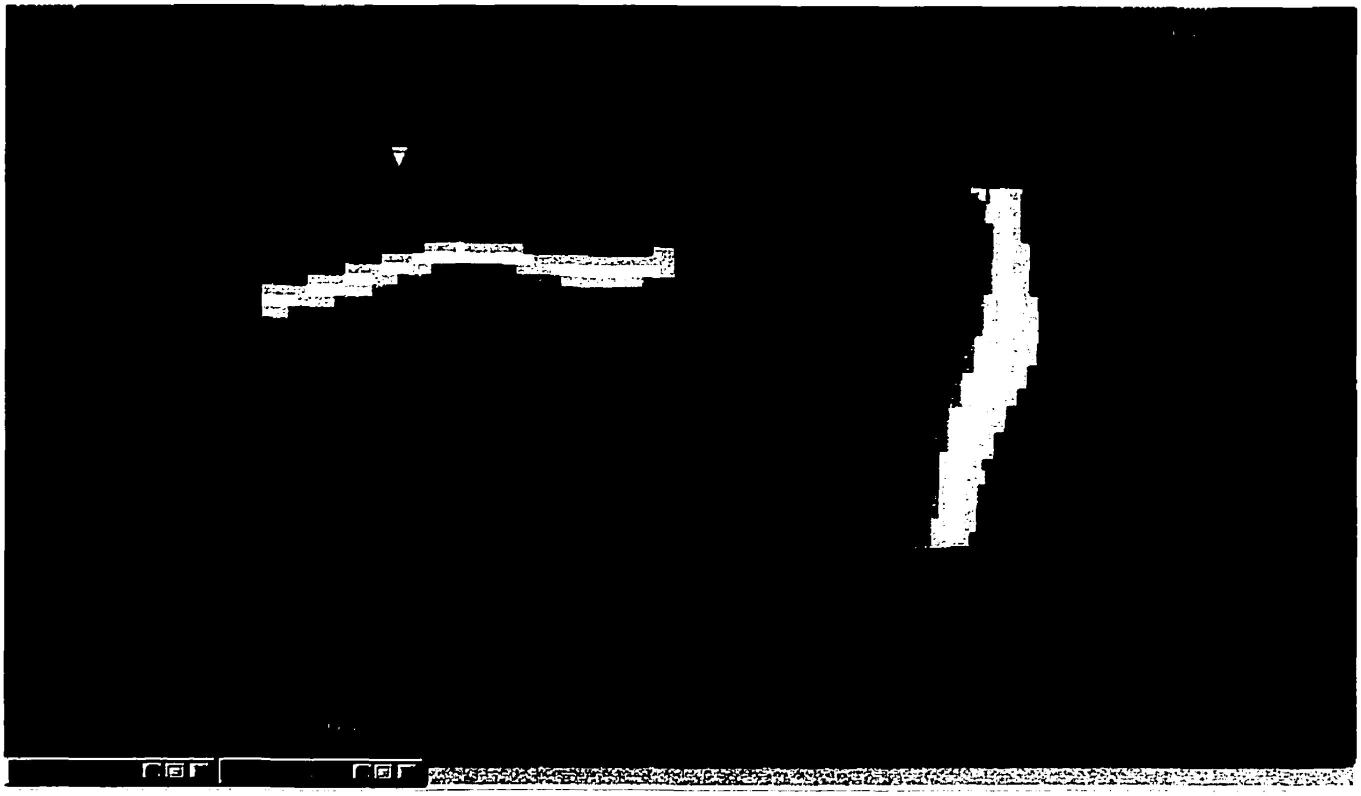
Figure 5.15 Contaminant concentrations for case III



5.3.4 Case IV Location of contaminant and a heat source in zone A, exhaust in zone B

An obstacle, which is also a heat generating source, is located in zone A. The influence of heat sources in airflow and contaminant distribution in rooms is evaluated in this section. Figures 5.16 and 5.17 show the air velocity and contaminant distributions for this case set-up.

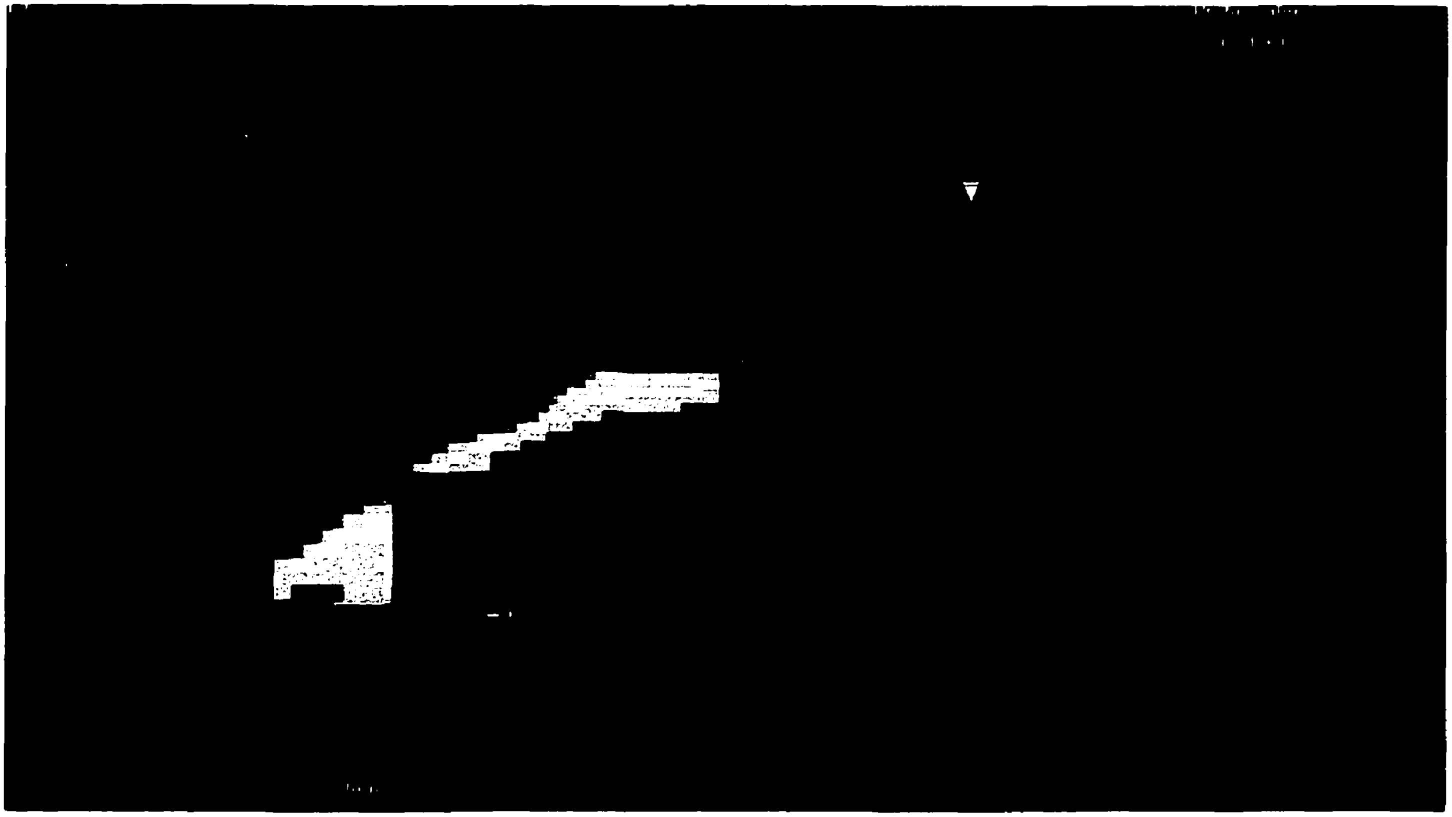
Figure 5.16 Air velocity contours for case IV



The presence of a heat source, as shown earlier in this study results in increased air velocities in both zones of the office.

The contaminant concentrations however remain higher in the zone with the heat source as shown in Figure 5.17. This has also been an observed phenomenon in the previous chapter of the study. The contaminant concentrations however increase gradually reaching higher levels close to the ceiling in zone A. A small percentage of contaminant infiltration is also observed in zone B.

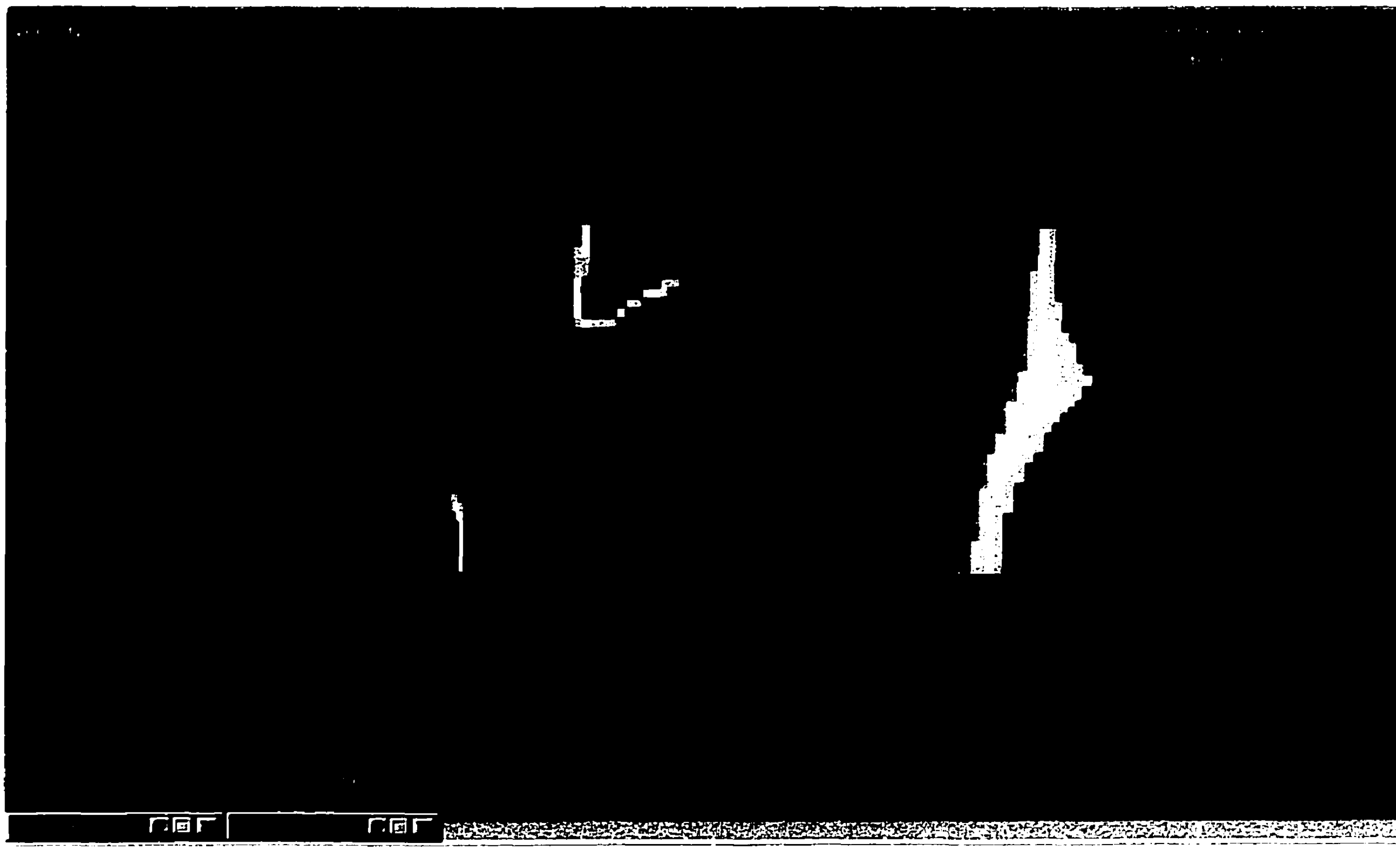
Figure 5.17 Contaminant concentration contours for case IV



5.3.5 Case V Inlet located in the ceiling of zone A, contaminant source and heat source in zone A

The inlet location is varied in this case and a heat source as in the previous case is located in the same zone as the contaminant source (zone A). Figures 5.18 and 5.19 show the velocity and contaminant distribution contours for this case.

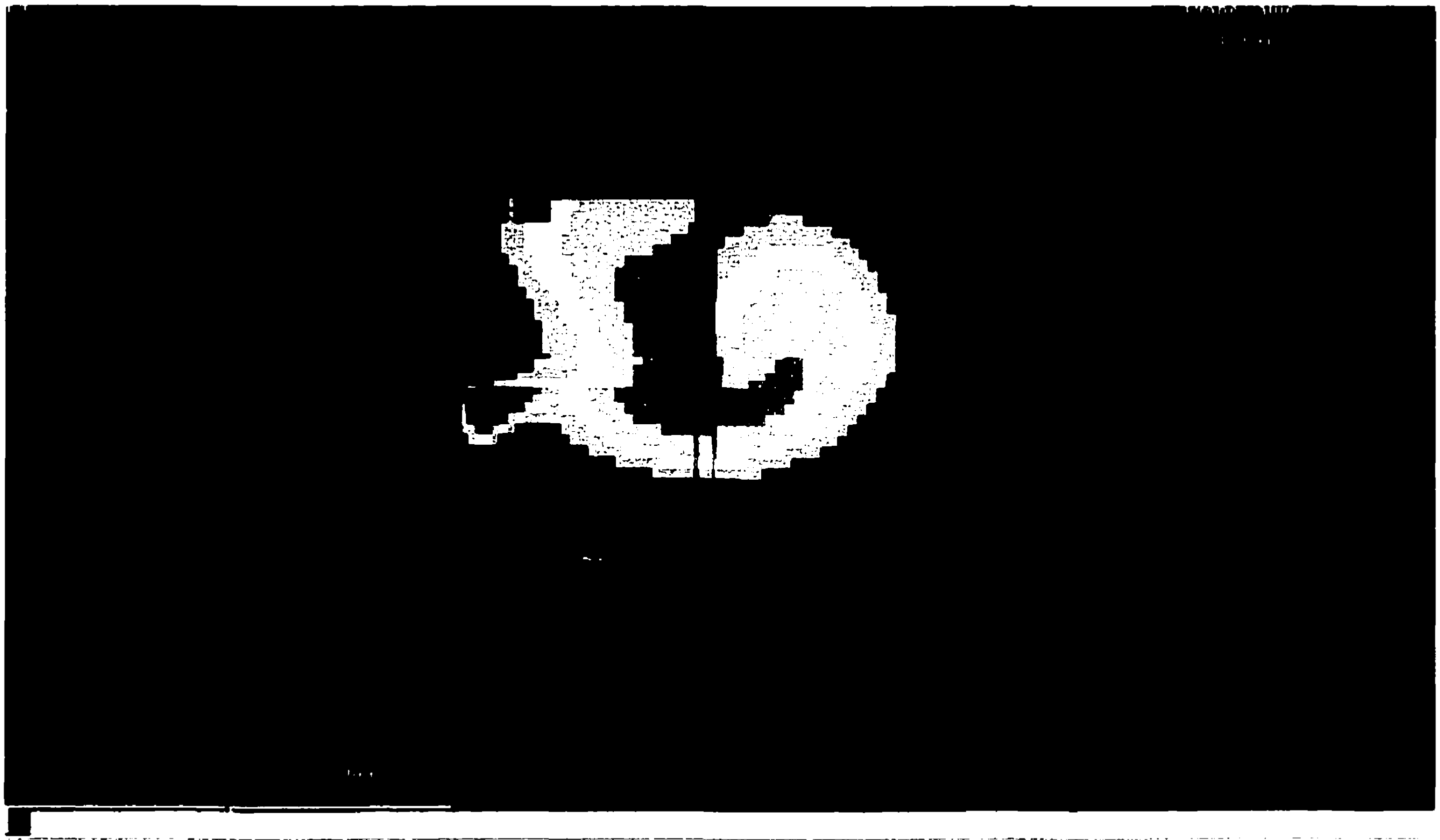
Figure 5.18 Velocity contours for case V



Air velocity is high in both zones. The heat source as in the previous case creates elevated air velocity around it and in zone B.

The contaminant levels are quite low in the occupant levels. But the contaminant does spread in to both the zones. The distribution of the contaminant is more in zone A as compared to zone B.

Figure 5.19 Contaminant contours for case V



The values of the contaminant in zone A remain much lower in comparison to the case IV. The configuration of case IV was similar to case V except for the location of inlet. This indicates that this configuration of the inlet-outlet could better achieve contaminant containment than the one in case IV.

Discussion of results

The results presented in this chapter are significant in revealing the influence of obstacle placements, contaminant source location, inlet-outlet location and heat sources in the overall air distribution in rooms. The existence of optimal placement of the above mentioned factors have also been observed.

Table 5.2 Summary of the parametric study

Office configuration	**Air velocity**	**Contaminant movement**
Case I: Contaminant and exhaust in zone B	Good air circulation in both the zones	Low levels of contaminant in zone B and zero in zone A.
Case II: Contaminant in zone A and exhaust in zone B	Reasonably good air movement in both the zones.	Contaminant spreads into both the zones. Higher values than in case I
Case III: Contaminant and flow obstacle in zone A	Good air circulation.	Contaminant present in both the zones. Levels lower than in case II
Case IV: Contaminant and heat source in zone A	High levels of air velocity in both the zones	Increased contaminant levels in zone A possibly due to the location of the heat source.
Case V: Inlet located in the ceiling in zone A. Contaminant source and heat source in zone A	Good air circulation in both the zones.	Lower levels of contaminant in both the zones for the same set-up as in case IV except for the inlet location.

The importance of computer simulations in predicting the influence and optimization of such factors is highlighted by the results obtained by this study.

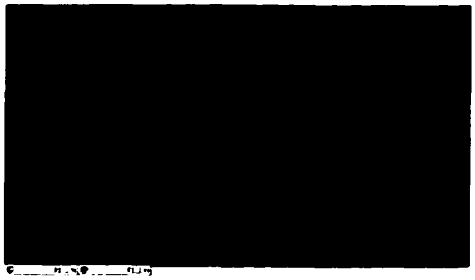
5.4 Evaluation of varying contaminant loads and ventilation flow rates on air quality in an office space

While the previous sections considered several alternatives to indoor space design and varying ventilation and contaminant load parameters, the space configurations were basic and did not depict the complexities of real situations. The following section will attempt to determine the capabilities of PHOENICS in assessing more complex situations with varying ventilation flow rates. This routine will evaluate the possibilities of energy conservation by reducing the airflow rates into each type of configurations under consideration.

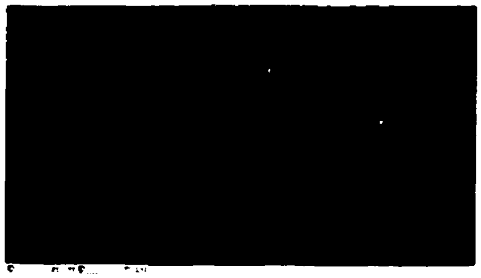
Four different space configurations and contaminant loads were considered for the following study. The inlet flow rates in each case, was varied between $0.05m^3/s$, $0.09m^3/s$ and $0.5m^3/s$. The office configuration in this section does not follow the pattern of Chen's (1999) study in order to enable the portrayal of a more complex situation. The model however is well validated at this point, due to the good matches in the results between simulated and experimental values that were obtained in comparison to the experimental study as presented in the previous sections.

Presented in Figure 5.20 are the four different space configurations that were considered. The office space in these cases consists of an open doorway that presents a pathway for interzonal interactions (which will be assessed further in Chapter 6).

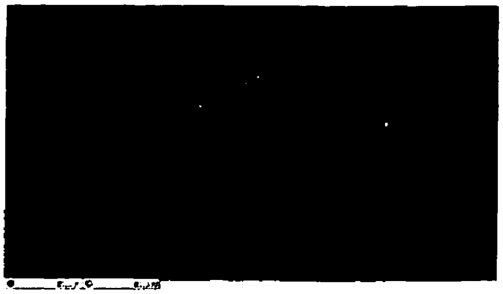
Figure 5.20 Office space configurations



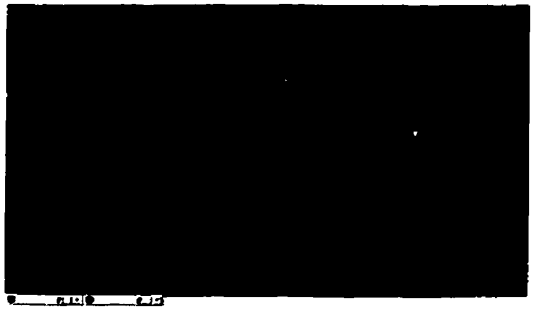
Configuration 1 (Case I)



Configuration 2 (Case II)



Configuration 3 (Case III)



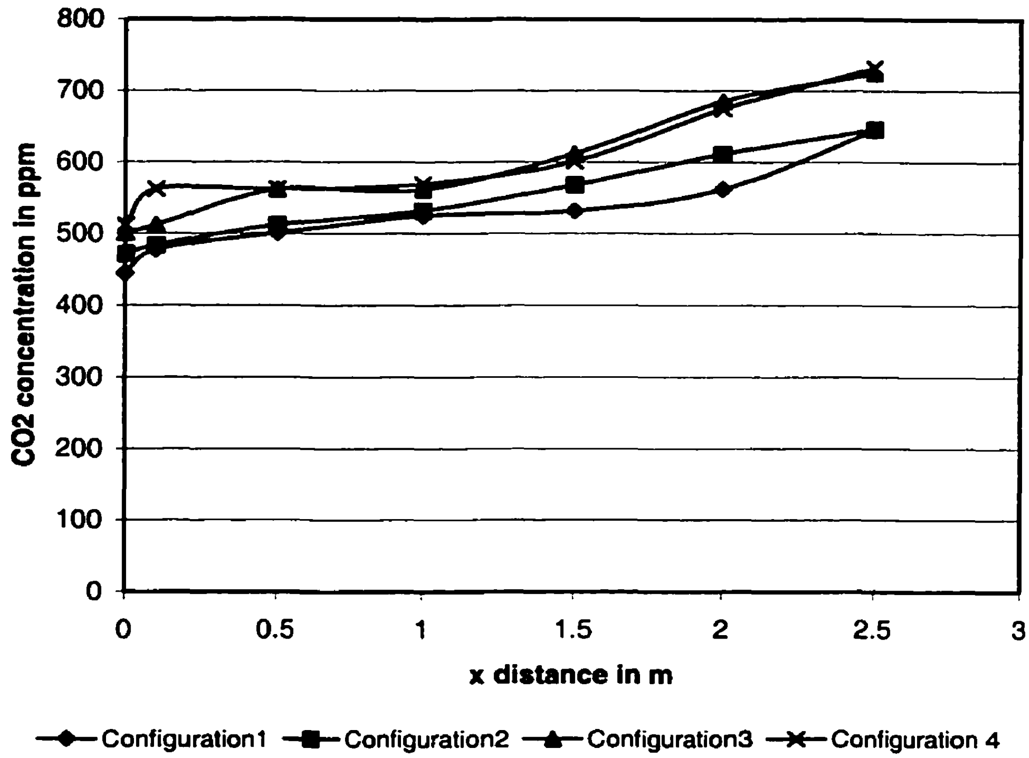
Configuration 4 (Case IV)

Case I has minimum flow obstacles (two partitions) and minimum contaminant sources the contaminant under consideration being carbon dioxide, which is being generated by the occupants at a rate of 15 L/h per source. Case II is similar to Case I, except for an increase in the number partitions from two to three. Case III and Case IV are similar to each other except for the absence of any partitions in case III. Both the cases considered have an increase in the contaminating sources (5) and partitions (4) in comparison to the previous cases. The inlet and outlet positions are fixed in all the four cases.

Presented below are graphs of comparative analysis of the varying inlet velocities for the four different configurations.

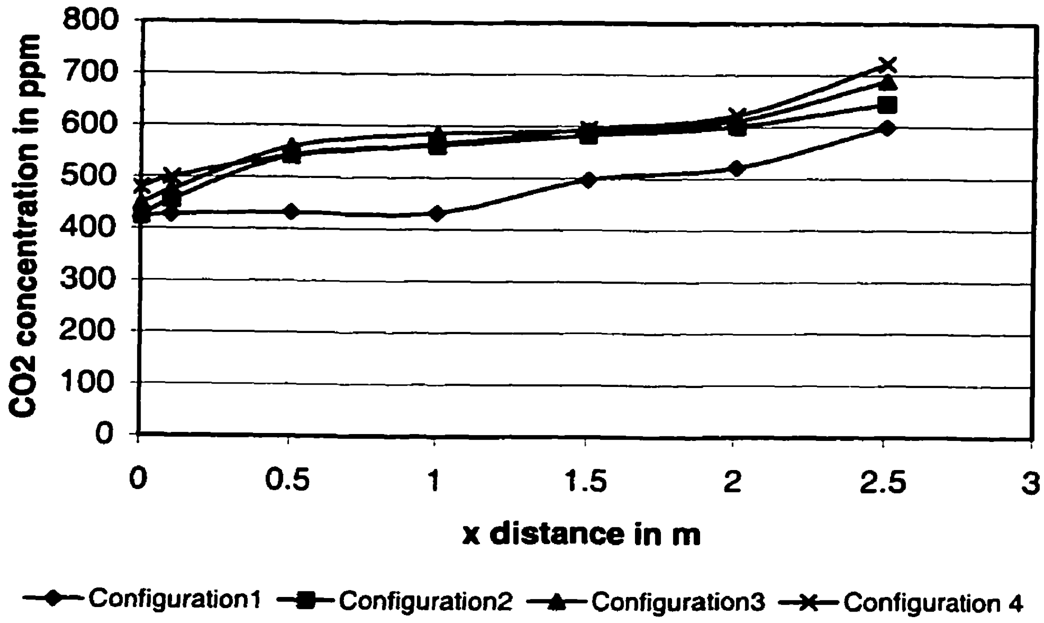
Inlet flow rate of $0.05m^3/s$

Figure 5.21 Carbon dioxide concentrations at an inlet flow rate of $0.05\ m^3/s$



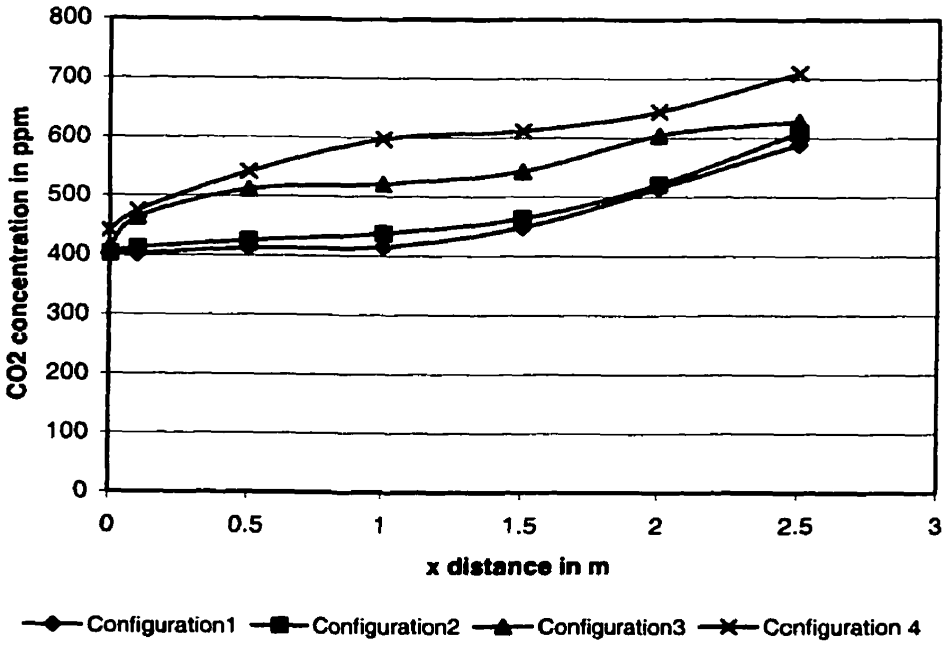
Inlet flow rate of 0.09 m^3/s

Figure 5.22 CO_2 concentrations at inlet flow rate of 0.09 m^3/s



Inlet flow rate of 0.5 m^3/s

Figure 5.23 CO_2 concentration at inlet flow rate of 0.5 m^3/s



While a ventilation flow rate of 0.5 m^3/s was found to be most effective in maintaining lower contaminant levels in the office space, it is seen that inlet velocities of 0.09 m^3/s and 0.05 m^3/s remain quite adequate in controlling the contaminant levels to lower values in the occupied zones. Tables 5.3 to 5.5 present values of contaminant levels at breathing levels of the occupants for the three different inlet velocity ranges.

Table 5.3 Carbon dioxide concentrations at flow rate of 0.05 m^3/s

Height in m	Configuration1 CO_2 in ppm	Configuration 2 CO_2 in ppm	Configuration 3 CO_2 in ppm	Configuration 4 CO_2 in ppm
0.5	501	512	562	562
1.0	525	532	562	569
1.5	532	568	612	601

Table 5.4 Carbon dioxide concentrations at flow rate of 0.09 m^3/s

Height in m	Configuration1 CO_2 in ppm	Configuration 2 CO_2 in ppm	Configuration 3 CO_2 in ppm	Configuration 4 CO_2 in ppm
0.5	432	542	559	542
1.0	435	562	585	565
1.5	498.1	583	592	595

Table 5.5 Carbon dioxide concentrations at flow rate of 0.5 m^3/s

Height in m	Configuration1 CO_2 in ppm	Configuration 2 CO_2 in ppm	Configuration 3 CO_2 in ppm	Configuration 4 CO_2 in ppm
0.5	412	425	512	542
1.0	415	438	522	598
1.5	449	464	544	612

From the tables 5.3 to 5.5, it is seen that the lowest flow rate of $0.05m^3/s$ with the most optimal design of 5 occupants and partitions does not exceed the levels of recommended indoor CO_2 of 800 ppm in the occupied zones. This ventilation rate could thus be the recommended value for configuration 4. But it is important to remember that PHOENICS simulations were performed at a steady state and it is always critical to get information on the transient contaminant concentrations in commercial buildings such as offices to determine the accumulated concentrations of the contaminants over time. Based on that, then it can be determined if there is a specific time during which increased flow rates into the occupied zones may be required. Multizone models are better suited for computing such transient state contaminant data.

6. COMPARATIVE ANALYSIS

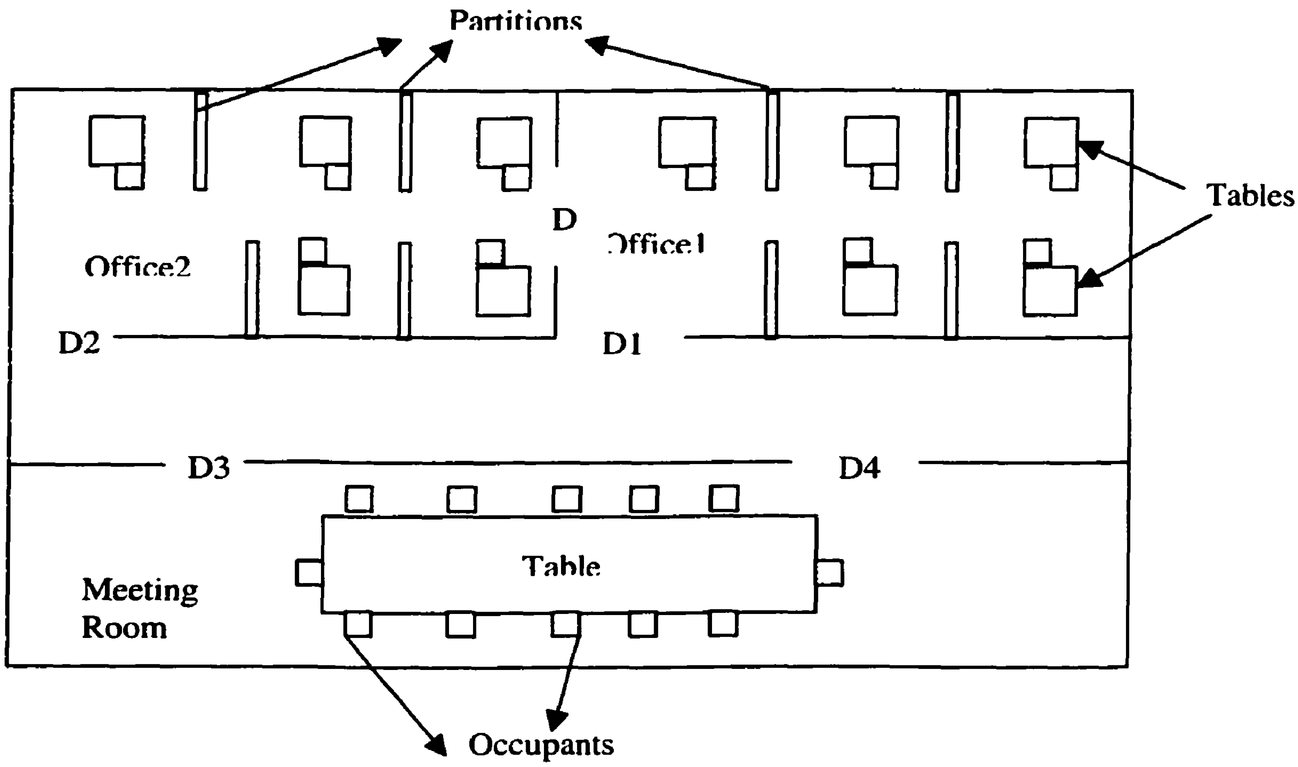
6.1 Introduction

It is critical to understand at what levels the two models PHOENICS and CONTAM compare and analyze their performance capabilities in detail before applying them in a coupled analysis. It is thus important to use the two models to assess the same office configuration. The previous chapters in this thesis have considered more individualistic applications of the two models on varying space configurations. Based on this knowledge it may be easier to use the two models in a coupled analysis.

6.2 Office Configuration

The office layout shown in the Figure 34 contains two office spaces and a meeting room. A corridor separates the offices 1 and 2 from the meeting room. A door is located between office 1 and 2. The interior space configuration of office 1 and office 2 is based on the space design of configuration 4 from Chapter 4 (see Section 4.3.2.3) of this thesis work. The space design of the meeting room consists of a long table with chairs for the occupants as shown in Figure 6.1.

Figure 6.1 Floor plan of the office space



In this section the adequacy of the ventilation rate into the office space is evaluated by changing the contaminant loads. The objective was to determine whether the designed flow rate maintains good indoor air quality in all the zones of the office under minimum, medium and maximum contaminant loads. In PHOENICS it is difficult to predict transient concentrations of contaminants. In this study, simulations with PHOENICS have been restricted to steady state analyses. In CONTAM, the doorways leading in and out of each zone have been considered as a zone in order to determine the contaminant exchange at the point of interaction between the zones. Transient contaminant concentrations have been computed using CONTAM. Three different scenarios based on a typical office schedule have been considered. The details of each of the scenarios are described in section 6.3. The arrival time or close to departure time when the contaminating sources are minimal, the peak load during mid-morning, afternoon periods and a specific case of heavily contaminated office space such as a meeting room and the overall interactions in different zones that could occur due to such an increase in the levels of contaminating sources. For all the cases, there is no specific fan schedule, i.e. the supply fans are on throughout the 8-hour work day.

6.3 Input Data

The input data for the two programs have been listed in the tables shown below. ASHRAE Std. 62 (1999) recommends 10 L/s/person as the design standard for ventilation systems for office spaces. This section will try to evaluate whether this is a good recommendation for the office in consideration. A better idea might be obtained with the coupled analysis, which will be studied in Chapter 7. For the specified office space the recommendation of 10 L/s translates to about 220 L/s per floor based on a maximum occupancy of 22 persons per floor under normal occupancy conditions (Table 6.3). While providing adequate airflow into a building is extremely beneficial from an indoor air quality perspective, it increases energy consumption and the environmental impacts associated with providing this energy (Persily *et al.*, 1994). The recommended rate of 0.22 m^3/s (10 L/s) per floor has been considered in this chapter.

Input Data for CONTAM

Table 6.1 Input data for CONTAM

Input Data	Input Value
1. Ambient Data a) Temperature b) Wind speed	 0°C 3 m/s
2. Leakage Area Data (based on a pressure drop of 4 Pa, discharge coefficient 1.0, flow exponent of 0.6) (Persily 1994) a) Exterior Walls b) Interior Walls c) Interior Doors d) Floors	2.9 cm^2/m^2 2.0 cm^2/m^2 75 cm^2 0.4 cm^2/m^2
3. Volume of each zone a) Office 1 b) Office 2 c) Meeting Room d) Corridor	 140 m^3 140 m^3 280 m^3 56 m^3
4. Sources of Contamination	Carbon dioxide – people as generating sources at a rate of 15 L/h/source/occupant
5. HVAC data	An air handler with a supply airflow capacity of 0.22 m^3/s serves the office spaces and the meeting room (designed based on 22 occupants, occupancy rate)

Input Data for PHOENICS

Table 6.2 Input data for PHOENICS

Input Data	Input Value
1. Room Dimensions	
a) office1 – Length, width, height	10m, 4m, 3.5m
b) office2 – length, width, height	10m, 4m, 3.5m
c) meeting room – length, width, height	10m, 8m, 3.5m
d) corridor – length, width, height	2m, 8m, 3.5m
2. Inlet values	
a) Flow rate	0.22 m^3/s
b) Temperature	17.0°C
3. Heat sources (per source)	
a) Occupants	75 W
b) Lighting	34 W
c) Computer	108 W
4.Sources of Contamination	Carbon dioxide – people as generating source at a rate of 15 L /h /occupant

Table 6.3 Occupancy Schedule

Input Parameters	Input Values
1. Ventilation Flow Rate	0.22 m^3/s
2. CO_2 Source	15 L/h/person
3. Occupants	
a) Minimum Occupancy (Case I)	6 occupants (3 in office 1 and 3 in office 2)
b) Normal Occupancy (Case II)	10 occupants (5 in office 1 and 5 in office 2)
c) Maximum Occupancy (Case III)	22 occupants (5 in office 1, 5 in office 2, and 12 in meeting room)
4. Space Occupancy Schedule	
a) Office 1 and Office 2	8 am – 9 am ---- Minimum Occupancy 9 am – 10 am --- Normal Occupancy 10 am – 11 am --- Maximum Occupancy 11 am – 4 pm --- Normal Occupancy 4 pm – 6 pm --- Minimum Occupancy
b) Meeting Room	8 am – 10 am ---- Empty (No Occupants) 10 am – 11 am --- 12 Occupants 12 pm – 5 pm --- No Occupants

6.4 Steady State Simulation Results

6.4.1 Airflow Simulations

CONTAM

The airflow simulations remain the same in all three cases, since the air intake design remains the same during all three simulations.

Table 6.4 Airflow rates in kg/s

Zones	Airflow rate (kg/s)
Office 1 to Office 2 (through doorway), D	0.015
Office 1 to Corridor (through doorway), D2	0.018
Office 2 to Corridor (through doorway), D1	0.00985
Meeting room to Corridor (through doorway), D3	0.012
Meeting room to Corridor (through doorway), D4	0.015

PHOENICS

Table 6.5 Air Velocity in m/s at a height of 1.2 m from the floor of the office

Zones	Air Velocity in m/s Case I	Air Velocity in m/s Case II	Air Velocity in m/s Case III
Doorway between office 1 and 2, D	0.0018	0.0079	0.0098
Doorway between office 1 and corridor, D1	0.0065	0.0086	0.01
Doorway between office 2 and corridor, D2	0.0015	0.0032	0.005
Doorway1 between corridor and meeting room, D3	0.0016	0.0053	0.0059
Doorway2 between corridor and meeting room, D4	0.006	0.0098	0.012

Presented in Tables 6.4 and 6.5 are the computed air flow rates by CONTAM and air velocities by PHOENICS respectively. While the CONTAM predictions remain the same for the three cases, the PHOENICS computations of air velocities vary for the three different scenarios. The airflow results for PHOENICS computations have been presented at a height of 1.2 m from the floor level. It is seen that in PHOENICS simulations there exists a difference in the values for the three scenarios since PHOENICS takes into account the variations in the indoor space configurations such as heat sources, flow obstacles, etc. The air velocity values increase in the various zones for cases II and III in the PHOENICS computations. In Table 6.6, a comparison of CONTAM predictions and the PHOENICS predictions for cases II and III are presented. Case III represents the maximum occupancy period in the office building. CONTAM predictions ranged from 16.7% to 50% variations with case II of PHOENICS air velocity predictions in comparison with the predictions of PHOENICS for case III where the values differed from 5.7% to 38.8% as shown in Table 6.6. For case I the CONTAM predictions differed from the PHOENICS predictions were higher ranging from 18.8% to 70% in the various zones.

Table 6.6 Comparison of the computed air velocity values

Zones	Air Velocity (m/s) CONTAM predictions	Air Velocity in m/s Case III PHOENICS predictions	% Diff.	Air Velocity (m/s) CONTAM predictions	Air Velocity in m/s Case II PHOENICS predictions	% Diff.
Office 1 to Office 2 (through doorway), D	0.006	0.0098	38.8	0.006	0.0079	24
Office 1 to Corridor (through doorway), D2	0.008	0.01	20	0.008	0.0086	7.0
Office 2 to Corridor (through doorway), D1	0.004	0.005	20	0.004	0.0032	-25
Meeting room to Corridor (through doorway), D3	0.005	0.0059	16.7	0.005	0.0053	5.7
Meeting room to Corridor (through doorway), D4	0.006	0.012	50	0.006	0.0098	38.8

6.4.2 CO_2 predictions

CONTAM Predictions

The simulation of CO_2 concentrations in various zones as computed by CONTAM is shown in the Table 6.7 for the three cases. It is seen that the average range as computed by CONTAM remains within the specified limit of 800 ppm for the first two cases. The values increase a little over 800 ppm for the third case. The predicted CO_2 values for the three cases for each of the zones increase by approximately 50 ppm in most of the zones as seen in Table 6.7. There is a significant increase in CO_2 concentration between case 2 and case 3 for the meeting room where the values increases by as much as 256 ppm.

Table 6.7 CO_2 concentrations in the various zones, ppm

Zones	CO_2 concentration (ppm) Case I (min. with 3 occupants in office 1 and 2)	CO_2 concentration (ppm) Case II (normal occupancy with 5 occupants each in office 1 and 2)	CO_2 concentration (ppm) Case III (maximum occupancy in offices 1 and 2 and 12 occupants in meeting room)
Office 1	649	695	702
Doorway between office 1 and 2, d1	642	645	740
Office 2	672	702	709
Doorway between office 1 and corridor,d2	591	622	650
Doorway between office 2 and corridor, d3	562	593	660
Corridor	587	625	754
Doorway1 between corridor and meeting room, d4	545	560	701
Doorway2 between corridor and meeting room, d5	542	559	697
Meeting room	542	549	805

PHOENICS Predictions

The carbon dioxide concentrations presented in Table 6.8 depict an average value that was calculated from the values selected at 12 different points of the meeting room, 8 different points in office 1 and in office 2, 6 point in the corridor and 5 points in each of the doorway zones. The points were selected such that an entire zone was well represented so that a good average value could be obtained. An average value thus calculated allows for a reasonably accurate comparison with the average value obtained using CONTAM (Table 6.8). The CO_2 computations made by PHOENICS are higher than the values predicted by CONTAM in all the zones and for all the cases.

The difference in values between the various zones for different case scenarios and the variations in a particular zone for each of the scenarios is more obvious in the PHOENICS predictions. In the corridor the difference in values for case 2 and case 3 predicted by CONTAM is 154 ppm where as the increase in value between the two cases predicted by PHOENICS is 202 ppm. It seems that the increased levels of CO_2 in the meeting room is better analyzed by PHOENICS. CONTAM predicts a very small increase for 7 ppm between cases 1 and 2 in the meeting room where as in PHOENICS the average values are not only higher but the difference in values between the two cases is as much as 72.8 ppm. This is probably due to the increased levels in office 1 and 2 during the normal occupancy period.

Table 6.8 Average CO_2 concentrations in ppm, PHOENICS predictions

Zones	CO_2 concentration (ppm) Case I	CO_2 concentration (ppm) Case II	CO_2 concentration (ppm) Case III
Office 1	710	735	769
Doorway between office 1 and 2, D	730	739	811
Office 2	709	713	746
Doorway between office 1 and corridor, D1	657	735	786
Doorway between office 2 and corridor, D2	713	763	776
Corridor	698	699	901
Doorway1 between corridor and meeting room, D3	620	685	793
Doorway2 between corridor and meeting room, D4	592	646	793
Meeting room	588	660	894

Table 6.9 shows the maximum values that were computed in each of the zones using PHOENICS. While in CONTAM only an average value for each zone is calculated, in PHOENICS the variations in every part of the zone is obtained which allows the engineer to be aware of the maximum values that may be encountered in a specific situation and hence it is possible to prevent the occurrence of high contaminant levels in a specific zone.

Table 6.9 Maximum CO_2 levels predicted by PHOENICS in the various zones of the office, in ppm

Zones	CO_2 concentration (ppm) Case I	CO_2 concentration (ppm) Case II	CO_2 concentration (ppm) Case III
Office 1	730	787	792
Doorway between office 1 and 2, D	745	798	815
Office 2	712	725	800
Doorway between office 1 and corridor, D1	733	792	800
Doorway between office 2 and corridor. D2	713	795	801
Corridor	615	725	925
Doorway1 between corridor and meeting room, D3	645	722	828
Doorway2 between corridor and meeting room, D4	605	717	801
Meeting room	595	712	912

An average value computed by CONTAM fails to provide details of such maximum levels of CO_2 concentration as in the case of the meeting room and the corridor where the values are greater than 900 ppm.

6.4.3 Discussion of Results

Table 6.10 Comparison of computed CO_2 in ppm (values for the three cases)

Zone	CONTAM Case I	PHOENICS Case I	% Diff	CONTAM Case II	PHOENICS Case II	% Diff.	CONTAM Case III	PHOENICS Case III	% Diff
Off1	649	710	8.6	695.3	735	5.4	701.5	768.9	8.8
Off2	672	708.5	5.2	702.3	712.5	1.4	709	745.5	4.9
MR	542	587.5	7.7	549	660.3	16.9	805	893.6	9.9
Corr.	587.3	697.5	15.8	625.2	698.5	10.5	754	900.9	16.3

Table 6.10 provides a comparative analysis of the CO_2 levels predicted by the two programs for the three cases. It is seen that CONTAM under predicts contaminant levels for all three cases in the various zones of the office. Variations in indoor space are however noted in the PHOENICS predictions.

The difference in predictions is due to the detailed format of analysis that is computed by PHOENICS while CONTAM depicts only the average contaminant concentrations in the zones. With CONTAM, the effect of the presence of flow obstacles, heat sources, etc. is not seen in the predicted results. It is seen in Table 6.10 that in the corridor and the meeting room the difference in the two predictions are greater than 10% in most cases with a maximum value of 16.9%. In Table 6.9 it is seen that PHOENICS is also able to predict the maximum levels of CO_2 that are obtained in the different zones such as 912.5 ppm that is encountered in the meeting room and a value of 925 ppm is predicted in the corridor.

6.5 Role of multizone models in IAQ analysis

Chapter 6 has shown the advantages of using PHOENICS over CONTAM in a direct comparative analysis that was performed using the two models.

- Also it was observed that only an average value of contaminant concentration could be obtained using CONTAM while PHOENICS is able to predict the maximum value that may be obtained in a specific point or several points in a zone
- PHOENICS is able to recognize the variations in a specific space design better than CONTAM and is thus able to predict the resulting contaminant concentrations and air velocities that are caused by such changes
- Interzonal contaminant exchange is also better predicted by PHOENICS

Despite the advantages of PHOENICS over CONTAM, CONTAM may still be the better model that may be suitable while considering large and complex buildings with varying levels of interactions with the indoor and outdoor environment. Although several recent articles (Musser, 2001, Carpenter, 1996, and Ayari *et al.*, 2000) have pointed towards the shortcomings of multizone models in predicting accurately the complexities of the indoor environment and the marked improvement in prediction accuracy using CFD models, the factors that are listed below still make the multizone models a better choice for practicality based on design and time considerations.

1. In multizone models, the depiction of complex commercial buildings such as offices that involve several zones, floors, etc. are easy to handle with respect to the input data requirement in general.

2. A number of zones can be modeled.
3. An overall idea of air movement and contaminant concentrations in buildings are obtained based on several different levels of interactions such as the outdoor environment, indoor environment, ventilation systems etc.
4. The computation time requirement for a single case set-up is much less compared to CFD models. Some of the cases discussed in this study such as the one discussed in Chapter 6 required about 7 hours for every case that was set up
5. It is easy to perform transient state simulations compared to CFD models where it is almost impossible to perform such simulations in complex situations. Transient state simulations are a very critical part of indoor air analysis since they provide information on the variation of air velocity and contaminant concentration distribution over time.

Based on the above considerations, it is seen that models like CONTAM are a very critical and integral part of IAQ analyses. But it has also been determined that CFD models are much more accurate in predicting the indoor environment. Therefore a coupled analysis is seen as an improvement over the existing multizone modeling technique. The appropriate coupling of these two models could drastically improve the predicting capabilities of multizone models and thus might make way for a powerful and more accurate simulation technique. The focus of the coupled analysis that is considered in this thesis is to use the ability of PHOENICS to recognize spatial variations and to apply the predictions of PHOENICS based on these changes to improve the predictions of CONTAM. This is considered an important step towards a more accurate simulating environment that can help generate meaningful results. The details of the coupled analysis are discussed in Chapter 7.

7. COUPLING TECHNIQUE

7.1 Introduction

Chapters 4, 5, and 6 have evaluated the capabilities of PHOENICS and CONTAM and compared the two programs in order to identify their strengthens and weaknesses. Both programs were found to have specific application areas. PHOENICS performed better where the intrazonal influences were greater on the overall flow structure in the office. The inclusion of PHOENICS as a part of CONTAM simulations may therefore be very critical for obtaining accurate results. CFD models are too complex in their input requirements and their computational time to be the major contributor for such a coupled analysis. Multizone models on the other hand provide an overall picture of the building interaction at various levels. Hence in this thesis work a technique to improve the simulating capabilities of the multizone model, CONTAM will be described. Schaelin *et al.* (1993) and Musser (2001) have done some preliminary work in this area using a similar technique. Schaelin *et al.* (1993) evaluated the location of contaminants and some design considerations such as location of doors on the overall airflow and contaminant distribution in a building. CFD program, PHOENICS was used to evaluate the results of such changes on the airflow and contaminant distribution in individual zones. A comparison between the predictions made by multizone model COMIS and PHOENICS was presented in individual zones. Musser (2001) conducted a similar study where the varying configurations of two zones were evaluated using multizone model and CFD model individually of each of the zones. One of the zones was then changed to a heavily contaminated zone and again the models were used one at a time so that a comparison of the two models could be obtained. It was found that significant variations were obtained when the contaminant concentration increased in one of the zones with the CFD model. The space configurations considered in both the studies were simple with just one or two zones with no flow obstacles. Variations of contaminant sources were considered by Musser while the study by Schaelin discussed varying locations of windows and doors. While their research was restricted to a single level data transfer with the CFD model providing evidence of good design values such as the prescribed airflow rate and its effect on air distribution in the various zones, in this study more detailed type of analysis will be conducted on a complex indoor space configuration with the interaction occurring in more than one level. The values from one program, PHOENICS have been considered as input for multizone program, CONTAM so as to enhance its predicted results. It must however be mentioned that at this point a coupled analysis may not necessarily mean less computational time effort since PHOENICS would definitely require a lot of computational time. But it is however recognized that PHOENICS alone would require considerably more time when complex situations are considered and the fact that it is extremely difficult to perform transient state calculations for such situations.

7.2 The Coupling Technique

The overall objective of the coupled analysis was to develop a technique where the predictions of CONTAM could be enhanced by the inclusion of PHOENICS in its analysis.

Technique 1:

The basic step is wherein the interactions of CONTAM with the outdoors environment is considered and the effect of changes on the indoor environment is studied using PHOENICS. This is probably one of the easiest approaches to be applied wherein the predictions of the multizone model can be improved by altering the design requirements based on the PHOENICS predictions. This approach has been used by Ayari *et al.* (2000), and Musser (2001)

Procedure:

a) A specific design consideration such as the adequacy of the recommended supply airflow rate is tested using CONTAM. The CONTAM simulation is run with input data such as volume of individual zones, contaminant source strengths, leakage data, outdoor air conditions, HVAC data.

b) CONTAM output of zonal airflow rates and contaminant concentrations are obtained

c) CONTAM output data such as zonal contaminant concentration and inlet velocities are used as input data for PHOENICS

d) PHOENICS output of air velocity and contaminant concentration distribution in each of the zones in the occupied space is obtained.

e) At this point, based on the PHOENICS output of the detailed distribution of contaminants in each and every zone, the question that is asked is whether the prescribed airflow rate was sufficient in maintaining the contaminant level under the recommended levels (for examples under 800 ppm for carbon dioxide).

f) If the above criterion was satisfied then the suitability of the prescribed airflow rate is determined.

g) If the contaminant distribution in all the zones were well under the specified limits then a lower flow rate may be prescribed with the repetition the procedures in technique 1. If the contaminant distribution in the zones is over the specified limit then the prescribed supply airflow rate may be increased and the scenario tested again for satisfactory indoor air quality based on the contaminant level in the zones.

h) This approach can be used while considering the suitability of ventilation systems, locations of flow obstacles, and location of contaminant sources.

i) Technique 1 is extended further in this work (compared to previous research) where the impact of a specific design consideration, supply airflow rate has been tested over a 8-hour period using CONTAM

Technique 2

Current research has applied technique 1 in simulation studies. In the current study, however a new technique is proposed where a direct exchange of data between the two models has been suggested.

<u>Procedure</u>

a) Technique 2 has been used to assess suitability of supply airflow rates and fan schedules in this study.

b) A specific flow rate is prescribed as the CONTAM input data similar to technique 1.

c) CONTAM simulation run is executed with the required input data as in the previous case.

d) The output values from CONTAM such as the zonal contaminant concentration levels and zonal airflow rates are then used as input data for PHOENICS

e) PHOENICS determines the detailed distribution of contaminant distribution based on the inlet velocity and initial value of the contaminant. The values obtained by PHOENICS are steady state values.

f) The average concentration, minimum concentration (initial concentration), maximum concentration of the contaminant is then determined and compared to the value obtained from CONTAM.

g) CONTAM, as seen in Chapter 6 under predicts the concentration of contaminants in comparison to PHOENICS values.

h) Hence the initial concentration (at 9 am, Section 7.3.2) obtained by PHOENICS is then fed back to the CONTAM and transient state calculation was conducted. This value is used to improve the results obtained by CONTAM over an 8-hour period in which the program is now able to predict higher values of contaminant comparable to the values obtained by PHOENICS (maximum concentration, average concentration)

i) Thus a technique is obtained by which CONTAM results may be improved while considering critical design considerations. It is important to note that in this study the implementation of the data exchange has been achieved manually.

7.3 Variations in the supply airflow rates: Technique 1 and Technique 2

Technique 1 has been the commonly used format to couple multizone and CFD models in most of the studies (Ayari *et al.*, 2000, Musser, 2001). CONTAM and PHOENICS are used to study the impact of varying airflow rates on the detailed air velocity and contaminant distributions in each zone. The interaction in this case takes place at only one level where the data from PHOENICS is used to determine the suitable design airflow for the building and to increase the accuracy in successive predictions using CONTAM. However, in the current research an exchange of data between the two programs will be conducted in order to enhance CONTAM's predictions.

The coupled analysis will first use the CONTAM model to determine the specific airflow rate that is computed at the inlet zone of each of the occupied spaces. This value is then used as the input for PHOENICS where the inlet velocity is used accordingly. The variation of airflow and contaminant distribution characteristics in each of the zones based on the respective inlet velocities are then determined using PHOENICS. CONTAM is also used to show the transient contaminant concentration variations over an 8-hour period. This coupling technique is characterized under the first category wherein the exchange of data between the two programs is taking place at only one level.

The simulation is further extended to include technique 2 which involved the exchange of data between PHOENICS and CONTAM and a comparison between the two predictions are then made. Three different air intakes, 100%, 50% and minimum (25%) of the prescribed airflow have been tested using CONTAM at the normal occupancy level (5 occupants in office 1, 5 occupants in office 2 and none in meeting room). The airflow rates that actually go into each of the zones as computed by CONTAM are used as an input value for the inlet flow rates for PHOENICS. The adequacy of such prescribed airflow rates and energy conservation measures on the indoor air quality is determined using PHOENICS by obtaining the details of air velocity and CO_2 distribution in the individual zones. Once the desired airflow rate has been determined, the transient contaminant distribution characteristic is evaluated using CONTAM. The design airflow into the office is the prescribed airflow rate of 10 L/s per person according ANSI ASHRAE Std. (1999).

In Chapter 6, the errors of determining indoor air characteristics with CONTAM alone was examined. Hence it is important to evaluate major design techniques, such as varying the amount of airflow in buildings using a more detailed approach such as with PHOENICS in order to properly examine the adequacy of airflow into each of the zones.

While reducing the amount of supply airflow rate will definitely have a positive impact on the energy consumption, the negative effects of such a reduction based on specific indoor configurations, contaminant loads and locations of flow obstacles has been discussed in an earlier chapter (Chapter 3). Hence the importance of coupled technique in determining the suitable outdoor air intake design is discussed in this section.

7.3.1 Case I 100% of the design airflow rate

Table 7.1 CO_2 concentration for 100% air intake (steady state concentrations at 9am)

Zones	CO_2 in ppm
Office 1	562
Office 2	500
Meeting Room	512
Corridor	650

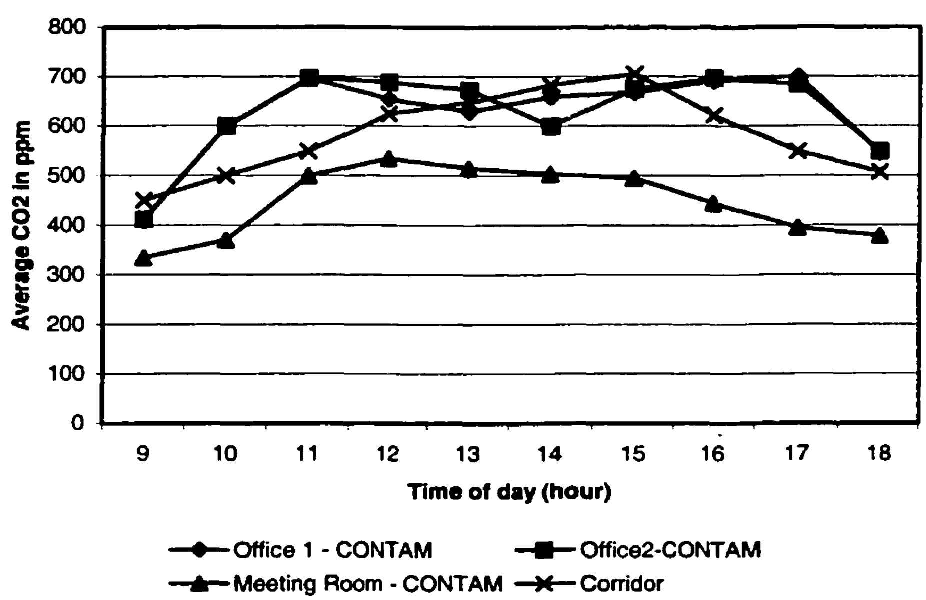
Table 7.2 CO_2 concentration for 100% air intake (maximum concentrations, steady state)

Zones	CO_2 in ppm
Office 1	815
Office 2	822
Meeting Room	712
Corridor	785

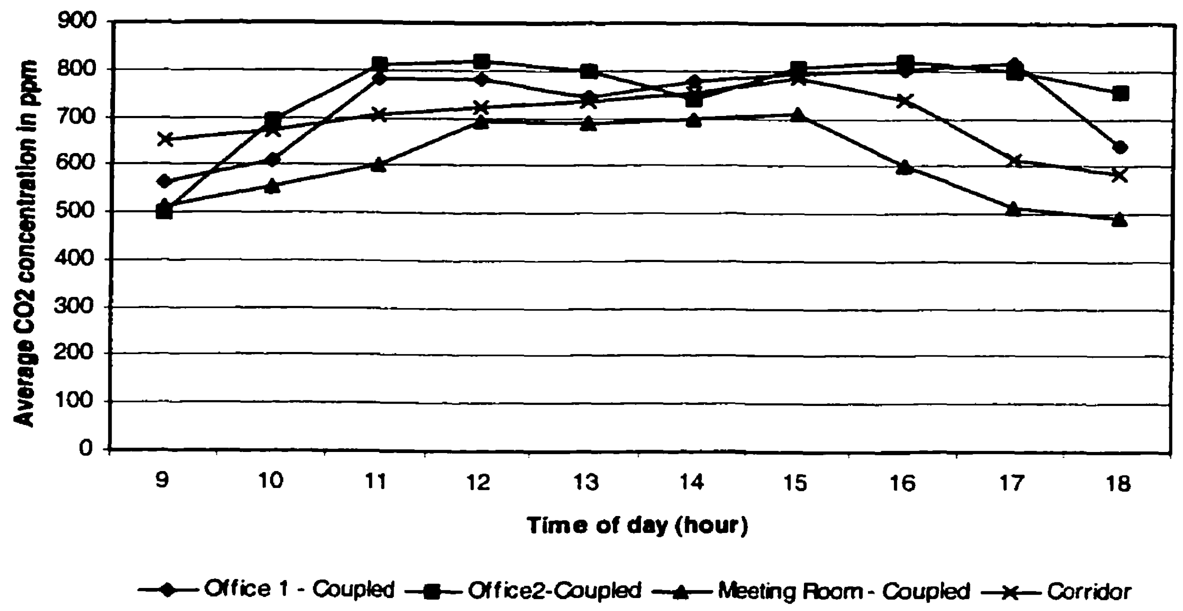
Table 7.1 gives the values of carbon dioxide concentrations that were predicted in each of the zones at 9 am using PHOENICS. Table 7.2 provides the maximum value of

CO_2 predicted by PHOENICS for this specific case. Figures 7.1 a and b depict the variations in CO_2 concentration over an 8-hour period using CONTAM values alone. In Figure 7.1 b, the initial values for CONTAM input are varied according to the steady state values anticipated in each of the zones based on the PHOENICS computations. It is seen that the maximum levels computed by PHOENICS are encountered at the later part of the day, around 3 pm.

Figure 7.1 Comparison of coupled analysis and CONTAM analysis for 100% air intake

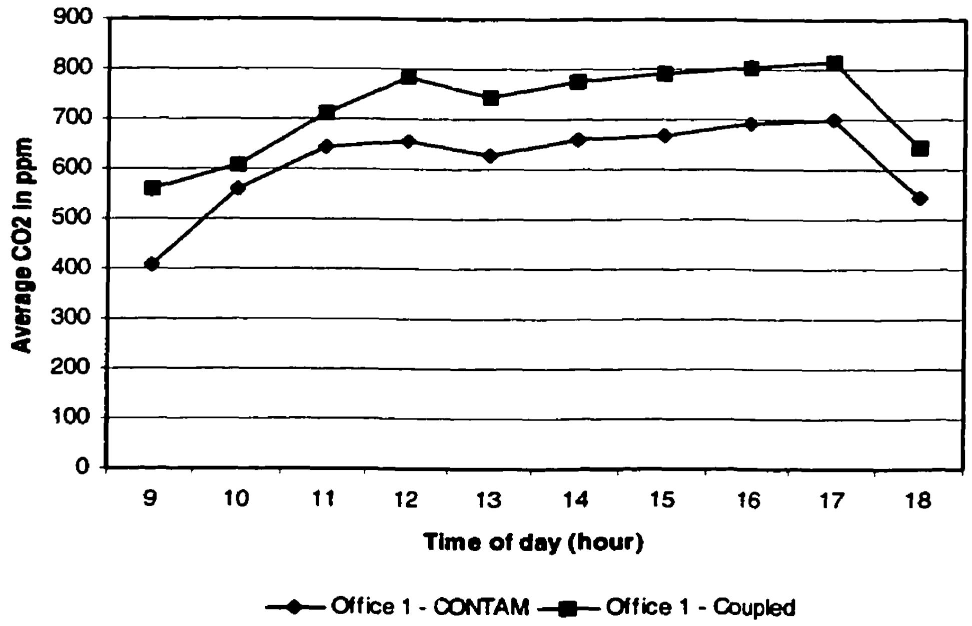


a) CONTAM Predictions

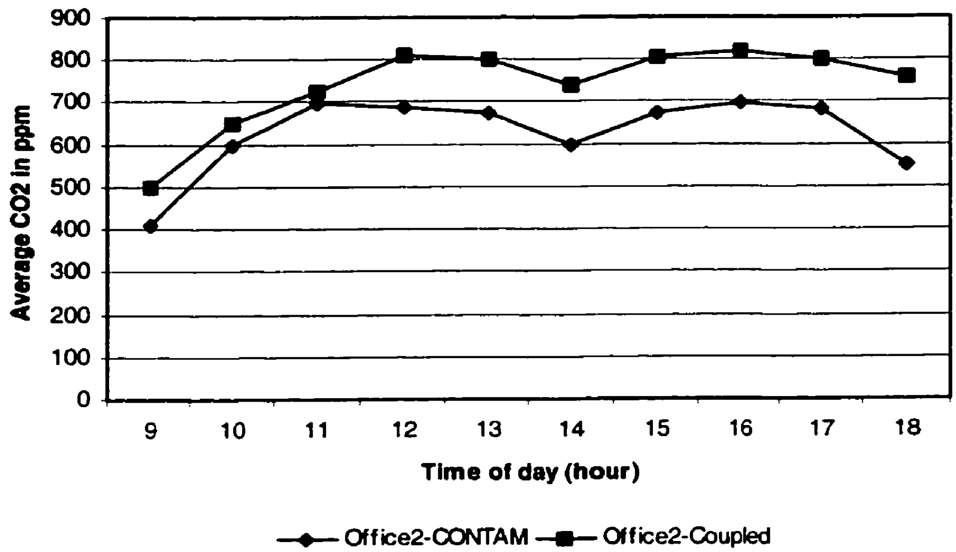


b) Coupled Predictions

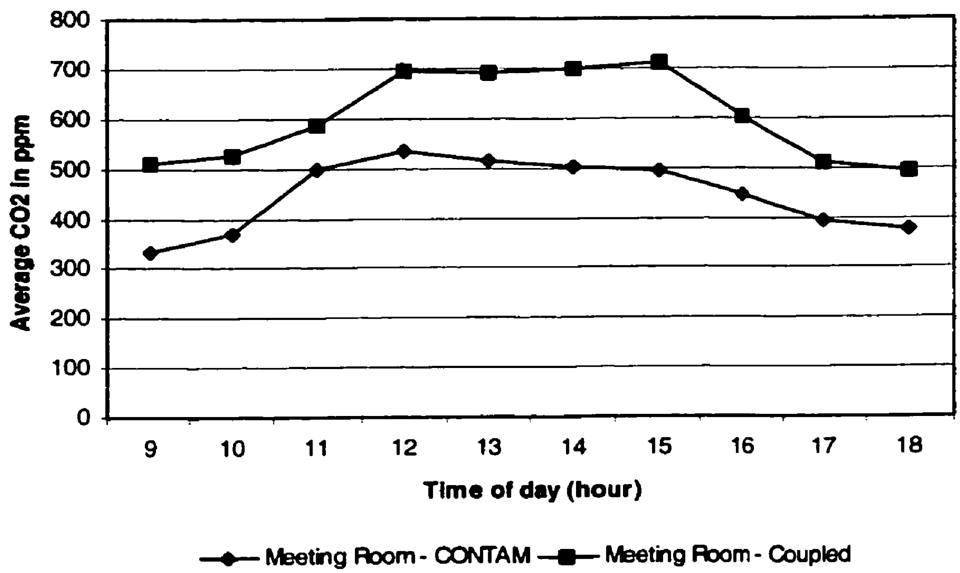
Figure 7.2 Comparison of CO_2 concentrations: CONTAM and Coupled Predictions (100% air intake)



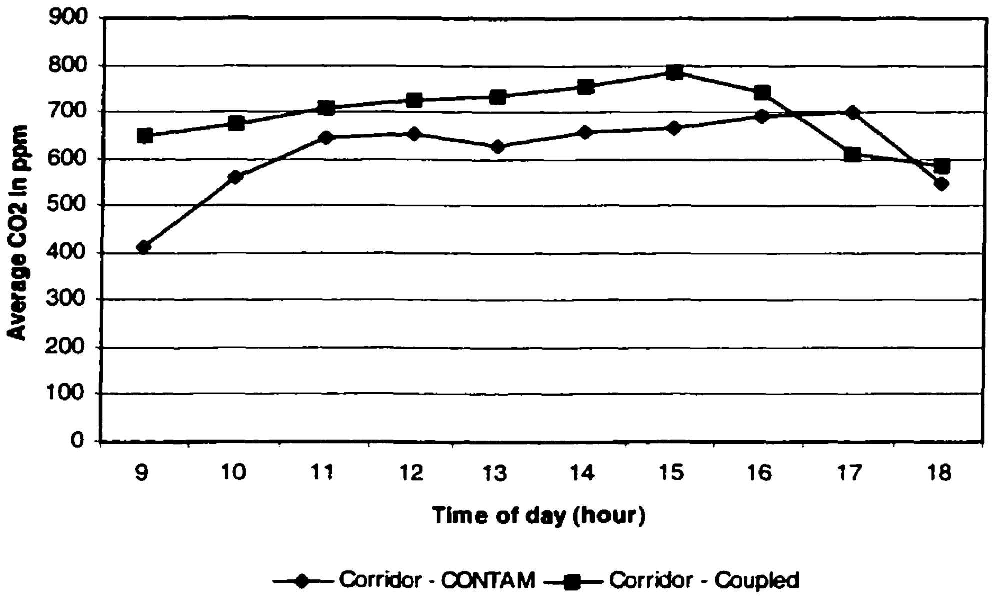
a) Office 1



b) Office 2



c) Meeting Room



d) Corridor

Figures 7.2 a, b, c, and d provide the detailed comparison between the CO_2 predictions made by CONTAM and coupled technique.

7.3.2 Case II 50% of design airflow rate

In this case the contaminant levels start exceeding 800 ppm in most of the zones except the meeting room (Tables 7.3 and 7.4).

Table 7.3 CO_2 concentration in ppm (steady state concentrations at 9 am) (50% air intake)

Zones	CO_2 in ppm
Office 1	650
Office 2	625
Meeting Room	575
Corridor	800

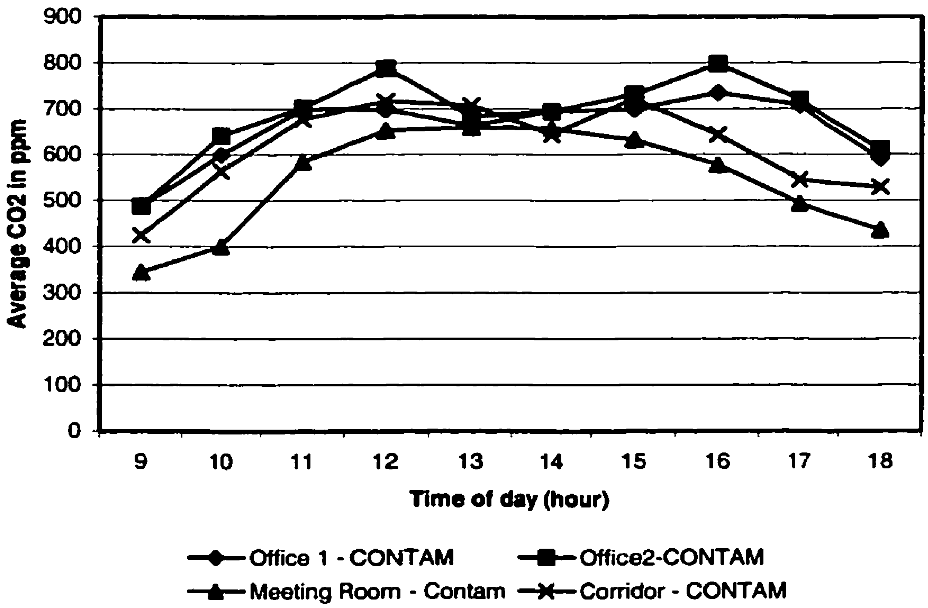
Table 7.4 CO_2 concentration in ppm (maximum values) (50% air intake)

Zones	CO_2 in ppm
Office 1	920
Office 2	900
Meeting Room	765
Corridor	900

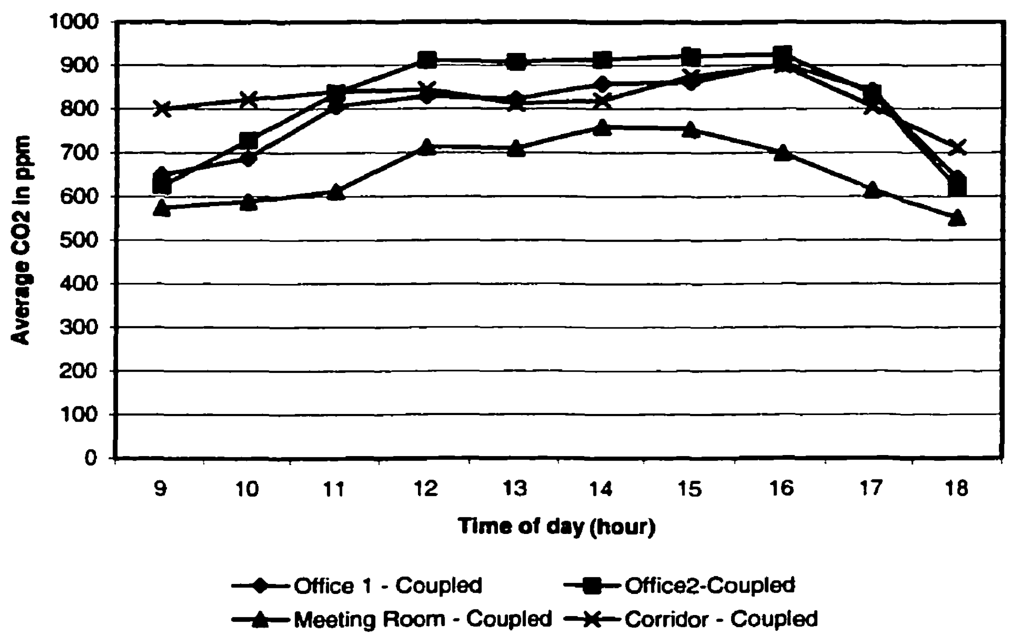
It is seen from Figure 7.3 that the higher contaminant levels are again encountered in the later part of the day. Such results aid in designing fan schedules for occupied spaces with regular and known occupancy schedules. Such implementations are major contributors to reductions in energy usage. This has been further evaluated in Section 7.5

where an additional heavily contaminated zone has been included to the office configuration.

Figure 7.3 Comparison of coupled analysis and CONTAM analysis for 50% air intake



a) CONTAM predictions

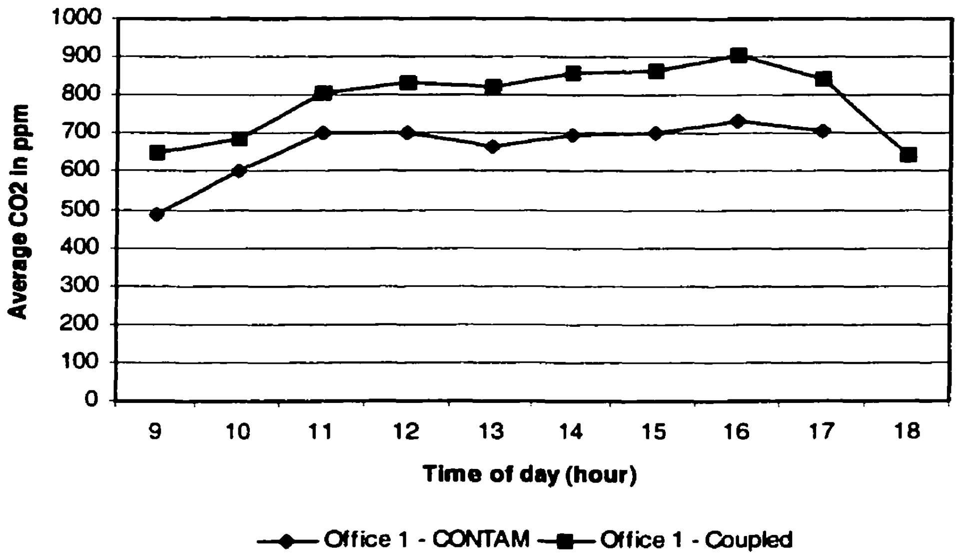


b) Coupled Predictions

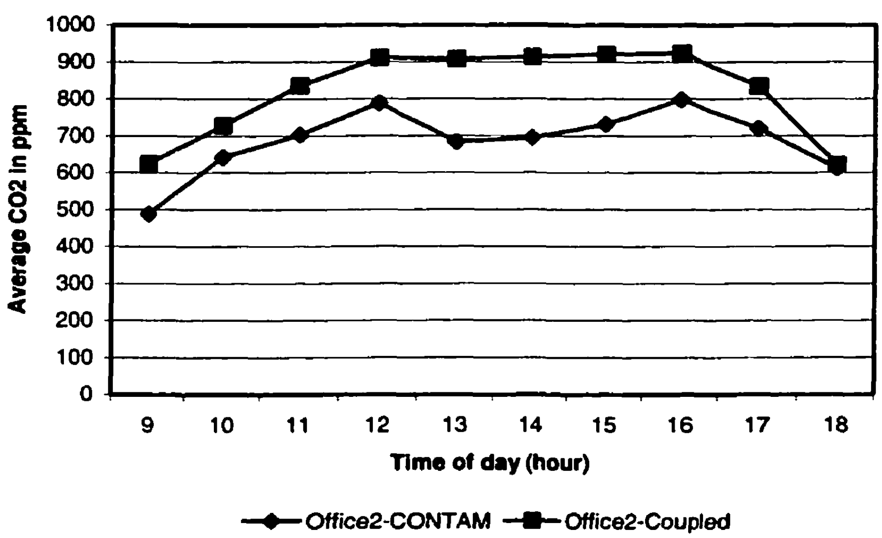
Figures 7.4 a, b, c, and d show the comparison in the values predicted by CONTAM alone and by PHOENICS. It is seen that there is a definite improvement in the predicted values using the combined model.

Figure 7.4 Comparative analysis between CONTAM and Coupled Predictions

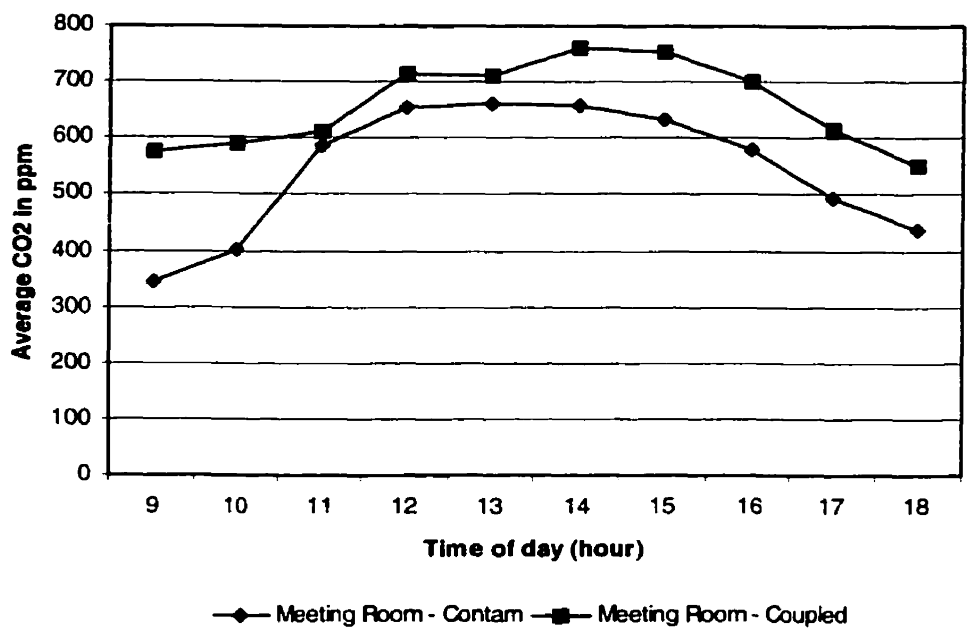
(50% air intake)



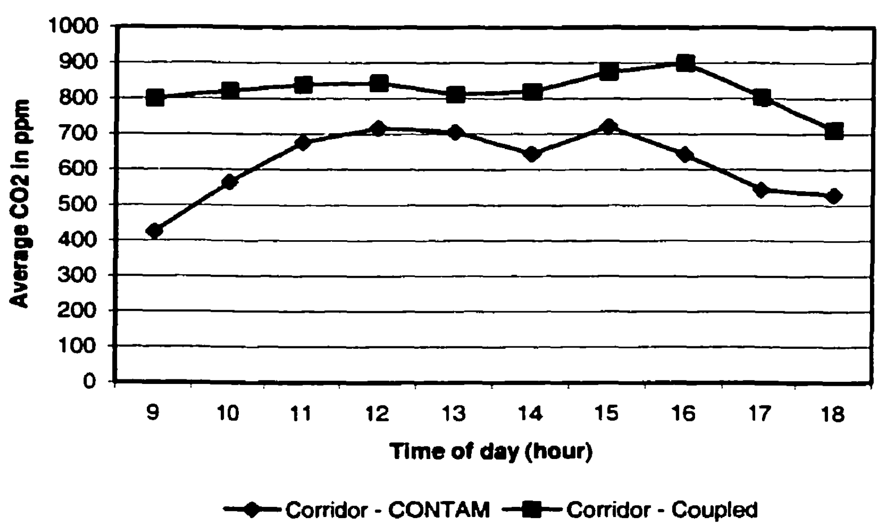
a) Office 1



b) Office 2



c) Meeting Room



d) Corridor

7.3.3 Case III 25% of design airflow rate

In this case the CO_2 levels reach well over 800 ppm in most zones of the office indicating the unsuitability of the application of this airflow rate with no additional specification of fan or occupancy schedules. The main focus of the simulation in this section was to determine the improvement in prediction abilities of CONTAM with the knowledge of detailed airflow characteristics in the office using PHOENICS.

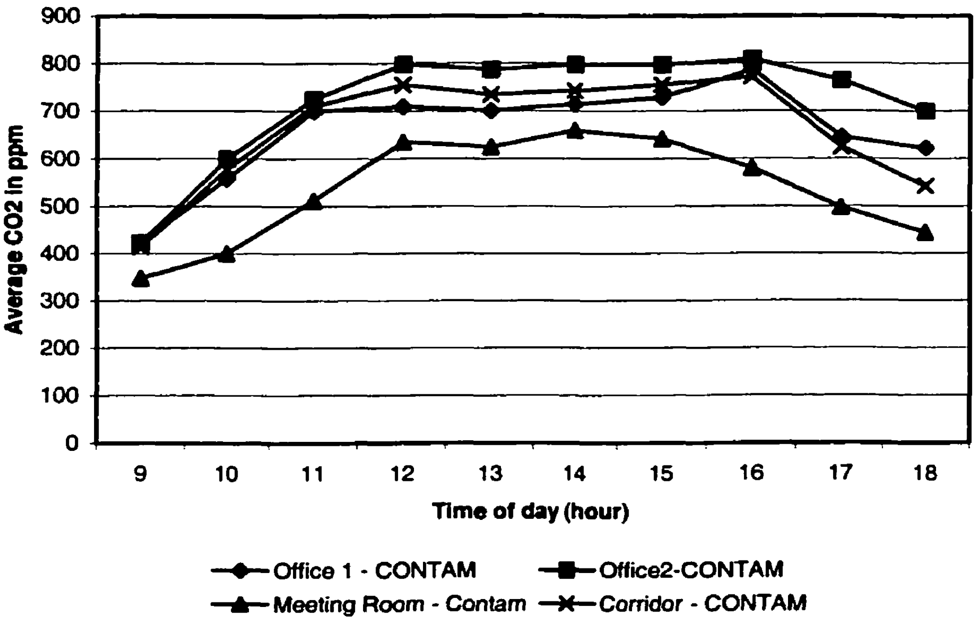
Table 7.5 CO_2 concentration in ppm (steady state values obtained at 9 am using PHOENICS) (25% air intake)

Zones	CO_2 in ppm
Office 1	745
Office 2	800
Meeting Room	601
Corridor	850

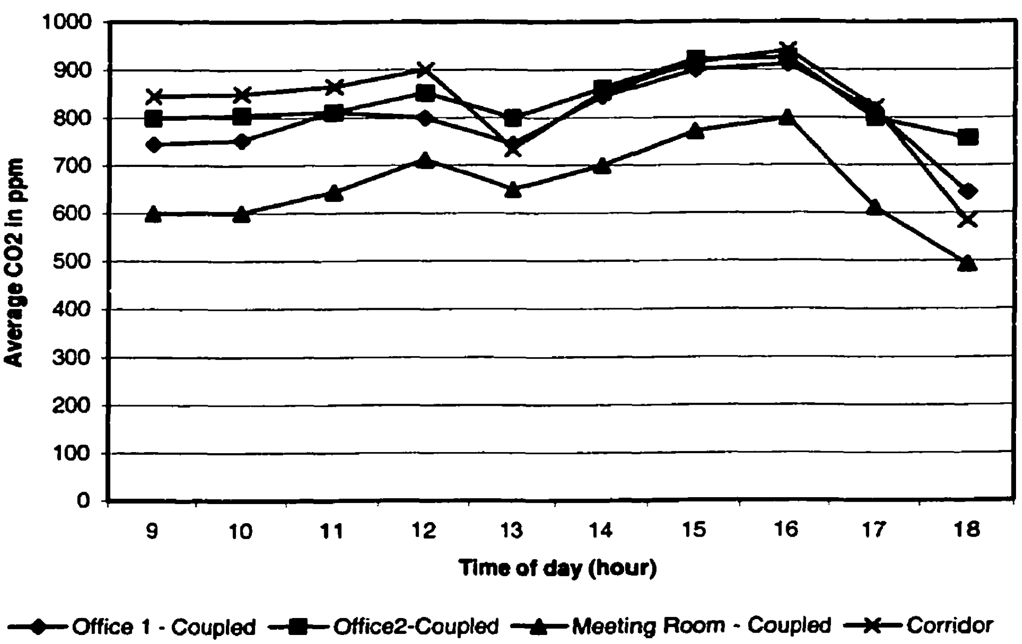
Table 7.6 CO_2 concentration in ppm (maximum values) (25% air intake)

Zones	CO_2 in ppm
Office 1	904
Office 2	912
Meeting Room	800
Corridor	940

Figure 7.5 Comparison of coupled analysis and CONTAM analysis for minimum air intake



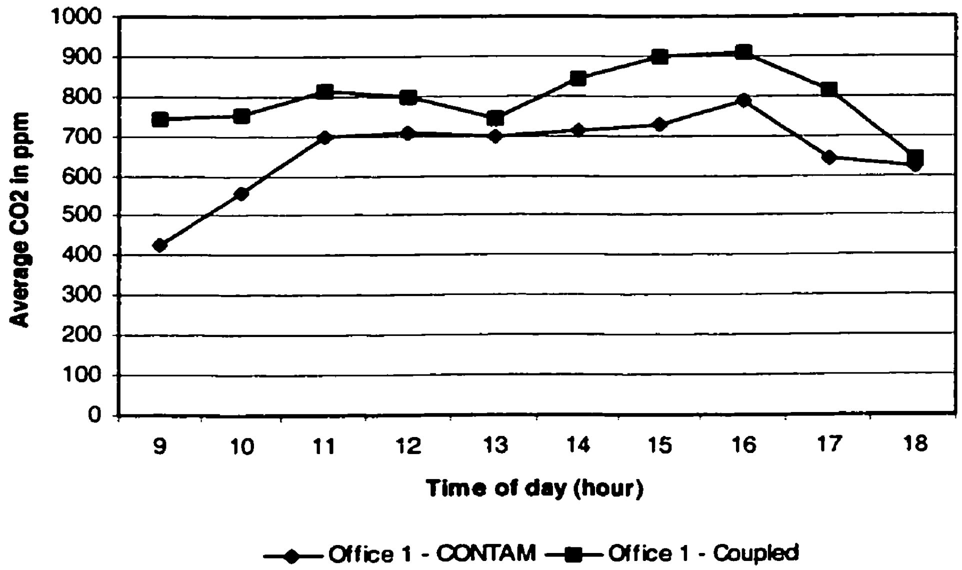
a) *CONTAM predictions*



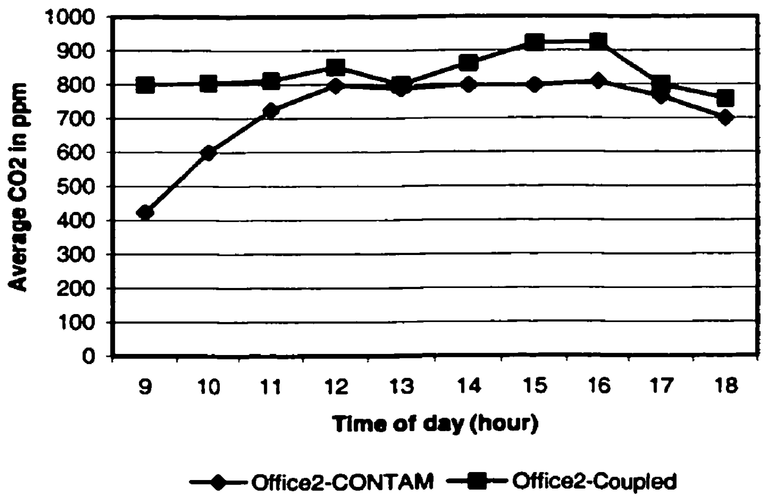
b) Coupled predictions

The 8-hour average follows the same patterns as in the other two cases, except in this case higher CO_2 levels are encountered in most of the zones past 11 am.

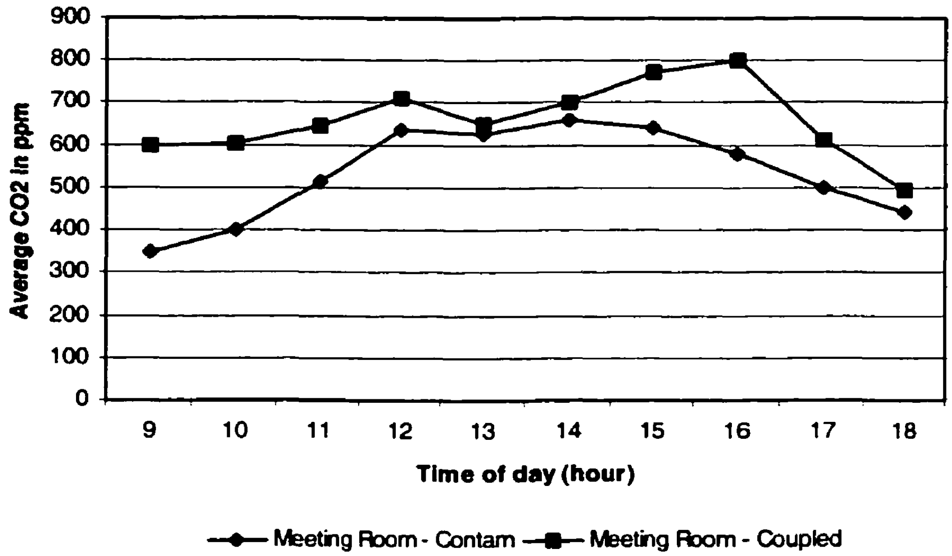
Figure 7.6 Comparison of CO_2 concentration: CONTAM and Coupled Predictions (25% air intake)



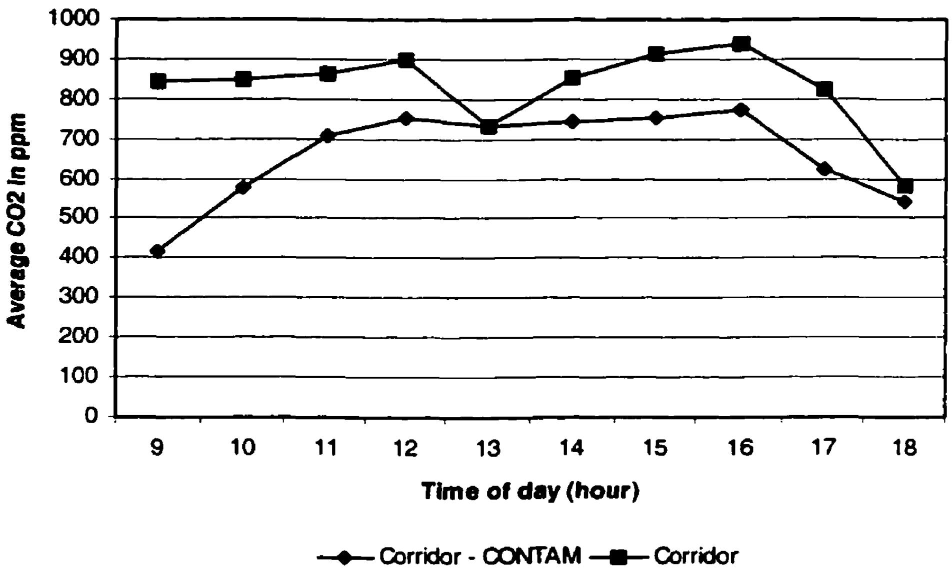
a) Office 1



b) Office 2



c) Meeting Room



d) Corridor

7.3.4 Discussion of Results

As seen in the simulations in sections 7.3.1 – 7.3.3, the knowledge of the details of contaminant levels in the zones of the office from the PHOENICS computations enable better design choices and improve the predictions of the multizone model, CONTAM. It is seen that in the absence of the coupled predictions, CONTAM tends to under predict the concentration levels. Such erroneous outcomes may result in improper selection of design supply airflow rate.

Technique 1 helped predict the unsuitability of 50% and 25% supply airflow rates based on the computed concentration values by PHOENICS, Table 7.4 and Table 7.6. In these two cases the maximum values predicted by PHOENICS exceeding 800 ppm and hence would make these two design values inappropriate.

The simulation case is further extended i.e. technique 2, where the steady state values obtained by PHOENICS were used as input values to predict transient state calculations using CONTAM. The comparative graphs for various zones showed that there was definite difference in the predictions made by the two techniques with the CONTAM only technique under predicting values by as much 40% in certain cases (in comparison with the values predicted by PHOENICS, Table 7.1 and 7.2, Table 7.3 and 7.4, and Table 7.5 and 7.6). Thus it is observed that technique two is able to give a better idea of the CO_2 distributions over the 8-hour period with the values obtained closer to PHOENICS predictions.

7.4 Variations in occupancy schedules and fan schedules (Technique 2)

7.4.1 Introduction

The previous section discussed the impact of varying supply airflow rates on the air quality of the office space. The advantage of using the coupled analysis in this situation was examined. Two cases are considered under this section. The first one is where the occupancy schedule varies with a higher level of CO_2 in the meeting room at a specific period of the day. Again in this situation as in the previous section and Chapter 4, no fan schedule is considered, i.e, with the fan on throughout the 8-hour working day operating at the specified supply flow rate.

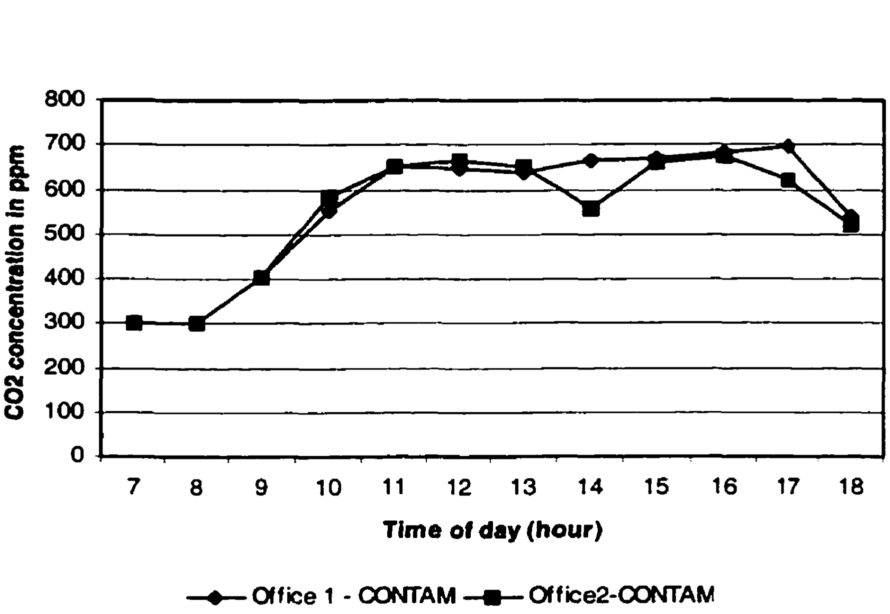
In the second situation, a more complex situation is considered where the interaction between the two programs is considered at more than one level. The office configuration used in Chapter 5 is considered in this chapter as well. In this study, a fan schedule is specified for the supply fans of the office based on the occupancy schedules and the expected contaminant concentration level as determined in the previous section and chapter.

7.4.2 Occupancy Schedules

7.4.2.1 No meeting room schedule

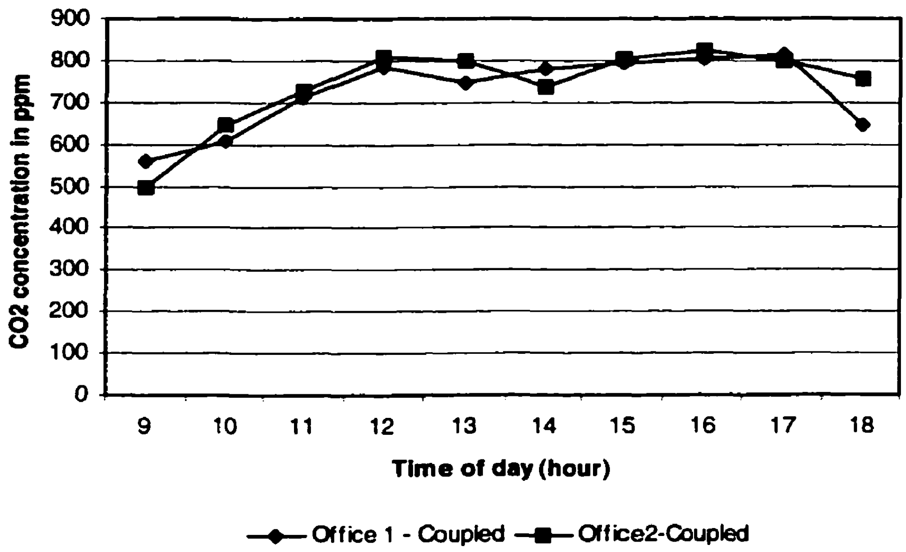
When there is no meeting room schedule specified it is seen that there is no major difference in the predicted values.

Figure 7.7 CONTAM predictions with no meeting room schedule



Figures 7.7 and 7.8 show the transient state predictions of varying CO_2 concentrations in the office spaces 1 and 2. Since the meeting room schedules have been excluded in this simulation, the meeting room has not been included in the graphs. It is seen that the variation in CO_2 concentration between the two techniques differ with the CONTAM values being less than 50 ppm from the predicted values of the coupled technique. The difference in predictions, increase towards late afternoon with the variations exceeding 100 ppm. This could be due to the accumulated errors in the predictions made by CONTAM towards the later part of the day.

Figure 7.8 Coupled predictions: No meeting room schedule



7.4.2.2 Meeting Room Schedule

Transient state predictions of the varying CO_2 levels in the office building based on a typical office schedule is simulated in this section. The occupants begin arriving at around 8 am. Normal occupancy is expected at around 9 am. Meeting time with peak occupancy is expected from 10 to 11 am. CONTAM is used to compute the varying carbon dioxide concentration over an 8 - hour period between 8 am to 4 pm (Please see Chapter 6, Table 6.3). There is no fan schedule or outdoor air intake schedule specified for this case.

Figure 7.9 CONTAM predictions, with meeting room schedule

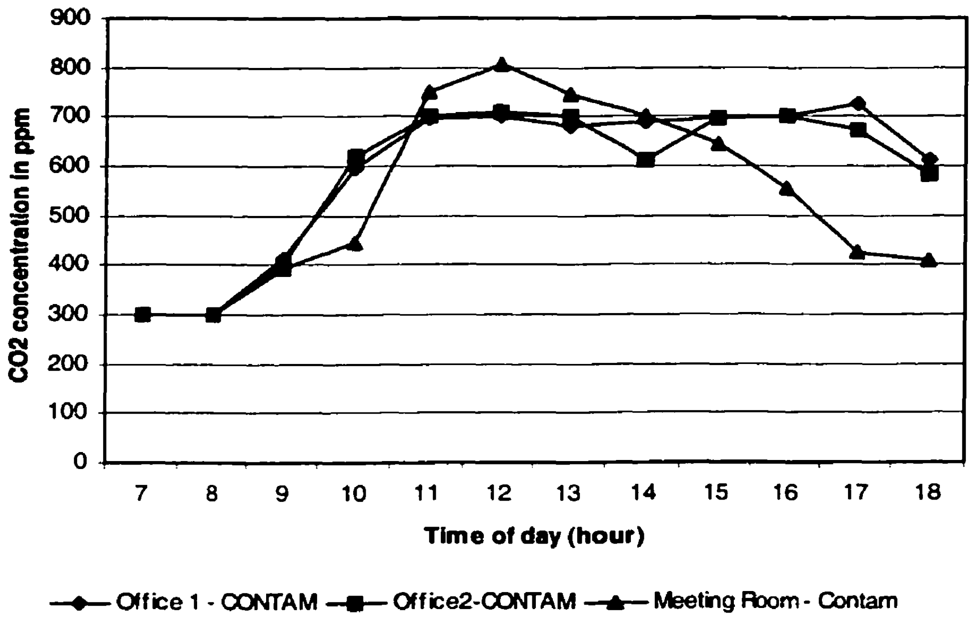


Figure 7.9 depicts the 8-hour variation in carbon dioxide levels in the office. Three important zones of the building, office 1, office 2 and the meeting room are shown in the graph. It is seen that the CO_2 levels in office 1 and 2 begin to increase from the assumed outdoor concentration level of 300 ppm beginning at 8 am. The levels remain low until 9 am, when they begin to increase depicting the normal occupancy level in the office. The meeting room shows a sudden increase in CO_2 levels between 10 to 11 am, the normal scheduled meeting time when the occupancy levels are maximum. The levels in the two office spaces also show an increase during this time due to the possible interaction with the meeting room. There is a slight decrease in the CO_2 levels during the lunch hour in the two offices while the meeting room shows a gradual decrease in the contamination levels over the period of time. The levels in office 1 and 2 again increase after 1 pm and continue to increase until 3 pm when again the levels start to go down as the occupants in the office depart from the workplace.

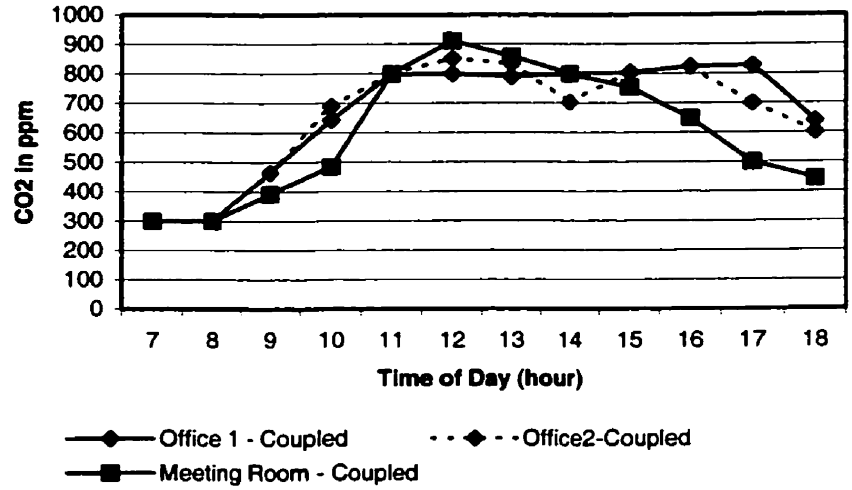
Figure 7.10 shows the variation in the values based on an average value calculated from the PHOENICS predictions for each of the zones. It is seen that in most of the zones the values predicted by CONTAM are far less than the predictions of PHOENICS. Since PHOENICS takes into account the presence of heat sources, flow obstacle, flow path locations, its predictions may have a far better impact in the subsequent analysis of the contaminant levels encountered in an 8-hour period. This knowledge may be especially critical in the present circumstance where a sudden increase in contaminant sources is encountered at a specific time.

Table 7.7 PHOENICS predictions of average CO_2 concentration levels

Zones	CO_2 concentration (ppm) Case 1	CO_2 concentration (ppm) Case 2	CO_2 concentration (ppm) Case 3
Office 1	710	735	769
Doorway between office 1 and 2, D	730	739	811
Office 2	709	713	746
Doorway between office 1 and corridor, D1	657	735	786
Doorway between office 2 and corridor, D2	713	763	776
Corridor	698	699	901
Doorway1 between corridor and meeting room, D3	620	685	793
Doorway2 between corridor and meeting room, D4	592	646	793
Meeting room	588	660	894

The predictions of PHOENICS for the peak occupancy period have been incorporated into the transient calculations of CONTAM.

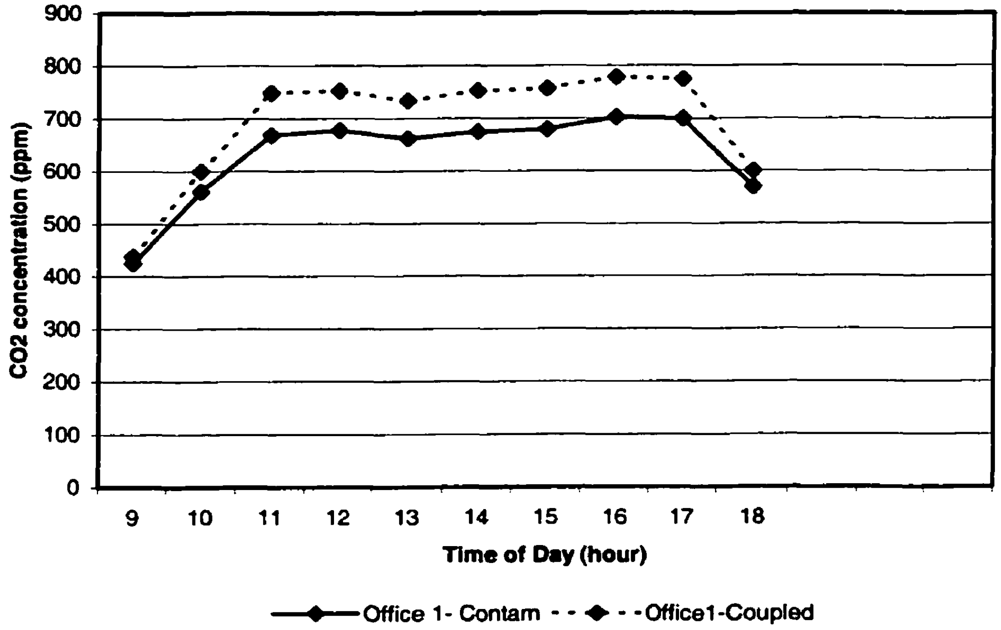
Figure 7.10 Coupled predictions, with meeting room schedule



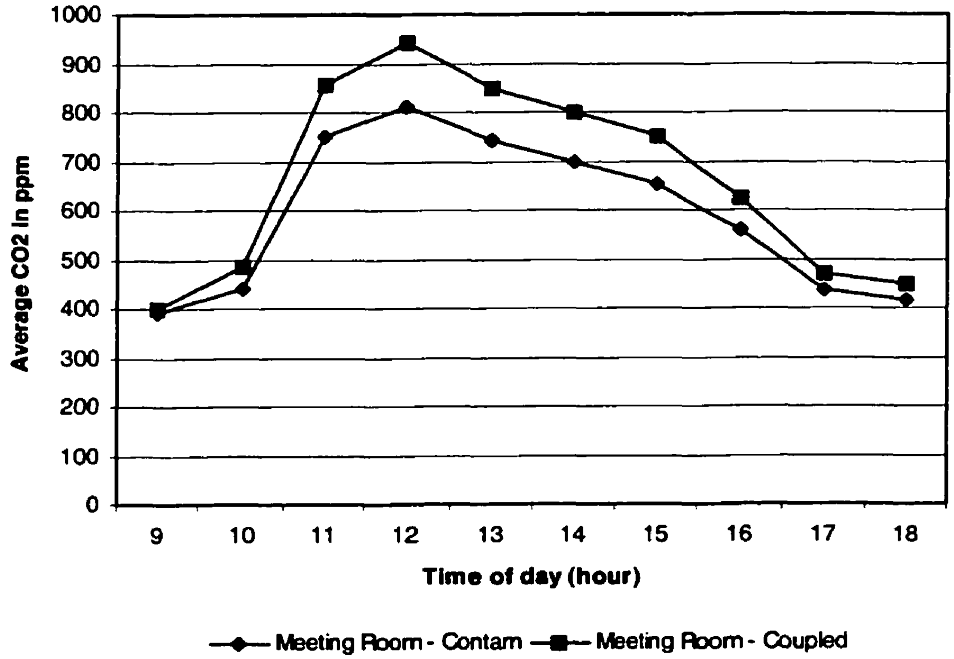
7.4.2.3 Discussion of Results

Figures 7.11 a and b compares the values for CONTAM and coupled predictions over an 8-hour period. It is seen that the values vary greater than 7% in some cases reaching as high as 18%. The existence of a heavily contaminated zone, such as the meeting room tend to cause errors in the CONTAM predictions. The coupled technique seems to compute better values and patterns of the office space taking into account the increased values encountered following the peak occupancy period.

Figure 7.11 Comparison of the two prediction techniques



a)

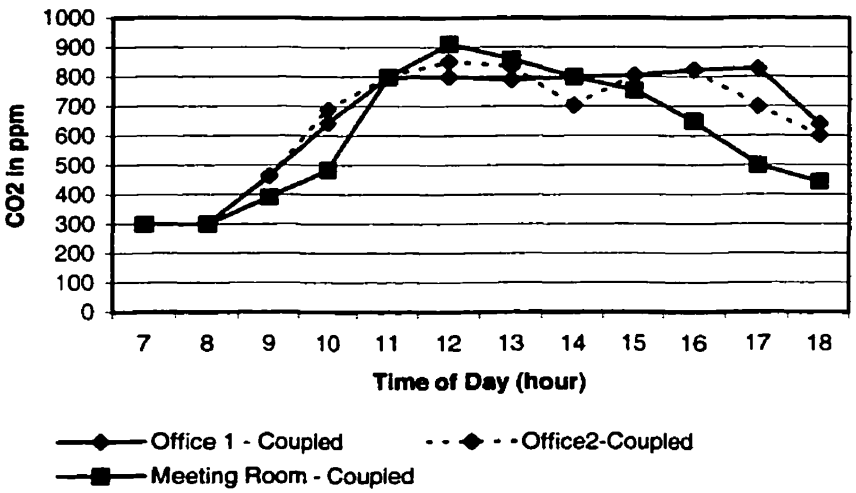


b)

7.4.3 Fan Schedule

In this section a supply fan schedule is suggested based on the anticipated CO_2 concentration. The computations from the coupled technique are considered in order to decide the fan schedule. Section 7.3 discussed the variations of supply flow rates without applying a fan schedule. In this section, supply fan schedules are suggested for the meeting room. Figure 7.12 depicts the carbon dioxide concentration levels based on the coupled analysis from the previous section. It is observed that the prescribed airflow rate of 10 L/s per person with the fan on condition still creates high levels of CO_2 concentration in the office with the meeting room schedule. Hence in this section the design airflow into the office is increased to 15 L/s per person and fan schedule will be considered in order to bring down the energy costs.

Figure 7.12 Coupled technique predictions: with meeting room schedule



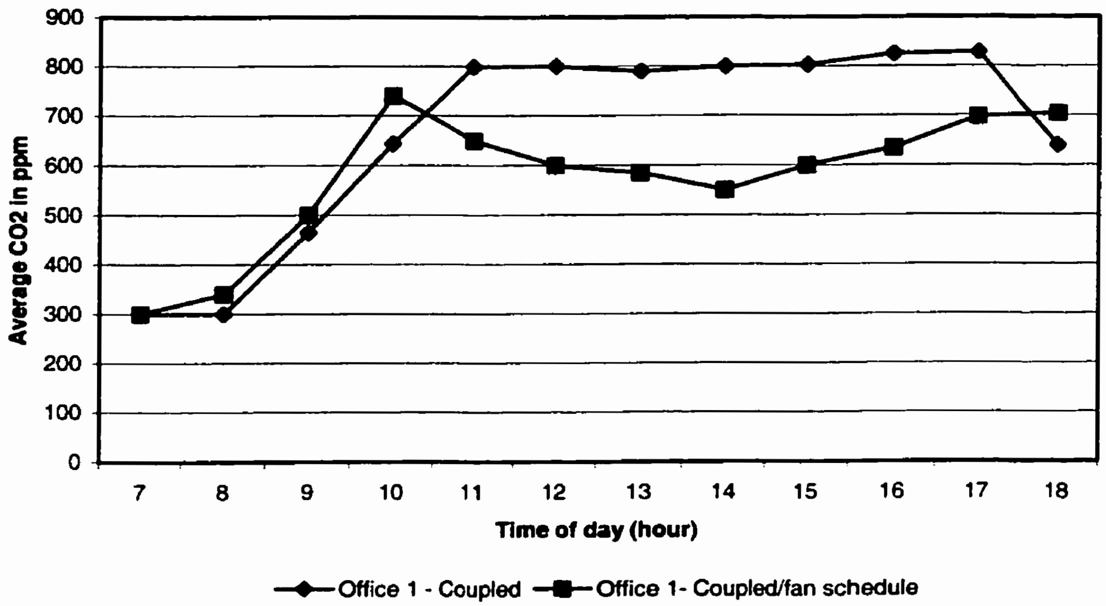
The CO_2 levels increase gradually from 8 to 10 am with the maximum value of 700 ppm encountered in office 1 at 10 am. The values then steadily increase between 10 am to 12 pm with the values rising above 800 ppm in all three zones of the office with a maximum of 925 ppm in the meeting room. While the values in the meeting room slowly and steadily decrease after this, in office 1 and 2 the values reduce slightly until 2 pm and then again reduce with another peak occurring at 3 pm. The values then decrease with values varying between 405 ppm in the meeting room to 608 ppm in office 1.

The fan schedule for the two zones, office 1 and meeting room are different based on the occupancy schedule of the office. The supply fan to the office spaces, 1 and 2 are kept at minimum levels from 8 am to 10 am when the occupancy rate is still varying from minimum to normal levels. From 10 am to 12 pm when maximum occupancy in encountered in the office, the fans are kept on at maximum level. Since the levels of CO_2 are still relatively high in the office spaces, the fans are still operated at full capacity until 2 pm and from then on it is operated at half capacity. For the meeting room, a different schedule is adopted. The supply fan is operated at minimum capacity until 10 am. From 10 am to 1 pm, it is operated at maximum capacity but after 1 pm, the fan is shut down

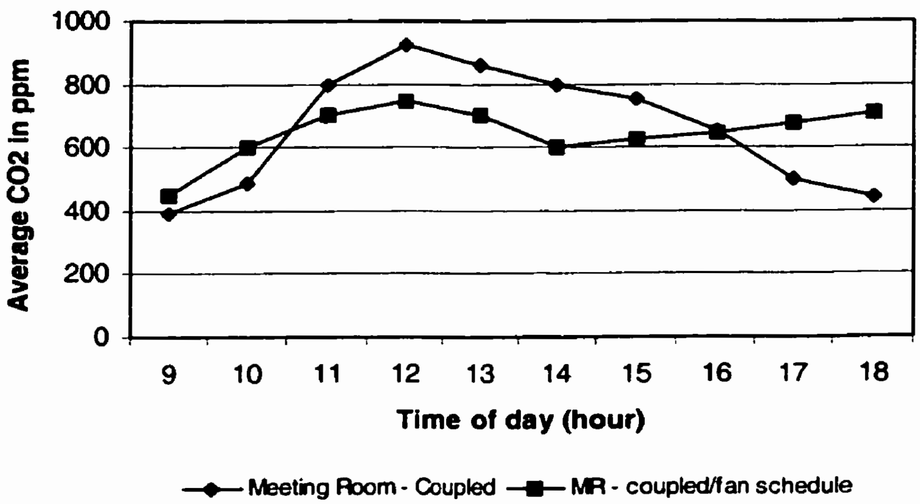
7.4.3.1 Discussion of Results

Figure 7.13 shows the comparison of computed coupled technique values with and without fan schedules. In the first case the values in the meeting room reach up to 925 ppm around 12 pm. The concentrations in office 1 also reach over 800 ppm at several times during the 8-hour period. With the fan schedule it is seen that the pattern of CO_2 distribution varies considerably but does not exceed 800 ppm.

Figure 7.13 Comparison of CO_2 concentrations with and without fan schedule



a)



b)

The meeting room and office 1 have increasing levels of CO_2 between 8am to 10 am when the fans are operating at minimum capacity. From 10 am till 12 pm the levels lower considerably due to the fans being operated at maximum capacity. This trend continues for office 1 where the values continue to fall until 2 pm. After this the values increase very gradually since the fans are still operating at 100% capacity and approach a value of approximately 700 ppm by 6 pm. The meeting room continues to drop until 2 pm then there is a rapid increase in the concentration of CO_2 due to the fan operating at a minimum capacity. The values, however does not increase beyond 712 ppm by 6 pm. It is critical to have the HVAC operational before the office begins to operate again the successive day, in order to clear out the residual contaminants from the building.

Figure 7.14 Predictions of CONTAM with the meeting schedule

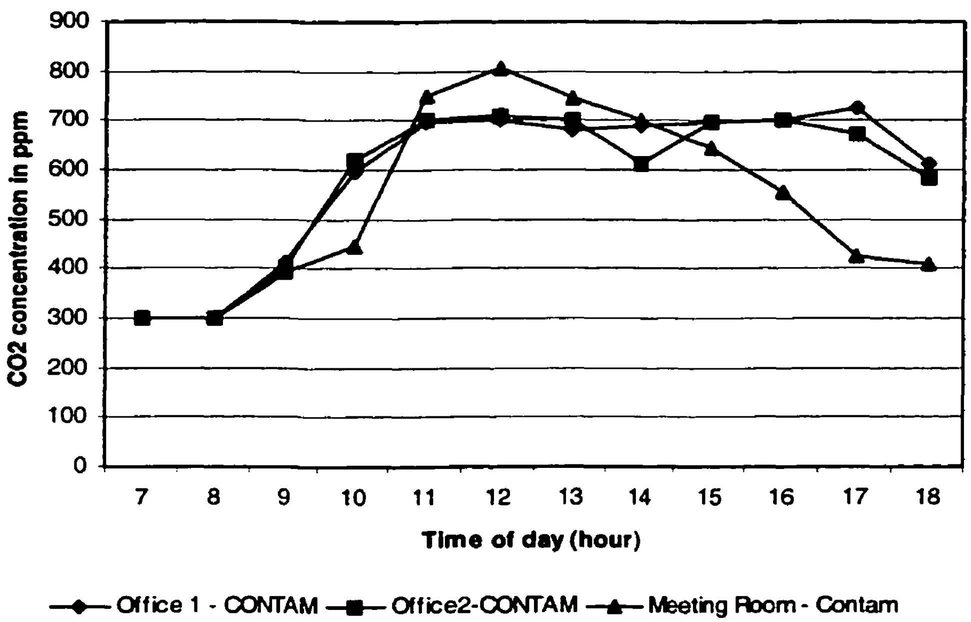


Figure 7.14 shows the predictions of CONTAM for the fan on condition with the original design airflow of 10 L/s per person. It is seen that the concentration of CO_2 seems to be contained very well even with the inclusion of the meeting room schedule. The use of the coupled technique not only helped identify the inadequacy of the

prescribed flow rate but also helped in prescribing a suitable fan schedule that could save energy costs while maintaining the desired indoor air quality in the office space.

8. CONCLUSIONS AND FUTURE WORK

8.1 Conclusion

Computational techniques are powerful research tools for indoor air quality analysis in buildings.

Multizone models such as CONTAM are popular tools of research of the indoor environment and have been widely used by studies to determine indoor airflow characteristics of buildings. Such models provide an overall picture of the airflow characteristics of the building taking into account the various factors that affect it. Multizone models have found their applications in complex situations of indoor air quality analysis as the literature search revealed and the results obtained in these studies were found to be fairly accurate. However several studies have also pointed towards the need for a more accurate technique to satisfy the growing instances of indoor air quality problems in buildings. So in this thesis work, a detailed analysis of the multizone model, CONTAM was conducted and the advantages and shortcomings were identified through an in-depth parametric study.

CFD models like PHOENICS have become an important part of indoor air research due to its ability to determine detailed flow structure of individual zones based on the presence or absence of sources of contamination, heat generating sources, their locations, and locations of inlets and outlets. Such knowledge has become invaluable in identifying problem areas within buildings and to determine suitability of certain design considerations. However the previous work with this model has been restrictive and applied to simple cases with mainly individual zones due to the innumerable input data involved and the time commitment being very large. In this thesis work however an attempt has been made to study a more complex situation with varying indoor environmental conditions. A parametric study that examined several different situations of contaminant source locations, strengths, locations of heat sources, and inlet-outlet locations along with varying inlet velocities was studies in detail.

In this work a direct comparison of the two models was conducted to determine the flow characteristics and the contaminant distributions in an office building. The results from this study were very useful to identify the positive and negative aspects of the two models. The CONTAM program was found to be crucial to indoor air quality assessment since it considers outdoor environmental as well as indoor environmental factors for its analysis. But the program was found to generate erroneous results in situations where the intrazonal characteristics had a major influence on the airflow and contaminant distributions. While the CFD model remained the better technique to identify intrazonal flow characteristics it is difficult to apply this model to interact with the data from the outdoor environment and where innumerable zones and several floors are involved. Also the time requirement for complex situations is extremely high. The multizone model was identified as the more feasible option for indoor air quality analysis.

A few studies have attempted to enhance the simulating environment by coupling the two models. However, the work has remained at a preliminary level. One of the focuses of this thesis work was to implement a good coupling technique that would use the advantages of the two models to generate meaningful results. The objective of the coupling technique was the enhancement of simulating capabilities of the multizone model, CONTAM. Hence the CFD model, PHOENICS, was used to increase the accuracy of CONTAM predictions. The focus was on the distribution of a single contaminant, carbon dioxide from the occupants in an office building. It has been shown in this work that it is important to identify the areas for which such an application would be effective. Not all situations require a coupled analysis. However, it was also determined that in situations where coupling was found to be necessary, the predictions of the multizone model, CONTAM alone generated erroneous results. Having identified such areas, a detailed study was made to evaluate the extent of improvement that could be achieved over the results from just using the CONTAM model. This thesis work has considered a more complex level of coupling technique in comparison to the previous work. The few studies that have addressed this issue have considered the coupling at a basic level where the detailed values from PHOENICS was used to determine the suitability of certain design considerations (Schaelin *et al.*, 1993, and Musser, 2001) without actual transfer of data between the two models. But in this study this aspect has been considered at a preliminary level. The more accurate and detailed values computed by PHOENICS have been used to update the initial concentration data for CONTAM in order to improve the successive results generated. It was found that the results obtained sometimes differed from the original by as much as 20%. This was found to be a fairly good improvement over the previous technique.

Table 8.1 Summary of Results

Thesis Contribution	Summary of Results
1. In-depth analysis of PHOENICS	Partition height, width and the presence have an influence on the air movement and contaminant distributions. Presence or absence of contaminant sources enhance air movement as do the presence of heat sources.
2. Comparative analysis of PHOENICS and CONTAM	CONTAM under predicts the contaminant concentrations while PHOENICS is able to provide accurate results based on the local influences in a space.
3. Development of a coupling technique to enhance the prediction capabilities of CONTAM	Enhancement of the simulation capabilities of CONTAM with the input from PHOENICS in order to better predict indoor environmental variations.

8.2 Future Work

This thesis study has addressed a very important link to the development of a powerful research tool for indoor air quality analysis. Such a model could result in simulating the realistic world in a better way and offer solutions to problems that are more meaningful. The coupling between the two models, CONTAM and PHOENICS was tested at a complex level. It was found that this technique when applied to the appropriate situations could generate results that were at least 20% more accurate than with CONTAM alone. In this study, the interactions between the two models were considered at specific times of a day over the 8-hour period. Also the actual transfer of data was made manually. The two models were not being operated on an automatic interaction approach. It would be extremely useful and less time consuming to develop such a technique in the future to further enhance the simulation environment and accuracy in predicted results. While considering complex indoor environments where the local influences in zones have a significant influence on the overall airflow characteristics in an occupied space and constantly vary in their design or loads over time it may be important to have an hour to hour exchange of data between the two models to make the results more meaningful. In this thesis study, the meeting room schedule (section 7.3, section 7.4) created a variation in the local influence during a limited period. Hence at this point the one time data exchange between the two models did provide reasonably good results. The hour-hour exchange between the two models is a major study in itself and beyond the scope of the current study. However it is seen as a critical step in improving the simulation environment.

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APPENDIX

A. CONTAM MULTIZONE MODEL

A.1 Introduction

This appendix describes briefly the multizone model CONTAM. The theory for CONTAM has already been discussed in detail under chapter 3 of this thesis work. In this section a description of the program and its assumptions will be provided.

A.2 CONTAM

CONTAMW is a multizone indoor air quality and ventilation analysis computer program.

Airflows: infiltration, exfiltration, and room-to-room airflows in building systems driven by mechanical means, wind pressures acting on the exterior of the building, and buoyancy effects induced by the indoor and outdoor air temperature difference. *Contaminant Concentrations*: the dispersal of airborne contaminants transported by these airflows; transformed by a variety of processes including chemical and radio-chemical transformation, adsorption and desorption to building materials, filtration, and deposition to building surfaces, etc.; and generated by a variety of source mechanisms, and/or *Personal exposure*: the predictions of exposure of occupants to airborne contaminants for eventual risk assessment.

CONTAMW can be useful in a variety of applications. Its ability to calculate building airflows is useful to assess the adequacy of ventilation rates in a building, to determine the variation in ventilation rates over time and the distribution of ventilation air within a building, and to estimate the impact of envelope air tightening efforts on infiltration rates. The prediction of contaminant concentrations can be used to determine the indoor air quality performance of a building before it is constructed and occupied, to investigate the impacts of various design decisions related to ventilation system design and building material selection, and to assess the indoor air quality performance of an existing building. Predicted contaminant concentrations can also be used to estimate personal exposure based on occupancy patterns in the building being studied. Exposure estimates can be compared for different assumptions of ventilation rates and source strengths.

(Information from the CONTAM website)

A.3 Information Source

For more information on how to use the software and for access to free downloads please refer to the following website:

http://www.bfrl.nist.gov/IAQanalysis/CONTAMWdesc.htm

B. COMPUTATIONAL FLUID DYNAMICS SOFTWARE, PHOENICS

B.1 PHOENICS

This appendix describes the CFD software, PHOENICS. Its name is an acronym for *Parabolic Hyperbolic Or Elliptic Numerical Integration Code Series*, wherein "parabolic", "hyperbolic" and "elliptic" are the names which mathematicians use for the underlying equations. (PHOENICS Journal). PHOENICS is a general purpose CFD code launched by CHAM (Concentration, Heat and Momentum Ltd.)

A detailed discussion of theoretical background for this software has been provided in chapter 3.

B.2 Source for Information

Further information on the software can be obtained from the CHAM website at the address provided below.

http://213.210.25.174/phoenics/d_polis/d_info/phover.htm

This website provides an in depth review of the software with many citations of applications and examples.

C. AVERAGE VALUES FOR PHOENICS STUDY

C.1 Introduction

In chapter 6, comparative analysis of PHOENICS and CONTAM was presented. The carbon dioxide concentration values computed by PHOENICS was averaged over a number points (8 points for offices 1 and 2, 12 point for the meeting room, and 6 points in the corridor) at heights of 1.1 m and 1.5 m from the floor. In order to determine whether the selected number of points were adequate in representing the entire zone, additional calculations were made. Case III, (Chapter 6, Section 6.4.2) which represented the maximum case scenario was used to calculate an average value based on additional points that were taken at 5 different heights in each of the zones (0.6m, 1.2 m, 1.8 m, 2.3 m, and 3.2 m)

Figure C1 Locations used in average value computations for PHOENICS

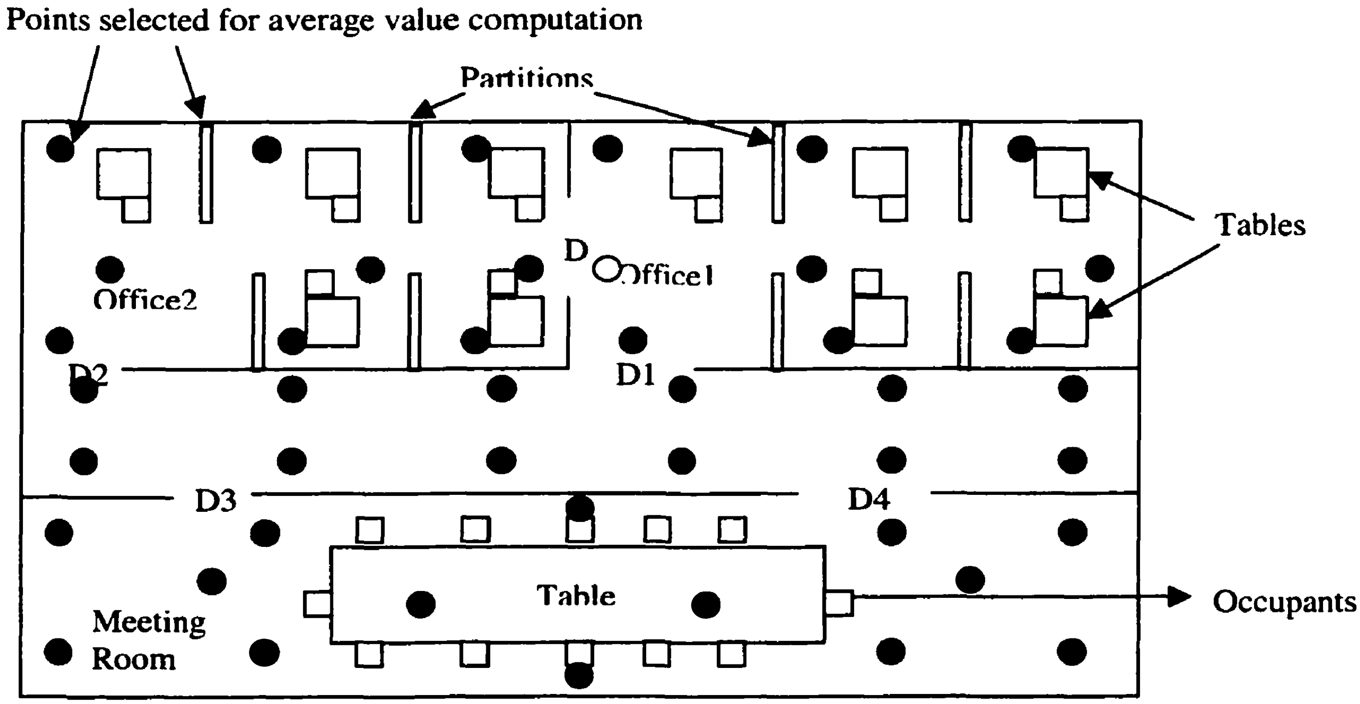

Table C1 Number of selected points for average value calculations

Zone	Number of Points
1. Office 1	45
2. Office 2	45
3. Corridor	60
4. Meeting Room	70

C.2 Results

The average values obtained using additional points in each zone in the corridor and the meeting room, were within 5% of the original average calculations. Hence, the average values calculated in chapter 6 are considered a fair representation of the carbon dioxide levels in the zones of the office.

Table C2 Comparison of the average values computed by PHOENICS

Zone	Average CO_2 value (from Table 6.8), in ppm	Average CO_2 value (new value), in ppm
Office 1	769	766
Office 2	746	750
Corridor	901	889
Meeting Room	894	888