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Development and Calibration of a Multi-Zone Model to Predict the Distribution of Contaminant in a Residential Building Using CONTAM Software

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DEVELOPMENT AND CALIBRATION OF A MULTI-ZONE MODEL TO PREDICT THE DISTRIBUTION OF CONTAMINANT IN A RESIDENTIAL BUILDING USING CONTAM SOFTWARE

by

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Nomenclature

A	area of an opening; cross-sectional area of a room
b	source term in a mass continuity equation
b'	source term in the linear form of mass continuity equation for a zone in a Multi-zone program
B	vector of source terms in an assembled momentum conservation equation
Bc	vector of source term in an assembled species conservation equation
Be	vector of source terms in an assembled energy conservation equation
C	nonlinear flow coefficient; ratio of inflow opening area to the cross-sectional area of a room; contaminant concentration
C	average contaminant concentration
$\mathbf{C_d}$	Discharge coefficient
$\mathbf{C_o}$	Observed Concentration
$\mathbf{C_p}$	Predicted Concentration
$\mathbf{C_p}$	Wind pressure coefficient
ERV	Energy Recovery Ventilation
F	Airflow rate
FB	Fractional Bias of the mean concentrations
FS	Fractional Bias based on variance
G	Generation rate
h	height
H	reference height
i	index of the zones for a multi-zone program; input parameter for *C*
ic	index of the flow paths linking zone i and zone c
ij	index of the flow paths linking zone i and zone j
j	index of the zones for a multi-zone program
L	Effective Leakage area
m	mass of the air

Nomenclature (Continued)

NMSE Normalized Mean Square Error.

MERV Minimum Efficiency Reporting Value.

n flow exponent.

P Absolute pressure

Q Volumetric flow rate

Q_r Predicted airflow rate

R Gas constant of air

Re the Reynolds number

S source term

T temperature

V given volume

W width; velocity in Z direction

a exponent for wind velocity profile

Outline of Thesis

Chapter I - The introductory chapter presents the context of the indoor air quality work and the development of the simulations software as a powerful tool of indoor modeling to predict contaminant concentrations. This section provides a summary of the entire thesis. It is followed by a discussion on the basis of the thesis research. This section summaries the importance of modeling in indoor air quality and how it started being used as a useful and inexpensive tool.

Chapter II - Literature review contains a review of the literature related to the managing of indoor air problems through computer simulations and how the amount of certain pollutants can affect the quality of people in indoor areas.

Chapter III - Basic definitions needed in all the development of the research, such as: the major assumptions of multi-zone software, the impact of the wind, temperature, and other relevant aspects that have an important impact in the airflows of air inside the buildings.

Chapter IV - The mathematical model of the simulation, explaining the basis for contaminant dispersal analysis through the conservation of mass for all species in a control volume, as well as the airflow analysis that have been developed to compute the building airflows which are necessary for contaminant analysis.

Chapter V – Research site and methods gives the details of the site and the data source used in the development of the research such as: physical plant, cooling and heating system, contaminant data, meteorological data and sampling features, as well as the input for the modeling and the scenarios used for the simulation.

(Continued)

Chapter VI – Results for the airflow test and the simulations completed for House 1 are presented in this chapter, as well as the validation of the models based on the ASTM guide D5157, Standard Guide for Statistical Evaluation of Indoor Air Quality Models. (ASTM, 1991).

Chapter VII - Discussion covers the airflow test characteristics of the House, the air zone changes rates and the inter-zonal airflow, and how they can affect the dispersion of contaminants. Also it covered the tunings made for the calibration of the model to ensure the accuracy of the information obtained through the simulations. And finally it mentioned some limitations in the use of the software to avoid in future studies.

Chapter VIII – Conclusion chapter presents the summary of the work of the calibration of the model using the CONTAM software and the interactions of the elements needed for the development of it.

Abstract

DEVELOPMENT AND CALIBRATION OF A MULTI-ZONE MODEL TO PREDICT THE DISTRIBUTION OF CONTAMINANT IN A RESIDENTIAL BUILDING USING CONTAM SOFTWARE

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The use of computer simulations is a powerful alternative in the Indoor Air Quality (IAQ) study due to the efficient performance and the amount of it is able to obtain. Multi-zone modeling is one of the most popular computing methods for IAQ study, thus can provide the knowledge of indoor airflow, temperature and contaminant concentration distributions.

The study was conducted in TX Air House 1 using CONTAM software developed by U.S. National Institute of Standards and Technology (NIST) which is one of the most widely used airflow and indoor modeling program. The model was developed and calibrated to predict the contaminant distribution in residential buildings.

In order to validate the results used in this work, statistical tools such as correlation coefficient, normalized mean square error and others were used to evaluate the accuracy of Indoor Air Quality (IAQ) prediction.

Flow parameters and HVAC characteristics are the basis for the analysis and understanding of building airflow and tracer gas behavior. Dropping the number of individual flow parameters and tuning in on the HVAC characteristics during calibration,

allowed to reduce the error and elevated the accuracy of the model, since the zones have similar airflow dynamics and tracer gas behavior.

Wind speed and wind direction could have significant influences in the distribution of the contaminant. The slight variations over time, the small amount of cross contamination between zones, and the physical conditions such as the tightness of the building, were observed to not allow these factors to have a real influence on the distribution of the contaminant.

1. Chapter One: INTRODUCTION

Indoor air quality has received more attention lately due to its importance in the public health scope; although this is a critical component emerging in significance, a large amount of information is lacking in this field.

Since the price of oil increased, the world changed its perspective on energy and started to save it by making the buildings more sealed thus, tending to minimize the supply of outdoor fresh air and resulting in the accumulation of indoor air contaminants. As a result, the indoor environmental quality became more problematic increasing reports of health problems related to poor indoor environments (Gretchen & Jagdish, 2012).

People on average spend vast majority of their time in indoor environments where they are continually exposed to indoor air pollutants. In fact, the US Environmental Protection Agency (USEPA) estimates that the average person receives 72 percent of their chemical exposure at home, which means that the places what are considered safest, paradoxically, expose them to the largest amount of potentially hazardous pollutants.

Investigators have reported a high prevalence of symptoms that are associated with poor Indoor Environmental Quality (IEQ). These concerns are often referred to as “Sick Building Syndrome” (SBS). Some symptoms are headache, fatigue, dizziness, and symptoms of irritation in eyes, nose, throat, and lower airways among the simple symptoms; however epidemiological studies have demonstrated that some cases of adverse health effects such as childhood leukemia, neurological disorders, non-Hodgkin’s

Lymphoma, and respiratory symptoms were strongly associated with indoor contaminants (Hyun-Min & Park, 2008).

Over the past years there have been changes in building materials, mechanical and electrical appliances and products used indoors. These materials and products emit different chemicals including solvents, unreacted monomers, and additives. Taken together, these changes have altered the kind and concentrations of chemicals that occupants are exposed to in their homes, workplaces and schools. Levels of other indoor pollutants have increased and remain high (e.g., phthalate esters, brominated flame-retardants, nonionic surfactants and their degradation products). Many of the chemicals presently found in indoor environments were not present 50 years ago. (Weschler, 2008)

Due to the increasing of the exposition to the chemicals inside residential buildings, the development of the indoor air modeling has been growing lately, because of the powerful role that simulations has in the Indoor Air Quality (IAQ) study, since it has an efficient, and flexible performance that allow to obtain extensive information for IAQ analysis.

Predicted contaminant concentrations can be used to determine the indoor air quality performance of a building before it is constructed and occupied. They can also be used to estimate personal exposure based on occupancy patterns in the building being studied. Consequently, the accurate and prompt identification of contaminant sources allow to remove the sources, isolate and clean the contaminated spaces reducing the long-term impact that it could have on people.

The prediction of contaminant concentrations can be used to determine the indoor air quality performance of a building, to explore the impacts of various design related to ventilation system design and building material selection. However in the modeling field it is important to know how accurate is the information obtained through a model, therefore, the calibration of the multi-zone model provides higher confidence in analyzing IAQ issues during diverse operation, or in formulating response plans and evaluating the effectiveness of possible mitigation actions when the building is subject to either accidental or intentional air-borne contaminant releases. In such cases, the programs have to be calibrated, i.e., the numerous model parameters need to be tuned so that simulated output closely matches observed system performance under some baseline conditions.

2. Chapter Two: LITERATURE REVIEW

2.1 History Indoor Air Quality

The main purpose of a building is to create comfortable environments capable to protect the human being from distinct elements coming from outside; these constructions need to be adequate for people who spend the majority of their time in indoor spaces, since now people are estimated to work and live up to 90% of their time inside; paradoxically buildings don't always protect them, too many spaces are more polluted than outdoor air; since sometimes the presence of molds, fungi, dust and toxic gases are trapped or growing on the inside exceeding the outdoor concentrations. (Burrough & Hansen, 2008).

By protecting ourselves from the outside, the man has confined himself inside an area with high concentrations of distinct substances creating an interior environment with a new atmosphere that could affect the health of the people which is exposed to contaminants for long-time.

Sundell (2004) presented a review of the history of indoor air quality and how this concept began up to the present also explained some determinant factors affecting indoor air quality.

Salthammer (2010) complemented Sundel's work by presenting a brief history and some indoor references values for different substances as well as strategies for the verification of guidelines.

Bernardino Ramazzini (1633-1714) started with the study of occupational diseases; as a result he was regarded as the father of occupational medicine, later his work was followed by Percivall Pott (1775) who published a work on chimney sweeps (Sundell, 2004). The Industrial Revolution brought a deterioration of human health within closed environments, mainly affecting factory workers quality of life; being exposed to the mechanical, chemical and, industrial processes of the 18th and 19th centuries.

The findings of associations between health effects and working in heavily polluted areas, started to be known in the age of the industrial revolution. At that time work dealing with questions of ventilation and the consequences of the lack of ventilations t, (Thomas Tredgold 1824).

(Heyman, 1881), also studied homes and concluded that natural ventilation cannot be relied on if we want to live on "clean" air. Pettenkofer and other researchers of this era often stated that source control is a prerequisite for good hygiene, and published about air exchange in dwelling houses. (G, 2010)

At the turn of the 20th century, Ellen Richards presented the potential health risks of poor IAQ, and the negative mental and economic consequences. She also emphasized the potential hazards and benefits of indoor air, since houses were the cause of many people's illnesses. Dust and inadequate ventilation, she claimed, contributed to pneumonia, tuberculosis and other illnesses (Kwallek, 2012).

After 20 years, the American Society of heating and ventilating Engineers (ASHVE) recommended ventilation standards, in 1915 and around the 1930s there was e a little scientific effort within the field of ventilation, IAQ, and health in non-industrial premises. (Sundell, 2004)

Yaglou (1936) studied the influence of bio-effluents on perceived air quality, and his work derived guidelines for ventilation which complemented the previous studies and the urgent need to establish a standard on ventilation.

In the late 1960s problems related to radon and formaldehyde became known, and converted prevalent in the early 1970s. House dust mites and SBS in the late 1970s and in the last decade, allergies and health issue related to indoor air again enter the scientific agenda. (Sundell, 2004)

Wittman (1962) described the emission of formaldehyde occurring from particle board; it required 15 years before an indoor environmental, guideline value for formaldehyde of 0.1 ppm was established.

In 1967 the Standard No. 62 “ventilation for acceptable Indoor Air Quality” was issued which took the work of Yaglou and Fanger into consideration (Salthammer, 2010).

In 1970 due to the high oil prices and the energy crisis, there was a need to build energy efficient construction, thus improving energy conservation, but there was a reduction in the exchange between outdoor fresh air and indoor air. This decrease of fresh air intake resulted in higher levels of chemical emissions by synthetic materials and chemical products that are broadly used in these airtight buildings.

Consequently, the decrease of ventilation rates and the increase of the presence of synthetic sources have allowed a rise in the concentrations of volatile organic compounds (VOCs) and semivolatile organic compounds (SVOCs). These high concentrations have been related to the sick syndrome in the occupants during the last three decades (Junfeng & Kirk).

Fangers (1992) emphasized the impact that load of pollution sources such as building materials, carpets and computers, the impact of ventilation and indoor air humidity have on people.

Studies on exposure in indoor environments and health effects have been conducted, and have shown there is strong evidence of the relation between IAQ and lung cancer, allergies, other hypersensitivities such as sick building syndrome (SBS), and multiple chemical sensitivity and respiratory infections. This new topic is very important in order to develop mechanisms to detect or prevent the detriment of indoor air (Sundell, 2004).

2.2 Indoor Air Quality

Indoor air quality is the physical effect of exposures of people inside of the building they are occupying and is frequently expressed in accordance to the ventilation rate (in L/s per person and L/s per m^2 floor area) or in concentrations for specific compounds. These concentrations are influenced by the sources present in indoor environments, outdoor sources and sources present in HVAC systems or surrounding spaces (Bluyssen, 2009).

Indoor air is thought to be the same as indoor climate, and therefore related to thermal comfort aspects such as too warm or too cold, however by the time the thermal condition has changed its importance inside the structures, since the environment inside is always more polluted from indoor sources than from outdoor air and have developed certain conditions affecting people inside. This was and is the basis of the need for ventilation and for concerns on indoor air quality (Sundell, 2004).

Frequently ventilation systems are set to minimize the amount of fresh air entering and circulating within the building. Heating, ventilating and air conditioning (HVAC) systems play a critical role in maintaining a clean indoor environment. However, inadequate design and operation of the HVAC system(s) can have negative effects on the indoor air quality, as well as the occupant’s health.

(Clause and Beko, 2010) presented some considerations about indoor air quality and what are the biggest challenges after 20 years of research in the area, also they showed some opportunities to improve structurally one of the youngest disciplines.

2.3 Indoor Contaminants and Sources

The main causes of Indoor Air Quality problems are airborne contaminants that can be generated inside or penetrate interior environments with passive or active airflows increasing the exposition to them and the concentrations indoors. Indoor air quality is determined by a range of conditions and the interactions of “sources” and “sink” and air movement among rooms and between the building and outside.

Unfortunately, people cannot identify IAQ as easily as thermal comfort, making indispensable develop methods of controlling IAQ to guarantee an adequate indoor air quality. However every indoor environment is case dependent in that each building cannot be generalized to each other, making each scenario unique.

We know today that indoor concentrations of some pollutants are influenced by outdoor concentrations. However for many other pollutants, such as formaldehyde and phthalates, indoor levels mainly are the result of indoor sources.

(Bluyssen, 2009) described the indoor air quality factors and its complexity associated with the characteristics of the contaminants as well as the type of source and how they can interact this makes it to understand the different processes of diffusion, sorption, evaporation and deposition of the pollutants over time.

Sources of pollutants may be building materials, furnishings or the HVAC system, consumer products, office or equipment; however a source can also emit compounds that are produced by contact with other compounds, consequently the mix of pollutants in indoor environments can be transformed due to chemical reactions, modifying the chemical composition of indoor air and hence occupants chemical exposures.

In indoor environments any source emits pollutants that come into the indoor air of a place that may lead to decreased levels of acceptable indoor air quality; those pollutants can react with each other or with pollutants from other sources, creating new pollutants.

The mode of emission of contaminant inside indoor environments is complex, because the mechanisms such as: diffusion, sorption, and evaporation are not well understood; besides there are sources in the indoor environment that release compounds which are absorbed onto indoor surfaces, those compounds can desorbed, react with compounds on the new source, and re-emit (secondary emission). There is another issue in the emission over time. Depending on the compound emitted, a different pattern of emission over time can occur, however a better understanding could result in predictions and explanation on the emission behavior to be predictable (Bluyssen, 2009).

The geometry and structure of a building, as well as the heating, ventilating, and air conditioning system have a huge influence on the building indoor conditions. Partitions, furniture and passageways between indoor spaces can also distort the airflow and the contaminant distributions (Liu & Zhai, 2007).

According to the complexity of the behavior of the contaminants inside indoor environments it is necessary to contemplate different IAQ means to control them. Although increasing ventilation seems the most recommended, there are several studies that have shown that increased air changes per hour have little or no correlation to some pollutants; this is the case with some voltaic organic compounds and radon (Burrough & Hansen, 2008).

2.4 Managing Indoor Air Quality

Sick Building Syndrome is used to describe acute symptoms which can affect the health of the occupants of a building and are associated to the fact that people spend time in a particular construction. The symptoms usually are resolved once the person leaves the structure or the source is controlled (Fotoula, 2011).

The most common symptoms known as Sick Building Syndrome (SBS) are: discomfort, headaches, nausea, dizziness, sore throats, dry or itchy skin, sinus congestion, nose irritation, excessive fatigue, incidence of asthma attacks and nasal allergy symptoms. Sometimes, more vague symptoms are presented such as difficulty in concentration, sensitivity to odors and personality changes. In this case the construction has developed a condition that can make the occupants uncomfortable, irritated or even ill.

The most common theories about the cause of sick building syndrome are related to factors such as: building materials, since some materials allow micro-organisms to grow on or in them, or the building materials may have chemicals or other substances in them or off - gassed; poor sanitation; ozone, organic solvents and formaldehyde in the atmosphere; office equipment, furnishings and other materials and products located or used in the building which can produce fumes; air borne chemical fumes or gasses from anything in the building; building air conditioning; inadequate ventilation; pollutants from inside or outside the building that were circulated by the air conditioning system and other environmental factors (Janis, 2006)

There are only three techniques for the control of all indoor air pollutants: dilution in which the ventilation brings in outdoor air has a strong benefit of diluting indoor contaminants rather than a negative effect of bringing in outdoor pollutants, since the concentration is related to the air change rate and the source strength; the next technique is extraction which are basically filtration and air cleaning of airborne contaminant, although some air cleaners are highly effective at particle removal; the air cleaners are generally not designed to remove gaseous pollutants (Liu & John, 2008); and finally the last technique is source control which basically is the elimination or removal or substitution at the source, this is the most effective way to improve indoor air quality because it eliminates individual sources of pollution or reduces their emissions in many cases. Source control usually requires some type of investigative procedure to determine precise source components.

Accurate prediction of source location can help determine and implement proper indoor environmental control measures, such as, shutting down the room with the source, supplying fresh air to the room, or exhausting dirty air out of the room.

2.5 Modeling Indoor Air Pollutant

With the advances in computer technology, computer simulations have become a dominant alternative in the IAQ study due to the efficient performance and large information that is able to obtain that is used for IAQ improvement.

Rapid advancements have been made in the field of environmental engineering that have allowed the development of new modeling techniques. Software developments over the past two decades have led to simulation techniques being applied to integrated building and HVAC systems. Axley James (2007) reviewed the historical development of the multi-zone airflow modeling theory explaining the approach upon which Multi-zone building airflow analysis may be based and how the analysis can be proven to be reasonably reliable, accurate and computational effective.

Simulations are used to prevent under or over-utilization of resources and to optimize system performance as well as reduce the probabilities of failure in the development of systems being suitable for prediction and optimization research. It's involving a large numbers of variables, and the models of simulations can be reconfigured and experimented that usually in an investigational approach is impossible as they are too expensive or impractical to do in the system.

Kadiyala and Kumar (2012) validated indoor air quality modeling using acceptable criteria for statistical proof in public transit buses. The research showed the importance of corroborating modeling techniques to ensure the accuracy in the results, since one of the serious limitations in the current literature is that very few studies have used measures to guarantee the reliability of the newly developed indoor air quality models.

Methods to model transport phenomena in physical systems are divided in two main categories, macroscopic or microscopic. The macroscopic systems, are based on idealizing systems with finite sized control volumes in which , momentum, or energy transport are described in terms of ordinary differential conservation equations (Axely, 2007)

Microscopic methods are based on continuum description of mass, momentum, and energy transport defined in terms of partial differential conservation equations that are frequently applied to portions of a physical system. Two computer simulations models are highly used in the study of building indoor environmental quality, which are multi-zone and Computational Fluid Dynamics (CFD) (Axely, 2007).

Indoor concentrations of airborne contaminants can be estimated by basic principles, where they are functions of penetration efficiency, air exchange rate (AER, also termed air change rate), decay rate, indoor source strength, and unit volume (Long et al., 2001; Pepper and Carrington, 2009). However for effective control and improvement measures, it is important to have an accurate and prompt identification of contaminant spaces. Liu and Zhai (2007) reviewed inverse modeling methods for indoor airborne pollutant tracking Liu and Zhai (2007) discussed the use of inverse modeling to identify potential indoor pollutant sources with limited pollutant sensor data. The study reviews various inverse modeling methods for advection– dispersion problems.

Liu and Zhai (2007) verified the feasibility and accuracy of the adjoint probability method for indoor pollutant tracking introducing the principles of the probability-based inverse modeling method and the corresponding equations as well as the CFD based inverse modeling algorithm. The method and algorithm were demonstrated and verified by two examples cases.

Another study made by Liu and Zhai (2008) describes the principles of the probability – based adjoin inverse modeling method and formulates a multi-zone model based inverse prediction algorithm in attempt to track indoor contaminant source location for buildings with many compartments.

2.5.1 Computational Fluid Dynamics (CFD)

Computational fluid dynamics models provide the spatial distribution and temporal evolution of air pressure, velocity, temperature, humidity, contaminants, and turbulence intensity by numerically solving the conservation equation mass, momentum energy, and species concentrations; however one of the major problems associated with CFD is that simulations are not fast enough to meet building design and control purposes (Xiang & Zhiqiang, 2007).

CFD model is only applied for indoor spaces where contaminant concentration is significantly non-uniform and for the rest of the spaces in building multi-zone software are applied. CFD model can predict fate and transport characteristics of indoor pollutants that allow the designers to create appropriate indoor layouts, effective sensor locations, and safe rescue path emergencies.

For many realistic problems, contaminant source conditions are unknown and need to be first identified through limited sensor outputs and then the forward CFD simulation can be conducted to reveal the contaminant release history and predict its development trend with and without proper control measures.

2.5.2 Multi-zone

Multi-zone models incorporate mass, energy and contaminant interactions among exterior, heating, ventilation and air conditioning (HVAC) systems, and pertinent zones inside the studied building. This type of simulation can calculate air exchange and contaminant migration within a room of a building and between a building and outdoors.

Multi-zone models treat rooms of a building as zones with uniform properties connected by flow elements, or links. The links represent airflow paths such as doors, windows, wall cracks, fans, and ducts and thus can provide a quick prediction of airflow and contaminant distribution in the whole building; as a result multi-zone model-based inverse modeling can locate the spaces with potential contaminant sources as well as determining the relevant source characteristics. Consequently for buildings with large rooms, identifying which room contains contaminant sources may be sufficient for contaminant control.

Among various multi-zone models, CONTAM developed by the U.S. National Institute of Standards and Technology (NIST), is one of the most extensively used and validated multi-zone programs (Liu & John, 2008).

CONTAM is a popular tool to determine building air infiltration, exfiltration, and room to room airflows driven by wind pressures on building exteriors, buoyancy effects related to the indoor and outdoor air temperature difference, and mechanical ventilation. It also predicts the dispersal of airborne contaminants and can be used to calculate personal exposure to contaminants.

(Townsend, 2009) Calibrated a computer model for residential ventilation systems and used the calibrated model to extend the results obtained in previous field testing. The main purpose of this study was evaluating ventilation systems that were not present in the houses tested by Hendron and to provide the capability to extend the results of field testing in one location under one set of environmental conditions to many locations under many sets of environmental conditions.

(Wang & Dols, 2010) introduced the algorithm for two methods of connecting CONTAM and CFD0, the external link for performing external airflow analysis, and the internal link for implanting a CFD zone in a CONTAM airflow and contaminant transport network. In this work they showed the embedded CFD zone is very useful for analysis of short-time contaminant transport, especially for evaluation of occupant exposure.

(Syder, 2010) proposed a methodology to calibrate multi-zone airflow model in a building. In this study it was found that the macro zones in the CONTAM software provided a robust manner of calibrating a complex model, since the zones reduce the number of individual flow parameters that need to be tuned during calibration.

(Firrantello, 2007) presented a calibration methodology based on measured heating, ventilation, and air-conditioning (HVAC) airflow rates and inter-zonal airflow direction; this has been partially validated using collected field data.

2.6 Types of Modeling

The modeling process can be divided into three different types, according to the characteristics of the problem.

1. **Type 1**, the direct problem or “forward problem”: given input and system parameters, find out of the model.

2. **Type 2,** the reconstruction problem or “inverse problem”: given system parameters and output, find out which input has led to this output.

3. **Type 3,** the identification problem or “inverse problem”: given input and output, determine the system parameters that agree with the relationship between input and output.

The model’s multi-zone and CFD models can predict airflow and contaminant distributions based on given inputs (boundary conditions) and system parameters (building and system characteristics), which is a direct or forward problem.

2.7 Validation of Indoor Air Quality Model

One of the important prerequisites for an indoor air quality (IAQ) model to be acceptable for use predicting the associative components is to perform statistical validation of the model. Statistical validation of the IAQ model performance can be done in three ways: operational model evaluation, dynamic model evaluation, and probability model evaluation.

(Kadiyala & Kumar, 2012) focused on the operational model evaluation, examining the performance of nine ANN-based $PM_{10.0}$ IAQ models by application of the ranked statistical performance measures using four different software programs.

Besides, (Kumar, 2012) provided a comprehensive review of all existing statistical performance measures, summarized the mathematical equations on computing the various statistical performance measures.

(Emmerich, 2006) Presented a review of empirical validation studies of the application of multi-zone indoor air quality (IAQ) models to residential scale buildings. This review focuses on empirical verification efforts, although Herrlin listed three techniques of model validation:

1. Analytical verification—comparison to simple, analytically solved cases
2. Inter-model comparison—comparison of one model to another
3. Empirical validation—comparison to experimental tests

There are some difficulties in validating multi-zone airflow models. These include input uncertainty (particularly of air leakage distribution) and attempting to simulate processes that cannot be modeled (e.g., using a steady-state airflow model to simulate the dynamic airflow process).

(Herrlin, 1992), showed but the number of cases a complex multi-zone model can simulate are unlimited, an absolute validation is impossible. However, validation efforts are still important to identify and eliminate large errors and to establish the range of applicability of the model. Therefore, a model's performance should be evaluated under a variety of situations. Herrlin, 1992 also emphasizes that it is important to recognize that a model's predictions will always have a degree of uncertainty.

2.7.1 Analytical Verification

Analytical verifications are routinely performed to check a numerical solution. For example, CONTAM has been checked for a number of analytical cases including airflow elements in series and parallel, power law airflow elements, quadratic flow elements, stack effect, wind pressure, doorway elements, duct elements, fan elements, contaminant dispersal, a contaminant filter, and a simple kinetic reaction. Therefore, analytical verification is of limited value in determining the adequacy of a multi-zone IAQ model for practical applications.

2.7.2 Inter-Model Comparison

Inter-model comparison provides a relative check of the assumptions and numerical solutions of different models. As with analytical verification, inter-model comparisons are of limited value in evaluating a model's adequacy for practical applications. However, good inter-model comparisons also enable generalization of empirical validation conclusions beyond the specific model studied.

Once again, power law flow elements and airflow elements were used to connect the four interior zones with each other and the ambient zone. A single wind speed and ambient temperature condition were applied. It should be noted that both inter-model comparisons discussed test the models for only a very limited range of conditions.

2.7.3 Empirical Validations

Empirical validation tries to compare model assumptions and numerical solutions with a more absolute standard. However, the standard is only as accurate as the measurements used to produce also the standard agreement between measurements and predictions could result from compensating errors in the model.

ASTM guide D5157, Standard Guide for Statistical Evaluation of Indoor Air Quality Models (ASTM 1991), provides information on establishing evaluation objectives, choosing datasets for evaluation, statistical tools for assessing model performance, and considerations in applying the statistical tools.

ASTM D5157 provides three statistical tools for evaluating the accuracy of IAQ predictions and two additional statistical tools for assessing bias. Values for these statistical criteria are provided to indicate whether the model performance is adequate. The measures for assessing agreement between predictions include the following:

1. The correlation coefficient of predictions vs. measurements should be 0.9 or greater.
2. The line of regression between the predictions and measurements should have a slope between 0.75 and 1.25 and an intercept less than 25% of the average measured concentration.
3. The normalized mean square error (NMSE) should be less than 0.25. NMSE is calculated as.

$$\boldsymbol{NMSE} = \sum_{\boldsymbol{I=1}}^{\boldsymbol{N}} (\boldsymbol{C_{pi}} - \boldsymbol{C_{oi}})^{\boldsymbol{2}} / \boldsymbol{n C_o C_p} \quad \text{Equation (1)}$$

Where

Cp***:*** predicted concentration
Co***:*** observed concentration.

And, the measures for assessing bias include:

4. Normalized or fractional bias (FB) of the mean concentrations. Fractional bias should be 0.25 or lower and is calculated as

$$\boldsymbol{FB} = \boldsymbol{2}(\boldsymbol{c_P} - \boldsymbol{C_o})/(\boldsymbol{c_P} + \boldsymbol{C_o}) \quad \text{Equation (2)}$$

5. Fractional bias based on the variance (FS), which should be 0.5 or lower. FS is calculated as

$$\boldsymbol{FS} = \frac{2(\sigma^2 c_P - \sigma^2 C_o)}{\sigma^2 c_P + \sigma^2 C_o} \quad \text{Equation (3)}$$

3. Chapter Three: BACKGROUND

3.1 Major Assumptions of Multi-zone Models

Multi-zone models implement mathematical relationships to model airflow and contaminant related phenomenon and therefore incorporate assumptions that simplify the model from that of the modeled phenomenon (Walton, 2013).

1. **Well-mixed zones**: this assumption refers to the treatment of each zone as a single node, wherein the air has uniform (well-mixed) conditions throughout. These conditions include temperature, pressure and contaminant concentrations.
2. **One-Dimensional Convection/Diffusion Zones**: all zones were considered to be well-mixed, i.e., having a uniform concentration. However, zones can be preconfigured by the user to be one-dimensional convection/diffusion zones in which contaminants can be allowed to vary along a user-defined axis.
3. **Duct Systems**: typically, during contaminant simulation, there are similarities between duct junctions and well-mixed zones and between duct segments and airflow paths. In this case the volumes of the duct junctions are determined from the duct segments to which they are connected.
4. **Conservation of mass**: when performing a steady-state simulation, the mass of air within each zone is conserved by the model. This implies that air can neither be created nor destroyed within a zone. However, when performing a transient simulation, CONTAM now provides the option of allowing the accumulation or reduction of mass within a zone due to the variation of zone density/pressure and the implementation of non-trace contaminants within a simulation.
5. **Trace contaminants**: trace contaminants are those that are found in low enough levels that they do not affect the density of air within a zone.

6. **Change in the density of air:** The program will allow for contaminants to reach levels that would, in actuality, affect the density, but the program will still treat them as if they were trace contaminants.
7. **Airflow paths:** airflow elements provided by CONTAM is modeled using either a powerlaw or quadratic relationship between airflow and pressure differences across the flow path.
8. **Source/sink models:** CONTAM provides several different source/sink elements or representations of contaminant generation/removal processes.

3.2 Ventilation and Infiltration

Ventilation is intentional introduction of air from outside into the building and it can be natural or mechanical ventilation. Between natural ventilation elements are: open windows, doors, grilles, and any other intentional building envelope penetration and it is driven by differential pressure.

On the other hand Infiltration is the flow of outdoor air into a building through cracks and other unintentional openings and through the normal use of exterior doors for entrance and exit. Infiltration is also known as air leakage into a building.

Ventilation and infiltration differ significantly in how they affect energy consumption, air quality, and thermal comfort, and they can vary with weather conditions, building operation, and use.

3.3 Driving Mechanisms for Ventilation and Infiltration

Natural ventilation and infiltration are driven by pressure differences across the building envelope caused by wind and air density differences due to temperature differences between indoor and outdoor air.

Mechanical air-moving systems also induce pressure differences across the envelope through operation of appliances, such as combustion devices, leaky forced-air thermal distribution systems, and mechanical ventilation systems. The indoor and outdoor pressure difference at a location depends on the magnitude of these driving mechanisms as well as the opening in the building envelope (ASHRAE, 2009).

3.4 Stack Pressure

Stack Pressure is the hydrostatic pressure caused by the mass of a column of air located inside or outside a building. It can also occur within a flow element, such a duct or chimney that has vertical separation between its inlet and outlet. The hydrostatic pressure in the air depends on density and the height of interest above a reference point.

Sherman (1991) showed that any single-zone building can be treated as an equivalent box from the point of view of stack effect, if its leaks follow the power law. The building is then characterized by an effective stack height and neutral pressure level (NPL) or leakage distribution.

Stack pressure differences are positive when the building is pressurized relative to outdoors, which causes flow out of the building. Therefore, in the absence of other driving forces and assuming no stack effect within the flow element themselves, when indoor air is warmer than outdoors, the base of the building is depressurized and the top is pressurized relative to outdoors; when indoor air is cooler than outdoor, the reverse is true.

3.5 Description of Wind in Buildings

Wind pressure is the most important driving force for airflow through the building envelope since wind creates a distribution of static pressure on the building's exterior surface that depends the wind direction, wind speed, air density, surface orientation and surrounding conditions. Wind pressure is generally positive on the air windward side of the building, and negative on the leeward sides (ASHRAE, 2009).

Air movement around buildings is three-dimensional turbulent flow. A more accurate approach than surface-averaged pressure coefficient is to account for variations in wind pressure coefficients by location over a building surface. Swami and Chandra (1988) presented a correlation of wind pressure coefficients for high-rise buildings, where the value of C_p *(wind pressure coefficient)* was determined for a specific point on the building facade instead of being averaged over the entire facade. Since it may only apply to high-rise buildings and cannot represent average ones, the correlation has not been incorporated into CONTAM.

C_p *(wind pressure coefficient))*, is a function of location on the building envelope and wind direction. Most pressure coefficient data are for winds normal to building surfaces. Unfortunately, for a real building, this fixed wind direction rarely occurs, and when the wind is not normal to the upwind wall, these pressure coefficients do not apply.

Walker and Wilson (1994) developed a harmonic trigonometric function to interpolate between the surface average pressure coefficients on a wall that were measured with the wind normal to each of the four building surfaces. This function was developed for low-rise building that are three stories or less in height.

The measured data used to develop the harmonic function from Akins et al. (1979) and Wiren (1985) show that typical values for the pressure coefficients are $C_p(1)= 0.6$, $C_p(2)= -0.3$, $C_p(3) = C_p(4)= -0.65$. Because of geometry effects on flow around a building application of this interpolation functions is limited to low-rise buildings of rectangular plan form with the longest wall less than three times the length of the shortest wall.

3.6 Buoyancy-Driven Airflows with Temperature Gradients

Besides the effects of wind pressure, buoyancy-driven airflows are also common in natural ventilation. In simulations of buoyancy-driven flows, zone temperature is a crucial factor. Since the current version of CONTAM does not include the calculation of energy conservation, a uniform temperature must be manually specified for each zone.
An improper setting of the zone temperature may result in inaccurate or even wrong results. The temperature can also stratify along the height of a zone and the assumption of a uniform temperature is invalid.

3.7 Trace Gas Measurements

Several tracer gas measurement procedures exist (including the ASTM Standard E741 test method) involve an inert or nonreactive gas used to label the indoor air. The tracer is released into a building and the concentration of the tracer gas is monitored and related to the building's air exchange rate. All tracer measurement techniques are based on a mass balance of the tracer gas in the building. Assuming the outdoor concentration is zero and the indoor concentration is well mixed (ASHRAE, 2009).

4. Chapter Four: MATHEMATICAL MODEL

The central concern of indoor air quality analysis is the prediction of airborne contaminant dispersal in buildings. Airborne contaminants disperse throughout buildings in a complex manner that depends on the nature of air movements in-to, out-of, and within the building system; the influence of the heating, ventilating, and air-conditioning (HVAC) systems; the possibility of removal, by filtration, or contribution, by generation, of contaminants; and the possibility of chemical reaction, radio-chemical decay, settling, or sorption of contaminants.

The basis for contaminant dispersal analysis is the application of conservation of mass for all species in a control volume (c.v.). A control volume is a volume of air which may correspond to a single room, a portion of a room, or several well-coupled rooms (a CONTAM zone) or the ductwork (where a junction, under the well-mixed assumption, has half the volume of each of the adjacent duct segments).

4.1 Properties of Air

In CONTAM air is treated as an ideal gas with properties computed from the ideal gas law. The density of air is given by

$$\boldsymbol{\rho = m/V} \quad \text{Equation (4)}$$

$$\boldsymbol{\rho = \frac{P}{RT}} \quad \text{Equation (5)}$$

Where,

m: $the\ mass\ of\ the\ air$
v: $a\ given\ volume$
P: $the\ absolute\ pressure$
R: $the\ gas\ constant\ for\ air$
T: $the\ absolute\ temperature$

The mass of air in control volume *i* is the sum of the masses of the individual contaminants in the (c.v).

$$\boldsymbol{m_i} = \sum_\alpha \boldsymbol{m_i^\alpha} \quad \text{Equation (6)}$$

The concentration of contaminant α in c.v. *i* is defined as

$$\boldsymbol{C_i^\alpha} = \boldsymbol{m_i^\alpha}/\boldsymbol{m_i} \quad \text{Equation (7)}$$

4.2 Contaminant Concentrations

Within CONTAM a contaminant may be added to c.v. *i* by:

a) Inward airflows through one or more paths at the rate $\sum_j F_{j=i}(1 - n_j^\alpha)C_j^\alpha$ where F_{j-i} is the rate of air mass flow from c.v. *j* to c.v. *i* and n_j^α is the filter efficiency in the path.
b) species generation at the rate G_i^α

A species may be removed from the c.v. by:

a) outward airflows from the zone at a rate of $\sum j\, F_{i-j}C_i^\alpha$ where F_{i-j} is the rate of air mass flow from c.v. *i* to c.v. *j*, and
b) Species removal at the rate R_α, iC_α, i where $R_{\alpha,i}$ is a removal coefficient.

Combining these processes into a single equation for the rate of mass gain of species α in c.v. i gives:

$$\frac{dm_i^\alpha}{dt} = \sum j\, \boldsymbol{F_{j-i}}\left(\boldsymbol{1} - \boldsymbol{n_j^\alpha}\right)\boldsymbol{C_j^\alpha} + \boldsymbol{G_j^\alpha} + \boldsymbol{m_i} \sum_\beta \boldsymbol{K^{\alpha\beta}} \boldsymbol{C_i^\beta} - \sum_j \boldsymbol{F_{i-j}} \boldsymbol{C_i^\alpha} - \boldsymbol{R_i^\alpha}\, \boldsymbol{C_i^\alpha} \quad \text{Equation (8)}$$

The transient conservation of species mass in a control volume is given by:

mass of contaminant α in c.v. i at time $t + \Delta t$ = mass of contaminant α in c.v. i at time $t + \Delta t \times$(rate gain of contaminant α - rate loss of contaminant α).

Or in equation from as:

$$\boldsymbol{\rho_i V_i C_i^\alpha}|_{t+\Delta t} \approx \boldsymbol{\rho_i V_i C_i^\alpha}|_t + \Delta \boldsymbol{t} \left[\sum j\, \boldsymbol{F_{j-i}}\left(\boldsymbol{1} - \boldsymbol{n_j^\alpha}\right)\boldsymbol{C_j^\alpha} + \boldsymbol{G_j^\alpha} + \boldsymbol{m_i} \sum_\beta \boldsymbol{K^{\alpha\beta}} \boldsymbol{C_i^\beta} - \sum_j \boldsymbol{F_{i-j}} \boldsymbol{C_i^\alpha} - \boldsymbol{R_i^\alpha}\, \boldsymbol{C_i^\alpha}\right]_{t+\delta t} \quad \text{Equation (9)}$$

4.3 Numerical Calculation of Contaminant Concentrations

There are different solutions for Equation 6 that can be characterized by the choice of $\boldsymbol{\delta t}$ to determine the rate of gain or loss. CONTAM has traditionally chosen $\boldsymbol{\delta t} = \Delta \boldsymbol{t}$ and Equation 6 becomes:

$$\boldsymbol{\rho_i V_i} + \Delta \boldsymbol{t}\left(\sum_j \boldsymbol{F_{i-j}} - \boldsymbol{R_i^\alpha}\right)\boldsymbol{C_i^\alpha}\Big|_{t+\Delta t} \approx \boldsymbol{\rho_i V_i C_i^\alpha}|_t + \Delta \boldsymbol{t} \left[\sum j\, \boldsymbol{F_{j-i}}\left(\boldsymbol{1} - \boldsymbol{n_j^\alpha}\right)\boldsymbol{C_i^\alpha} + \boldsymbol{G_i^\alpha} + \boldsymbol{m_i} \sum_\beta \boldsymbol{K^{\alpha\beta}} \boldsymbol{C_i^\beta}\right]_{t+\Delta t} \quad \text{Equation (10)}$$

All concentrations C_i^α at time $t + \Delta t$ are functions of various other concentrations also at $t + \Delta t$. This is the *standard implicit method*, and it requires that a full set of Equations must be solved simultaneously.

The number of equations, N, equals the number of species times the number of control volumes. In a traditional Gauss elimination (or LU decomposition) solution the computation time is proportional to N3, making it impractical for large problems.

CONTAM offers three solution methods which take advantage of matrix sparsity to handle cases with large numbers of equations. These are a direct skyline algorithm, an iterative biconjugate gradient (BCG) algorithm, and an iterative successive over relaxation (SOR) algorithm (LU decomposition is provided only for testing and benchmarking). The skyline algorithm is very fast for problems of intermediate size but can be slow for large problems. The SOR algorithm requires much less memory and may be faster for large problems unless there are convergence difficulties. In such cases use the BCG solution, although it may also experience convergence difficulties. It can be useful to test the different methods to determine which will give optimum performance before doing a long transient simulation.

4.4 Airflow Analysis

Over the years many methods have been developed to compute building airflows which are necessary for contaminant analysis.(Feustel and Dieris, 1992) report 50 different computer programs for multizone airflow analysis. Note that "zones" go by many other names in these programs, e.g., nodes, cells, and rooms are common alternatives. The airflow calculations in CONTAM are based on the algorithms developed in AIRNET [Walton 1989a and 1989b]

4.4.1 Basic Equations

The air flow rate from zone j to zone i , $F_{j,i} = f(P_j - P_i)$

The mass of air,$m_i(Kg)$ in zone i is given by the ideal gas law

$$\boldsymbol{m_i} = \boldsymbol{\rho_i V_i} \quad \text{Equation (11)}$$

Where,

V_i: Zone volume (m^3)

ρ_i: Zone pressure (Pa)

T_i: Zone Temperature (K), and

R: 287.055 (J/Kg*K) (gas constant of air)

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

$$\frac{\partial \boldsymbol{m_i}}{\partial \boldsymbol{t}} = \boldsymbol{\rho_i} \frac{\partial \boldsymbol{V_i}}{\partial \boldsymbol{t}} + \boldsymbol{V_i} \frac{\partial \boldsymbol{\rho_i}}{\partial \boldsymbol{t}} = \sum \boldsymbol{F_{j,i}} + \boldsymbol{F_i} \text{ Equation (12)}$$

Where,

m_i: Mass of air in zone i
$F_{i,j}$: Airflow rate (Kg/s) between zone j and zone$i$: positive values indicate flows from j to i and negative values indicate flows from i to j.

4.4.2 Airflow Elements

Infiltration is the result of air flowing through openings, large and small, intentional and accidental, in the building envelope. Simulation programs require a mathematical model of the flow characteristics of the openings. For a general introduction see Chapter 27 of (ASHRAE 2005) and section 2.2 of (Feustel 1990).

Flow within each airflow element is assumed to be governed by Bernoulli's equation:

$$\Delta \boldsymbol{P} = \left(\boldsymbol{P_1} + \frac{\boldsymbol{\rho V_1}^2}{\boldsymbol{2}}\right) - \left(\boldsymbol{P_2} + \frac{\boldsymbol{\rho V_2}^2}{\boldsymbol{2}}\right) + \boldsymbol{\rho g}(\boldsymbol{z_1} - \boldsymbol{z_2}) \text{ Equation (13)}$$

Where,

ΔP: Total pressure drop between points 1 and 2.
P_1, P_2: Entry and exit static pressures.
V_1, V_2: Entry and exit velocities.
ρ: Air density
g: Acceleration of gravity (9.81 m/s^2)
z_1, z_2: Entry and exit elevations.

The following parameters apply to the zones: pressure, temperature (to compute density and viscosity), and elevation. The zone elevation values are used to determine stack effect pressures. When the zone represents a room, the airflow elements may connect with the room at other than its reference elevation.

4.4.3 Powerlaw Flow Elements

Most infiltration models are based on the following empirical (powerlaw) relationship between the flow and the pressure difference across a crack or opening in the building envelope:

$$\boldsymbol{Q} = \boldsymbol{C}(\Delta\boldsymbol{P})^{\boldsymbol{n}} \text{ Equation (14)}$$

The volumetric flow rate, *Q* [m³/s], is a simple function of the pressure drop, *P* [Pa], across the opening. A common variation of the powerlaw equation is:

$$\boldsymbol{F} = \boldsymbol{C}(\Delta\boldsymbol{P})^{\boldsymbol{n}} \text{ Equation (15)}$$

Where the mass flow rate, *F (*kg/s), is a simple function of the pressure drop. A third variation is related to the orifice equation:

$$\boldsymbol{Q} = \boldsymbol{C_d}\boldsymbol{A}\sqrt{\frac{\boldsymbol{2\Delta P}}{\boldsymbol{\rho}}} \text{ Equation (16)}$$

Where,

$C_{d:}$ discharge coefficient, and
A: orifice opening area.

Theoretically, the value of the flow exponent should lie between 0.5 and 1.0. Large openings are characterized by values very close to 0.5, while values near 0.65 have been found for small crack-like openings.

The CONTAM functions for powerlaw elements calculate flows using both the laminar and the turbulent models and select the method giving the smaller magnitude flow.

4.4.4 Leakage Areas

The powerlaw model can be used with the component leakage area formulation which has been used to characterize openings for infiltration calculations [ASHRAE 2001, p. 25.18]. The leakage area is based on a series of pressurization tests where the airflow rate is measured at a series of pressure differences ranging from about 10 Pa to 75 Pa. The effective leakage area is based on a rearrangement of equation

$$\boldsymbol{L} = \frac{\boldsymbol{Q_r}\sqrt{\boldsymbol{\rho}/\Delta\boldsymbol{P_\gamma}}}{\boldsymbol{C_d}} \quad \text{Equation (17)}$$

Where,

L= equivalent or effective leakage area [m^2],
ΔP_r= reference pressure difference [Pa],
Q_r= predicted airflow rate at P_r (from curve fit to pressurization test data) [m^3/s], and
C_d= discharge coefficient.

There are two common sets of reference conditions:

C_d = 1.0 and P_r = 4 Pa
or
C_d = 0.6 and P_r = 10 Pa.

4.4.5 Ducts

The theory of flows in ducts (and pipes) is well established and summarized in Chapter 35 of the *2005 ASHRAE Fundamentals Handbook* [ASHRAE 2005] The Analysis is based on Bernoulli's equation and its assumptions. The dynamic losses due to fittings and so forth are given by

$$\Delta \boldsymbol{P_d} = \boldsymbol{C_d}\frac{\rho V^2}{2} \text{ Equation (18)}$$

Where, *Cd* = dynamic loss coefficient. Total pressure losses are given by

$$\Delta \boldsymbol{P} = \Delta \boldsymbol{P_f} + \sum \Delta \boldsymbol{P_d} \text{ Equation (19)}$$

Since F = VA, where A is the cross section (or flow) area,

$$\boldsymbol{F} = \sqrt{\frac{2\rho A^2 \Delta P}{\frac{fL}{D} + \sum C_D}} \text{ Equation (20)}$$

CONTAM calculates the friction factor using the nonlinear Colebrook equation.

4.4.6 Constant Flow Fans

One particularly simple but useful airflow element sets a constant flow between two nodes. Since the flow is constant, the partial derivatives of flow with respect to the node pressures must be zero. The constant flow element does not contribute to the Jacobian, (A), but it does add to the right side vector, (B).

CONTAM provides two constant flow elements: one for constant mass flow and one for constant volumetric flow.

5. Chapter Five: RESEARCH SITE AND METHODS

5.1 Research Site

The study area corresponds to the research-houses built at the University of Texas at Tyler by the department of TxAIRE They were created for the development of projects that provide a better understand of energy efficiency and all related topics.

House are located inside the campus of the University of Texas at Tyler as shown in Figure 1 and described in Table 1.

Figure 1. House Location

Table 1. Coordinates House 1

Longitude	95°15'33.35"W
Latitude	32˚18'52".49N
Altitude	540 msnm

5.1.1 House Characteristics

The two TXAIRE houses are identical; the only difference is the attic of the houses, House 1 has a vented attic, in which the insolation and air barriers are located in the ceiling that separates the house from the attic, and for the purpose of this research, the house selected for this work was number 1 due to a time constrain of time that allowed just a House 1 study. The House has and ERV and HVAC systems which allow comparisons of the performance of both systems in different seasons. Figure 2 shows an exterior view of House 1.

Figure 2. Research House.

5.1.2 Floor Plan

Figures 3 and 4 show the plan of the house and the mechanical drawing, which show information about the heating, ventilating and air conditioning system that allow analyzing the whole system and how the airflows and exchange of air are performed under the house features which have a direct influence on the indoor air quality of the air performance.

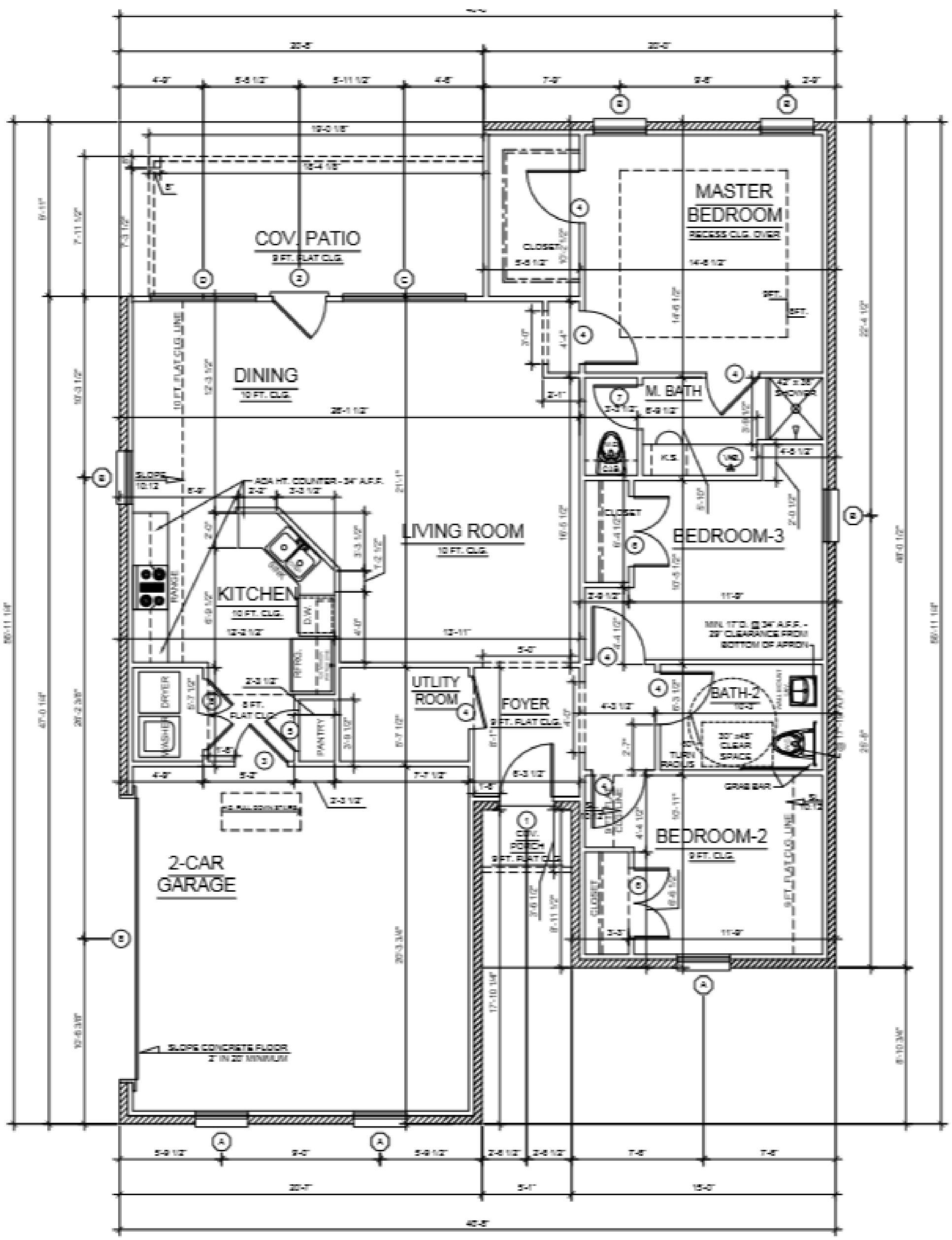


Figure 3. Floor Plan

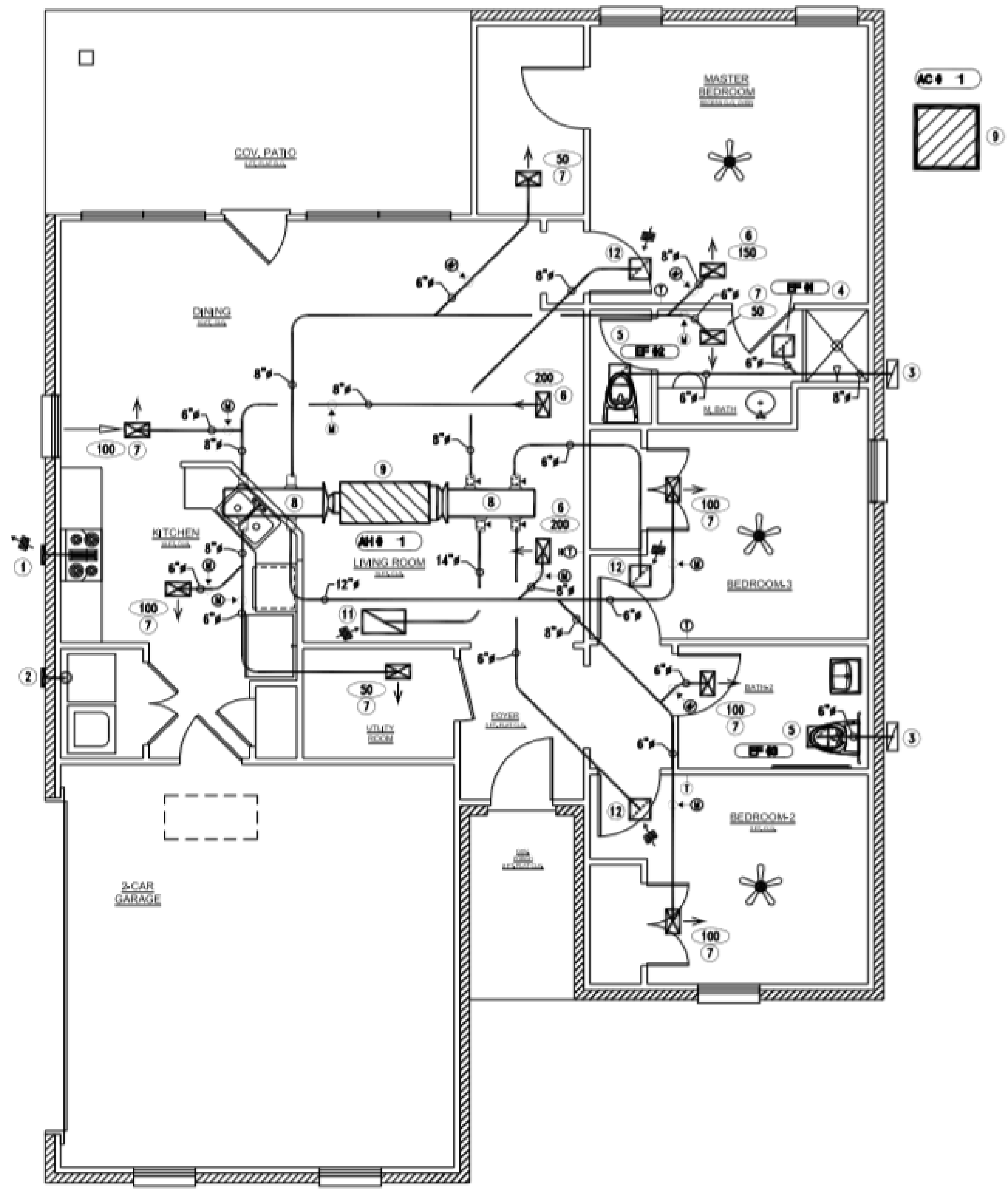


Figure 4. Ventilation System

5.2 METHODS

5.2.1 Data Source

Figure 5 shows the data sources used in this research. There were five main sources of data: cooling and heating system; meteorological data; physical plant; contaminant concentration data and sampling. Each of these data sources is described in more detail in the sections that follow.

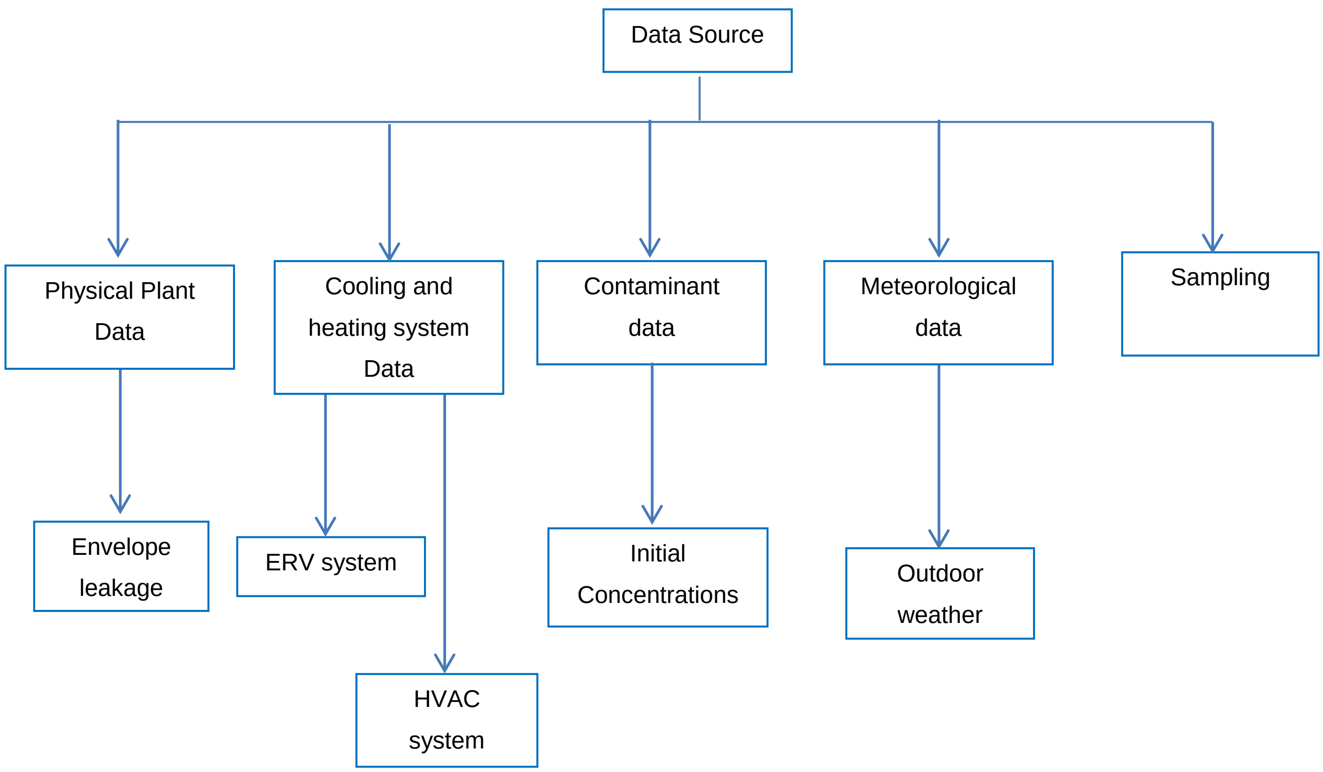


Figure 5. Data Sources used for the research

5.2.1.1 Physical Plant

The floor area is a significant factor to consider when predicting air infiltration which is one of the primary factors affecting indoor air quality and energy consumption. High infiltration rates can decrease harmful exposures to pollutants of indoor origin, or they can increase exposures to pollutants that originate outdoor. Table 2 shows the characteristics of the house and the total surfaces area and volume.

Table 2. Physical Characteristics of the House

Zone Name	Floor Area (ft^2)	Max Height (ft)	Volume (ft^3)	Exterior Wall Area (ft^2)	Exterior Surface Area (ft^2)
Living Room	750	10.0	7220	472	1972
Master Bedroom	337	9.0	2766	433	1107
Bedroom 3	159	8	1272	100	418
Bathroom	64	8	512	50	178
Bedroom 2	165	9	1485	315	645
Total	1475	44	13255	1370	4320

5.2.1.1.1 Envelope Leakage

Air leakage data from literature as well as values used in previous studies were used in this research, this is very important since this data shows individual and whole building zone air exchange rates and determines airflow rates and pressure differences between zones. These inter-zone airflow rates are useful for predicting pollutant transport within buildings with well mixed zones (ASHRAE, 2009). Table 3 shows the airflows elements used for the simulation of the building.

Table 3 Airflow elements of the building

General ceiling, typical value
HVAC ceiling penetration, tight value
Attic door, tight value
Bathroom door, closed, including frame and undercut, manuf. home
Closet door, closed, tight value
Closet door frame, tight value
Door, exterior, wood, frame, tight value
Door, exterior, single, tight value
Door, exterior, sliding glass, tight value
Exterior door frame
Garage door, closed, tight value
Door, interior closed, including frame and undercut
Door, interior, closed, tight value
Hall doorway, typical value
Attic floor
Ceiling-joint joint, tight value
Floor-wall joint, tight value
Wall-wall joint, tight value
Electrical outlet, tight value
Plumbing penetration, interior, tight value
Garage roof, tight value
Attic vent, based on attic floor area, typical value
Bathroom exhaust vent, tight value
Kitchen exhaust vent, tight value
Wall, interior, typical value
Window frame, wood, tight value
Window

5.2.1.1.2 Heating and Cooling System

The TX Air House has an Energy Recovery Ventilation (ERV), which exchanges the energy contained in exhausted building or space air using it to treat the incoming outdoor ventilation air in residential and commercial HVAC systems. During the warmer seasons, the system pre-cools and dehumidifies while humidifying and pre-heating in the cooler seasons.

Also, House 1 has the heating, ventilation, and air conditioning (HVAC), in which the three central functions of heating, ventilating, and air-conditioning are interrelated especially with the need to provide thermal comfort and acceptable indoor air quality. HVAC systems provide ventilation, reduce air infiltration, and maintain pressure relationships between spaces.

5.2.1.1.3 ERV System

The ERV system takes outdoor air at a rate of 165 CFM. The zones which are by the air supplied are: master bedroom, Bedroom 3, and Bedroom 2, in this system there are 4 exhaust ducts which are located in the kitchen and the Foyer, and two bathrooms area. Table 4 shows the airflows of each supply and exhaust points, and Figure 6 the appearance of it.

Figure 6. Energy Recovery Ventilator (ERV)

Table 4 Supply and exhaust terminals of ERV

ZONE	SUPPLY (CFM)/EXHAUST (CFM)
MASTER BEDROOM	58 (S)
MIDDLE BEDROOM	46 (S)
FRONT BEDROOM	61 (S)
ENTRYWAY EXHAUST	64 (E)
KITCHEN EXHAUST	101 (E)

5.2.1.1.4 HVAC System

The HVAC system has a fan with a capacity of 1200 CFM. This system does not take any air from outside and therefore the recirculation of the system is 100%. Table 5 shows the airflows of each terminal in the HVAC system.

Table 5 Supply and return terminals of HVAC

ZONE	SUPPLY (CFM)/EXHAUST (CFM)
MASTER BATHROOM	176 (S)
MIDDLE BATHROOM	80 (S)
MAIN	943 (S)
EXHAUST	334 (E)
RETURN	866 (R)

5.2.1.1.4.1 Ducts

Only horizontal segments can be displayed on the ContamW SketchPad, but vertical segments can be implemented as well. Each duct segment is referred to as *duct flow element*. *Duct flow elements* describe the mathematical relationship between flow through and pressure drop along the duct, the flow resistance or forced flow characteristics, cross-sectional geometry, and optional leakage per unit length of a duct.

Table 6 shows the values used in the software for the duct sections which are based on (ASHRAE, 2009).

Table 6. Duct characteristics

Type of duct	Relative Elevation	Terminal Loss coefficient	Free face Area	Duct Area
Circular	8.5 ft	0.8	0.33 ft^2	0.338 ft^2

5.2.1.1.4.2 Filters

The air filters remove particles from the air stream to keep the air conditioning system clean and to remove particles from the air. As the filters get loaded with particles, the filter becomes more efficient, but it also increases resistance and reduces airflow. The system will not perform as well thus affecting the efficiency of the system and the building air.

The Minimum Efficiency Reporting Value (MERV). The ratings are based on the ability to filter out undesirable particles from the air. This allows comparing distinct filters through a numerical value ranging from 1 (lowest efficiency) to 20 (highest efficiency) and indicates how well the filter captures and holds dirt and dust of a specified size range. Table 7 presents the rating of the filters in the duct system of the Tx Air House 1.

Table 7. Filters of the Return terminals

TYPE OF FILTER	LOCATION	MERV
Air Purification System	ERV	12
Filter M3	RETURN TERMINALS	10

5.2.1.1.5 Contaminant Data

Airborne contaminants are dispersed throughout buildings due to several transport mechanisms. The concentration contaminants were taken in the Tx Air House 1.
Table 8 shows the characteristics of the species or contaminants will be used during the simulation.

Table 8 Characteristics of CO_2

CONTAMINANT	MOLECULAR WEIGHT (Kg/Kmol)	EEFECTIVE DENSITY (Kg/m^3)	DIFFUSION COEFFICIENT cm^2/s	SPECIFIC HEAT KJ/(KgK)
CO_2	44.02	1.91	0.00019	0.83

5.2.1.1.6 Meteorological Data

Meteorological data has an essential impact in the distribution and dispersion of contaminant. The principal parameter in the movement of contaminants by the atmosphere is the wind, its speed and direction of wind, which are interrelated with temperature gradients. Meteorological data from the local station located in the House was used for the advance of the research. Table 9 shows the average of the meteorological variables measured for the sampling day.

Table 9. Average of meteorological parameters

Temperature Outside	Hi Temperature	Low Temperature	Humidity Outside	Wind Speed	Wind Direction
73	73	73	84	3.01	337

5.2.1.1.7 Outdoor Weather

Figures 7 through 10 show the weather characteristics.

Figure 7. Temperature

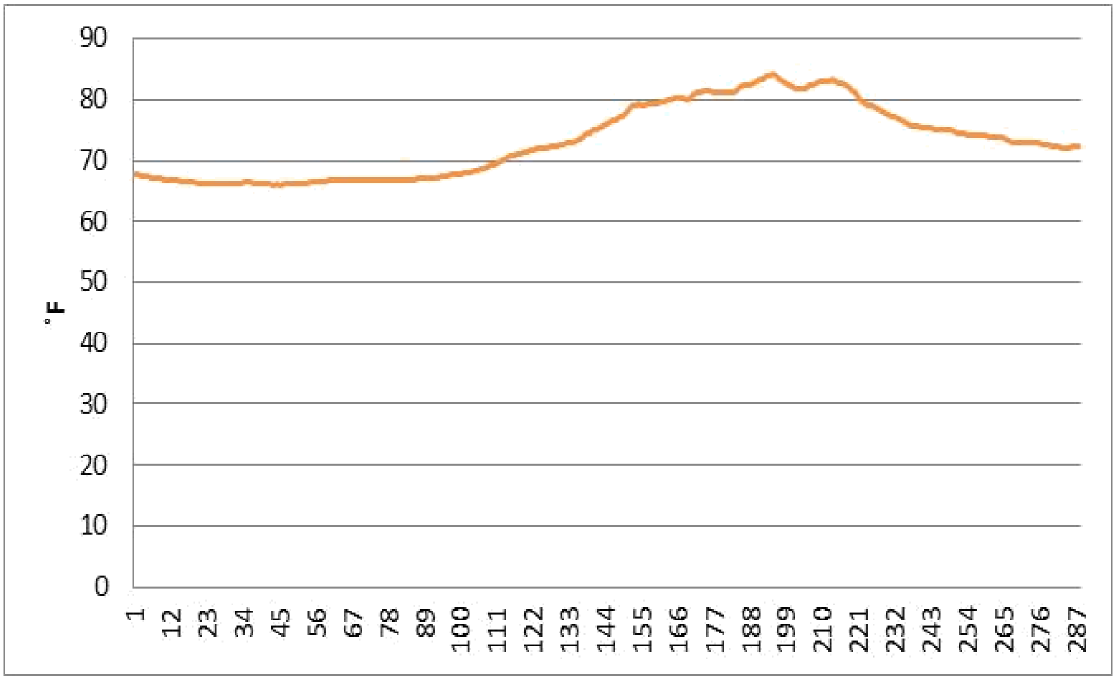


Figure 8. Relative Humidity

Figure 9. Wind Speed

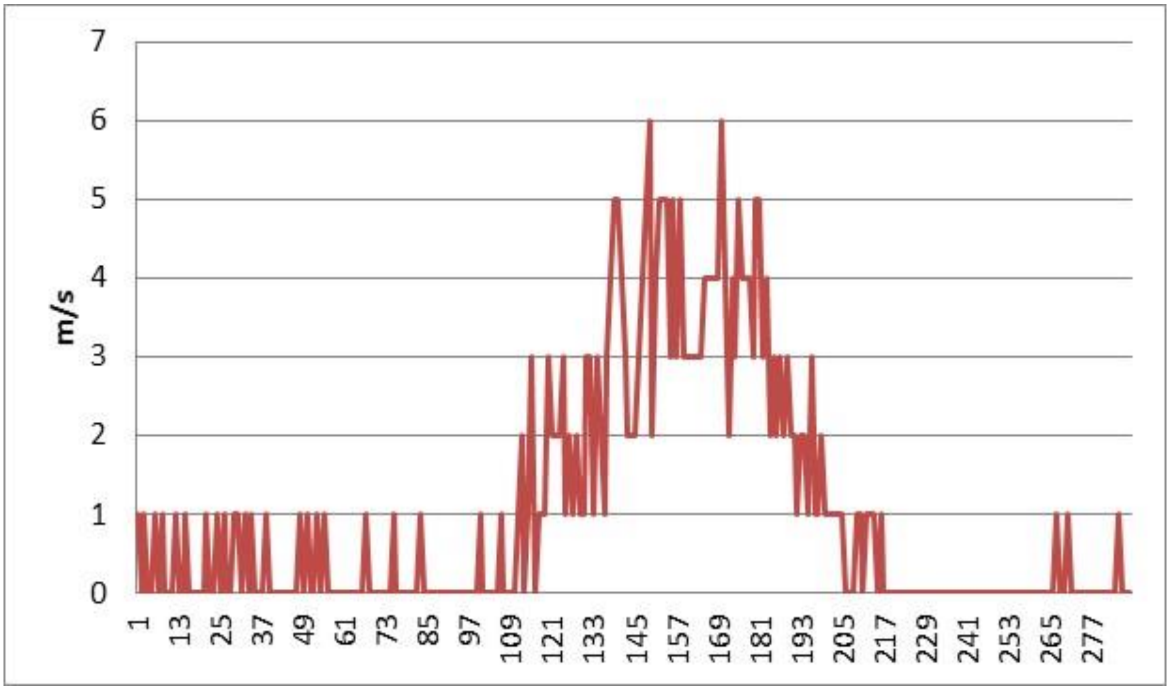
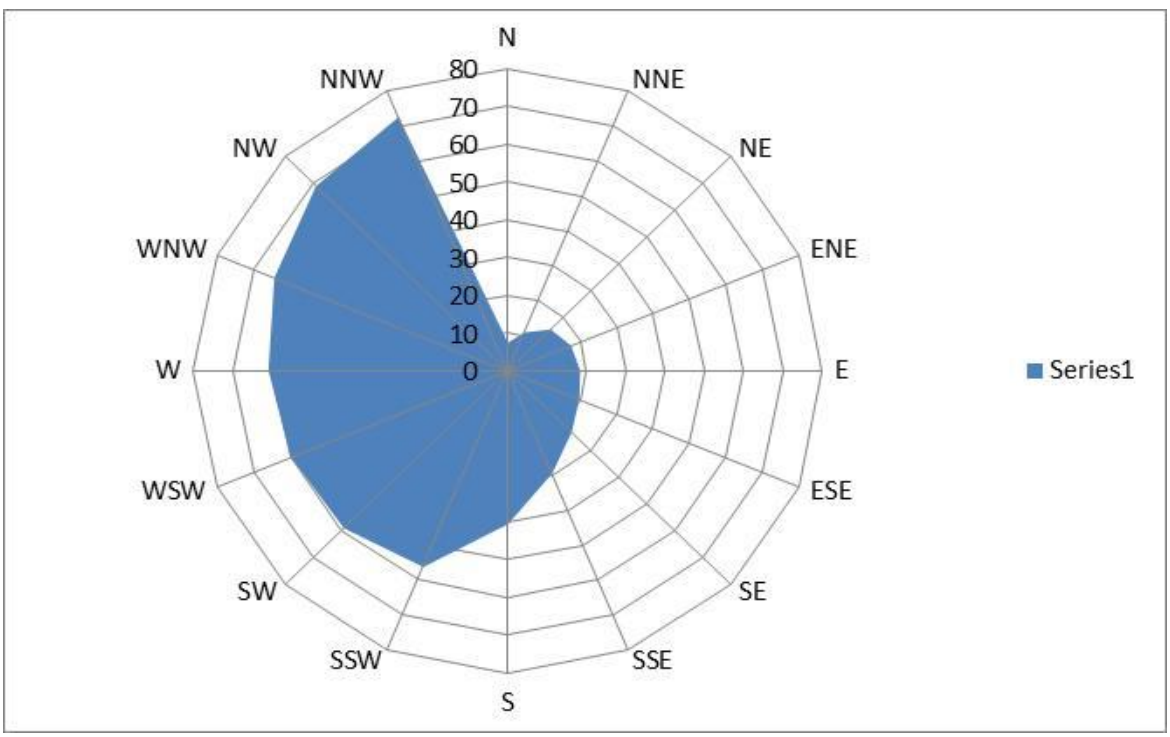


Figure 10. Wind Direction



5.3 Sampling

Calibration exercises were performed in the House 1 of the department of Tx-Air to collect tracer gas data, CO_2 releases need to be performed in the building and CO_2 sensors were placed throughout the building to record CO_2 concentrations.

To start the test, the CO_2 tank was opened in the Master Bedroom with the appropriate ventilation system operating to reach reasonable steady-state conditions, according to the design experiment.

The samples were taken on October 11, 2013 in Tx-Air House 1 with the CO_2 Tank generator and the Flow meter Omega Model: FL2001. Figure 11 and 12 show the equipment used during the testing and Table 10 shows the different experiments designed for the research.

Figure 11. Flow Meter

Figure 12. CO_2 Tank

The sample collection was located at 5 ft above the floor to approximate human exposures; also it was collected in the Master Bedroom where there is good air circulation.

This area was selected due to the high activity use and the potential pathway doors, vents, windows, walls, ventilation grilles, and the possible mixing height of the air of the building.

The gas was released with steady – injection at a flow rate of 1.0 SCFH during the experiment; however some calculations were required, since the airflow-meter was for the air, not CO_2.

Table 10. CO_2 airflow

Airflow air	Density of CO_2	Airflow CO_2
1.0 CFM	2.814 Kg/m^3	1.313×10^{-3} Kg/s

Table 11 shows the characteristic of each scenario, the time and duration.

Table 11. Time and characteristic of experiment

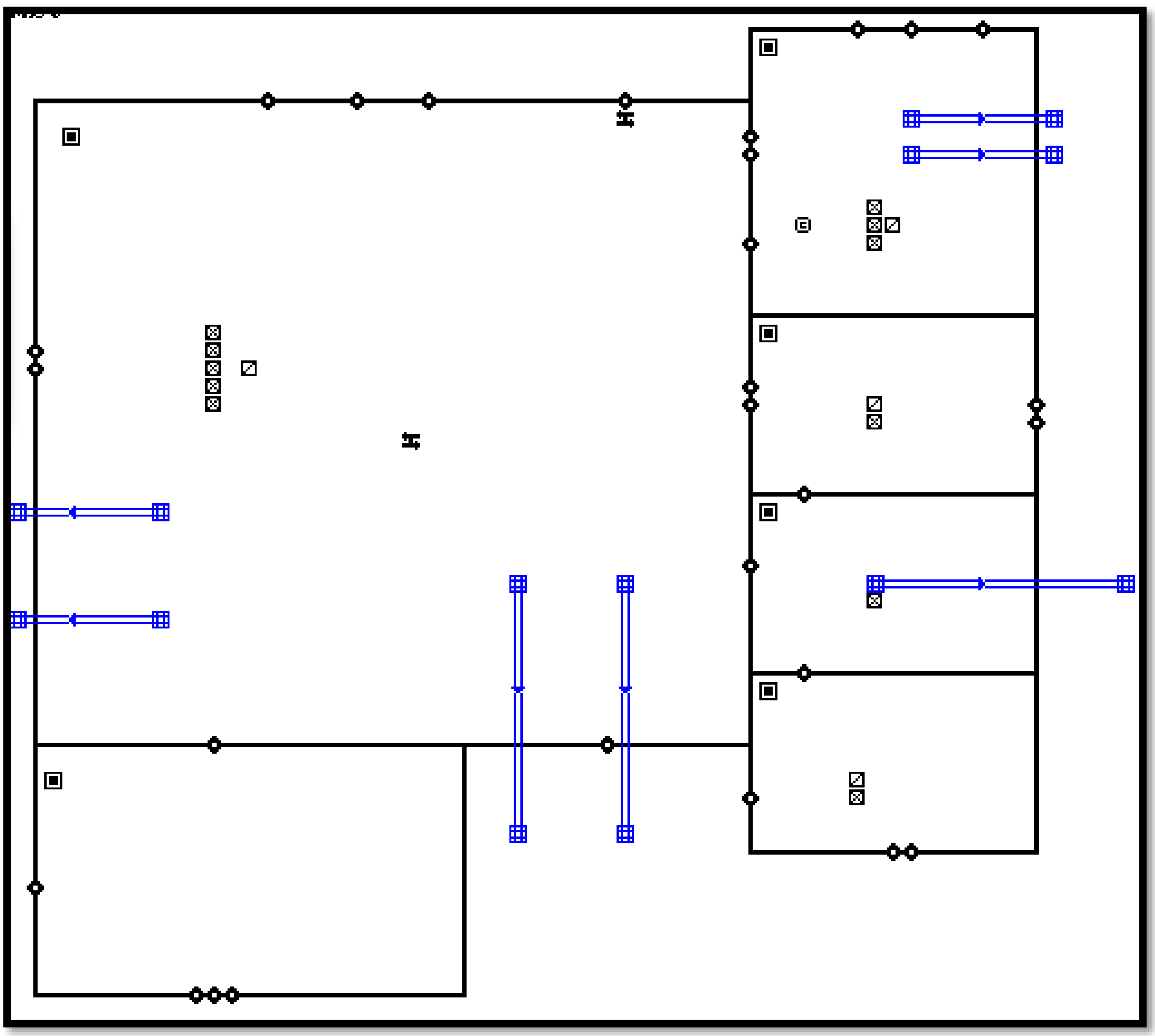
EXPERIMENTS	CONDITIONS	TIME
Experiment 1	Recirculation ON ERV 100%	9:25 to 1:30
Experiment 2	Recirculation OFF ERV 100%	1:50 to 3:55
Experiment 3	Recirculation ON ERV OFF	4:05 to 6:10

5.4 Model Input

5.4.1 Building Zones

The Tx Air House was divided into 6 zones since the multi-zone CONTAM model treats rooms of building as zones with uniform properties. It was necessary divide the building into complete zones to allow the program to predict the concentrations and the airflows in the house Figure 13 shows the sketchpad of the building with supply and return terminals, and Figure 14 explained the connotation of the symbols in the sketchpad.

Figure 13. Schematic Representation and Building Components



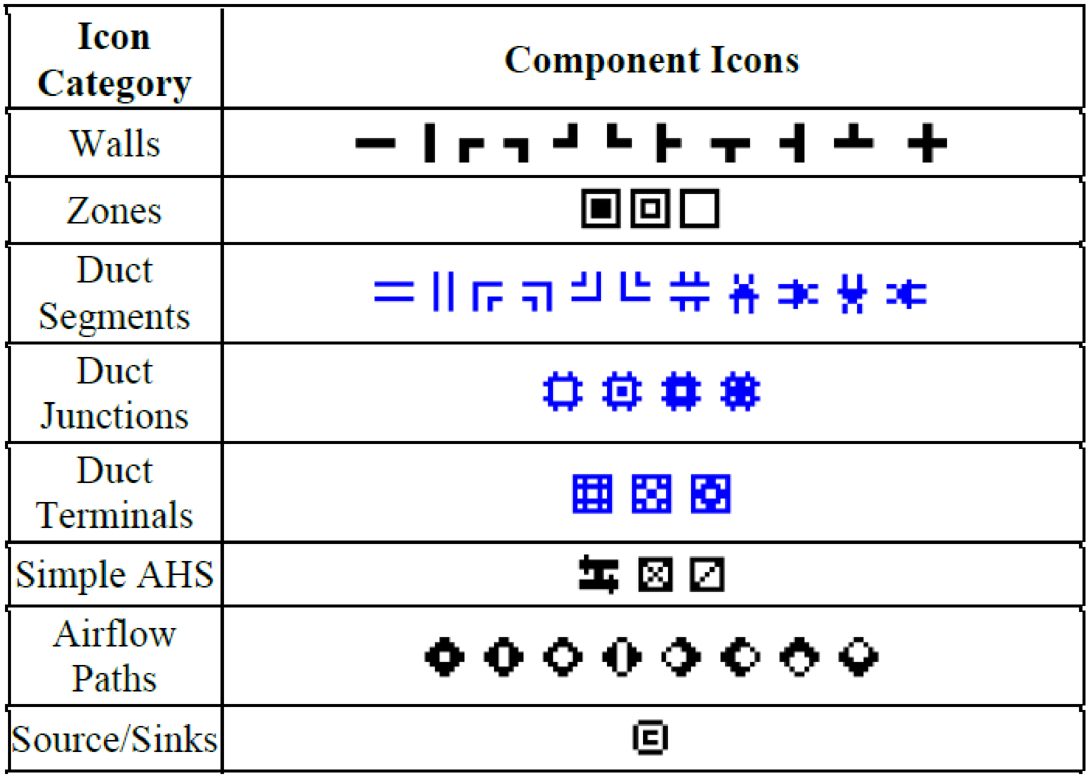


Figure 14. Symbols Representation

5.4.2 Flow Paths

Table 12 Flow Paths

Type of Element	Mathematical Model
One-way Flow using Power law Models	Leakage Area Data
	Orifice Area Data
Fan and Forced Flow Models	Constant Volume Flow

5.4.3 Simulation

Airflow Test

The Airflow test generates data related to building ventilation. The data is used to gauge the reasonableness of model inputs before beginning analysis of a building.

All simulations were performed as steady contaminant dispersion and steady-state airflow simulations. This means that the building's pressure distribution, volumetric airflow rates through each flow path and contaminant concentrations are calculated and remain fixed for one set of conditions.

Table 13 presents the initial concentrations for the different simulations.

Table 13. Initial Concentrations

EXPERIMENTS	LIVING ROOM	BEDROOM 2	BEDROOM 3	BATHROOM	MASTER BEDROOM	ATTIC
1	386	335	419	404	398	298
2	407	342	426	426	419	291
3	415	338	424	436	428	285

6. Chapter Six: RESULTS

6.1 AIRFLOW TEST

Table 14 Airflow Test Results

PARAMETER	VALUE	UNITS
Building Air change rate	0.387	ach
Ambient Temperature	60	˚F
Pressure	99348.9	Pa
Wind speed	2.42	m/s
Wind Direction	337	degrees
Conditioned Zones	18612.2	ft^3
Ducts & AHS (conditioned)	62.1	ft^3
Unconditioned Zones	984.3	ft^3

Table 15 Air change per hour in the system

ZONE	C/U	SUPPLY	RET/EXH	CIRC TOT	P [PA]	T [C]	VOL [m^3]
ATTIC	U	0	0	0.02	-0.4	28.2	27.9
MASTER BEDROOM	C	7.3743	5.0002	4.37	2.1	23.9	93.9
MAIN	C	**7.9209**	**8.3997**	**8.92**	-0.8	23.9	209
MIDDLE BEDROOM	C	2.8226	4.3583	4.36	0.3	23.9	44.3
BATH 2	C	1.8747	0	**9.85**	0.7	23.9	17.8
FRONT BEDROOM	C	2.329	2.078	5.08	3	23.9	46
GARAGE	C	0	0	0.02	0.8	23.9	115.9

Table 16 Inter-zonal Airflows

from\to	Attic	Main	Master Bedroom	Middle Bedroom	Bathroom	Front Bedroom	Garage
Attic	0	0	0	0	0	0	0
Master Bedroom	0	119.308	0	0	0	0	0
Main	0	0	162.277	38.6873	52.0887	0	18.827
Middle Bedroom	0	0	0	0	0	0	0
Bathroom	0	0	0	24.6331	0	107.456	0
Front Bedroom	0	0	0	0	107.456	0	0
Garage	0	1.3434	0	0	0	0	0
Ambient	0.3575	0	0	0	0	0	0

6.2 VALIDATION

CONTAM could provide inaccurate results in the simulations with non-uniform momentum effect, temperature, and contaminant concentration. Before executing all the experiments it was necessary to validate the information provided by the software.

Hence, this chapter first verifies the accuracy of the model through the data measured in the TxAir House. Results were evaluated statistically using ASTM D5157-97 Standard Guide for Statistical Evaluation of Indoor Air Quality Models (ASTM 2008). ASTM D5157 has three criteria relevant to evaluating the results of this work.

It was necessary for the validation to examine the concentrations obtained versus the concentrations predicted by the simulation, and establish the correlation coefficient, the normalized mean square error (NMSE) and the Fractional bias. The results are presented in the Tables 18 through 20. And the Tables 21 through 23 presents the final measured and predicted concentrations.

Table 17. Statistical Evaluation of Experiment 1

CONTAMINANT	Living Room	Bedroom 2	Bedroom 3	Master Bedroom	Bathroom	Attic
r > 0.9	0.9907	09985	0.968	0.9995	0.999	1.0
M 0.75 to 1.25	0.987	0.9949	0.992	0.9991	0.999	1.0
b/Co < 0.25	0.02	0.03	0.04	0.02	0.04	0.07
NMSE < 0.25	0.066	0.047	0.135	0.022	0.091	0.260
FB < 0.25	-0.036	-0.031	-0.052	-0.021	-0.043	-0.072
FS < 0.5	-0.017	-0.009	0.017	-0.001	0.000	0.00
Maximum Error	4.248	3.420	5.564	2.355	4.776	7.915
Minimum Error	3.109	2.716	4.437	1.872	3.858	6.299
Average Error	3.6	3.0	5.1	2.097	4.2	6.987

Table 18. Statistical Evaluation of Experiment 2

CONTAMINANT	Living Room	Bedroom 2	Bedroom 3	Master Bedroom	Bathroom	Attic
r > 0.9	0.9626	0.978	0.982	0.9947	0.9905	0.9993
m 0.75 to 1.25	0.9732	0.9409	0.965	1.01	1.0027	1.006
b/Co < 0.25	0.018	0.020	0.005	0.044	0.047	0.052
NMSE < 0.25	0.000	0.041	0.044	0.024	0.053	0.073
FB < 0.25	-0.046	-0.040	-0.041	-0.031	-0.045	-0.053
FS < 0.5	-0.016	-0.100	-0.053	0.034	0.015	2.000
Maximum Error	5.611	4.960	5.007	3.261	5.030	5.457
Minimum Error	3.438	2.635	3.161	2.602	4.025	4.744
Average Error	4.4	3.91	4.02	3.0	4.4	5.2

Table 19. Statistical Evaluation of Experiment 3

CONTAMINANT	Living Room	Bedroom 2	Bedroom 3	Master Bedroom	Bathroom	Attic
r > 0.9	0.9939	0.9804	0.9924	1.0	0.9704	1.0
m 0.75 to 1.25	1.0048	1.012	1.003	0.9365	0.91	1.0
b/Co < 0.25	0.045	0.073	0.111	0.111	0.159	0.489
NMSE < 0.25	0.040	0.029	0.020	0.199	0.043	0.077
FB < 0.25	-0.039	-0.033	-0.028	0.087	-0.041	-0.055
FS < 0.5	0.0156	0.0449	0.000	0.101	-0.101	0.00
Maximum Error	4.266	4.062	5.230	2.827	4.699	5.440
Minimum Error	3.529	2.777	4.421	2.454	3.428	5.028
Average Error	3.838	3.3	4.8	2.725	4.0	5.314

Table 20. Results Experiment 1

	LIVING ROOM		BEDROOM - 2		BEDROOM-3		BATHROOM		MASTER BEDROOM		ATTIC	
TIME	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**
9:25	408.62	393.74	340.98	330.10	459.85	435.98	413.88	394.11	434.23	424.48	303.54	284.19
9:30	417.82	402.94	343.61	333.73	433.25	412.38	429.31	409.54	460.83	452.08	305.84	286.49
9:35	418.8	403.92	347.87	335.99	431.28	407.41	446.38	427.14	466.41	456.66	307.16	287.81
9:40	422.74	407.86	347.22	335.34	434.23	412.36	452.62	432.85	456.56	445.81	304.2	284.85
9:45	424.38	409.50	345.58	335.70	428.98	405.11	481.52	461.75	459.85	450.64	295.99	276.64
9:50	427.67	412.79	345.58	334.70	432.26	410.39	487.1	467.33	467.4	458.65	301.25	281.90
9:55	427.34	412.46	363.64	352.76	432.26	412.39	480.86	461.09	457.55	447.80	294.02	274.67
10:00	431.61	416.73	375.13	364.25	432.92	412.05	463.79	444.02	469.7	459.95	294.68	275.33
10:05	431.61	416.73	380.71	369.83	434.89	411.02	473.97	454.20	469.37	459.67	297.63	278.28
10:10	434.56	419.68	381.37	370.49	433.58	412.71	467.07	447.30	471.34	460.59	296.32	276.97
10:15	443.43	428.55	358.05	347.17	437.85	413.98	483.82	464.05	477.91	468.16	300.92	281.57
10:20	462.14	447.26	356.08	346.20	432.26	410.39	486.44	467.67	474.29	464.54	303.54	284.19
10:25	463.46	445.58	359.04	347.16	435.22	411.35	473.97	454.20	475.61	465.86	298.62	279.27
10:30	467.07	449.19	356.08	344.20	431.61	410.74	483.49	463.72	489.73	479.98	290.74	271.39
10:35	470.03	455.15	357.72	347.84	430.29	406.42	481.85	462.08	487.1	477.35	291.07	271.72
10:40	448.68	433.80	363.64	352.76	438.83	416.96	478.23	458.46	507.46	497.71	286.8	267.45
10:45	462.47	447.59	367.58	356.70	439.82	415.95	493.34	473.57	472.65	462.90	288.11	268.76
10:50	454.26	439.38	371.19	360.31	435.22	413.35	484.47	464.70	472	462.25	288.77	269.42
10:55	458.2	443.32	367.9	357.02	447.7	427.83	487.1	467.33	473.64	463.89	290.41	271.06
11:00	462.14	447.26	368.23	357.35	443.76	422.89	478.89	459.12	470.03	460.28	290.08	270.73
11:05	470.35	455.47	371.84	360.96	442.44	418.57	476.92	457.15	467.4	457.65	279.9	260.55
11:10	465.43	450.55	368.56	357.68	445.4	423.53	479.88	460.11	461.16	451.41	286.8	267.45
11:15	468.71	453.83	368.89	358.01	440.8	420.93	478.89	459.12	462.47	452.72	278.59	259.24
11:20	466.08	451.20	373.16	362.28	441.13	420.26	472.98	453.21	461.49	451.74	279.57	260.22

(Continued)

	LIVING ROOM		BEDROOM - 2		BEDROOM-3		BATHROOM		MASTER BEDROOM		ATTIC	
TIME	MEASURED	PREDICTED	MEASURED	PREDICTED	MEASURED	PREDICTED	MEASURED	PREDICTED	MEASURED	PREDICTED	MEASURED	PREDICTED
11:25	463.46	448.58	368.89	358.01	441.46	417.59	474.95	455.18	460.17	450.42	284.5	265.15
11:30	466.74	451.86	362.32	351.44	434.23	413.36	472.98	453.21	457.88	448.13	287.46	268.11
11:35	459.19	441.31	365.93	355.05	443.43	419.56	471.34	451.57	459.52	449.77	289.1	269.75
11:40	458.2	440.32	360.68	349.80	452.29	430.42	471.01	451.24	455.25	445.50	289.43	270.08
11:45	458.53	439.65	361.01	351.13	453.61	429.74	475.94	456.17	454.59	444.84	266.11	246.76
11:50	459.85	441.97	361.34	349.46	470.35	449.48	467.4	447.63	455.58	445.83	268.74	249.39
11:55	465.1	447.22	364.62	352.74	444.74	420.87	476.26	456.49	457.55	447.80	268.74	249.39
12:00	470.03	452.15	363.64	353.76	437.19	415.32	474.29	454.52	458.53	448.78	265.45	246.10
12:05	458.2	440.32	367.58	356.70	448.35	424.48	474.29	454.52	456.23	446.48	268.41	249.06
12:10	454.92	437.04	358.71	347.83	442.44	420.57	494.98	475.21	454.92	445.17	260.53	241.18
12:15	458.53	439.65	355.75	344.87	436.53	416.66	489.07	469.30	449.01	439.26	267.1	247.75
12:20	449.34	430.46	357.4	346.52	443.76	422.89	486.44	466.67	448.35	438.60	264.8	245.45
12:25	446.05	428.17	369.55	358.67	436.2	412.33	487.1	467.33	441.13	431.38	254.29	234.94
12:30	444.41	425.53	389.25	378.37	435.88	412.01	462.47	442.70	447.37	437.62	258.23	238.88
12:35	443.76	428.88	376.77	365.89	446.38	422.51	459.85	440.08	452.95	443.20	267.1	247.75
12:40	456.23	441.35	348.86	337.98	444.41	420.54	474.29	454.52	456.89	447.14	258.56	239.21
12:45	471.67	456.79	347.22	336.34	446.05	422.18	463.13	443.36	452.95	443.70	254.62	235.27
12:50	464.11	449.23	346.23	335.35	445.73	421.86	459.52	439.75	463.13	453.38	256.92	237.57
12:55	478.56	463.68	339.34	329.46	438.17	414.30	468.38	448.61	470.68	460.93	253.31	233.96
13:00	476.26	461.38	336.05	325.17	440.47	419.60	453.61	433.84	486.77	477.02	244.44	225.09
13:05	447.7	432.82	336.05	325.17	446.05	422.18	466.41	446.64	490.71	480.96	251.99	232.64
13:10	449.01	434.13	336.38	326.50	444.41	422.54	483.49	463.72	465.43	455.68	254.95	235.60

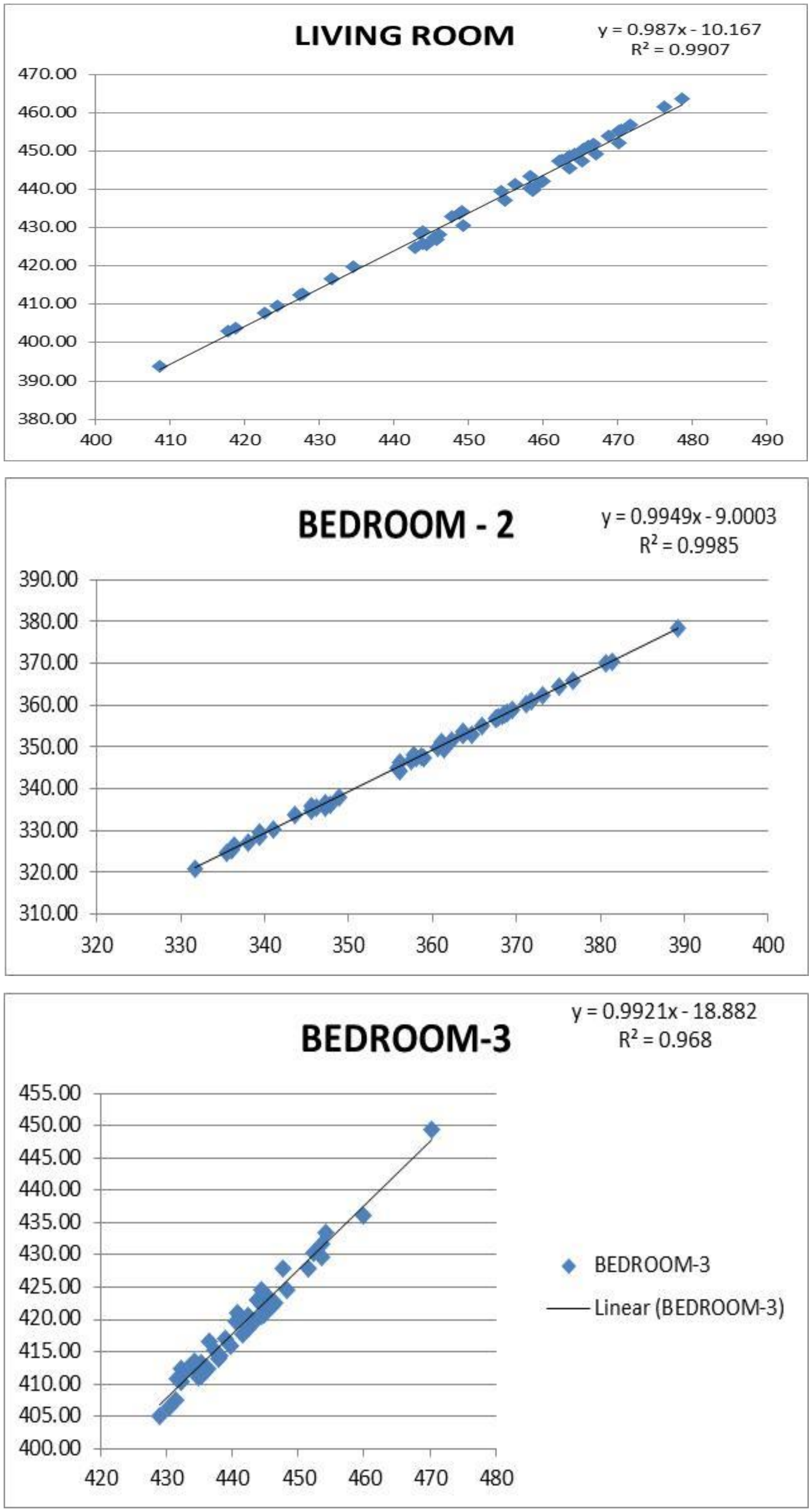
Table 21. Results Experiment 2

	LIVING ROOM		BEDROOM-2		BEDROOM-3		BATHROOM		MASTER BEDROOM		ATTIC	
TIME	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**
13:50	445.4	424.63	339.01	325.13	442.44	428.46	473.31	452.43	464.77	450.79	256.92	244.26
13:55	444.08	422.31	334.08	322.20	431.28	416.30	483.49	461.82	472.65	459.31	261.84	249.18
14:00	455.58	435.81	325.87	312.99	423.4	405.42	492.35	468.47	478.23	463.25	262.83	250.17
14:05	465.43	444.66	323.9	308.02	442.44	425.46	498.92	476.04	482.5	467.16	245.75	234.09
14:10	461.16	439.39	312.41	298.53	441.46	422.48	500.56	478.89	484.8	470.82	243.78	231.12
14:15	459.85	439.08	314.38	300.50	440.47	420.49	503.19	479.31	486.11	472.77	242.8	230.14
14:20	466.08	445.07	313.72	302.84	439.16	420.18	504.5	483.62	480.2	465.22	240.17	227.51
14:25	466.74	445.97	309.78	299.90	413.55	394.57	503.19	482.31	482.83	467.49	247.72	235.06
14:30	473.97	448.20	310.77	298.89	409.28	391.30	501.55	480.67	484.47	470.49	251.01	238.35
14:35	464.44	443.67	304.53	291.65	407.64	393.66	517.31	496.43	485.79	472.45	250.35	237.69
14:40	466.08	447.31	300.26	288.38	404.02	390.04	518.62	497.74	478.89	463.91	246.08	233.42
14:45	466.08	445.31	301.57	289.69	402.38	388.40	518.62	496.95	476.59	461.25	246.41	233.75
14:50	458.53	442.76	314.05	302.17	396.8	382.82	519.94	496.06	479.88	465.90	242.14	229.48
14:55	465.1	444.33	320.62	307.74	401.4	387.42	499.25	476.37	476.26	462.92	245.1	232.44
15:00	462.14	441.37	338.35	322.47	398.77	384.79	491.7	470.03	473.31	458.33	234.59	221.93
15:05	462.47	441.70	327.19	318.31	403.04	389.06	489.73	465.85	470.68	455.34	237.87	225.21
15:10	483.16	461.39	298.95	289.07	402.38	388.40	486.77	465.10	469.37	455.39	237.87	225.21
15:15	493.67	473.90	286.8	275.92	390.56	376.58	474.62	450.74	512.71	499.37	231.96	219.30
15:20	477.25	456.48	290.08	280.20	398.44	383.46	484.47	463.59	487.1	472.12	239.51	226.85
15:25	480.86	459.09	289.43	277.55	396.14	380.16	486.11	465.23	488.09	472.75	241.81	229.15
15:30	455.91	438.14	295.66	287.78	395.16	377.18	485.79	464.91	501.22	487.24	241.16	228.50
15:35	460.17	439.16	298.95	291.07	400.41	381.43	492.68	471.80	470.35	457.01	243.45	230.79
15:40	458.53	438.76	300.59	285.71	399.1	379.12	495.64	474.76	472.98	458.00	245.1	232.44
15:45	459.19	433.42	303.22	288.34	401.07	382.09	493.67	472.00	473.97	458.99	244.44	231.78

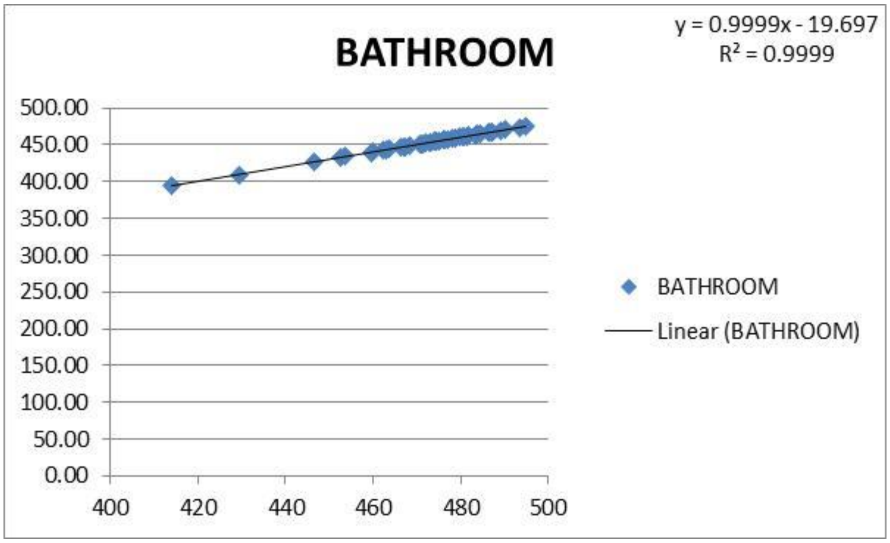
Table 22. Results Experiment 3

	LIVING ROOM		FRONT BEDROOM		MIDDLE BEDROOM		BATHROOM		MASTER BEDROOM		ATTIC	
TIME	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**	**MEASURED**	**PREDICTED**
4:05	385.64	370.76	336.71	325.17	420.11	400.08	407.31	392.33	397.79	386.92	305.19	289.27
4:10	381.7	366.82	332.11	321.11	417.49	395.81	407.96	393.98	396.47	385.60	316.68	300.76
4:15	372.17	356.29	324.23	314.69	445.07	425.39	396.8	379.82	384.65	373.78	312.74	296.82
4:20	378.08	363.20	324.56	313.02	445.73	425.70	393.19	378.21	388.59	377.72	312.08	296.16
4:25	387.28	372.40	331.13	319.59	437.85	416.17	404.35	388.37	393.19	382.32	299.6	283.68
4:30	383.99	368.11	330.47	319.47	439.82	420.14	403.7	387.72	392.86	381.99	298.29	282.37
4:35	385.96	372.08	334.74	325.20	415.52	395.49	406.65	389.67	398.44	387.57	300.59	284.67
4:40	389.58	375.70	332.77	321.23	420.11	398.43	407.64	389.66	401.07	390.20	300.59	284.67
4:45	390.23	376.35	333.43	319.89	420.44	400.76	407.64	388.66	399.76	388.89	296.98	281.06
4:50	383.34	368.46	338.02	327.02	418.47	398.79	405.99	389.01	400.08	389.21	297.96	282.04
4:55	385.64	370.76	331.13	321.59	414.53	394.50	423.4	405.42	395.49	384.62	296.65	280.73
5:00	384.98	369.10	335.72	324.18	415.52	393.84	427.01	408.03	395.81	384.94	299.6	283.68
5:05	383.99	369.11	343.61	332.61	413.22	393.54	424.05	407.07	392.2	381.33	296.32	280.40
5:10	378.08	363.20	343.61	334.07	415.84	395.81	425.37	410.39	393.19	382.32	295.99	280.07
5:15	385.64	369.76	356.08	345.08	418.8	397.12	400.41	383.43	394.83	383.96	297.96	282.04
5:20	388.92	375.04	339.66	330.12	419.79	400.11	403.37	385.39	399.1	388.23	301.57	285.65
5:25	393.19	379.31	337.37	325.83	419.13	399.10	404.02	385.04	399.1	388.23	300.92	285.00
5:30	402.38	387.50	328.83	317.29	414.53	392.85	400.08	385.10	390.23	379.36	293.69	277.77
5:35	404.68	389.80	326.86	314.86	413.55	393.87	398.44	384.46	409.61	398.74	294.68	278.76
5:40	404.35	389.47	328.83	319.29	415.19	395.51	397.79	382.81	410.92	400.05	294.02	278.10
5:45	410.26	394.38	323.58	312.04	414.53	394.50	394.5	380.52	411.9	401.03	293.37	277.45
5:50	381.37	366.49	329.81	318.81	413.22	393.54	395.81	378.83	443.1	432.23	292.71	276.79
5:55	383.67	368.79	335.07	325.53	421.43	401.75	402.05	387.07	398.44	387.57	298.62	282.70
6:00	385.96	370.08	338.02	326.48	423.4	401.72	403.37	386.39	399.76	388.89	301.25	285.33

Figure 15. CO_2 concentrations measured vs. predicted. Experiment 1



(Continued)


BATHROOM
y = 0.9999x - 19.697
R² = 0.9999
500.00
450.00
400.00
350.00
300.00
250.00
200.00
150.00
100.00
50.00
0.00
400
420
440
460
480
500
BATHROOM
Linear (BATHROOM)


MASTER BEDROOM
y = 0.9991x - 9.3214
R² = 0.9995
510.00
500.00
490.00
480.00
470.00
460.00
450.00
440.00
430.00
420.00
420
440
460
480
500
520
MASTER BEDROOM
Linear (MASTER BEDROOM)

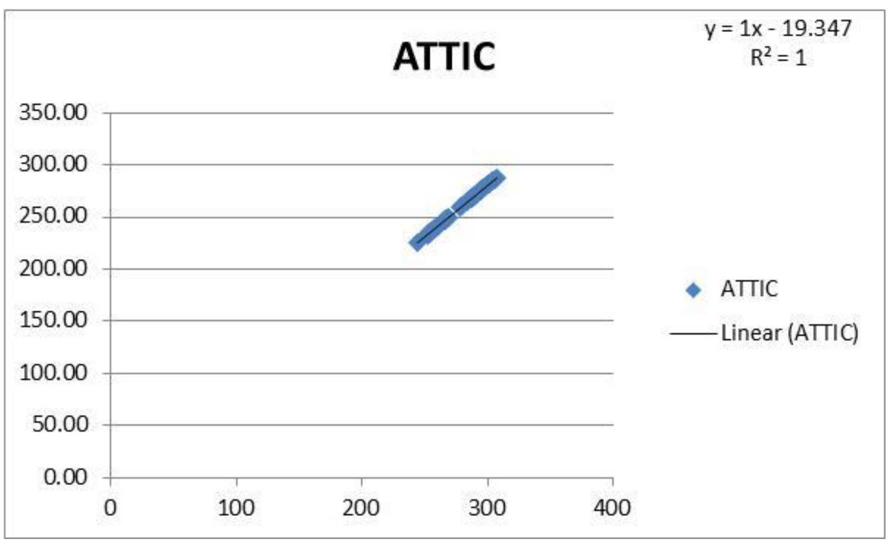
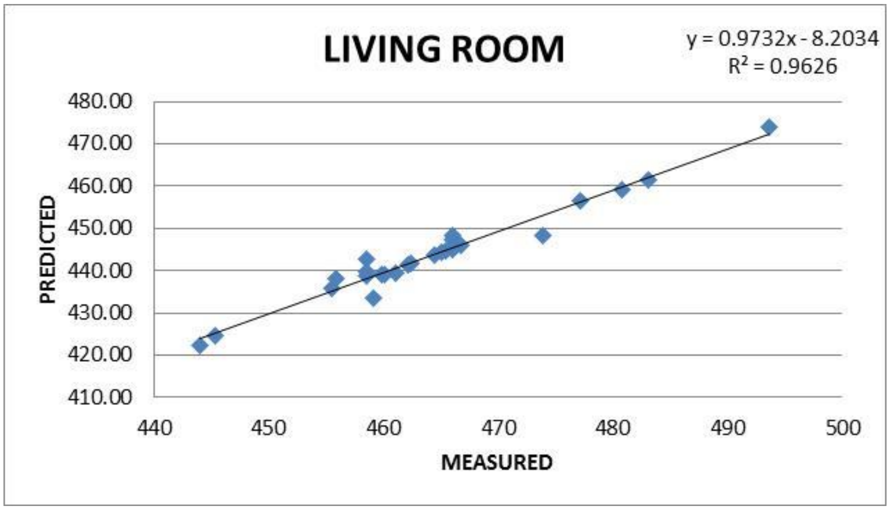
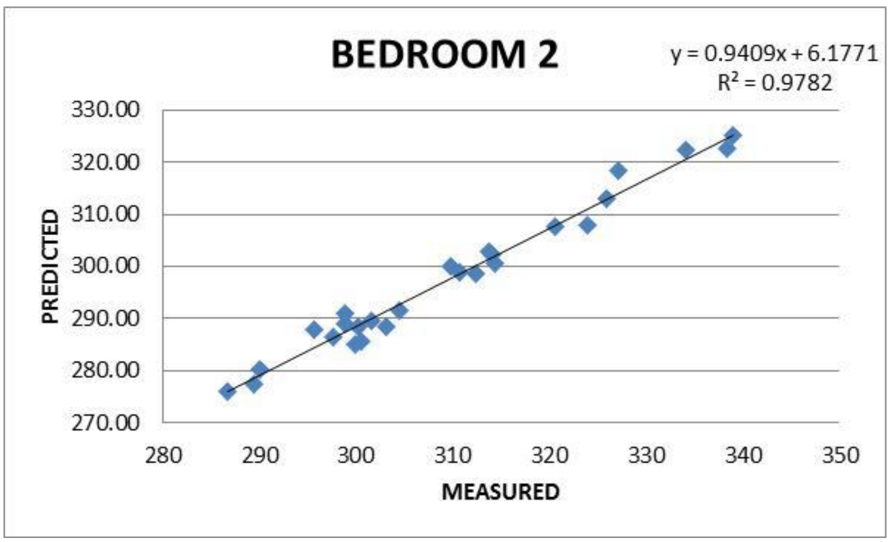
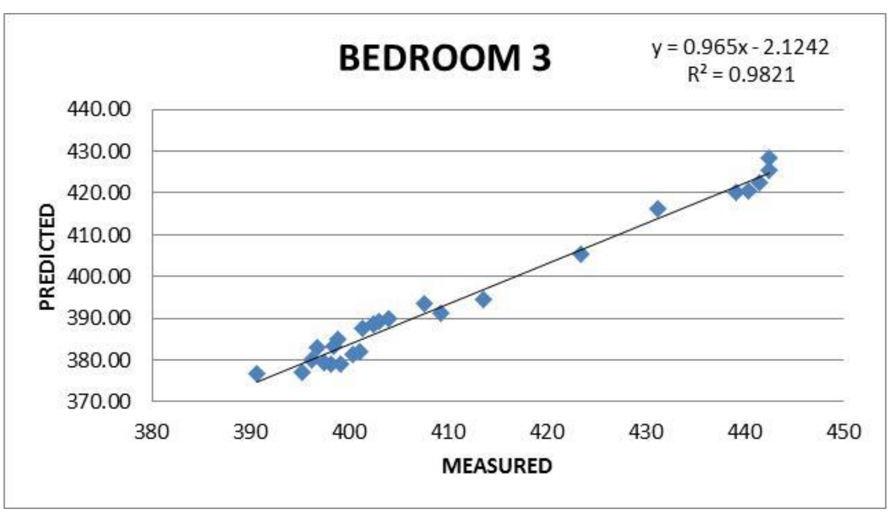

ATTIC
y = 1x - 19.347
R² = 1
350.00
300.00
250.00
200.00
150.00
100.00
50.00
0.00
0
100
200
300
400
ATTIC
Linear (ATTIC)

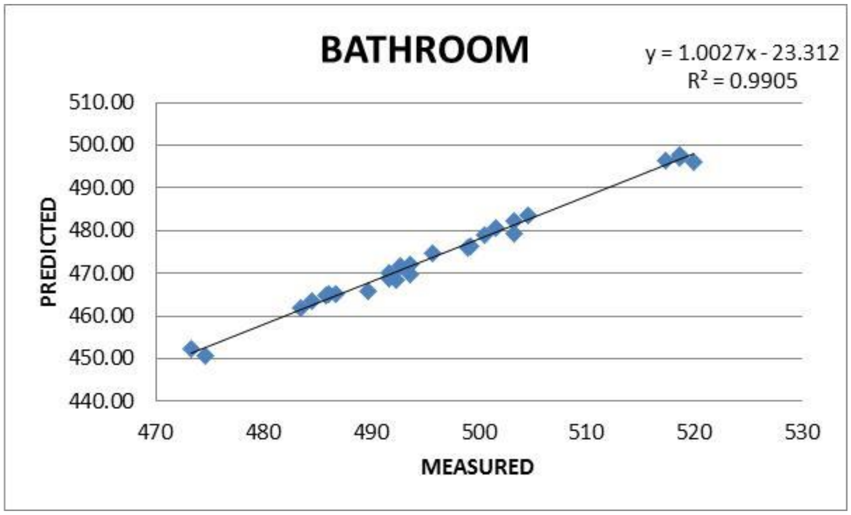
Figure 16. CO_2 concentrations measured vs. predicted. Experiment 2

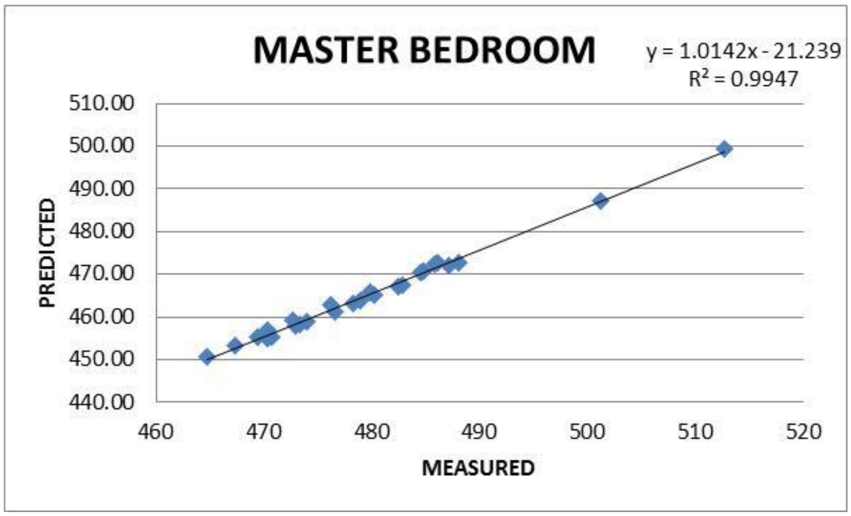






(Continued)


BATHROOM
y = 1.0027x - 23.312
R² = 0.9905
510.00
500.00
490.00
480.00
470.00
460.00
450.00
440.00
PREDICTED
470
480
490
500
510
520
530
MEASURED


MASTER BEDROOM
y = 1.0142x - 21.239
R² = 0.9947
510.00
500.00
490.00
480.00
470.00
460.00
450.00
440.00
PREDICTED
460
470
480
490
500
510
520
MEASURED

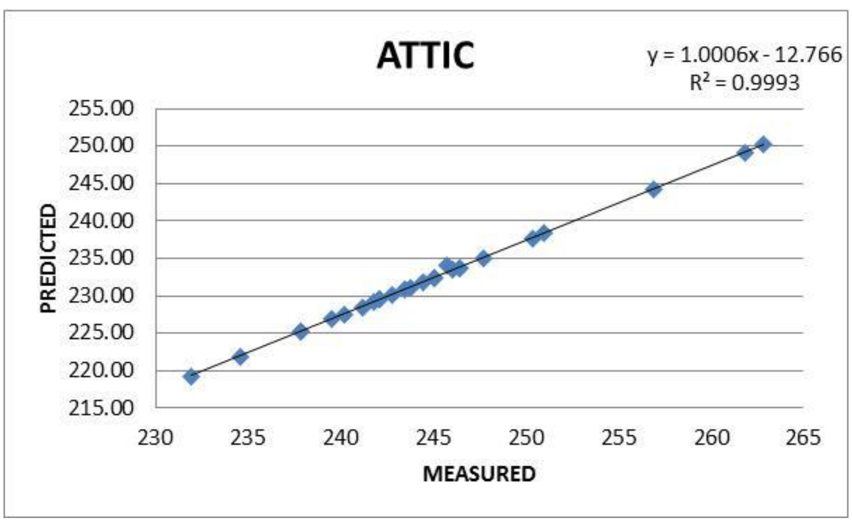
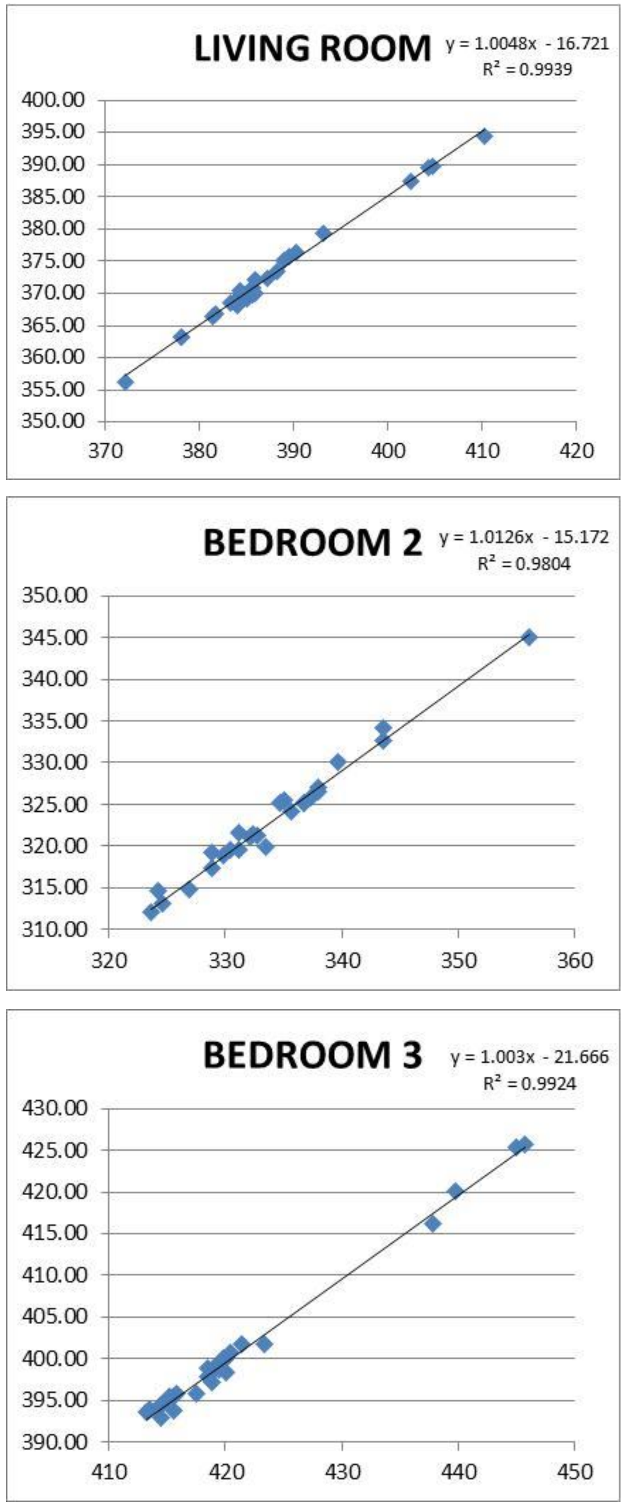
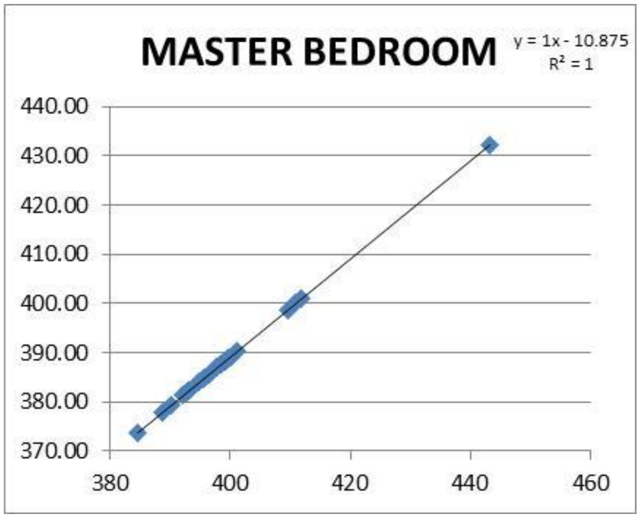

ATTIC
y = 1.0006x - 12.766
R² = 0.9993
255.00
250.00
245.00
240.00
235.00
230.00
225.00
220.00
215.00
PREDICTED
230
235
240
245
250
255
260
265
MEASURED

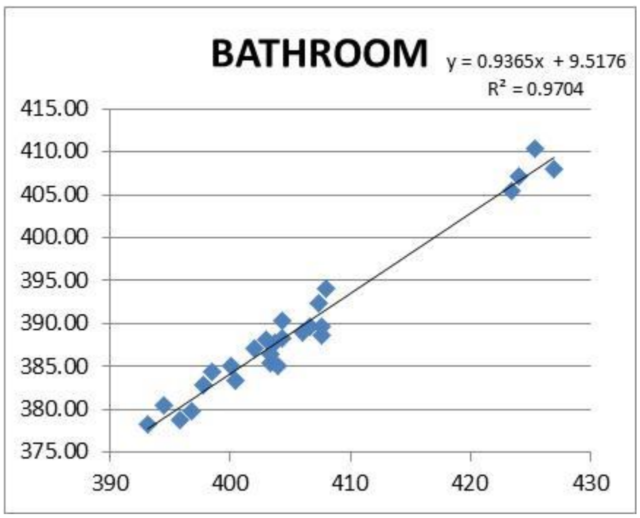
Figure 17. CO_2 concentrations measured vs. predicted. Experiment 3



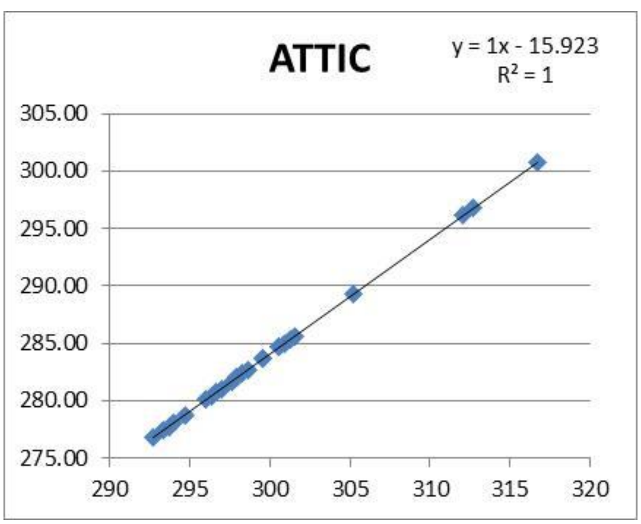
(Continued)



MASTER BEDROOM
y = 1x - 10.875
R² = 1
440.00
430.00
420.00
410.00
400.00
390.00
380.00
370.00
380
400
420
440
460



BATHROOM
y = 0.9365x + 9.5176
R² = 0.9704
415.00
410.00
405.00
400.00
395.00
390.00
385.00
380.00
375.00
390
400
410
420
430



ATTIC
y = 1x - 15.923
R² = 1
305.00
300.00
295.00
290.00
285.00
280.00
275.00
290
295
300
305
310
315
320

7. Chapter Seven: DISCUSSION

This chapter covers the analysis of the results obtained though the study. The results are presented and discussed as the Airflow Test of the House, calibration data and the validation of the final model.

7.1 Airflow Test

With the results of the airflow test it was possible to determine the infiltration value of the house which was 0.387 ach. According to the American Society of Heating, Refrigeration, and Air Conditioning Engineers (ASHRAE) this accomplishes the minimum ventilation rates in building providing acceptable indoor air quality of 0.35 ach for residential, and also the value match with the typical infiltration values in housing in America, since from tightly constructed housing with seasonal average air Exchange rates as low as 0.1 air changes per hour (ach) to loosely constructed housing with air exchange rates as great as 2.0 ach (ASHRAE, 2009). Table 14 shows the results of the airflow test.

7.1.1 Zone Air Change Rates

The individual zone air change rates for the different ventilation system in House 1 show low air change rates throughout all zones, with the lowest being in the Master and Middle bedroom zones.

The ERV showed huge air change rate increases in the bedrooms but was about the same as the other ventilation system in the Living Room zone.

Table 16 shows the air changes rates per zone as well as the exhaust/return, outdoor airflows, and airflows from the system.

Results for the zones indicate that the maximum air change rates in the supply system are in the Living Room zone and Master Bedroom.

The Main or Living zone has the maximum amount of return because in this zone there is the exhaust terminal of ERV and also the return of the HVAC system, making this area an important exchange part in the house.

The Master bedroom has the largest area, therefore the amount of air exhausted from the system is larger than other zones of the building increasing the exchange of air form this room.

Outdoor air change rates were calculated as the total flow of outdoor air into the building (including both air leakage through the exterior envelope and outdoor air intake via the mechanical ventilation system) divided by the building volume. Attics were not included in the building volume.

In the Attic there is no supply, return or exhaust since a diffuser is not located in this part of the house, and however there is an amount of outdoor air due to infiltration from the outside.

This outside air supply tends to increase the positive air pressure in the room with respect to the exterior; this causes fluctuations in the positive pressure (with respect to the exterior) in the zones.

The vented attic air change rate was about 0.02 ach and this can be explained by referring to the meteorological station information which indicates that the wind speed during the sampling period was 3.01 m/s.

7.1.2 Inter-zonal Airflows

Table 17 shows the intern-zonal airflows, where the airflow from the Main area to the Master Bedroom is the highest for the HVAC system and the impact of the direction of the Exhaust ventilation system.

Airflow from the Garage to the Main or Living Room zone was the lowest for the ventilation system since the ERV system was design to supply air to the bedrooms and exhaust from the Main or Living Room zone. Thus the living zone, negative and the bedrooms become positive.

The highest inter-zonal airflow was found between the main zone and the Master bedroom. Since the ERV system and the HVAC system supply air to the zones and the zones contain the larger area of the house, these results are well founded.

7.2 Airflow Simulation Results

The development of the CONTAM models for the TX Air House 1 and their association into airflow and contaminant transport behavior are described in this chapter. The development of the models presented a number of challenges and other issues that are worth discussion and address, the need for additional studies in the future.

The method used in this research was to analyze the degree of match between the predicted concentrations and measured CO_2 concentrations by, studying the plots for each macro-zone. The quality of the match between the two curves can be evaluated visually and statistically.

7.2.1 Validation

Statistical indices (including correlation coefficient, slope and intercept for regression line standard error of the estimate, normalized mean square error, and fractional bias) were calculated for the zones of the House to make quantitative comparisons regarding the level of agreement between measurements and predictions of transient pollutant concentrations.

Tables 18, 19 and 20 summarize the reported correlation coefficients between the predicted and observed data sets. (r) Ranges from -1 to +1, with -1 indicating an inverse relationship, 0 indicating no relationship, and +1 indicating strong relationship between the two datasets. ASTM suggests that r values greater than 0.9 generally indicate adequate model performance with respect to the correlation coefficient, which was found in the data analyzed in this study. All the relationships are positive an adequate performance.

Also a slope was founded between the suggested range of 0.75 and 1.25 as the DS 157. Thus the regression between the predicted and the measured values matched well.

It is recommended that $\frac{b}{C_o} < 0.25$ where C_o is the mean value of the observed data. This generally indicates adequate performance with respect to the regression, and was found in these results.

The NMSE is a measure of the magnitude of the error between the predicted and observed data sets value of less than 0.25 indicates a satisfactory performance of the model.

The Fractional Bias (FB) is a measurement of the bias of the mean concentrations of the predicted data. Value less than 0.25 indicates an acceptable performance of the model with respect to FB.

The Index of variance bias (FS) was found to be less than 0.5 in all the data sets confirming satisfactory performance of the model.

Good performance was seen between the modeling results and the CO_2 gas results. As described before, the greatest agreement was obtained for experiment 2 even though all the models presented a good fit between the measured and predicted concentrations.

Several methods of plotting the resulting tracer gas release data were evaluated. It was found that CO_2 concentrations curves for individual rooms were the most capable for analyzing the gas changes. There were no important changes in the predicted concentrations which confirm good results of the model versus the concentrations measured in the house.

The overall goal of these tracer gas simulations was to be able to identify macro-zones that do not change under varying conditions.

Figures 15, 16 and 17 show the individual CO_2 concentration curves for each room of the building for every set of conditions described in Table 11.

Since there were different scenarios or simulations but the same releases occurred, it became apparent that the release location could have a significant impact on which rooms are affected by contamination, and also the Inter- zonal airflow behavior impact in the distribution of the contaminants inside the building.

Wind speed and wind direction could have significant influences in the distribution of the contaminant. However the slight variations over time, the small amount of cross contamination between zones, and the physical conditions such as the tightness of the building, were observed to not allow these factors to have a real influence on the distribution of the contaminant.

The macro-zones identified did not show significant changes under the various conditions for both the airflow-based and tracer gas-based analyses. This confirms that the airflow dynamics are dominated by the HVAC in the slight variations in tracer gas behavior as well as cross contamination between zones.

The differences of the concentrations of the contaminant need to be evaluated as significant for occupant exposure and the type of calibration is performed since the type of contaminant varies and the impact on human health as well, this dynamics need to be specified by the researcher in the scope of the study.

7.2.2 Calibration Data

Some differences between predicted and measured concentrations remain after tuning the flow parameters, thus possible measurement errors and uncertainties for factors impacting room air changes and source rate need to be investigated (i.e., HVAC airflow rates, room volumes, and outside air percentages, and additional sources).

All locations had higher predicted concentrations than measured, showing the model was over predicting the concentrations; therefore it was necessary to adjust the system volume, instead of the room volumes which were estimated from floor the plans. Since an increase in the system volume results in a decrease in the predicted concentrations making bigger difference between the predictions and the measurements are smaller.

Assuming the HVAC airflow rates were measured accurately, it was initially hypothesized that these differences must be attributed to airflow into and out of the room via the exterior envelop or inter-zonal airflow paths. Consequently, adjustments to the flow parameters (coefficients and exponents) for these airflow paths was tried. The flow exponent was varied from the default of 0.65 to 0.5 and 0.7. This represents the range of typical flow exponents recommended by Walton and Dols (2008).

Other sources of inconsistencies between measured and predicted behavior could include uncertainties or errors in HVAC airflow rate or leakage in the system, CO_2 concentration measurements, errors in the development of the PCW model and the consequences of the well-mixed assumption which need to be explored for improvement of the model.

The ERV and HVAC airflow rates, were changed ad was the source airflow, which showed a difference in the predicted concentrations for the measurement location of the macro-zones. The leakage exponent did have a positive impact in the curve however it was not really significant in improving the model.

The well-mixed assumption of the multi-zone model may also be a significant source of error. It is possible that the CO_2 sensor was placed in a location where it recorded concentrations that were not representative of the room average due to the small temperature difference between the outside air and the return air. Therefore, it is valid to assume that the initial concentration used in the model may have an error.

7.3 Limitations of Study

The CONTAM models of the reference buildings provide important tools to evaluate the ventilation and IAQ performance of various buildings. However, there are a number of limitations to the CONTAM models that need to be considered and addressed in the future. The CONTAM simulations maintained a constant indoor air temperature and used the minimum amount of outdoor ventilation air specified for each zone (or HVAC system) thus simplifying the system, without taking into account the ERV unit that complements the HVAC system. Thus, future applications of CONTAM to these models may consider varying supply airflow rates and indoor temperatures.

For this study, there was just one source taken into account. For future simulations it is important to recognize more possible sources that may improve the simulation results of the model.

The software has some issues with the hydrostatic pressure calculation as well as the average air density in duct stack calculation, varying the leakage and the pressure drop in the duct system.

8. Chapter Eight: CONCLUSION

The process of calibrating a model is critical in simulations for predicting contaminant dispersion and estimating personal exposure. Therefore it is important emphasize the accuracy of the model to obtain precise results.

Reducing the number of individual flow parameters that need to be tuned during calibration reduces the error and elevates the accuracy of the model since the zones have similar airflow dynamics and tracer gas behavior.

Flow parameters and HVAC characteristics are the base for the analysis and understanding of building airflow and tracer gas behavior. Tuning the model for these factors improved accurate of the model.

In the experimental design method, the same location release was used for the different experiments; therefore it would be useful to see different releases places to confirm if the contaminant distribution is governed by the internal airflow dynamics.

Altering the flow parameters in the airflow paths of macro-zones during calibration did not seem to significantly improve the match between measured and predicted tracer gas curves.

Due to minor variations in observed wind direction and wind speed, it was concluded that wind direction and speed had little impact on the concentration curve. However, the leakage had a large impact when there was wind resulting from wind induced infiltration which was low for this building.

The time and cost involved in performing a model calibration study inevitably limits the scope, allowing presentation of results in the model for only small options between large building features, airflows, and contaminant concentrations which could be applied.

Future studies can address meteorological variations, active contaminants, or specialized situations such as ambient pollutant entry, small time scales, and non-trace contaminants.

ASTM Standard Guide 5157 provides a significant tool for statistical evaluation of multi-zone models, since different model applications require different levels of accuracy. Some studies include only averages of percent differences between measured and predicted values, reducing the amount of information on the effectiveness of the model at predicting airflows and concentrations, exaggerating large relative differences for small absolute values.

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