THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Influence of building envelope on indoor air quality

Field measurements, analysis, and method development related to indoor odors

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"Ideas are like rabbits.
You get a couple and learn how to handle them,
and pretty soon you have a dozen."
- John Steinbeck

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Abstract

The ventilation system should provide occupants with fresh air while removing excess pollutants from the building. However, increasing ventilation may inadvertently draw more pollutants into the occupant area or prove ineffective in altering emission rates from building materials and furnishings. If not addressed properly, this can make raising the ventilation rate inefficient, resulting in unnecessary heat losses or, in the worst case, reduced indoor air quality. This thesis addresses two previously insufficiently understood situations of contaminant transport within buildings, both manifested as unpleasant indoor smells: contaminant transport from adjacent compartments and early-stage emissions of air pollutants in new buildings.

The former, inspired by school buildings in Sweden demolished due to 'moldy' smells, was thoroughly explored in my Licentiate thesis, *Contaminant Transport by Air Infiltration from Crawl Space to Occupant Area-Numerical Simulations and Field Measurements in Swedish schools*, and is presented here as a summary.

The latter focuses on indoor air quality in new buildings, which often have initial high volatile organic compound (VOC) levels, typically perceived as a 'new smell.' In Sweden, it is common to run the ventilation system at full rate for several months as a remedy due to the negative effects of high VOC levels on occupants. However, the drawback of this strategy is the risk for overventilation with unnecessary energy losses. Two methods, 'VOC-passport' and 'Ventilation threshold', are developed to assess how ventilation can improve indoor air quality in more energy-efficient ways.

Results show that with VOC-passport, it is possible to simulate dynamic variations in VOC concentrations in new buildings based on passive VOC measurements and building physics modeling. With this method, it is possible to find an optimal ventilation strategy for low VOC concentrations and minimal energy losses. In addition, an analytical analysis of the diffusion of VOCs in materials shows that if ventilation rates exceed a certain threshold, further increases will not affect the emission rate. A quantified ventilation threshold is useful for setting the ventilation rate regarding optimal off-gassing and an important complement to the VOC-passport.

Keywords material emissions, indoor air quality, odor, VOC, ventilation

List of publications

Appended publications

This thesis is based on the following publications:

Paper I F. Domhagen, P. Wahlgren, C-E. Hagentoft, Method for Detecting Contaminant Transport through Leakages in a Condemned School In *International Building Physics Conference*, 2018.

Paper II F. Domhagen, P. Wahlgren, C-E. Hagentoft, Impact of weather conditions and building design on contaminant infiltration from crawl spaces in Swedish schools – Numerical modeling using Monte Carlo method *Building Simulation*, 2021.

Paper III F. Domhagen, S. Langer, A. S. Kalagasidis, Modeling VOC levels in a new office building using passive sampling and humidity measurements *Building and Environment*, 2023.

Paper IV F. Domhagen, S. Langer, A. S. Kalagasidis, Theoretical threshold for estimating the impact of ventilation on materials' emissions *Under review*.

Paper V F. Domhagen, S. Langer, A. S. Kalagasidis, Dynamics of VOC emissions from a new material *Under review*.

Notes on my contributions

The list below states my major contributions to each of the appended papers.

Paper I: I tested and developed a method for leakage search. I analyzed the results and drafted the manuscript in collaboration with my supervisors.

Paper II: I developed the infiltration model used in the simulations and performed all calculations. I analyzed the results and drafted the manuscript in collaboration with my supervisors.

Paper III: Measurements and planning of measurements were performed in collaboration with my supervisors. I developed the numerical model and performed the calculations. I analyzed the results and drafted the manuscript in collaboration with my supervisors.

Paper IV: The idea of a theoretical threshold was mine, and I derived the analytical model. I performed the calculations and made a comparison with the literature. I authored the manuscript in collaboration with my supervisors.

Paper V: Measurements and planning of measurements were performed in collaboration with my supervisors. I performed most of the analysis and authored the manuscript in collaboration with my supervisors.

Other relevant publications

These publications are relevant to the thesis, and I have authored or coauthored them during my PhD studies:

[a] A. S Kalagasidis, F. Domhagen, S. Langer, Early-stage concentrations of formaldehydes and TVOC in a new low-energy building
In *E3S Web of Conferences*, volume 172. EDP Sciences, 2020.
doi: 10.1051/e3sconf/202017206007.

[b] F. Domhagen, P. Wahlgren, C-E. Hagentoft, Pressure distribution around the thermal envelope – a parametric study of the impact from wind and temperature on contaminant transport within a building
In *E3S Web of Conferences*, volume 172. EDP Sciences, 2020.
doi: 10.1051/e3sconf/202017211004.

[c] F. Domhagen, P. Wahlgren, C-E. Hagentoft, Contaminant transport through the thermal envelope: Evaluation of airflows based on numerical modeling and field measurements
In *ASHRAE Topical Conference Proceedings*. ASHRAE, Inc., 2019.

Acknowledgments

This thesis summarizes my research conducted at the Division of Building Technology at Chalmers University of Technology. Under the guidance of two supervisory teams, I conducted two distinct research projects: contaminant transport by infiltration and emission in new buildings. The research was funded by the Swedish Energy Agency, SBUF, Formas, and Lokalförvaltningen in Gothenburg.

I would like to express my gratitude to all my supervisors who have supported me throughout my time as a PhD student. I am grateful to Paula Wahlgren and Carl-Eric Hagentoft for their support and guidance in pursuing my Licentiate degree. I would like to sincerely thank Angela Sasic Kalagasidis for her endless support, enlightening discussions on building physics, and for fostering my growth as a researcher. Additionally, I am deeply thankful to Sarka Langer for her efforts in bridging my knowledge gaps in chemistry, offering invaluable insights, and always being so positive and encouraging.

I am also grateful to Mia Alm at Lokalförvaltningen for her valuable insights and for granting access to several school buildings used for studies in both of my research projects. I am thankful to Per Löveryd, Olle Nyström, and their colleagues at Akademiska hus for making the office field measurements possible. Additionally, I appreciate Stefan Setterlund at Lokalförvaltning for providing me with data from the ventilation system.

I would also like to acknowledge and express my thanks to all my colleagues at the division. Thank you for all the coffee breaks with interesting discussions, sports activities during lunch breaks, support, and encouraging working environment. A special note of gratitude to Ali Naman Karim for being such a good friend, colleague, and roommate.

Above all, my deepest thanks go to my wife Malin and our two daughters, Hilde and Liv, for their unwavering love, joy, and support.

Fredrik Domhagen
Göteborg, September 2023

List of Symbols

A	area of emitting material, m^2
ACR	air change rate, h^{-1}
AH	absolute humidity, $\mathrm{g\,m}^{-3}$
AH*	model for concentration with a humidity dependent source, $\mu\mathrm{g\,m}^{-3}$
AH*-DE	model for concentration with a humidity dependent and decaying source, $\mu\mathrm{g\,m}^{-3}$
c	concentration, $\mu\mathrm{g\,m}^{-3}$
c_0	initial concentration, $\mu\mathrm{g\,m}^{-3}$
c_p	specific heat capacity of air, $\mathrm{J\,kg}^{-1}\,\mathrm{K}^{-1}$
c_s	concentration in supply air, $\mu\mathrm{g\,m}^{-3}$
DE	model for concentration with a decaying source, $\mu\mathrm{g\,m}^{-3}$
D_m	diffusion coefficient in the material, $\mathrm{m}^2\,\mathrm{s}^{-1}$
E	emission rate, $\mu\mathrm{g\,s}^{-1}$
K_{ma}	partition coefficient, 1
Q	heat flow, W
R^2	Pearson correlation coefficient, 1
R_a	ventilation rate, $\mathrm{m}^3\,\mathrm{s}^{-1}$
$RMSE$	root mean square error, 1
S	lumped source strength, $\mu\mathrm{g\,s}^{-1}$
S_i	source model parameters (i=1,2,3,4,5) determined by curve fitting
T	temperature, K or °C
t	time, s or h
t_c	time constant, s or h
$TVOC$	total concentration of VOC
V	volume, m^3
V_e	effective volume, m^3
VOC	volatile organic compound
x	distance, m
ρ_a	density of air, $\mathrm{kg\,m}^{-3}$

Contents

Part I

Summary

Chapter 1

Introduction

Inadequate indoor air quality can have detrimental impacts on health, work productivity, and overall perceptions of the indoor environment [1]. Numerous indoor pollutants, including volatile organic compounds (VOCs), ozone, radon, bacteria, and mold, contribute to this issue [2–5]. Among these pollutants, VOCs are generally considered to be one of the main pollutants [6] and may originate from various sources such as solvents, paints, aerosol sprays, furnishings, disinfectants, and building materials [7, 8]. Notably, some VOCs, such as formaldehyde and certain aldehydes, have a low odor threshold [9], which means they are sensed at low concentrations and may cause discomfort or annoyance among occupants. This, in turn, negatively influences how people perceive the indoor air quality. Some odorous contaminants, although not in harmful concentrations, can impact the cognitive performance of individuals within a building. Consequently, maintaining low levels of VOCs and other potentially unpleasant air pollutants generally leads to improved cognitive functioning and overall well-being among occupants [10–12].

The source of contaminants is sometimes related to the thermal envelope by emissions from materials or is influenced by the thermal envelope through its impact on contaminant transport from within the construction to the occupant zone. In addition, contaminants may be a result of elevated moisture levels or moisture damage [13–15]. In new buildings, there is often a characteristic ”new-smell”, caused by non-occupant related VOCs emitted from new building materials and products. This ”new-smell” is typically higher when the building is new and diminishes gradually to acceptable levels after several months [16–20].

The building owner is responsible for taking action when there are problems with indoor air quality, and increasing the ventilation rate is often the first measure taken [21]. For example, in new buildings in Sweden, it is common practice to run the ventilation system at full rate for 6-12 months to reduce the levels of ”new-smell”. However, such a general approach may not be the most efficient, depending on the nature and location of the contaminant source. Increasing the ventilation rate also increases energy loss, and may, in some cases, worsen the indoor air quality if it leads to more contaminants being

drawn into the occupant space.

To determine the optimal strategy (if the contaminant itself cannot be removed), it is crucial to consider the location and nature of the contaminant source. If the source is located in adjacent non-occupant areas of the building, for example, inside a crawl space or cold attic, the transportation of contaminants is affected by air infiltration and pressure distribution in the building [22–24]. Increasing the ventilation or adding another vent opening may therefore affect the indoor air quality in ways that are difficult to predict. In addition, the impact of air leakages in the building envelope on the operation of the ventilation system is rarely, if ever, addressed in practice (through the design or operation of the ventilation system).

As for elevated VOC levels in new buildings, excessive ventilation rates may not considerably impact emission rates, meaning that increased ventilation does not substantially reduce the off-gassing time [25, 26]. If the purpose of increased ventilation rates is to keep VOCs at acceptable levels, then intermittent ventilation may prove to be a better option, where ventilation rates are increased during occupancy hours and decreased during non-occupancy hours. However, the challenge with such a strategy is to determine appropriate ventilation rates and the duration of pre-ventilation time, which can vary from several minutes to several hours [27].

In office buildings, variable ventilation volume (VAV) systems are commonly used to reduce energy loss, with carbon dioxide (CO_2) often serving as a control signal to manage ventilation and decrease occupancy-related pollutants. However, CO_2 cannot effectively indicate non-occupancy-related pollutants [28] and is therefore not suitable as a control signal for the ventilation system when there is a need to reduce VOC levels related to material emissions. Further, modern ventilation systems sometimes come with real-time metal oxide semi-conductive (MOS) sensors that are capable of detecting various odorous VOCs generated by events, such as cleaning and cooking. However, these sensors are not designed to indicate the presence of specific harmful contaminants, as they cannot distinguish between different VOCs [29–31], and they react less strongly to emissions from building materials [30]. Although there are promising results for improving these sensors in the future [32, 33], the usability of the sensors available today is uncertain regarding monitoring VOC concentration decay from new materials in buildings.

A different approach to estimating the required ventilation rate is to model the emission levels dependent on the ventilation rate. Various methods have been proposed that utilize emission data from the National Research Council Canada (NRC) database rate [34–36]. For example, in a method proposed by Ye et al. [36] the ventilation requirement is divided into two steps: the first addresses initial high emission rates, while the second addresses lower long-term emissions. This division aims to prevent over-ventilation during later stages when emission rates have decreased. The authors acknowledge the importance of the material emission database as a valuable resource, but they note its limitations in terms of covering all materials available in the market. To enhance accuracy, the authors suggest obtaining more representative emission data encompassing a wider range of materials. Despite these uncertainties,

this study emphasizes the importance of considering material emissions when adjusting ventilation rates. However, continued research and improvements in emission data collection are essential for enhancing the precision and feasibility of such ventilation rate adjustments.

Rather than just arbitrarily increasing the ventilation rate when facing indoor air quality problems, it would be better to use mechanical ventilation together with knowledge about the thermal envelope in more resourceful ways so that issues with indoor air quality can be efficiently solved without unnecessary ventilation losses. Consequently, there is a need for practical methods that do not depend on knowledge about the physical properties of specific contaminants, which can be used to handle odorous emissions in new and old buildings.

1.1 Aim

The aim of my research is to investigate how the thermal envelope affects odorous contaminants in buildings. In particular, it addresses the relation between materials that can act either as contaminant sources or influence contaminant transportation within the building and ventilation. The aim of this research is divided into two topics: **contaminant transport by air infiltration** and **emissions in new buildings**. The first topic required investigation of how air leakage distribution, climate (wind and temperature), and ventilation affect the transportation of contaminants within the building. This work was carried out and thoroughly discussed in my Licentiate thesis and is presented here as a summary in Chapter 2. The second topic required an investigation of the relation between ventilation and VOC emissions, ”new-smell”, in new buildings, and development of a feasible method for dealing with early VOC emissions in new buildings. This topic is the focus of this thesis.

In addition, for both topics, there is a focus on applicability in real-world situations. Since there is a need for practical methods for dealing with odorous emissions in buildings, the developed methods aim to be feasible in practical situations.

Figure 1.1 shows an overview of my research project and illustrates the separation of the two topics. The right-hand side of Figure 1.1 shows the focus of this thesis.

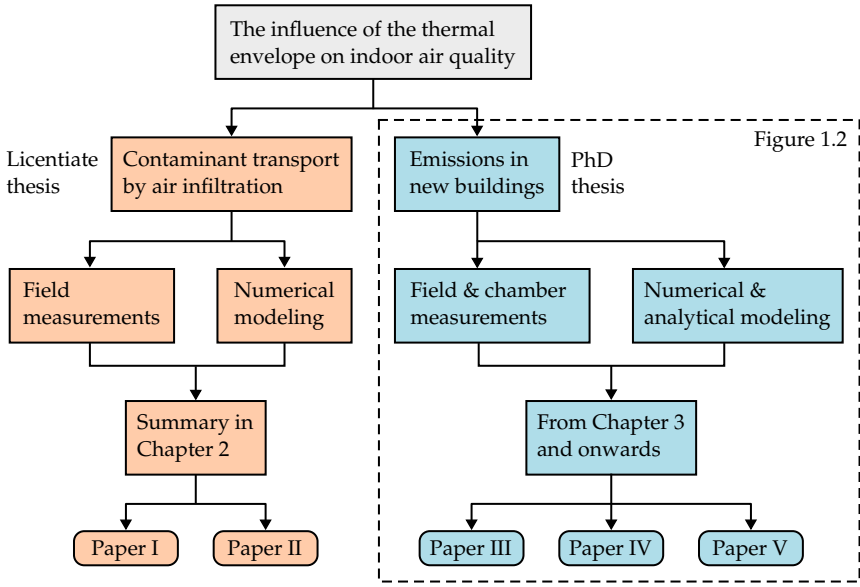

Figure 1.1: Overview of my research. The dashed rectangle marks the work that is the main focus of this thesis.

1.2 Scope

The scope of this thesis can be separated into the following topics:

- Development of a method, **VOC-passport**, that combines passive measurements of VOCs with temperature, humidity, and ventilation measurements to calibrate a numerical method that predicts VOC concentration dependent on ventilation rates.
- Development of an analytical model that can be used to determine a **theoretical ventilation threshold** from which increased ventilation does not considerably increase emission rates.

For an overview of the scope and methods, see Figure 1.2.

1.3 Methodology

The work in this thesis is based on various methods that can be divided into two distinct categories:

- **Measurements** in the field and test chamber
- Numerical and analytical **modeling**

For measurements of VOC concentrations in the office building, Figure 1.3, I used passive sampling in accordance with ISO standards [37, 38], which

provides average concentrations of individual VOCs over several days. There are two major motivations for using this method. First, the method is well known and standardized in the ISO-standard, which means that it is easily implemented in practical situations. Second, measuring average concentrations over several days means that steady long-term emissions from materials are captured, while stronger, short-term emissions are averaged out. This is further described and discussed in Section 3.1.

In the field measurements, supply air flows and temperature and humidity levels in the rooms, were conveniently measured using loggers integrated into the ventilation system.

For measurements of VOC emissions from the new carpet inside the test chamber (Figure 1.3), I used passive and active sampling in accordance with ISO standards [37–40]. While passive sampling, as described above, is useful for capturing long-term emissions, active sampling is used instead to capture the initial decline in emission rate that is typically observed for new materials.

The pressure drop across a damper in the exhaust ventilation channel was used to calculate the ventilation exhaust rate, and a combined humidity and temperature logger was used for measuring temperature and humidity.

To derive the analytical equations, I used mathematical analysis, aided by the symbolic computation functionalities in MATLAB [41] and MATHCAD [42]. All numerical computations were performed in MATLAB [41].

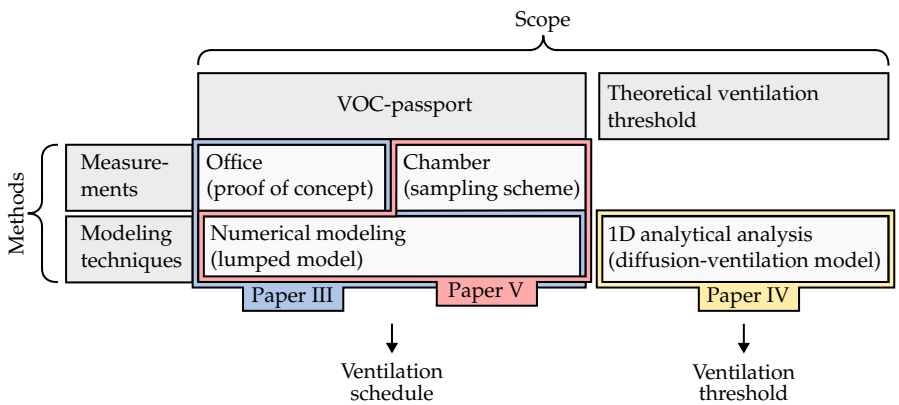

Figure 1.2: Overview of the scope and methods of the thesis.

Figure 1.3: Left: exterior and interior photos of one of the office rooms. Right: photo of the inside of the test chamber.

1.4 Limitations

The VOC emissions in this thesis are non-occupant related and are emitted by new materials. VOCs are not targeted for their potential negative health effects or how common they are in new buildings. Likewise, the health effects associated with elevated VOC levels are not considered. Specific VOCs are analyzed when they are suspected of working as indicators (or signals) for material emissions in a room. Mechanical ventilation rates are measured either as supply or exhaust ventilation. However, air leakage is not measured but is estimated based on experience and is included in the calculation of the total air change rate. The influence of temperature on emission rates is limited to air temperature. The concentration of VOC in the air supply was assumed to be negligible in the field measurements.

1.5 Thesis outline

Chapter 2 summarizes my Licentiate thesis, *Contaminant Transport by Air Infiltration from Crawl Space to Occupant Area: Numerical Simulations and Field Measurements in Swedish Schools*. This work focuses on contaminant transport from crawl spaces up to the occupancy area and how this transport is influenced by temperatures, wind, ventilation, and air leakage distribution. Two papers from the Licentiate thesis are also appended to this thesis, **Paper I** and **Paper II**.

In Chapter 3, I present the two sampling techniques, passive and active sampling, and the source and lumped models used in **Paper III** and **Paper V**. VOC-passport method and results from field measurements, based on **Paper III**, are described in Chapter 4. In Chapter 5, I present the work from **Paper IV** in which an analytical model that describes the relation between ventilation and emissions rates is developed. Chapter 6 describes the work in **Paper V**, where emissions from a new carpet are measured inside a test chamber. In Chapter 7, I discuss the work presented in Chapter 3-6 along with some ideas for improvement and further development. Conclusions

and suggestions for future research are listed in Chapter 8 and Chapter 9 respectively.

Chapter 2

Contaminant transport by air infiltration

Background

Some Swedish school buildings built in the 1960s and 1970s have indoor air quality problems. Poor indoor air quality is usually perceived as a bad odor and causes discomfort among pupils and teachers. Unfortunately, in many cases, it is difficult to find efficient solutions because the source of the problem is unknown. Many problematic schools are built with a crawl space foundation; the contaminant source is often suspected to be inside the crawl space.

Several types of contaminants, such as VOCs, bacteria, and radon, may be found in the indoor air in schools [2]. If the source of the contaminants is inside the crawl space and if there is a positive pressure difference across the floor construction, this can lead to an increased risk of indoor air quality problems on the first floor [22].

Increasing ventilation rates is often the first measure taken for any building with indoor air quality problems [21]. In buildings with crawl spaces, it is common to install an exhaust fan in the crawl space to prevent contaminated air from leaking into the classroom. Unfortunately, these measures do not always work, and sometimes the building is excluded of service for some time before being demolished.

Investigations on how wind, temperature, mechanical ventilation, and the thermal envelope affect indoor air quality and contaminant transport from crawl spaces to classrooms are performed in a series of four research papers [43–46]. The findings are summarized in my Licentiate thesis *Contaminant Transport by Air Infiltration from Crawl Space to Occupant Area: Numerical Simulations and Field Measurements in Swedish Schools* [47].

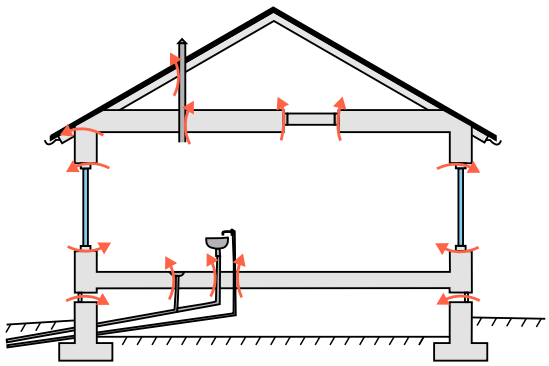

Figure 2.1: Principle drawing showing potential leakage paths in a building with a crawl space.

Methods

Leakage search with dry ice, or the ”icebox method”, is a method in which frozen carbon dioxide (dry ice) is used to determine if air leakage into the classroom originates from the crawl space or not. Solid carbon dioxide turns into a gaseous phase in which the gas is used as a tracer gas that is easily detected by measurement devices. This method proved useful for determining whether air leakage was coming from the crawl space or from elsewhere. The method is described in more detail in **Paper I**.

Simulations of contaminant transport through leakages were performed using a numerical infiltration model developed in the numerical computing platform MATLAB [41]. The purpose of this study was to investigate how the pressure difference across the floor construction and contaminant concentrations are affected by temperature, wind, and air permeability distribution. The model was used to investigate correlations between model parameters, such as air permeability and temperature, and to analyze measures, such as increased ventilation or use of an exhaust fan in the crawl space. I conducted investigations both as a case studies, [46], and also with Monte Carlo method described in **Paper II**. The purpose of the Monte Carlo simulations was to quantify the probability of impact on the concentration and pressure difference as the input parameters changed. In addition, I conducted field measurements of temperature, wind, and pressure differences across the floor construction between the classroom and the crawl space in two different school buildings.

Results and conclusions

The following paragraphs present the main results and conclusions.

Increasing mechanical ventilation is often the first measure taken when there are indoor air quality problems. However, increasing the ventilation rate may worsen the problem, depending on the air leakage distribution

and ventilation rates. Figure 2.2 shows the normalized concentration in the classroom and the normalized contaminant flow from the crawl space plotted against the exhaust ventilation for one building. In this example, the flow of contaminants reaches a maximum at approximately 1.1 $\mathrm{L\,s^{-1}\,m^{-2}}$; after that, increased ventilation will not draw more contaminants into the classroom and the concentration starts to decrease. This is only an example; however, it clearly shows that increased ventilation can lead to drawing more contaminants into the occupancy area and may also reduce contaminant levels.

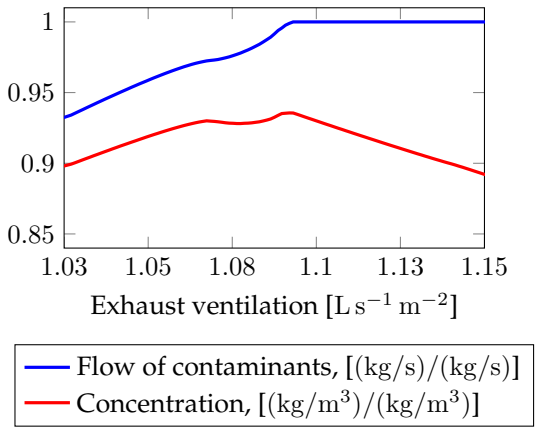

Figure 2.2: Contaminant flow through the floor construction and concentration of contaminants in the classroom plotted against increased mechanical exhaust airflow from the classroom. In this example, a ventilation of 1.03 $\mathrm{L\,s^{-1}\,m^{-2}}$ is based on the ventilation requirement for schools.

The Monte Carlo simulations show that concentrations increase in 17 % of the cases in the Gothenburg climate and in 24 % of the cases in the Östersund climate when exhaust ventilation is increased from 320 $\mathrm{L\,s^{-1}}$ to 330 $\mathrm{L\,s^{-1}}$. Therefore, it is important to measure the pressure difference across the floor construction when increasing the mechanical ventilation to ensure that the pressure difference does not increase. This must be done while measuring the pressure differences across the floor construction.

The impact of wind and temperature on pressure differences across floor constructions are investigated. The results show that the stack effect is an important driving force for pressure differences across floor construction, even in buildings with only one floor (and a crawl space). If there is no mechanical exhaust ventilation in the crawl space, there will be a positive pressure difference across the floor construction in relation to the occupancy area, during the majority of the heating season.

Moreover, wind affects the pressure difference, typically in the range of -2 Pa to +1 Pa depending on the building shape and wind direction. However, the wind also increases the air change rate in the building, which leads to decreased concentrations in the occupancy area.

Installing an exhaust fan in the crawlspace is a common measure for controlling the pressure difference. Simulations show that the exhaust fan should be adjusted to achieve a pressure difference of at least -5 Pa to ensure a negative pressure when the weather changes. However, the pressure difference is quite sensitive to changes in the airtightness of the crawl space; therefore, any additional openings after the fan has been adjusted may reduce the pressure difference considerably. Therefore, along with continued maintenance of the crawl space, it is important to maintain its airtightness, with monitoring the pressure differences across the floor. In cold climates, it is advisable to adjust the exhaust fan during chilly days when the stack effect is stronger. If this is not done, the negative pressure sustained by the exhaust fan may be reduced if the outdoor temperature drops.

Concluding remarks

When trying to solve indoor air quality problems where the contaminant source is suspected to be inside an adjacent compartment, such as a crawl space, it is important to account for the stack effect and air leakage distribution when taking any measures. For example, increased ventilation may worsen the problems if the pressure difference across the floor is not monitored, and exhaust ventilation may work only temporarily if the stack effect is not accounted for or if the airtightness changes.

Chapter 3

VOC measurements and modeling

This chapter describes the methods used for measuring VOC concentrations in the field and in the test chamber. In addition, the source and lumped models used in VOC-passport and for the analysis of measurement results are described.

3.1 Devices and sampling techniques

I use two sampling techniques, *active sampling* for measuring the average concentration during a few hours or less and *passive sampling* for measuring average concentrations over five to seven days. The main difference between the two methods is that with active sampling, an air pump pumps air in the room through the sampling tube, while passive sampling is based on diffusion principles.

VOCs were passively sampled on Tenax TA adsorbent tubes and analyzed according to ISO 16017-2 [37]. Aldehydes were passively sampled using DSD-DNPH Aldehyde Diffusive Sampling Devices and analyzed according to ISO 16000-4 standard [38]. Figure 3.1 shows the passive samplers as they are installed during the measurement. For active sampling, VOCs were collected on Tenax TA adsorbent tubes (Perkin Elmer) for 30 minutes using an air flow of 150 $\mathrm{mL/min}$ in accordance with ISO 16000-6 [40]. Aldehydes were sampled on Sep-Pak XpoSure Aldehyde Sampler according to ISO1600-3 standard [39] for 2 hours with an air flow of 1.5 $\mathrm{L/min}$. For passive sampling, VOCs were sampled on Tenax TA adsorbent tubes (Perkin Elmer) and analyzed according to ISO 16017-2 [37]. Aldehydes were sampled using DSD-DNPH Aldehyde Diffusive Sampling Devices (Supelco, Bellefonte, PA) and analyzed according to ISO 16000-4 [38]. After the sampling, both active and passive, the Tenax tubes were thermally desorbed and analyzed by gas chromatography/mass spectrometry (GC/MS), while analysis of the aldehydes included solvent extraction and liquid chromatography.

To determine of the air concentration of the target compounds, information about sample volumes and the compounds' masses is required. The volume in the active sampling was determined straightforwardly from the known air flow rate and sampling time. A diffusive uptake rate in $\mathrm{mL\,min^{-1}}$ is required for determining of the volume in passive sampling. The uptake rates are available from the literature, and the time is based on the start and stop times for the exposure of the respective sampler to air containing the air pollutants.

The VOCs were quantified as total volatile organic compounds (TVOCs) as toluene equivalents using the uptake rate and the response factor for toluene. Terpenes, α-pinene, 3-carene, and limonene were quantified using their compound-specific uptake rates and response factors. The uptake rate for 4-phenylcyclohexene was estimated from a comparison of the concentrations achieved by active and passive sampling and the known uptake rate of toluene, Section 6.2. The response factor for 4-phenylcyclohexene was determined by a targeted calibration. Quantification of the aldehydes was based on the uptake rates reported in the literature [48] and response factors from in-house calibration.

Figure 3.2 illustrates the principal difference between passive and active sampling. Passive samplers, collect VOCs for several days (5–7 days), and consequently, the analysis of the passive samplers gives the average concentration during the entire sampling period.

Emissions from materials, some time after a material has been introduced into a room and the initial easily accessible VOCs have been emitted, are relatively stable with a slow and continuous emission rate (compared to other types of sources). The benefit of passive sampling is that it captures continuous emissions that act over long timespans such as emissions from materials, while temporary sources, caused by humans are averaged out.

As shown in Figure 3.2, active sampling is performed for a shorter time, such as a few hours or less. This makes active sampling more useful for capturing faster more dynamic changes in concentration; for example, the initial decline in concentration shortly after a new material is introduced into a room.

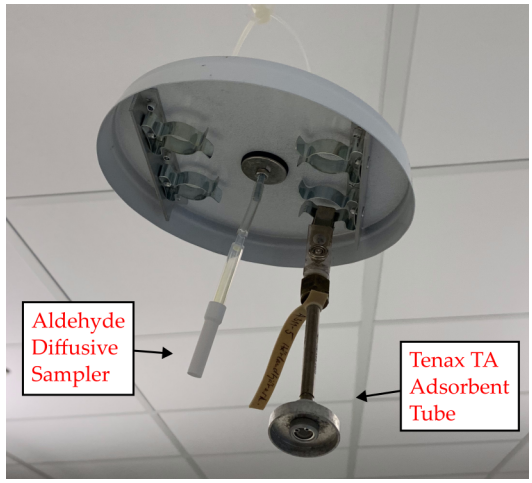

Figure 3.1: Photo of passive samplers installed underneath the ceiling during field measurements.

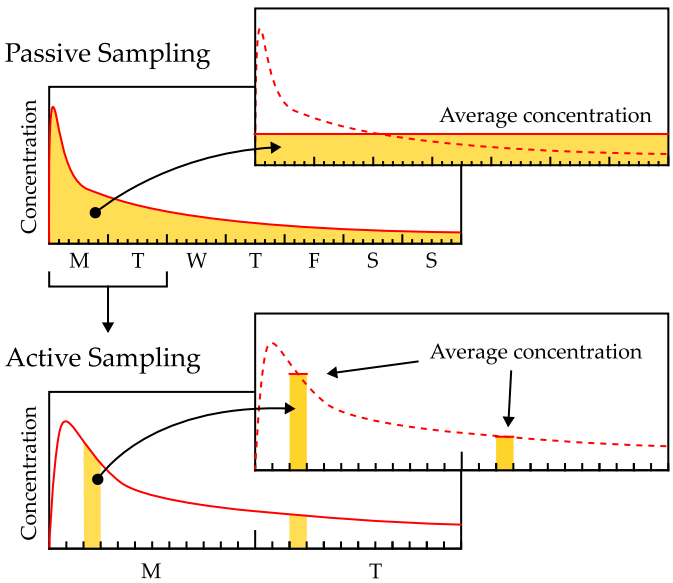

Figure 3.2: Illustration of the different timescales for which passive and active sampling are used.

3.2 Numerical models

The decline of VOC concentrations in newly constructed buildings is non-linear and depends on internal diffusion within the emitting material [49]. In addition, porous materials that absorb VOCs attenuate concentration fluctu-

ations in a room [50, 51]. Both these effects are of interest when modeling VOC concentrations in new buildings and should be accounted for depending on the timescale of interest.

There are generally two different types of models used to predict VOC concentrations in the indoor air, nonphysical and physical sound models. Nonphysical models are used to describe statistical regularities derived from measurements, for example, auto-regressive moving averages [52]. The major drawback of such models is the lack of transferability among different conditions, for example, when the geometry is changed in relation to the original experiment. Physical models are instead based on some fundamental physical processes in which material properties are determined from experiments. With physical models it is therefore possible to assess the levels of VOCs in a room even as conditions change.

Physical models vary in complexity. In less complex models, VOC is contained in gaseous form in the air in a room and is balanced against source and sink terms that are constant or vary depending on, for example, temperature. These models are, in this thesis, referred to as lumped models, meaning that the VOC concentration in the room depends only on time, while spatial variations are ignored. It is then possible to represent the VOC concentration in the room in a single point.

In addition, there are more complex models that utilize Fick's second law to describe the diffusion of VOCs inside materials (such as the model described in Chapter 5).

This chapter briefly describes the physical models used in **Paper III** and **Paper V**.

Models for the emission rate

The rate at which a material releases VOC is influenced by the temperature and humidity present in the room, where higher temperature or humidity results in increased emission rates [53, 54]. The effects of temperature and humidity are studied in **Paper III** and **Paper V**. The following expression relates the emission rate to temperature and humidity:

$$S\left(T, AH\right) = S_1 T^{0.75} \exp\left(S_2 AH - \frac{S_3}{T}\right) \tag{3.1}$$

where S_1, S_2, and S_3 are parameters determined by fitting the measured data.

Equation 3.1 was proposed by J. Xiong et al. [53]. However, in the original expression, humidity is expressed in terms of relative humidity rather than absolute humidity.

In **Paper III**, the results show no significant difference in terms of correlation between using relative humidity and using absolute humidity as input to Equation 3.1. Absolute humidity is therefore used as input because in contrast to relative humidity, it is decoupled from temperature. This simplifies analysis because the influences of temperature and humidity are easier to separate.

In addition, if the temperature variation (in degree Kelvin), as in the field measurements in **Paper III**, is relatively small compared to the variations in

absolute humidity, the effect of temperature may be ignored:

$$S\left(AH\right) = S_1 \exp\left(S_2 AH\right) \tag{3.2}$$

Emissions from new materials may exhibit both long-term and short-term characteristics. In the early stages, the release of VOC near the material surface results in high emission rates. This process is relatively brief, typically taking a couple of days to a couple of weeks, making it a short-term source [17, 55, 56]. However, VOC emissions originating from deeper within the material are hindered by diffusion, leading to lower emission rates that occur over several months [36]. The double exponential model describes both long-term and short-term emissions [55, 57]:

$$S\left(t\right) = S_1 \cdot \exp\left(-S_2 \cdot t\right) + S_3 \cdot \exp\left(-S_4 \cdot t\right) \tag{3.3}$$

where S_1, S_2, S_3, and S_4 are parameters determined by fitting the measured data.

VOC model for a ventilated space

The mass balance for VOC in a single room with a lumped source strength at a constant ventilation rate:

$$V_e \frac{\partial c}{\partial t} = R_a \left(c_s - c\right) + S \tag{3.4}$$

The solution of Equation 3.4 for a time-independent source is well known and reads:

$$c(t) = c_0 \cdot \exp\left(-\frac{R_a}{V_e}t\right) + \left(\frac{S}{R_a} + c_s\right)\left(1 - \exp\left(-\frac{R_a}{V_e}t\right)\right) \tag{3.5}$$

The effective volume, V_e, describes the total VOC short-term storage capacity, as the concentration in the room varies and includes buffering in both the indoor air and materials inside the room. This approach is analogous to the moisture buffering volume of a ventilated space [58, 59]. Each VOC may have different buffering properties; consequently, the effective volume may have different values for different VOCs inside the same room.

For the remaining equations we assume that the concentration of VOC in the supply air is negligible, c_s=0. In reality, background concentrations are never zero. However, because these models are adjusted based on measured values, any existing background concentration will be handled indirectly by the source term.

At steady state, Equation 3.5 becomes:

$$c = \frac{S}{R_a} \tag{3.6}$$

By substituting Equation 3.2 into Equation 3.5, we obtain an expression for the concentration in a ventilated space with a source that is humidity

dependent:

$$c(t) = c_0 \cdot \exp\left(-\frac{R_a}{V_e}t\right) + \frac{S_1 \exp\left(S_2 \cdot AH\right)}{R_a}\left(1 - \exp\left(-\frac{R_a}{V_e}t\right)\right) \tag{3.7}$$

Similarly, by substituting Equation 3.1 into Equation 3.5, we obtain an expression for the concentration in a ventilated space with a source that is temperature and humidity dependent. For a series of input data with varying temperature, humidity, and ventilation rate for each time-step the solution is expressed as:

$$\begin{aligned} c_i = c_{i-1} \cdot \exp\left(-\frac{(R_a)_i}{V_e}\Delta t\right) + \\ + \frac{S_1 \cdot T_i^{0.75} \exp\left(S_2 \cdot AH_i - S_3/T_i\right)}{(R_a)_i}\left(1 - \exp\left(-\frac{(R_a)_i}{V_e}\Delta t\right)\right) \\ i = 1, 2, ...N \end{aligned} \tag{3.8}$$

Here, Δt is the length of the time step and i is the index for each step and its corresponding temperature, absolute humidity, and ventilation rate.

As with Equation 3.4, an expression for the concentration in a ventilated space can also be derived for a time-dependent double exponential decay source. The solution is found by substituting Equation 3.3 into Equation 3.4 and solving the following equation (here the initial concentration is set to zero, $c_0 = 0$):

$$\begin{aligned} c(t, AH) = \Bigg[& S_1 \frac{\exp\left(-\frac{R_a}{V_e}t\right) - \exp\left(-S_2 t\right)}{V_e\left(S_2 - \frac{R_a}{V_e}\right)} \\ & + S_3 \frac{\exp\left(-\frac{R_a}{V_e}t\right) - \exp\left(-S_4 t\right)}{V_e\left(S_4 - \frac{R_a}{V_e}\right)} \Bigg] \cdot \exp\left(S_5 AH\right) \end{aligned} \tag{3.9}$$

If we ignore the influence of humidity on the emission rate, Equation 3.9 is simply:

$$\begin{aligned} c(t) = & S_1 \frac{\exp\left(-\frac{R_a}{V_e}t\right) - \exp\left(-S_2 t\right)}{V_e\left(S_2 - \frac{R_a}{V_e}\right)} \\ & + S_3 \frac{\exp\left(-\frac{R_a}{V_e}t\right) - \exp\left(-S_4 t\right)}{V_e\left(S_4 - \frac{R_a}{V_e}\right)} \end{aligned} \tag{3.10}$$

Chapter 4

VOC-passport

This chapter presents VOC-passport and results from field measurements conducted in a new office building. This chapter is based on **Paper III**. For an overview of its relation to the scope and methods of this thesis, see Figure 4.1.

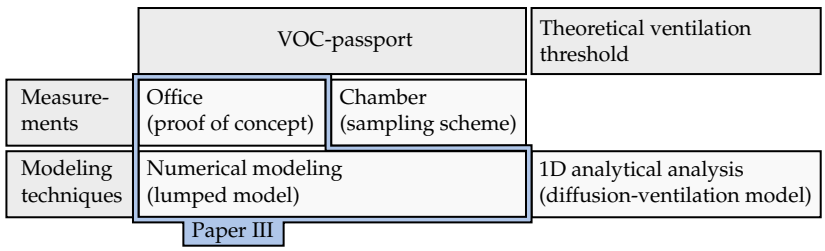

Figure 4.1: Paper III in relation to the scope and methods of the thesis.

Establishing an optimal ventilation rate (or ventilation schedule), considering energy consumption and emissions from materials, is a complex task that requires and understanding of the relationship between emission rates, buffering capacity, and ventilation rates within a room. The idea behind VOC-passport is to combine on-site measurements of early-stage VOCs with numerical simulations to predict how VOC concentrations change with changes in ventilation rate. Measurements using passive samplers are performed shortly after a new building is constructed, and the results from the measurements are used to calibrate a numerical model. A successfully calibrated model is then used to optimize a ventilation strategy for the building, so that VOC concentrations are maintained at acceptable levels with minimal ventilation losses.

The result from measurements and a successfully calibrated model is a certificate or passport for the building providing information on how material-related VOC concentrations relate to ventilation rates and how the building should be ventilated to achieve the desired VOC levels. Figure 4.2 shows an overview of the method including the following steps:

1. Temperature, absolute humidity and ventilation airflow rates are measured using sensors built into the ventilation system, and VOCs are measured using passive samplers as described in Section 3.1.

2. The average temperature, average absolute humidity, and median ventilation airflow rates are calculated for each sampling period, where a sampling period is the period during which passive samplers were used.

3. The source model, Equation 3.1, is calibrated by fitting against the lumped source strengths calculated from the measured VOC concentrations using Equation 3.6.

4. Model parameters (initial concentration and effective volume) in Equation 3.8 are determined by fitting simulation output to measured VOC concentrations.

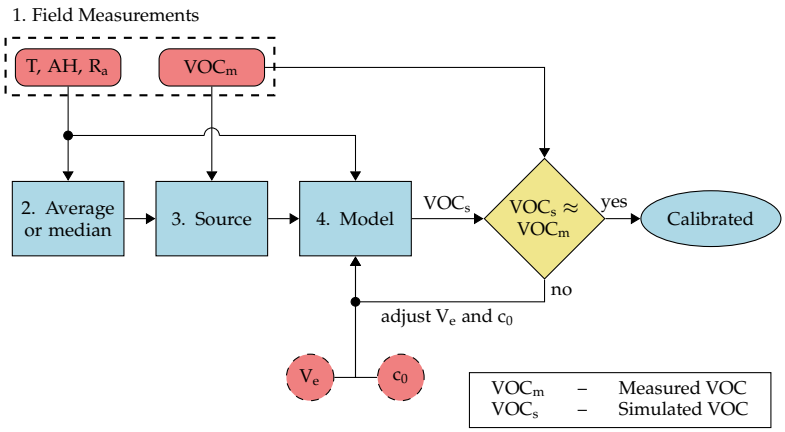

Figure 4.2: Flowchart showing an overview of the VOC-passport method.

4.1 Results of field measurements

This section presents results from field measurements conducted in one of two meeting rooms inside a new office building. Temperature, humidity, and ventilation rates are measured by sensors built into the ventilation system, while VOC concentrations are measured with passive samplers. For a complete description of the building, the reader is referred to **Paper III**. Figure 4.3 shows the results from the measurements of TVOC (total concentration of VOC), formaldehyde, aldehydes, terpenes, supply airflow, and absolute humidity in one of the rooms (room 2 in **Paper III**).

During sampling period 2, the ventilation rate is set close to zero, which results in a higher concentration during that period. The idea of having a clear peak in the VOC concentration was to facilitate finding an effective volume, V_e, for the room to use in the concentration model, Equation 3.8. This is to avoid

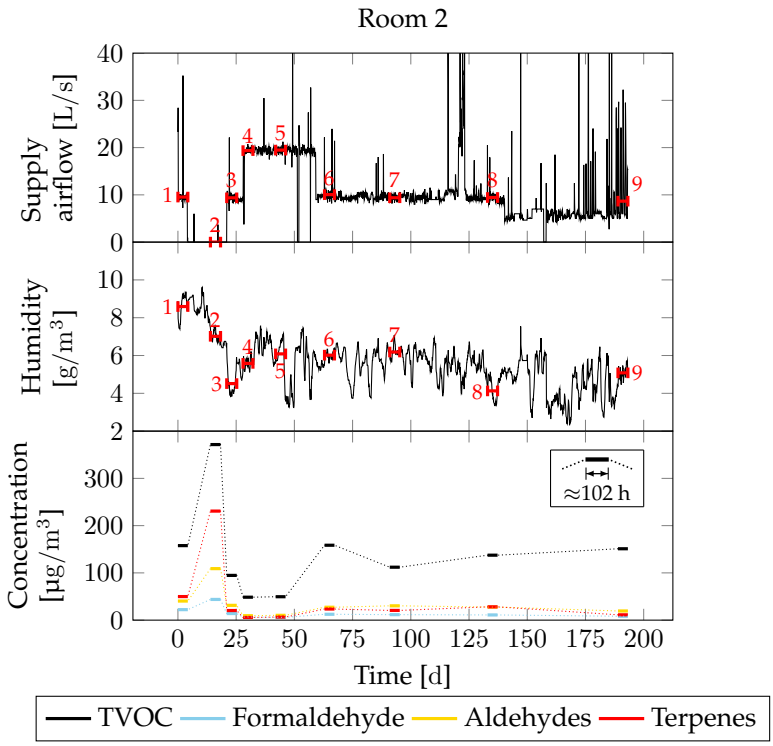

Figure 4.3: Measured supply ventilation, humidity and measured VOC concentrations in room 2. Sampling periods are numbered from 1 to 9. The horizontal bars show the measured average concentration during each measurement period and the dashed lines, between each measurement, are added to visualize trends. The length of each measurement period is 4 days and 6-8 hours (≈102 h).

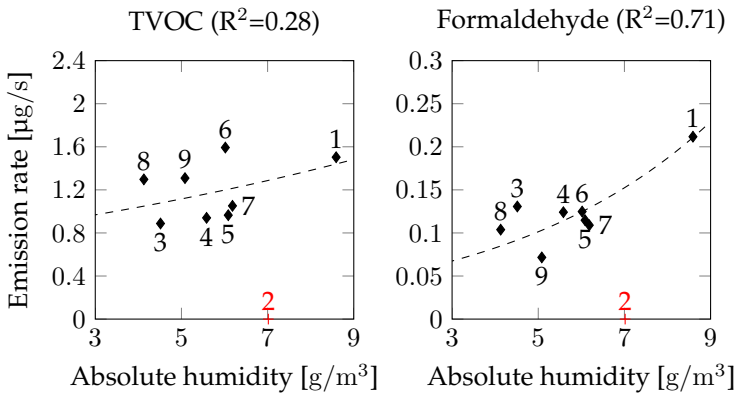

Figure 4.4: Calculated source strengths plotted against absolute humidity with model predictions for TVOC and formaldehyde. Dots are calculated using Equation 3.6, and the dashed line is calculated using Equation 3.1.

having only measurement periods where the concentration is in a steady state throughout the majority fo the time of the measurement. Moreover, having non-steady state measurements facilitates capturing the dynamic changes in concentrations.

Source strengths are calculated from measured data, formaldehyde, TVOC, temperature, absolute humidity, and ventilation rates. First, emission rates are calculated based on the median ventilation rate for each measurement period using Equation 3.6, with the assumption that there is no background concentration. Then, the coefficients S_1, S_2 and S_3 in Equation 3.1 are found by curve fitting using the function *fit()* in MATLAB [41]. The resulting function describing the emission rate dependent on temperature and absolute humidity with the emission rates (calculated from measured concentrations) shown in Figure 4.4. To simplify the visualization, and because the variation in temperature was relatively small compared to variations in humidity, emission rates in Figure 4.4 are plotted with the average temperature for the respective measurement period as input.

Further, the second measurement (the red cross in Figure 4.4, left and right) is excluded in the calculations. During this period, the ventilation rate was reduced to close to zero, and the source strength could therefore not be described using Equation 3.1.

The next step in VOC-passport is to calibrate the model by determining the unknown coefficients c_0 and V_e in Equation 3.8. This is done using the Global Optimization Toolbox in MATLAB to minimize the difference between the model output and the measured VOC concentrations. As shown in Figure 4.5, the measured concentrations are plotted together with the predicted concentrations of formaldehyde. The black line is the predicted concentration in the room, the blue lines represent the average predicted concentrations, and the red lines represent the measured concentrations.

The second measurement period had a relatively low ventilation rate,

which means that airflows that were not measured, such as air leakage, became a larger share of the total ventilation, which increased the sensitivity of the assumed air leakage. This measurement period, was therefore excluded when calibrating the model.

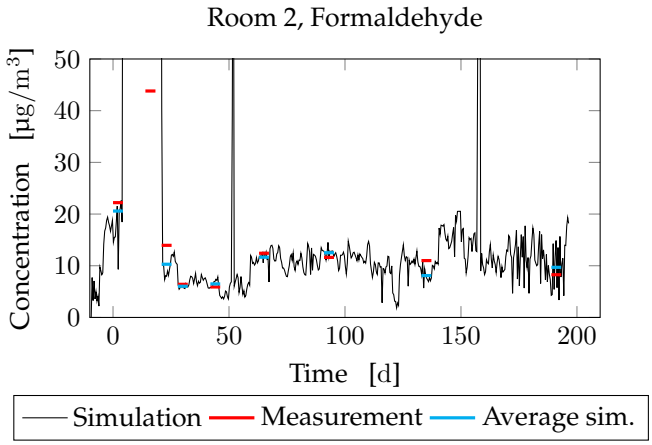

Figure 4.5: Model prediction and measured aldehyde concentrations. Input parameters: c_0=0 $\mu g/m^3$, V_e=37 m^3 and fitting degree: R^2=0.89.

4.2 Optimized ventilation – Example

With a known VOC storage capacity (effective volume, V_e) and a known source strength, the change in concentration in response to a change in ventilation rate can be simulated using Equation 3.8. The long-term exposure (1 year) of formaldehyde should not, according to the indoor air quality guidelines published by *Public Health England*, exceed 10 $\mu g\, m^{-3}$ [60]. To show how the calibrated model can be used to reduce ventilation losses while not exceeding a certain concentration, this value is used as an upper limit during office hours. Figure 4.6 shows a ventilation schedule where ventilation is increased during office hours and reduced outside office hours. This example shows how information about the buffering capacity of a room in relation to its emission rates can be used to determine the pre-ventilation time needed to keep formaldehyde levels below a certain limit if an intermittent ventilation schedule is used.

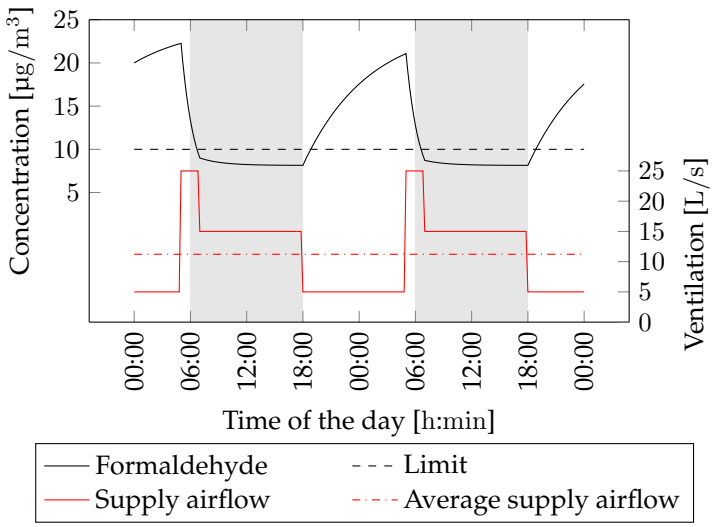

Figure 4.6: Example of optimized ventilation schedule to keep formaldehyde levels below 10 $\mu g\,m^{-3}$ during occupancy hours.

4.3 Potential energy savings

An estimation of the ventilation heat losses can be made using the following equation:

$$Q = (T_i - T_e) \cdot R_a \cdot \rho_a c_p \cdot (1 - \eta) \tag{4.1}$$

If we, for example, assume the following: indoor air temperature, T_i = 21°C, outdoor air temperature, T_e = -10°C and the efficiency of the heat recovery system, η = 75%, then, in the case where the ventilation is running at full rate (25 $L\,s^{-1}$) for 24 hours the total heat loss is 5.6 $kW\,h$. Assuming the same air temperatures, in the case of ventilation following the schedule shown in Figure 4.6, the total heat loss for 24 hours is 2.5 $kW\,h$. This is a reduction in ventilation heat loss of approximately 55% when using the VOC-passport method rather than running the ventilation at full rate.

Chapter 5

Theoretical ventilation threshold

In new buildings, ventilation is generally increased for reducing VOC concentrations to acceptable levels and increasing off-gassing of VOCs for faster depletion of emission sources [25]. However, the results from the literature are inconsistent regarding the latter. Studies have reported that increased ventilation increases off-gassing [61–63], but there are also studies reporting that off-gassing remains unchanged as the ventilation increases [25].

This chapter is based on **Paper IV** which presents an analytical model that can be used to study the relations among the emitting area, ventilation rate, time, and diffusivity of emitting materials. Figure 5.1 shows an overview of the paper in relation to the scope and methods of this thesis.

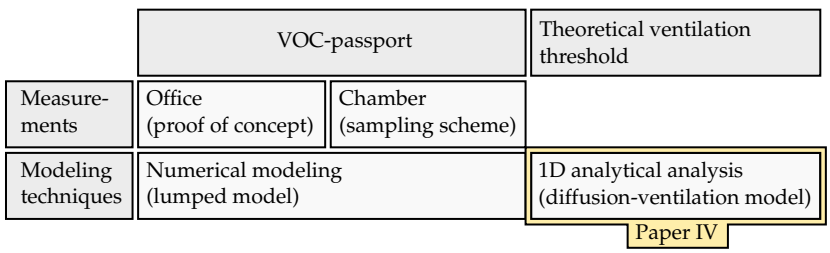

Figure 5.1: Paper IV in relation to the scope and methods of the thesis.

The mass transfer of VOCs between porous materials and indoor air depends on various physical processes. These processes include boundary diffusion, internal diffusion within the materials, and sorption at the interfaces between solid surfaces and air [64]. Sorption, in particular, involves microscopic mass transfer between a solid surface and the surrounding air, and its efficiency relies on the characteristics of both the adsorbate (VOC) and the adsorbent (material) [64].

Several mathematical models that account for diffusion and sorption in

porous materials have been developed [65]. The model developed in this chapter is based on the widely employed c_0-K-D model.[66–71] This choice is made due to the model's ability to offer a sufficiently precise depiction of VOC transport and storage while facilitating mathematical derivations.

5.1 Analytical model

The following assumptions are made while deriving the analytical model: the emitting material is assumed to be homogeneous and semi-infinite, diffusion within the materials is assumed to be one dimensional, the VOC emitted from the material is assumed to be well-mixed with the air in the room, and the storage capacity of the air in the room is ignored. Figure 5.2 shows a graphical representation of the model.

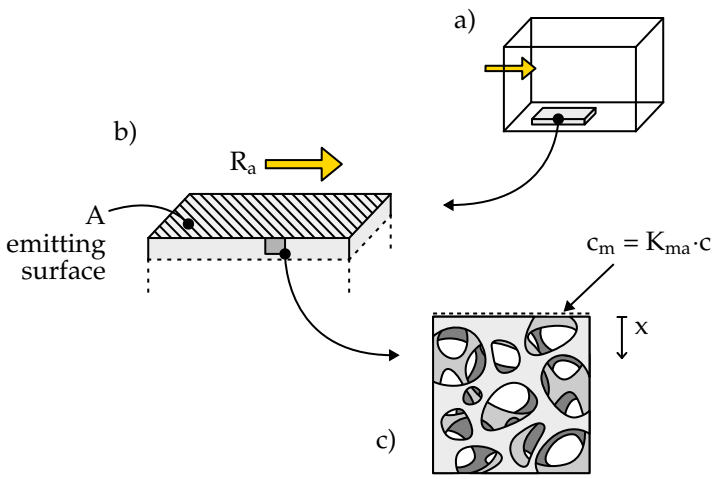

Figure 5.2: Graphical representation of the model. a) material placed inside a ventilated room; b) emitting surface area; c) internal surface area and interface between material and air.

The one-dimensional diffusion of VOCs in a homogeneous material is described using Fick's second law:

$$D_m \frac{\partial^2 c_m}{\partial x^2} = \frac{\partial c_m}{\partial t} \tag{5.1}$$

At the material–air interface, VOCs exist interchangeably in both the air and material phases. Because of the different reference volumes in the (porous) material and air, the corresponding VOC concentrations are linked by the partition coefficient K_{ma}:

$$c_m(t)|_{x=0} = K_{ma} \cdot c(t) \tag{5.2}$$

The initial concentration in the material and air is denoted as c_0:

$$c_m(x,0) = c_0 \tag{5.3}$$

The Robin boundary condition at the surface of the material in contact with the indoor air is expressed as follows:

$$-D_m \frac{\partial c_m}{\partial x}\bigg|_{x=0} + \frac{R_a}{A}\frac{c_m}{K_{ma}}\bigg|_{x=0} = \frac{R_a}{A}c_s \tag{5.4}$$

The concentration at infinite depth equals the initial concentration:

$$c_m(\infty, t) = c_0 \tag{5.5}$$

The solution for the above-described differential equation with the given boundary and initial conditions is found by using Laplace transformations, as expressed below:

$$\begin{aligned}\frac{c_m(x,t) - c_0}{c_s K_{ma} - c_0} = \operatorname{erfc}\left(\frac{x}{\sqrt{4D_m t}}\right) - \\ \exp\left(\frac{x}{\sqrt{D_m t_c}} + \frac{t}{t_c}\right)\operatorname{erfc}\left(\sqrt{\frac{t}{t_c}} + \frac{x}{\sqrt{4D_m t}}\right)\end{aligned} \tag{5.6}$$

The coefficient t_c [s] is a time constant that describes the relation among the emission area, diffusivity, and ventilation rate:

$$t_c = \frac{A^2 K_{ma}^2 D_m}{R_a^2} \tag{5.7}$$

Because we ignore the storage capacity of the air in the room and assume well-mixed air, the concentration in the room is:

$$c(t) = \frac{c_m(t)}{K_{ma}} \tag{5.8}$$

and the emission rate becomes:

$$E(t) = A\sqrt{D_m}\,(c_s K_{ma} - c_0)\cdot u(t, t_c) \tag{5.9}$$

where u expresses the change in the emission rate over time:

$$u(t, t_c) = \exp\left(\frac{t}{t_c}\right)\operatorname{erfc}\left(\sqrt{\frac{t}{t_c}}\right)\sqrt{\frac{1}{t_c}} \tag{5.10}$$

The function u has the following limit as t_c^{-1} approaches infinity:

$$\lim_{\frac{1}{t_c}\to\infty} u(t, t_c) = \frac{1}{\sqrt{t\pi}} \tag{5.11}$$

In Figure 5.3 $\sqrt{t_c}\cdot u$ is plotted against time for different values of t_c. The figure shows that for small time constants, t_c, and high ventilation rates, the

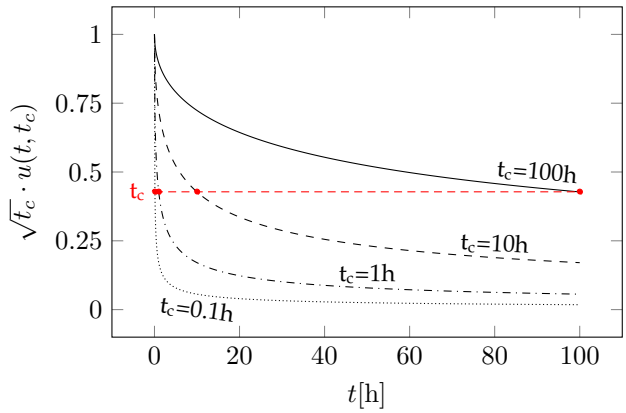

Figure 5.3: $\sqrt{t_c} \cdot u(t, t_c)$ plotted against t for different time constants, t_c.

concentration drops more rapidly than for large time constants, where the concentration decline is slower.

Figure 5.4 shows u plotted against $t_c^{-0.5}$ at different timescales. The reason for plotting u against $t_c^{-0.5}$ is that it facilitates interpretation in terms of ventilation rate, since, for example, doubling $t_c^{-0.5}$ is the same as doubling the ventilation rate. In Figure 5.4, we can see that at small timescales, the emission rate is more sensitive to changes in $t_c^{-0.5}$, while at long timescales, the emission rate becomes less sensitive at lower values of $t_c^{-0.5}$. For each timescale, there is a threshold at which changes in $t_c^{-0.5}$ stop having significant effect on the emission rate. As an example, for practical uses, a time scale of a couple of days to a week is reasonable. Then, from Figure 5.4, we can see that for values of $t_c^{-0.5} = 0.12$ and higher, an increase in ventilation will not considerably increase the emission rate. Therefore, increasing the ventilation rate further cannot be motivated by an increase in off-gassing for faster depletion of VOCs.

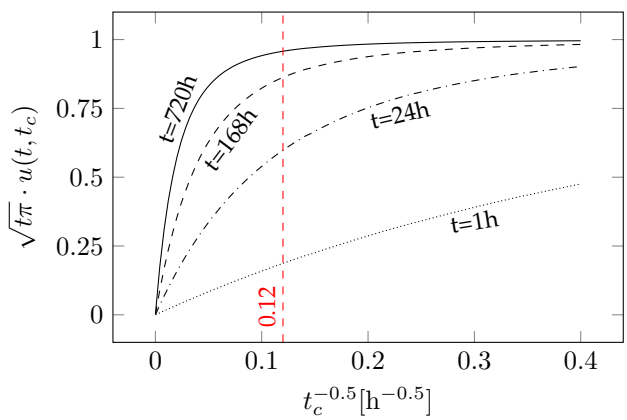

Figure 5.4: $\sqrt{t\pi} \cdot u(t, t_c)$ plotted against $\frac{1}{\sqrt{t_c}}$ at different timescales, t.

5.2 Ventilation threshold – an example

The proposed limit in Figure 5.4 can be used to calculate the ventilation threshold for a material with known material properties: D_m and K_{ma}. In **Paper IV**, a table with different materials and their properties is presented. As an example, we will perform a calculation based on the material (from the table) that results in the highest ventilation threshold. In this case, this is benzaldehyde in the gypsum board, which has $K_{ma}^2 D_m \approx 4 \cdot 10^{-3}$. Now, from Equation 5.7, and with $t_c^{-0.5} = 0.12$ the ventilation threshold becomes $R_a/A = 0.13\ \mathrm{L\,s^{-1}\,m^2}$. This value can then be interpreted as an upper limit, valid from one week after the material is installed, at which increasing the ventilation rate will not increase the rate of emissions.

The proposed ventilation threshold ($R_a/A = 0.13\ \mathrm{L\,s^{-1}\,m^2}$) is now compared with data from earlier studies. Results from [72], [73] and [74] are used because they present data from field measurements where emission rates are measured at different air change rates. However, the emitting area is not always mentioned explicitly, and in those cases, assumptions are made based on the description of the building. A detailed description of each compared case can be found in **Paper IV**.

Here, three cases are presented and summarized in Table 5.1. In case number 1, measurements of VOC are performed in two rooms with different ventilation rates, 1.5 $\mathrm{h^{-1}}$ and 3.5 $\mathrm{h^{-1}}$. It was found that the relative reduction of VOC was similar in both rooms, indicating that the different ventilation rates had negligible effects on the emission rates. The calculated ventilation threshold is 0.47 $\mathrm{h^{-1}}$, lower than both ventilation rates, indicating that the increased ventilation should not affect emission rates, as was observed in the study.

Similarly, in case 2, the relative reduction in VOC concentration was similar in two apartment buildings with the ventilation rates of 0.8 $\mathrm{h^{-1}}$ and 1.7 $\mathrm{h^{-1}}$. Here, the calculated ventilation threshold was 0.19 $\mathrm{h^{-1}}$, which is lower than the actual ventilation rates; therefore, increasing the ventilation did not affect the emission rates.

In case 3, measurements in a newly built house showed a correlation between ventilation and emission rates for two different air change rates, 0.32 $\mathrm{h^{-1}}$ and 0.14 $\mathrm{h^{-1}}$. The ventilation threshold for this case was 0.18 $\mathrm{h^{-1}}$, which is between the two measured ventilation rates. This means that a lower emission rate can be expected at air change rates of 0.14 $\mathrm{h^{-1}}$ compared to 0.18 $\mathrm{h^{-1}}$, which is in line with the conclusions from the study that TVOC concentration decreased by 30% at the lower ventilation rate.

The results from Table 5.1 indicate that ventilation thresholds are not higher than 0.5 $\mathrm{h^{-1}}$. For comparison, in the Swedish building code, buildings should be ventilated with a ventilation rate of 0.35 $\mathrm{L/m^2/s}$ [75], which at normal room height is about 0.5 $\mathrm{h^{-1}}$. This might explain why many studies conclude that the emission rate does not increase with increased ventilation; simply normal ventilation is in most cases higher than the threshold. In addition, for school buildings and offices, ventilation rates are often higher. For example, the Public Health Agency of Sweden recommends a ventilation rate of at least

Table 5.1: Summary of the comparison with measurements. A is the emitting area, *ACR* is the ventilation rates from the study, *Threshold* is the calculated threshold at which increasing the ventilation will not affect the emission rate, and *Outcome* specifies whether the emission rate was affected by the change in ventilation rate in the study.

Case No.	A [m^2]	ACR [h^{-1}]	Threshold [h^{-1}]	Outcome	Reference
1.	164[1]	1.5-3.5	0.47	Unaffected	[72]
2.	92[2]	0.8-1.7	0.19	Unaffected	[73]
3.	110	0.14-0.32	0.18	Affected	[74]

[1]The emitting area is estimated to be 2.5 times the floor area

[2]The emitting area is assumed to be the same as the floor area

$0.35\ \mathrm{L/m^2/s}$ +7 $\mathrm{L/s/person}$ [76].

The decisive parameters for the ventilation threshold are the diffusion coefficient, D_m, and the partition coefficient, K_{ma}, where higher values of $K_{ma}^2 D_m$ lead to a higher ventilation threshold; therefore, for example, the material and the VOC in a room with the highest $K_{ma}^2 D_m$ (and emitting area) will determine the ventilation threshold.

The ventilation threshold calculated in the example above is based on benzaldehyde in gypsum board, which has a high value for $K_{ma}^2 D_m$ compared to other materials, and consequently many other materials will result in a lower ventilation threshold.

Chapter 6

Sampling schemes

The emission characteristics of a VOC source are decisive for the choice of measurement method. Short-term emissions require short-term measurements, while long-term emissions can be captured using long-term measurements [77], such as passive sampling. New materials often exhibit both short-term and long-term emission characteristics. Initially, new materials release shallow VOCs originating near the surface. This process is relatively short and can therefore be regarded as short-term. On the other hand, emissions originating from deeper within the material are, due to diffusion within the material, emitted more slowly. This process acts on a longer timescale of several months [36] and is therefore regarded as long-term emissions.

In VOC-passport, passive samplers provide an average VOC concentration over 5–7 days, accounting for long-term emissions. When introducing a new material, VOC concentrations rise quickly and decline over days to weeks before they become steadier [17, 55, 56]. However, starting passive measurements too early risk disturbance by the initial concentration peak. For VOC-passport to be successful, it is important to avoid starting measurements too early, when the initial concentration impacts the results.

This chapter is based on **Paper V** where active and passive sampling is used to measure long- and short-term VOC emissions from a new carpet placed inside a dedicated test chamber. Figure 6.1 shows an overview of the paper in relation to the scope and methods of this thesis.

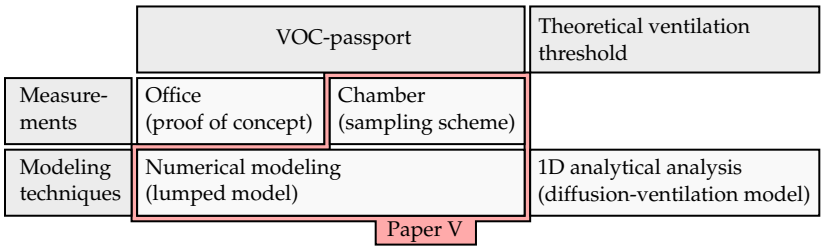

Figure 6.1: Paper V in relation to the scope and methods of the thesis.

6.1 VOC emission test chamber

Three carpet samples, each measuring $2.4\ \mathrm{m} \times 1.75\ \mathrm{m}$, were obtained from a single carpet roll as shown in Figure 6.2. The selection of the carpet roll was solely based on its distinct "new-smell." The carpet roll had plastic foil wrapping when it arrived at the shop, and the wrapping was not removed until shortly before cutting the carpet samples. The cut pieces were then tightly rolled together and thoroughly plasticized to preserve the VOC levels in the carpet prior to the experiments. The product description confirmed that the carpet was composed of polyamide with latex backing.

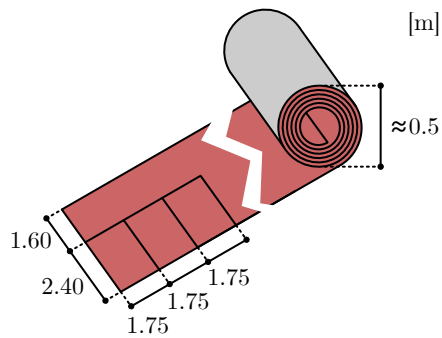

Figure 6.2: Carpet roll dimensions and how each piece of carpet was cut from the roll.

Measurements were performed inside the test chamber, as shown in Figure 6.3, with dimensions of $3.5\ \mathrm{m}$ in length, $2.4\ \mathrm{m}$ in width, and $2.3\ \mathrm{m}$ in height. The chamber was situated indoors as part of a specialized building designed for testing ventilation systems, hereafter referred to as the hall. The indoor location shields the chamber from outdoor conditions such as atmosphere and solar radiation, ensuring that its temperature depends solely on the indoor air temperature of the hall. The hall is ventilated with outdoor air and heated by radiators.

The ventilation system operates by employing an exhaust fan that connects

to the ventilation outlet of the hall, as shown in Figure 6.3. Using a damper, the ventilation rate can be adjusted to achieve the desired ventilation rate. Because the chamber is not airtight, any supply air that enters the chamber seeps in from the hall through leaks around the door and various joints in the chamber walls. Throughout the measurements, the ventilation rate was $3.5 \pm 0.3\ \mathrm{L\,s^{-1}}$ (ACR $\approx 0.65\ \mathrm{h^{-1}}$).

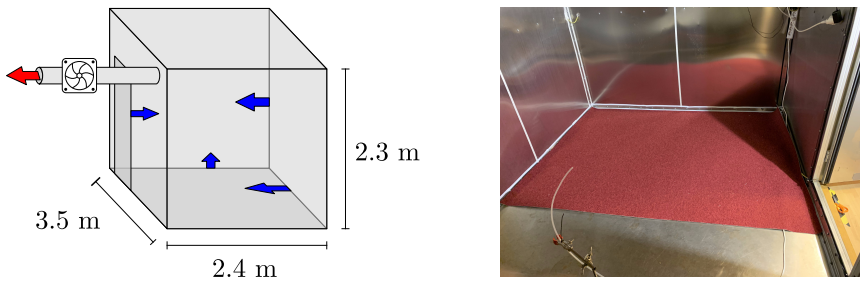

Figure 6.3: Left: Principle drawing of the measurement chamber. Right: Photograph from inside the chamber prior to the start of test condition 1.

Measurements were performed for three different test conditions, where each test condition lasted for four weeks; see Figure 6.4 for an overview. In addition, each test condition had its own unique setup in terms of the emission load or indoor conditions, as illustrated in Figure 6.5. Passive samplers collected VOC for one week at a time throughout all measurements and active (pumped) samplers collected VOC once each day during the first five days of each test condition (Monday to Friday).

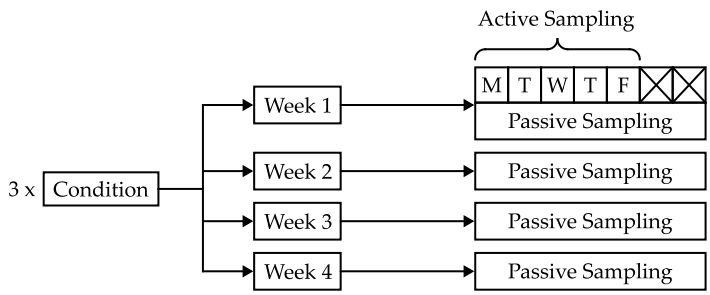

Figure 6.4: Schedule showing the order of the measurements, active and passive sampling, for each test condition.

The three measurement conditions are summarized as follows: ① One carpet test piece, 2.4 m × 1.75 m, covered half of the chamber. ② A second carpet test piece was added so that the entire chamber floor was covered by carpet. ③ Both carpet test pieces from the first and second test conditions were removed, and one new carpet test piece, 2.4 m × 1.75 m, was placed on

the floor. In addition, humidifiers were used to increase the air humidity in the test chamber.

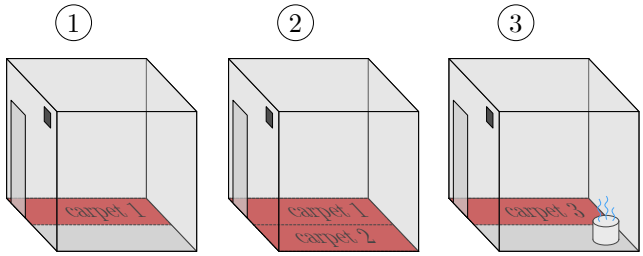

Figure 6.5: Three test conditions: ① the carpet covers half of the floor, ② one additional piece of carpet is added, and ③ a new carpet covers half of the floor, and the air humidity is increased.

6.2 Results of chamber measurements

Several VOCs were detected, and many of them came from the indoor air of the hall, as confirmed by analyzing the inlet air and empty chamber samples. Among these compounds, only 4-phenylcyclohexene (4-PCH) and benzaldehyde were found to be emitted exclusively from the carpet; and therefore, only these two compounds are included in the analysis. The compound 4-PCH is commonly found in indoor air emissions from polyamide carpets with latex adhesive backing, which is often associated with the smell of new carpets [78]. Benzaldehyde is frequently used in industrial processes as a precursor to plastic additives and dyes, and is used as a flavoring agent and fragrance [79].

Figure 6.6 and Figure 6.7 show the results from measurements of temperature, humidity, 4-PCH and benzaldehyde during test condition 1 and 3, respectively. For results from test condition 2, see **Paper V**. Usually, introducing a new source inside the chamber results in a concentrated peak followed by exponential decay. However, the first measurement of 4-PCH during test condition 1 (Figure 6.6) does not follow this trend, and it is unclear if this deviation is due to measurement error or if it has some other explanation.

Passive sampling requires an uptake rate to determine the sampled air volume, which is dependent on environmental conditions and is specific to each VOC. In this work, for benzaldehyde, an uptake rate of 38.2 $\mathrm{mL\,min^{-1}}$ is used [48]. However, no literature information was available for 4-PCH, and the reported uptake rate for toluene (0.32 $\mathrm{mL\,min^{-1}}$) [80] was therefore used. This approximation led to higher 4-PCH concentrations in the passive sampler results (Figure 6.6 and Figure 6.7), compared to active samplers. Active sampling uses a calibrated pump with a known airflow; these measurements are therefore considered more accurate. Thus, the uptake rate for 4-PCH was recalculated based on the average concentration in active measurements during test conditions 1 and 3. The recalculated uptake rate of 4-PCH was

0.65 $\mathrm{mL\,min^{-1}}$, and concentrations for 4-PCH using both the new estimated uptake rate and the uptake rate of toluene are presented in Figure 6.6 and Figure 6.7.

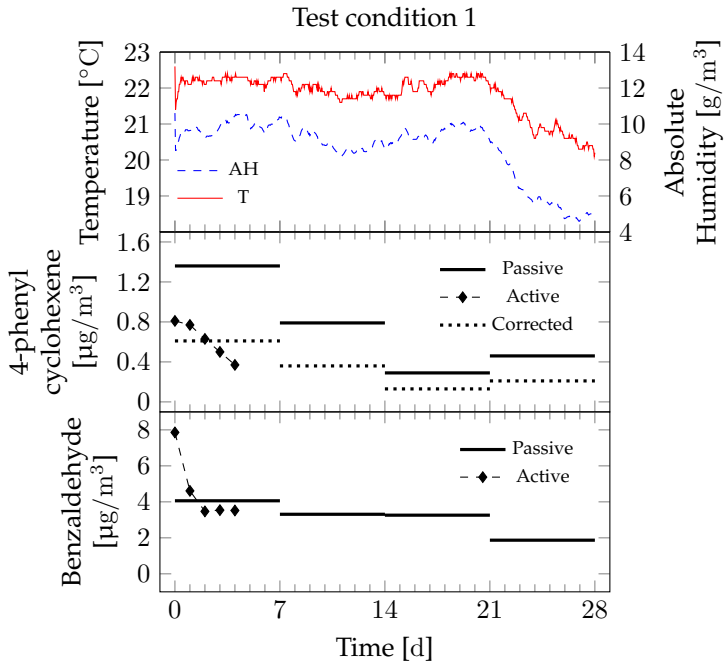

Figure 6.6: Temperature, absolute humidity, and passive and active measurements inside the chamber during test condition 1.

In Table 6.1 the correlation coefficient, R^2, and RMSE (root mean square error) for measurements were compared with the models described by Equations 3.7 (with initial concentration set to zero, $c_0 = 0$), 3.9 and 3.10. Because the air in the chamber is well-mixed because of the fans inside the chamber and the buffering capacities of the carpet and surfaces in the chamber is unknown, I assume that V_e equals the total air volume of the room (V_e=19.3 $\mathrm{m^3}$).

To simplify the interpretation of the results in Table 6.1, the equations used have the following names: Equation 3.7 is referred to as AH* because the source depends only on the humidity in the chamber, Equation 3.10 is referred to as DE because the source decays over time, and Equation 3.9 is referred to as AH*-DE because the source both decays over time and is dependent on the humidity in the chamber.

The double exponential models, Equation 3.9 and Equation 3.10 describe two emission processes: the rapid release of shallow and easily released VOC near the surface, followed by the slower release of VOC from within the carpet. Results demonstrate that by combining early active sampling with long-term passive sampling, both these processes can be captured. Moreover, both double exponential decay models, AH*-DE and DE (Equation 3.9 and

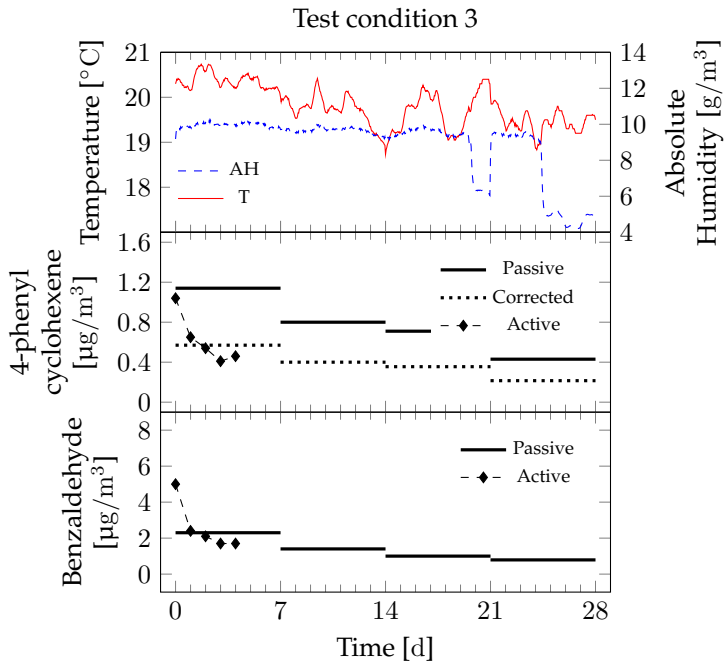

Figure 6.7: Temperature, absolute humidity, and passive and active measurements inside the chamber during test condition 3.

Equation 3.10), have correlation coefficients above 0.9 in all test conditions (see Table 6.1).

Table 6.1: R^2/RMSE for each test condition 1–3 and for three different models: only absolute humidity, AH* (only from passive samplers) Equation 3.7; only emission decay, DE Equation 3.10; and both absolute humidity and emission decay, AH*-DE Equation 3.9.

	Test Condition	**AH* (passive) [R^2/RMSE]**	**DE [R^2/RMSE]**	**AH*-DE [R^2/RMSE]**
Benzaldehyde	1	0.99/0.23	0.98/0.38	0.99/0.28
	2	1.0/0.05	0.99/0.05	1.0/0.03
	3	0.88/0.34	0.99/0.19	0.99/0.21
4-PCH	1	0.53/0.21	0.92/0.10	0.92/0.10
	2	0.92/0.07	-	-
	3	0.96/0.05	0.97/0.05	0.98/0.05

Figure 6.8 and 6.9 show the predicted emission rates and concentrations based on Equations 3.3 and 3.10. Figure 6.8 shows that the initial emission rate for benzaldehyde declines rapidly during the first two to three days. However, in test condition 2, the initial emission rate is lower compared to that in test conditions 1 and 3. Surprisingly, this occurs even though carpet 2 was added

while carpet 1 was still inside the chamber. It appears that the three pieces of carpet did not have the same initial concentration, even though they were plasticized before being placed in the chamber. One possible explanation is that, during transport and storage, some diffusion occurred despite the protective plastic wrapping, resulting in a concentration gradient across the carpet roll. Consequently, the outermost layer (one of the carpet pieces) may have a lower concentration and a smaller amount of easily accessible VOCs compared to the other two pieces when introduced into the chamber. Figure 6.2 illustrates that one carpet piece is large enough to cover the entire outer layer of the roll, while the other two pieces must be rolled behind it. Additionally, Figure 6.8 shows a slight difference in the initial values between test conditions 1 and 3, which is to be expected if there is a concentration gradient within the carpet roll, with one piece located behind the other. However, the most significant concentration drop would occur across the outermost layer of the carpet. Similarly, the initial concentration of 4-PCH should also be higher in test condition 1 compared to that in test condition 2, which is correct except for the first active measurement. As previously mentioned, the first measurement (test condition 2) does not follow an exponential curve and may be underestimated due to measurement error.

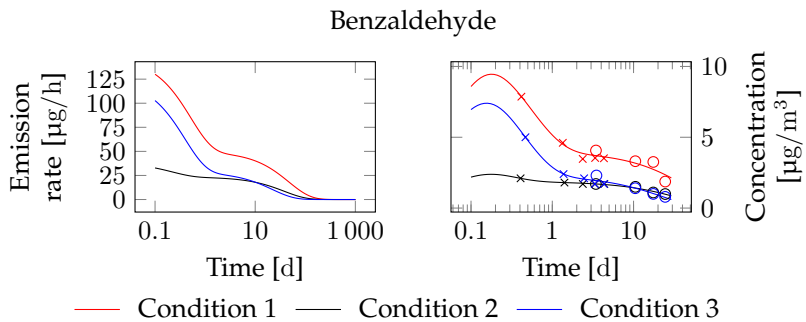

Figure 6.8: Predicted emission rates and concentrations plotted against measurements.

The depletion of shallow VOCs takes about 2–3 days for benzaldehyde and about 1-2 weeks for 4-PCH. To capture long-term, steadier emissions using passive sampling, measurements should not be initiated before the release of shallow VOCs is negligible; otherwise, there is a risk of overestimating the concentrations. Based on the chamber measurements, this process can take 1–2 weeks.

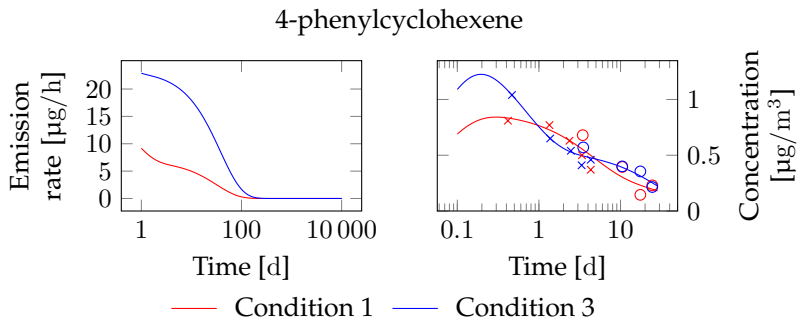

Figure 6.9: Predicted emission rates and concentrations plotted against measurements.

Chapter 7

Discussion

The circumstances for the field measurements, as described in **Paper III**, were in many ways optimal. The building service manager was interested in the study and had extensive knowledge about the building and its ventilation system, which was helpful throughout the study. In addition, I was allowed to control the ventilation rates in each room separately, which made it possible to set ventilation rates that were of interest for the study. Such circumstances are likely to be unusual in most building projects, and the implementation of VOC-passport might be more challenging and might need more detailed planning to be successful in typical building projects.

During the last year, I conducted field measurements in three different new school buildings. I have not yet completed the analysis of the measurements; consequently, the results have not yet been published. However, in contrast to the office buildings mentioned above, these buildings represent better typical new buildings. In this chapter, I will therefore discuss, based partly on experience from these field measurements, some potential challenges and ideas for improving VOC-passport. I will also discuss how the theoretical ventilation threshold can be used as a complement or alternative to VOC-passport.

Ideas for improving VOC-passport

One of the major challenges with VOC-passport is to ensure that measurements are made so that the data can be used for calibrating both the source model and the model for room concentration. Further, for model calibration, measurements during periods when the ventilation is turned off, such as measurement period 2 in Figure 4.3 are not needed.

Calibration of the source model is ideally performed when concentrations are relatively stable (steady state), while calibrations of the model for room concentration must be performed with unsteady measurements (to be able to capture dynamic changes in concentration). In buildings where it is possible to control the ventilation rates, this can be done by following the ventilation scheme proposed in Figure 7.1 – if, based on our experience with measure-

ments in the office building, we assume that after a change in ventilation rate concentrations become steady in less than a week. Then, any change in ventilation should be maintained for two weeks, where for the first week concentrations adapt toward a new steady state, while during the second week concentrations are steady. In the example in Figure 7.1, measurement periods ③ and ⑤ would be in steady states (and possibly also periods ①, depending on the ventilation rates prior to this period), and measurement periods ② and ④ would be changing (unsteady). Measurement periods that are in steady state could then be used to calibrate the source model, while all measurement periods, 1–5, can be used to calibrate the concentration model.

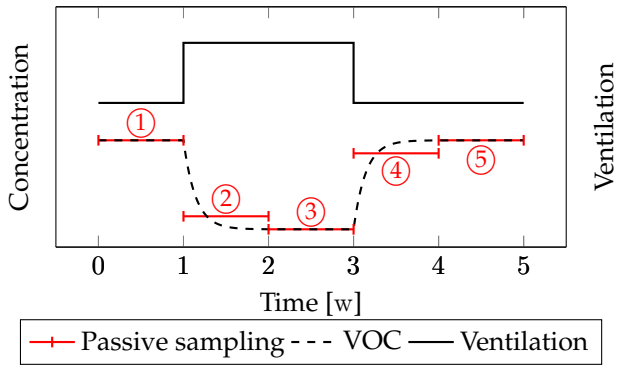

Figure 7.1: Idea for an improved ventilation scheme during measurements.

Applications of the theoretical ventilation threshold

Regarding the ventilation threshold, presented in **Paper IV**, there is a need for more research to further validate and better understand how it can be used and developed. However, it is still useful to reflect on its potential usability as an alternative, or possibly a complement, to the VOC-passport. A threshold for ventilation that can be estimated by appreciating the total surface of the emitting area in a new room (here, perhaps, equipment and furniture can be accounted for in terms of equivalent area) can be used as a guide for setting the ventilation rates. For example, if ventilation is lowered at nighttime (or outside occupancy hours), the ventilation threshold can serve as a set point for ventilation. With a lower ventilation rate below the threshold, off-gassing would not be maximized, while a higher ventilation rate above the threshold would lead to unnecessary ventilation losses.

The calculated ventilation thresholds in **Paper IV**, based on field measurements from the literature, were all below the ventilation requirements in the Swedish building code. If this is true for most buildings, it could mean that diffusion models are not necessary for modeling VOC emissions in the field because the concentrations in the room would be independent of the diffusion within materials. Then, decay models combined with models for capturing short-term buffering of VOC would be a more practical, and thus

better modeling approach.

However, uncertainties remain related to the theoretical ventilation threshold, and more research is needed. For example, in the above-mentioned examples, the threshold is determined for one VOC at a time (or the most critical one), and it is not certain how the threshold is affected when there are several critical VOCs being emitted.

Challenges with VOC-passport

Ideally, for VOC-passport to be successful, field measurements should be taken before the building is taken into service, but after the building is finalized. Given the results in **Paper V**, where it took 1–2 weeks before the initial, easily accessible VOCs were released, it seems as if several weeks might be needed to complete the measurements. This can be a challenge. Normally, the builder is on a tight schedule, which means that the building is taken into service shortly after its completion, and sometimes even before it is completely finished. In addition, both schools and offices are usually furnished before they are taken into service; since emissions from furniture are also important to capture, measurements need to be started after furnishing is completed.

When the building is still not completed, ongoing VOC-passport measurements can be disturbed if new sources, such as furniture, are continually added. In addition, if measurements are taken when the building is already occupied, additional occupant-related VOCs will be present in the indoor air. Another challenge is the disturbance from opening and closing doors or windows in the rooms where measurements are conducted, which affects the air change rate.

However, I noticed that most of the rooms have similar materials and furniture. Therefore, a possible approach to the challenges mentioned above would be to have one or a few representative rooms that are prioritized to be finalized first. These rooms can then function as representatives for the rest of the building. For this strategy to be successful, it is important to have effective communication among the building owner, the builder, the company responsible for furnishing, and any other contractor involved in the construction and management of the building.

Odor tests

Passive measurements of VOCs in the two rooms in the office building, as described in Chapter 4, were complemented by odor tests. This testing procedure involved a panel of individuals who collectively entered one of the rooms, sniffed the air, and evaluated the perceived odors using a questionnaire. These evaluations were conducted at specified times, and on several occasions. Unfortunately, it proved challenging to enlist willing participants for the panel, often resulting in only one or two attendees at the scheduled times. Consequently, the results obtained from these tests were inconclusive. Nevertheless, the limited data gathered from the questionnaires indicated a

correlation between perceived odors and measured VOC levels. The results from the questionnaire are published as a technical report [81].

Chapter 8

Conclusions

This thesis is divided into two topics: **contaminant transport by air infiltration** and **emissions in new buildings**. Common to both topics are unspecified disturbing odors related to the thermal envelope; the thesis focuses on practical methods that can be used in real-world situations to deal with these odors.

The first topic, **contaminant transport by air infiltration**, is addressed through an investigation of how air leakage distribution, climate (wind and temperature), and ventilation affect the transportation of contaminants within the building. This work was carried out and thoroughly discussed in my Licentiate thesis [47]. The main conclusions from this study are found in Chapter 2.

The second topic, **emissions in new buildings**, is covered by an investigation of the relationship between ventilation and VOC emissions as well as "new smell" in new buildings and includes a proposal for developing feasible methods for dealing with early VOC emissions in buildings. The main conclusions from the second topic are listed below:

- The proposed method, VOC-passport, which consist of passive sampling of VOC, measurements of ventilation rates, temperature and humidity and a numerical model is a promising tool for assessing VOC concentrations in new buildings.
- Ventilation rates and humidity have major impacts on VOC concentrations during the early stages, while typical air temperature is less important.
- The proposed analytical model can be used to understand the impact of ventilation rate on nonoccupant related VOC emissions in new buildings. With the model, a physics-based threshold of $0.13\ \mathrm{L\,s^{-1}\,m^{-2}}$ was identified, from which additional ventilation does not result in an increased emission rate. This estimated ventilation threshold is lower than typical (mechanical) ventilation rates, which explains why changes in ventilation rates often do not affect emission rates.

- Combining short-term active sampling in the initial few days with weekly passive sampling over a span of weeks proved successful for capturing both the rapid emission of shallow VOCs and the gradual release of VOCs from deeper inside the carpet material.

General conclusion:

- Increasing the ventilation rate, as a response to poor indoor air quality, always comes with the cost of increased energy usage. If the effect on contaminant transport or the type of contaminant source is not considered, there is always a risk that the measure will have a negligible or negative effect on indoor air quality.

Chapter 9

Future work

The methods, VOC-passport and ventilation threshold presented in this thesis require additional development and validation before they can be implemented in the field. Therefore, I suggest that future research focus on the following topics:

- The prospect of using VOC-passport for optimizing ventilation schedules in new buildings with regard to indoor air quality and energy usage is promising. However, more studies in the field (and laboratory) are needed for validation of the model itself and the optimized ventilation schedule. In addition, an improved strategy should be developed (as discussed in Chapter 7) for setting ventilation rates during the measurement to improve the fitness degree of the model.
- The VOC-passport method is in its current state not capable of accounting for the long-term decline in the emission rate. Further development of the model should focus on coupling with, for example, double exponential decay models.
- Further validation of the analytical model for calculating the ventilation threshold is needed. Repeated measurements in the laboratory and field are needed to understand how the threshold value is distributed in new buildings (or in different materials and material combinations). Laboratory measurements are needed to better understand the influence of surface convection.

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