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Impact of Climate Change on Indoor Air Quality of Residential Buildings in Belgium Over Summer Time

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I dedicate this work especially to my beloved Family.

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Thank you all,

Sincerely,

Mohsen Pourkiaei.

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Résumé

Les impacts du changement climatique sur la qualité de l'air intérieur (QAI) sont déterminés par un ensemble de facteurs influents. Ce système de régulation intègre les modifications des polluants atmosphériques et des conditions météorologiques (intérieures et extérieures), ainsi que le comportement des occupants et les caractéristiques des bâtiments. Par ailleurs, les plans d'action de rénovation des bâtiments visant à faire face à l'augmentation des phénomènes météorologiques extrêmes et aux demandes énergétiques correspondantes se traduisent par des bâtiments plus étanches à l'air, avec des taux de renouvellement d'air réduits et l'introduction de nouvelles technologies de chauffage, ventilation et climatisation (HVAC). Cette thèse de doctorat explore l'état futur de la QAI dans une maison à ventilation naturelle (avec ventilateurs d'extraction) en Belgique, selon divers scénarios climatiques projetés jusqu'en 2100. À cette fin, la recherche comprend trois sections principales (chapitre 2): I) l'étalonnage de capteurs à faible coût et les campagnes de mesure de la QAI (chapitres 3 et 4), II) le développement, la validation et l'étalonnage du modèle de QAI (conception multizone/multicontaminant dans CONTAM) (chapitre 5), et III) l'obtention des entrées futures du modèle de QAI (chapitre 6). En appliquant cette méthodologie à l'étude de cas choisi, des niveaux de QAI peuvent être prévus au milieu et à la fin du siècle. Enfin, pour fournir un outil d'aide à la décision pour objectiver l'évaluation des impacts du changement climatique sur la QAI, un indice hybride changement climatique-QAI (CAPI) a été conçu. Le CAPI intègre simultanément l'état de la qualité de l'air intérieur, la pollution de l'air extérieur et les vagues de chaleur. Les projections temporelles futures du CAPI jusqu'en 2100 ont montré une tendance à la baisse de la qualité de l'air intérieur dans le contexte d'une augmentation des épisodes de chaleur extrême. Les résultats du CAPI pour l'étude de cas choisie ont été calculés en considérant des dépassements des niveaux d'ozone.

Abstract

Impacts of climate change on the Indoor Air Quality (IAQ) are derived by a system of influential factors. This governing system incorporates the alterations of air pollutant and air weather conditions (indoors & outdoors), in parallel with occupants' behaviour and building characteristics. On the other hand, building retrofit action plans to tackle the increasing extreme weather events and corresponding energy demands, result in more air-tight buildings with reduced air exchange rates, and new Heating, Ventilation, and Air Conditioning (HVAC) technologies. This PhD thesis explores the future state of IAQ in a naturally ventilated house (with exhaust fans) in Belgium, under various climate scenarios projected up to 2100. To this end, the research includes three main sections (Chapter 2): I) IAQ low-cost sensor calibrations and IAQ measurement campaigns (Chapter 3&4), II) IAQ model development, validation, and calibration (multi-zone/multi-contaminant design in CONTAM) (Chapter 5), and III) Obtaining future inputs of the IAQ model (Chapter 6). By applying this methodology to a chosen case study, IAQ levels can be predicted in the middle and end of the century. Finally, to provide a decision supporting tool and objectivize the assessment of climate change impacts on IAQ, a hybrid climate change-IAQ index (CAPI) was designed. CAPI integrates the state of IAQ, outdoor air pollution, and heat waves simultaneously. Both experiments and future temporal estimates of CAPI till 2100 showed an increased trend of declining IAQ levels in the context of increasing extreme heat events. The CAPI results for the selected case study were calculated considering exceedances of ozone levels.

Abbreviations & Nomenclature

A	Indoor Surface Area
AC	Air Conditioner
ADAM	Adaptive Moment Estimation
AER	Air Exchange Rate
AI	Artificial intelligence
AIC	Akaike Information Criterion
ANN	Artificial Neural Networks
ANSI	American National Standards Institute
AP	Outdoor Air Pollution
AQ	(Outdoor) Air Quality
AQG	Air Quality Guidelines
AR	Assessment Report
ASHRAE	American Society of Heating, Refrigerating & Air-Conditioning Engineers
ASTM	American Society for Testing and Materials
b	Regression Intercept
b_0	y-intercept
BEM	Boundary Element Method
BIC	Bayesian Information Criterion
Bi-LSTM	Bi-Directional Long Short-Term Memory
b_k	Regression (slope) Coefficients for each Input
$C(0)$	Initial Concentration
$C(t)$	Concentration at Time t
C_a	outdoor concentration
CAPI	Climate change-Affected Poor IAQ
CAPS	Cavity Attenuated Phase Shift spectroscopy
C_b	Background Concentration
CC	Climate Change
$C_{F,out}$	Outdoor Concentration of molecule F
CFC	Chlorofluorocarbon

CFD	Computational Fluid Dynamic
C_h	Concentration in the HVAC system
CH_4	Methane
C_i	Indoor Pollutant Concentration in Zone *i*
C_i	Concentration of Species *i*
C_j	Concentration in Zone *j*
CLD	Chemiluminescence Detection
C_{max}	Maximum Concentration during the residence time
CNN	Convolutional Neural Network
CO	Carbon Monoxide
C_o	Observed Concentration
CO_2	Carbon Dioxide
C_p	Peak Concentration at the time t_p
C_p	Predicted Concentration
CTM	Chemical Transport Models
DAQFF	Deep Air Quality Forecasting Framework
DCE	Days of Climate Change Events
DCPI	Days of CC Correlated Poor IAQ
DL	Deep Learning
D_{xx}	Species Concentration Diffusion Coefficients
D_{yy}	Species Concentration Diffusion Coefficients
D_{zz}	Species Concentration Diffusion Coefficients
EBM	Energy Balance Models
EC	European Commission
ECD	Electron Capture Detector
ECMs	Earth System Models
E_F	Emission Rate of molecule F
E_i	Emission Source term
ELV	Exposure Limit Values
EPA	Environmental Protection Agency of US

ε	Stochastic Error (residuals)
FB	Fractional Bias
FDM	Finite Difference Method
FEM	Finite Element Method
FID	Flame Ionization Detection
FPS	Federal Public Service Health of Belgium
FS	Fractional bias based on variance
FTIR	Fourier-transform infrared spectroscopy
FVM	Finite Volume Method
f_x	Velocity Body Force terms
G	Emission Rate
GA	Genetic Algorithm
GCM	Global Climate Models or General Circulation Models
GHG	Greenhouse Gas
GRU	Gated Recurrent Units
HCHO	Formaldehyde
HFC	Hydrofluorocarbon
HPA	Health Protection Agency
HPLC	High-Performance Liquid Chromatography
HVAC	Heating, Ventilation, and Air Conditioning
HW	Heat Wave
IAC	Indoor Air Chemistry
IAQ	Indoor Air Quality
IEQ	Indoor Environmental Quality
IOM	Institute of Medicine
IPCC	Intergovernmental Panel on Climate Change
IR	Infrared (Solar Irradiance)
IRCEL-CELINE	Belgian Interregional Environment Agency
IRM	Royal Meteorological Institute of Belgium
ISSeP	Institut Scientifique De Service Public

K	Deposition Rate
k	Observations
$k_{F\text{-}J}$	Biomolecular Reaction Rate Constant Between molecules “F and J”
$k_{G\text{-}H}$	Biomolecular Reaction Rate Constant Between molecules “G and H”
K-S	Kolmogorov–Smirnov examination
LASSO	Least Absolute Shrinkage and Selection Operator
LBL	Lawrence Berkeley National Laboratory
LCS	Low-Cost Sensors
LOA	Limits of Agreement
LPT	Lagrangian Particle Transport technique
LSTM	Long Short-Term Memory recurrent networks
LULUC	Land Use and Land-Use Changes
M	Predicted Concentrations
M	Regression Slope
MAE	Mean Absolute Error
MAPE	Mean Absolute Percent Error
MAR	Modèle Atmosphérique Régional
MCMC	Markov Chain Monte Carlo
ML	Machine Learning
MLR	Multiple Linear Regression
MM	Meshless method
MOx	Metal Oxide
MS	Mass Spectrometry
MSE	Mean Square error
NCCN	National Crisis Center of Belgium
NDIR	Non-Dispersive Infrared Gas detection
NH_3	Ammonia
NIST	National Institute of Standards and Technology
NMAE	Normalized Mean Absolute Error
NMSE	Normalized Mean Square Error

NO	Nitrogen Oxide
NO_2	Nitrogen Dioxide
O	Observed Concentrations
O_3	Ozone
OH	Hydroxyl radical
P	Pressure
p	Level of Confidence
PA	Accuracy & Predictive Ability
PBT	Population Based Training
P_F	Formation Rate of molecule F due to gas-phase reactions
PFC	Perfluorocarbons
PIC	Particle-in-Cell method
PID	Photoionization Detectors
PLS	Partial Least Squares
PM_1	Particulate Matter 1 µm
$PM_{2.5}$	Particulate Matter 2.5 µm
PM_{10}	Particulate Matter 10 µm
PR	Precipitation
P_{ta}	Penetration factor for outdoor pollutants entering the indoors
$Q_{a,i}$	Airflow from the outdoors into zone *i*
$Q_{h,i}$	Airflow from the HVAC system into zone *i*
$Q_{i,a}$	Airflow from zone *i* to the outdoors
$Q_{i,h}$	Airflow from zone *i* into the HVAC system
$Q_{i,j}$	Airflow from zone *i* into zone *j*
$Q_{j,i}$	Airflow from zone j into zone *i*
r	Pearson Correlation Coefficient
R^2	Coefficient of Determination
RBF	Radial Basis Function
RCP	Representative Concentration Pathways
r_F	Loss Rate of molecule F

RFR	Random Forest Regression
RH	Relative Humidity
RMSE	Root Mean Square Error
Rn	Radon
RNN	Recurrent Neural Networks
r_s	Spearman's correlation
S	Source/sink terms
SA/V	Surface-Area-to-Volume ratio
SCF	Study Conceptual Framework
SD	Standard Deviation
SF_6	Sulphur hexafluoride
S_i	Pollutant removal term
SO2	Sulfur dioxide
SOA	Secondary Organic Aerosol
SSP	Shared Socioeconomic Pathways
T	Temperature
t	Time
TCD	Thermal Conductivity Detector
TMY	Typical Meteorological Years
TVOC	Total Volatile Organic Compound
u	Horizontal Velocity
UHI	Urban Heat Island effect
UKCP09	UK Climate Projections 2009
UV	Ultraviolet
v	Lateral Velocity
$v_{d,F}$	Deposition Velocity of F to indoor surfaces
V	Mixing Volume
V_i	Zone Volume
VOC	Volatile Organic Compound
w	Vertical Velocity

WD	Wind Direction
WHO	World Health Organization
WS	Wind Speed
x_i	Inputs
y	Output
y_F	Molar Yield
λ	Air Exchange Rate
λ	Ventilation Rate
ρ	Density
σ_{xx}	Normal Viscous Stress
σ_{xy}	Tangential (Shear) Viscous Stress term
σ_{xz}	Tangential (Shear) Viscous Stress term
τ	Residence Time

1. INTRODUCTION

INDOOR AIR QUALITY IN THE CONTEXT OF A CHANGING CLIMATE

1. Introduction

1.1. Background

Climate variability represents all the changes in the climate which take place longer than particular weather events, while the term "climate change" itself, targets those changes that remain for a longer time span, e.g., decades or more (significant, long-term changes in the global climate). Climate change comprises both global warming and its effects on Earth's weather patterns (Allen et al. 2018). There is now clear evidence that projected climate change will have major impacts on the indoor environments (Vardoulakis et al. 2015). The risks are not yet fully described quantitatively, but various outcomes, e.g., that higher temperatures higher indoor concentrations, are expected (changes in building materials emissions, natural air exchange rates (AERs), outdoor pollutants levels, occupancy behavior, etc.). Natural ventilation refers to the "ventilation occurring as a result of only natural forces, such as wind pressure or differences in air density, through intentional openings such as open windows and doors." (ASHRAE 2017). Higher outdoor ozone concentrations may lead to increased indoor chemistry and the formation of secondary products. Mitigation and adaptation policies are needed, and, before that, a better understanding of how buildings will be impacted and used is needed (Weschler 2000).

Climate change may affect Indoor Air Quality (IAQ) and associated health impacts via increases in indoor pollutants emissions, increases in indoor temperatures (altering the comfort and natural AERs), increasing or decreasing emissions of pollutants from outdoor sources (changes in ambient air pollution driven by climate change), changes in building construction and operations that alter AERs, and changing occupants' activity patterns and behaviors, including use of heating systems, windows and air-conditioning systems. These changes will be driven not only by climate change itself, but also by efforts to adapt to or mitigate climate change, and will occur in parallel with other societal trends, such as population growth and urbanization, that could impact the built environment and IAQ. Those most vulnerable to climate-related changes in the indoor

environment likely include the poor, the elderly, and children. While the challenges posed by climate change for IAQ are not qualitatively new (Field 2010), the complexity of future changes will offer new challenges.

IAQ, as a subset of Indoor Environmental Quality (IEQ), is mainly correlated to three influential domains (Pourkiaei & Romain 2023):

1) outdoor environment (weather and air pollution),

2) occupants' behavior and

3) the building itself (structure, material, utilities, etc.).

To be specific, IAQ is determined as characteristics of the air we breathe-in in the indoor environments, e.g., gaseous composition, humidity, temperature, and contaminants concentrations (ASHRAE 2024). The National Crisis Center of Belgium (NCCN), coordinated an extensive risk assessment in 2018, for Belgium territory with the time span of 5 years. Collective experts evaluated different risks based on their priority, probability and the influential strengths on population, society, environment and the economy. For the risk of 'large-scale deterioration of air quality', the analysis outcome was as following (NCCN 2018):

- Impact: low impact
- Probability: very likely

The very likely low impact "deterioration of air quality" impacts the IAQ of buildings.

The subject of "IAQ being affected by climate change" was brought to the literature by a specific report presented by R. Field in 2010, and just after it the exclusive report of "climate change, IAQ and health" by the U.S. Environmental Protection Agency (EPA) (Field 2010, Schenck 2010, Fisk 2015). Two years after, W. Nazzarof subjectively discussed the detailed consequences of climate change to IAQ, and established a bright baseline for future studies to answer this question: What are the effects of climate change on IAQ? (Nazaroff 2013).

Other distinguished qualitative studies include but are not limited to: The report of Institute of Medicine (IOM 2011), and Health Protection Agency (HPA) report on the effects of climate change (Vardoulakis et al. 2012, Vardoulakis et al. 2015). Figure 1.1., adapted from (IOM 2011), shows selected pathways through which climate change is likely to modify IAQ.

1.2. IAQ Definition

There have been many debates among IAQ specialists about the proper definition of IAQ and specifically what constitutes "acceptable" IAQ. By the definition of European Ventilation Industry Association (EVIA) "Indoor air quality (IAQ) is a term which refers to the air quality within and around buildings and structures, especially as it relates to the health and comfort of building occupants." (EVIA 2024). According to the definition proposed by US EPA, the IAQ is "the air quality within and around buildings and structures, especially as it relates to the health and comfort of building occupants.". By another definition presented by ASHRAE Technical Committee (TC) 1.6, IAQ refers to the "attributes of the respirable air inside a building (indoor climate), including gaseous composition, humidity, temperature, and contaminants.".

1.3. IAQ & Climate Change

In general, the level of chemical and airborne contaminants in buildings are mainly linked to ventilation characteristics (Air Exchange Rate (AER) of outdoor air into indoor), infiltration rates of outdoor air, and indoor emission/sink sources (Vardoulakis et al. 2020, Fazli 2021). Internal emission/sink sources are linked to occupants' behavior (transient & intermittent) and building elements (permanent). Also, household activities affect the indoor air pollutant removal rate by deposition, filtration, and exfiltration, while some re-suspensions may take place (Shrubsole 2012). Indoor emission sources include transient emissions from internal sources (i.e., construction materials, building equipment, and utilities), and intermittent emissions (i.e., burning fuel and candles, smoking, cooking, heating, and occupant behaviors) (Shrubsole et al. 2012, Sá et al. 2022). Indoor air pollutants comprise a wide variety of physical, biological, and

chemical contaminants, including but not limited to Carbon Monoxide (CO), Carbon Dioxide (CO_2), Volatile Organic Compounds (VOCs), Nitrogen Oxides (NO & NO_2), Particulate Matter (PM), and Ozone (O_3) (Gonzalez-Martin et al. 2021). Notably, CO_2 is not cataloged among the selected indoor pollutants by the World Health Organization (WHO), but it has been widely used as an indicator of adequate air ventilation where high indoor CO_2 levels indicate low AERs. High CO_2 levels show poor AERs and potential accumulation of indoor pollutants (Moreno-Rangel et al. 2018, ANSI/ASHRAE 2022, Persily et al. 2022).

Fig 1.1. Different scenarios that climate change may impact buildings and inhabitants. (Re-illustration from (IOM 2011), and original picture is adapted from (Su, undated)).

Future scenarios correlated with the indoor built environment include future climatological scenarios, future Greenhouse Gas (GHG) emissions, and future buildings' adaptation and

mitigation strategies regarding energy retrofit plans. It is known that these scenarios will impact the contaminant concentrations in residential buildings (Spengler 2012, Nazaroff 2013, Zhong & Lee 2017, Fazli et al. 2021). The abovementioned elements can also affect the indoor environment through heat and mass transfers between the interior spaces and the surrounding environment.

To meet the European 2050 climate-neutral targets, current policies suggest present premises must go through extensive retrofitting by utilizing sufficient insulation, high-performance Heating, Ventilation, and Air Conditioning (HVAC) systems, and enhanced air tightness (Shrubsole et al. 2012, Cornet et al. 2013). Such measures to air tightness and HVAC systems along with climate change itself, are projected to result in alterations of IAQ and personal exposure to airborne contaminants. However, IAQ directly affects public health and well-being (Son 2023). Correspondingly, to mitigate heat waves and peak pollution events residential building models need to consider changing ambient environments (Amaripadath et al. 2023). Figure 1.2. presents Key pathways linking climate change to IAQ and health (directly imported from Zhang et al. 2023: *Handbook of indoor air quality*. Springer Nature 2023)

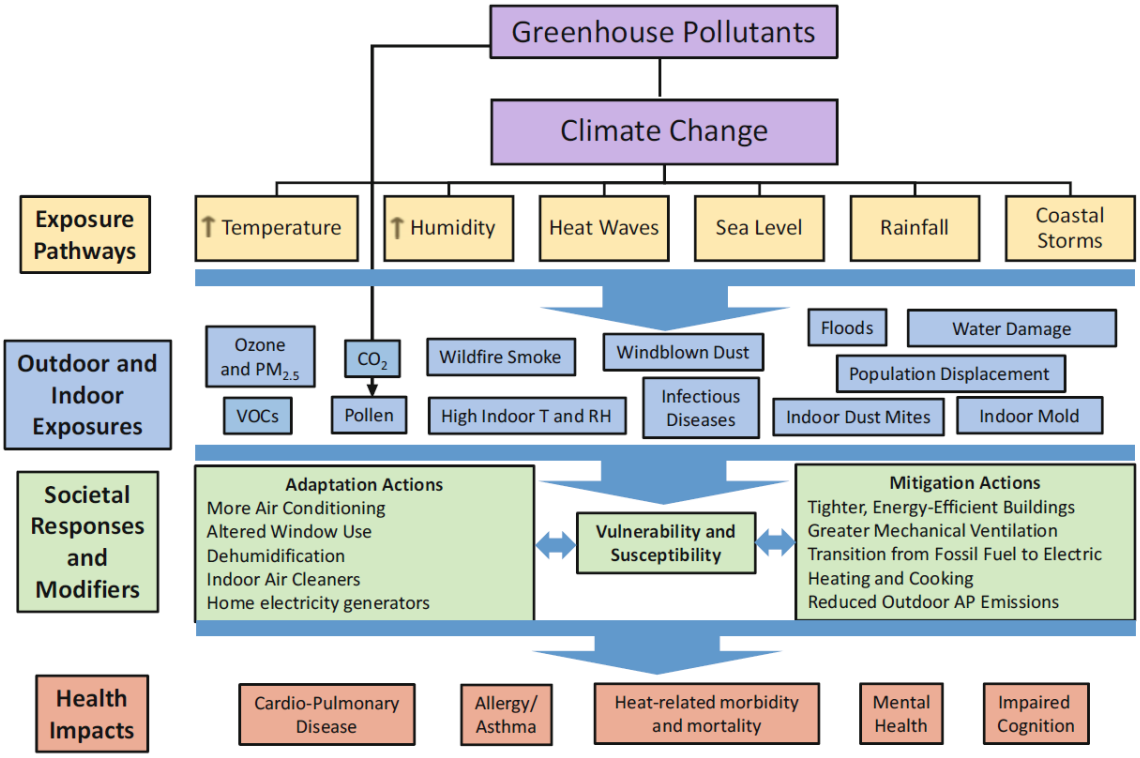

Fig 1.2. Key pathways linking climate change to IAQ and health (directly presented from Zhang et al. 2023: *Handbook of indoor air quality*. Springer Nature 2023)

1.4. Problem Statement

As global temperatures rise and extreme weather events become more frequent, the built environment faces new challenges in maintaining healthy indoor environments. Residential buildings, where individuals spend the majority of their time, are particularly vulnerable to the impacts of climate change on IAQ due to factors such as building design, ventilation systems, and occupant behaviors. The problem statement revolves around the need to understand the complex interactions between climate change and IAQ indicators (parameters), quantitatively, including temperature, humidity, air pollutants, and indoor comfort levels. Climate change can exacerbate indoor air pollution by altering outdoor air quality, variation in regional weather patterns along with increasing the frequency of heatwaves (changes of natural AER) and promoting the growth of indoor mold and allergens. Moreover, changes in building energy usage and ventilation patterns driven by climate adaptation strategies may inadvertently compromise

IAQ (More air tightened ↔ Less AER). Also, low maintained HVAC systems can be a source for some indoor pollutants.

This thesis seeks to build a methodology to investigate the relationship through which climate change affects IAQ (quantitatively) and provide a decision supporting tool to assist mitigation of potential risks and promote healthier indoor environments. By elucidating these relationships and developing targeted interventions, this research aims to contribute to the resilience and sustainability of residential buildings in the face of climate change impacts on IAQ.

1.5. Objectives And Research Questions

This Ph.D. research, as a part of OCCuPANt project (OCCuPANt, 2020), forecasts the impact of climate change on Belgian residential houses. Also, it provides a corresponding decision supporting tool to provide information on if and which adaptation measures are needed.

OCCuPANt, University of Liege project:

Impacts of climate change on the indoor environmental and energy performance of buildings in Belgium during summer.

On the strategic level, this research aims at contributing to a healthy and productive community by indicating the vulnerability of occupants in the indoor environment to the projected impacts of climate change. In other words, the research aims to safeguard human health, comfort, and productivity inside buildings despite a changing climate and achieve this most sustainably, by focusing on the IAQ analysis under different future climatological scenarios.

The effect of overheating and extreme heat events on IAQ in Belgium has remained unknown (one of primary OCCuPANt's motivations). In this sense, with a focus on the **summer time**, Ph.D. research objectives are as follows:

(i) Evaluating the application of low-cost air pollution sensors for long-term indoor measurement campaigns (essential for IAQ model development and design validation)

(ii) Developing a modeling-based research methodology for quantitative assessment of climate change impacts on IAQ

(iii) Implementation of the developed modeling-based research framework, along with accusation of required inputs, for both the basis year and the future state

(iv) Introducing a hybrid index to objectivize the climate change impacts on the IAQ (IAQ-CC index)

This research is crucial for understanding and mitigating the effects of climate change-induced overheating on IAQ during summer, ensuring occupant health and comfort in increasingly extreme temperatures. This Ph.D. research intends to answer the following main research question:

• *What are the likely impacts of climate change on the IAQ of residential Belgian houses in summers?*

The main research question can be broken down into several specific questions that need to be addressed initially. Those questions explore different research gaps that are identified and answered in different scientific publications. The specific research questions are as follows:

. ***RQ1.*** *How do current methods assess time-integrated IAQ information in residential buildings in temperate climates in the context of climate change?*

. ***RQ2.*** *How to efficiently employ low-cost sensors for IAQ model development?*

. ***RQ3.*** *How to determine future regional values of IAQ influential parameters following pre-defined scenarios of climate change?*

. ***RQ4.*** *How to quantify and evaluate the IAQ performance of buildings under the overheating impact of climate change, using a decision-supporting tool?*

The second chapter is dedicated to the research framework development. Implementation of each section of the framework is presented in the following chapters. Chapter three presents the IAQ measurement tools aimed at acquiring inputs for the base IAQ model and validating their accuracies. The calibration of low-cost sensor monitoring devices is included in this chapter also. In the fourth chapter, indoor measurement campaigns and their results are presented. In the fifth chapter, the study of the IAQ models, the development of the IAQ basis model (year 2021) in CONTAM, and its validation and calibration processes are presented. Chapter six is dedicated to the future IAQ model input preparation. Ultimately, the seventh chapter addresses the final results, discussions, and conclusions.

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2. RESEARCH FRAMEWORK DEVELOPMENT

2. Research Framework Development

2.1. Introduction

Developing a research framework for quantitative analysis of climate change impacts on IAQ is crucial for understanding and mitigating potential health risks. Climate change affects outdoor air quality, weather patterns, and building environments, all of which can significantly affect IAQ. This framework aims to systematically assess these impacts by integrating climate models, air quality simulations, and building performance evaluations. By quantifying the relationships between climate variables and indoor pollutant levels, the framework provides a robust basis for a methodology for predicting future IAQ scenarios under different climate change projections. Additionally, it assists identifying key factors influencing IAQ, such as changes in temperature (affecting the AERs), and infiltration rates, potential variations in occupants-building relationship, thereby informing the development of adaptive strategies to enhance indoor environmental health and resilience in the face of climate change. This chapter is an effort to answer the first research question (*RQ1*).

2.2. Literature Review

Flagship Studies Targeting Quantitative Assessments Of IAQ In A Changing Climate

This section (2.2.) is drafted with inspiration from reference Pourkiaei et al. 2024 (Systematic framework for quantitative assessment of IAQ under future climate scenarios; 2100s projection of a Belgian case study).

The modeling of IAQ has remained a fundamental subject within the scope of indoor air science and engineering for a long time (Heinsohn & Cimbala 2003). Before obtaining representative IAQ models, measurement campaign, and validation procedures must be performed. Large-scale temporal predictions can only be achieved through the utilization of models. Several underlying processes and elements in assessing IAQ outcome have been found in previous attempts to create

physical and chemical IAQ models, including emissions, infiltration/exfiltration and ventilation, chemical reactions, and surface interactions (sorption and deposition) (Abdalla & Peng 2021).

The recent literature provides valuable information on the various phenomena associated with future climatological scenarios and their potential impacts on IAQ. Nevertheless, it remains complex and diverse to obtain a quantitative approach for the assessment of interlinked and contradictory impacts of these future scenarios on indoor pollutant concentrations (Fisk 2015, Mansouri et al. 2022). The possible effects on IAQ are frequently ignored in discussions about building energy efficiency. Also, the adequate IAQ level is seen in contrast with efficient energy performance.

Energy-saving measures taken at the expense of IAQ reduction, increase the potential negative risks to occupants' productivity, comfort, and health. Hence, it is imperative to standardize the perception of climate change effects on IAQ by establishing the regulations and policies to be enforced in the building codes and retrofit mandates.

The first question considered in evaluating the scientific literature is: "Which studies have quantitatively assessed the impacts of climate change on IAQ?"

Taylor et al. employed EnergyPlus 8.0 integrated generic contaminant model to examine the indoor levels of $PM_{2.5}$ under various UK Climate Projections 2009 (UKCP09) scenarios in the London housing stock (Taylor et al. 2015). Their model takes into account the natural ventilation, infiltration of ambient outdoor $PM_{2.5}$ into indoors, $PM_{2.5}$ produced indoors through fixed trends of cooking and smoking, and reduced building permeabilities. The model doesn't consider any variations in outdoor air PM levels and assumes it at fixed levels. The predictions till 2050 indicated that flats have 0.7–0.8 times as much outdoor $PM_{2.5}$ infiltrating indoors compared to detached dwellings, but 1.8–2.8 times higher $PM_{2.5}$ from indoor sources.

Ilacqua et al. employed a steady-state single-zone mass balance model to estimate the climate change effects on future indoor air pollution "exposures", in terms of changing infiltration rates

(Ilacqua et al. 2017). Their model only takes into account the infiltration ratio of pollutants from ambient to indoors through the building leakages, and its correlation with future climate (temperature) scenarios. The model doesn't consider any ventilation type, occupant behavior, and variations in outdoor air pollution levels. The AER via infiltration was estimated by the Lawrence Berkeley National Laboratory (LBL) model (McWilliams & Jung 2006). The findings for a temporal range of 2040-2070 indicated a 5% decrease in infiltration rates would lead to a 2-23% relative rise in the level of indoor-originating contaminants, along with a 2-18% decrease in the level of outdoor-originating contaminants.

Chang et al. investigated the influence of climate change on the variations of indoor formaldehyde (molecular formulae: HCHO) levels, by IIAQ-CC model (a developed dynamic multimedia model based on mass balance equations) (Chang et al. 2018). The modeling was performed for the temporal range of 2010-2100. The outdoor concentration of formaldehyde was estimated by a model named KPOP-CC, which allocates meteorological data with IIAQ-CC. However, no available English language reference describing the KPOP-CC model was found. Future indoor formaldehyde levels were predicted by considering different scenarios of formaldehyde emission and window openings.

Salthammer et al. employed single-zone mass balance and one-dimensional heat transfer models to evaluate the impacts of climate change on PM levels and indoor climate, in a single-family house (Salthammer et al. 2018). The model didn't take into account the impacts of the building envelopes, airflow patterns, indoor emission sources, and mechanical ventilation systems. Also, they only made rough theoretical estimates of future outdoor PM levels based on past data statistics. For warm seasons until 2040, their model estimated a reduction of indoor $PM_{2.5}$ and PM_{10} concentrations by 22% and 34%, respectively. Zhao et al. (in continue of Salthammer et al. 2018) addressed the future outdoor air pollution concentrations (only for 24hr, O_3) without presenting the detailed method, in a recent study (Zhao et al. 2024). They have falsely claimed

that IPCC (Intergovernmental Panel on Climate Change) scenarios provide the change in annual mean concentrations. However, they don't discuss the fact that IPCC target contaminants are only GHGs (GHG surface air mole fractions of 43 species, including CO_2, CH_4, N_2O, HFCs, PFCs, halons, HCFCs, CFCs, sulphur hexafluoride (SF_6), ammonia (NF_3) (Chen et al. 2021a)), and their future annual mean emission rates are provided, not their regional concentrations (IPCC AR6, 2023, Meinshausen et al. 2020, Chen et al. 2021b).

Fazli et al. developed national residential energy and indoor air model, to predict energy use and IAQ, in the U.S. dwellings in the mid-21st century (Fazli et al. 2021). They developed a comprehensive single-zone mass balance model to estimate indoor pollutant concentrations. Their model takes into account infiltration, natural and mechanical ventilation, deposition, reaction, and pollutant removal by HVAC filters. They utilized CMAQ model to estimate future outdoor air pollution. The Community Multiscale Air Quality model or CMAQ, is a sophisticated three-dimensional Eulerian grid chemical transport model developed by the US EPA for studying air pollution from local to hemispheric scales. They considered a series of assumptions for future building characteristics (increased airtightness, implementation of electric stoves and HVAC systems), and population evolution (increased construction in building housing stock and population displacement), while other less predictable parameters were kept constant. Their results showed that indoor levels of PM_1, $PM_{2.5}$, and NO_2 would decrease due to reductions in both indoor and outdoor sources. Also, indoor levels of O_3 stemming from outdoor origins would rise, potentially increasing indoor chemistry reactions. Considering the results and learning lessons from the International Energy Agency (IEA) EBC Annex 86 "Energy Efficient IAQ Management in Residential Buildings" (Annex-86 2024), specially the subtask 4 (ST4): performance of smart ventilation (Kolarik & Guyot 2022, Guyot et al. 2023), the outcome of the literature analysis is presented in Table 2.1.

Table 2.1. Studies in the literature that quantitively assessed the IAQ under future climate scenarios.

IAQ-CC Study	IAQ model	Ventilation type	Future Climate Scenario	Future air pollution	Future building characteristics	Future Occupant activities	Pollutants
Taylor et al. 2015	EnergyPlus	natural	UKCP09	-	✓	✓	$PM_{2.5}$ (↑)
Ilacqua et al . 2017	single-zone mass balance	-	IPCC* A2	-	-	-	Rn, PM_1, $PM_{2.5}$, O_3, Carbonyl, NO_2, HNO_3 (↑↓)
Chang et al. 2018	mass balance	natural + mechanical	IPCC, RCP8	KPOP-CC	✓	✓	Formaldéhyde (↑↓)
Salthammer et al. 2018	single-zone mass balance	-	IPCC, RCP8	-	-	-	$PM_{2.5}$, PM_{10} (↓)
Fazli et al. 2021	single-zone mass balance	natural + mechanical	IPCC, RCP8	CMAQ	✓	-	PM_1(↓), $PM_{2,5}$(↓), NO_2(↓), O_3(↑), VOC(↑),
Zhao et al. 2024	single-zone mass balance	-	IPCC, SSP1,2,5	~	-	-	O_3, Limonene(↑↓) (24 hr)

* IPCC & its scenarios (RCP & SSP) are presented in section 6.1.1, in details.

2.3. Thesis Research Framework

A research framework provides a structured approach to guide the research process, ensuring that all relevant aspects are considered and addressed systematically. Secondly, it helps to clarify the research objectives, questions, and hypotheses, providing a clear roadmap for conducting the study.

After understanding the principles of research problem, the correlated literature and references were examined methodologically. It was realized that the net effect of climate change on indoor contaminant levels (correlated to occupants' exposure) is contingent upon various mechanisms beyond mere temperature rise. These mechanisms include the arrangement of emission sources (indoors or outdoors), behavioral responses, potential building modifications, and the climate change penalty on ambient air pollution and meteorological conditions.

Evaluation of a representative system in its future state as the main goal (research question), prioritize and mandate a modeling solution. Due to the lack of national representative IAQ designs in Belgium, developing a base IAQ design (case study) was targeted. To meet the requirements for a *validated IAQ design*, a series of experiments were considered for the design validation and calibration.

Complementarily, obtaining the future input variables and adjusting the research assumptions due to limitation factors were taken into account. It should be noted that the research framework was designed and developed in multiple steps during the thesis progress. Figure 2.1. illustrates the designed framework of this thesis for the quantitative assessment of climate change impacts on IAQ.

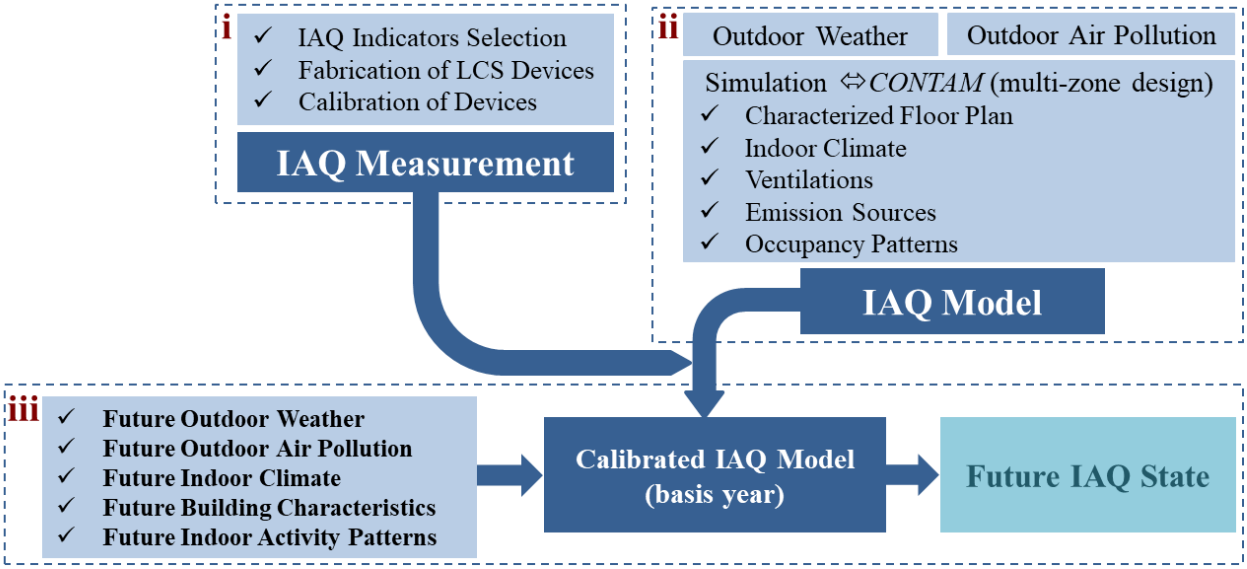

Fig 2.1. Intensive thesis framework for quantitative assessment of climate change effects on IAQ.

Selecting this approach requires series of assumptions as well as considering certain levels of uncertainties. In this method, the IAQ model should be fed by main future inputs including future outdoor air pollution, future AERs, future climate data, and future indoor climate. Also, other future parameters (occupants' behavior, building characteristics, ventilation, etc.) should be considered. The output results can go into as much detail as the IAQ model allows. Generally, well-developed IAQ models are capable to take into account ventilations, emissions, depositions, filtrations, and leakages, as well as defined chemical reactions based on formerly identified physical chemistry involved in the phenomena. Correspondingly, if a phenomenon is not identified, generalized or described in terms of scientific equations (e.g., atmospheric chemical interactions or surface emission rates among other physical-chemical factors, etc.); it is not going to be determined in the future modeling, either. Models, enable us to have a reliable temporal estimation through the events with current available knowledge of phenomena by the help of assumptions. The outcome analysis could be advanced, as far as the IAQ model is capable to simulate involved physical and chemical domains. Moreover, impacts of climate change vary on a regional basis (Lead 2008). Hence, the impacts of climate change on IAQ should be studied vary by region as well.

Figure 2.2. presents the research methodology of the project in terms of a study conceptual framework (SCF). SCF is the tool that ties all aspects of the study together, offering a coherent perspective to understand the research more holistically.

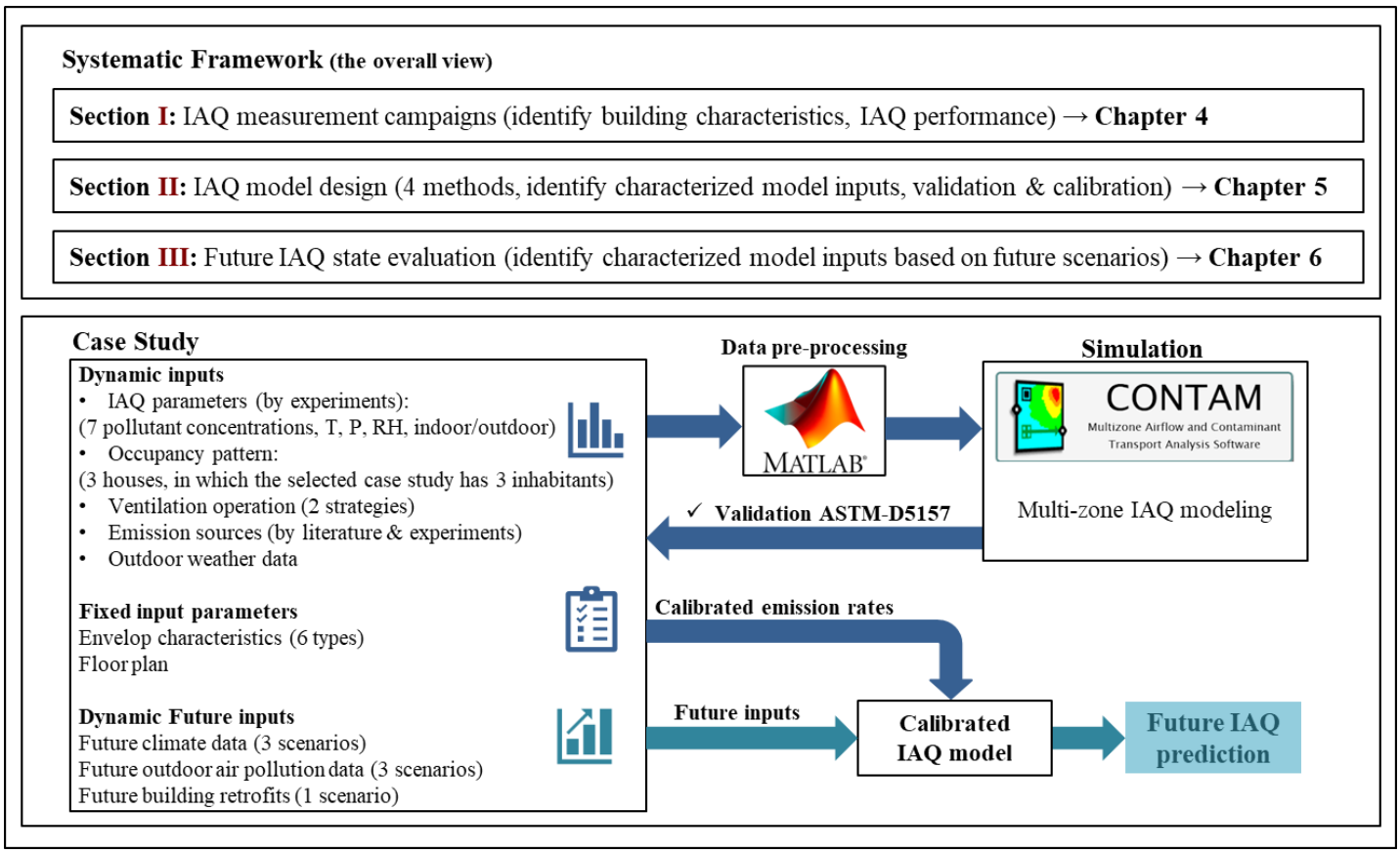

Fig 2.2. Study conceptual framework (SCF).

2.4. Conclusion

There are rising IAQ concerns about both GHG emissions and heatwave risks (direct/indirect), which are expected to take place to a greater extent in future climate scenarios. There is no common guidance to examine the climate change effects on IAQ quantitatively, to date. To overcome this lack, as the first step of this thesis a "thesis research framework" (see Figure 2.1.) and a "study conceptual framework" (see Figure 2.2.) were developed. In order to recap these frameworks into a more general road map that can be followed step by step (with various choices) to evaluate all influential factors computably, a systematic framework is presented in the Figure 2.3. (Pourkiaei et al. 2024). The first strength of this systematic framework is rooted in the robust literature study and consideration of all

accomplished distinct projects on the topic, worldwide. While the systematic framework presents multiple choices for researchers at each section and step, the thesis focus is on a time and cost-efficient approach selection for all three main steps of i) IAQ measurement, ii) IAQ model design, and iii) Future IAQ state evaluation. Different aspects of this modular systematic framework, and the selected solutions among those presented, will be discussed in the following chapters of the thesis. The primary objective of the proposed framework is to offer a wide variety of solutions for quantitative IAQ investigation across the board. It is noteworthy that, while implementing the framework on the selected case study, the research placed greater emphasis on the summer duration (due to project objectives concerning overheating - Chapter 4), the application of CONTAM IAQ model (for computing natural ventilation AERs - Chapter 5), and the pollutant O_3 (a highly influential contaminant for the hybrid index – Chapter 7).

Correlated publishment of this chapter:

Pourkiaei, M., & Romain, A. C. (2023). Scoping review of indoor air quality indexes: Characterization and applications. *Journal of Building Engineering*, 106703, https://doi.org/10.1016/j.jobe.2023.106703

Pourkiaei, et al. (2024). Systematic Framework for Quantitative Assessment of Indoor Air Quality Under Future Climate Scenarios; 2100s Projection of a Belgian Case Study. *Journal of Building Engineering*, 109611, https://doi.org/10.1016/j.jobe.2024.109611

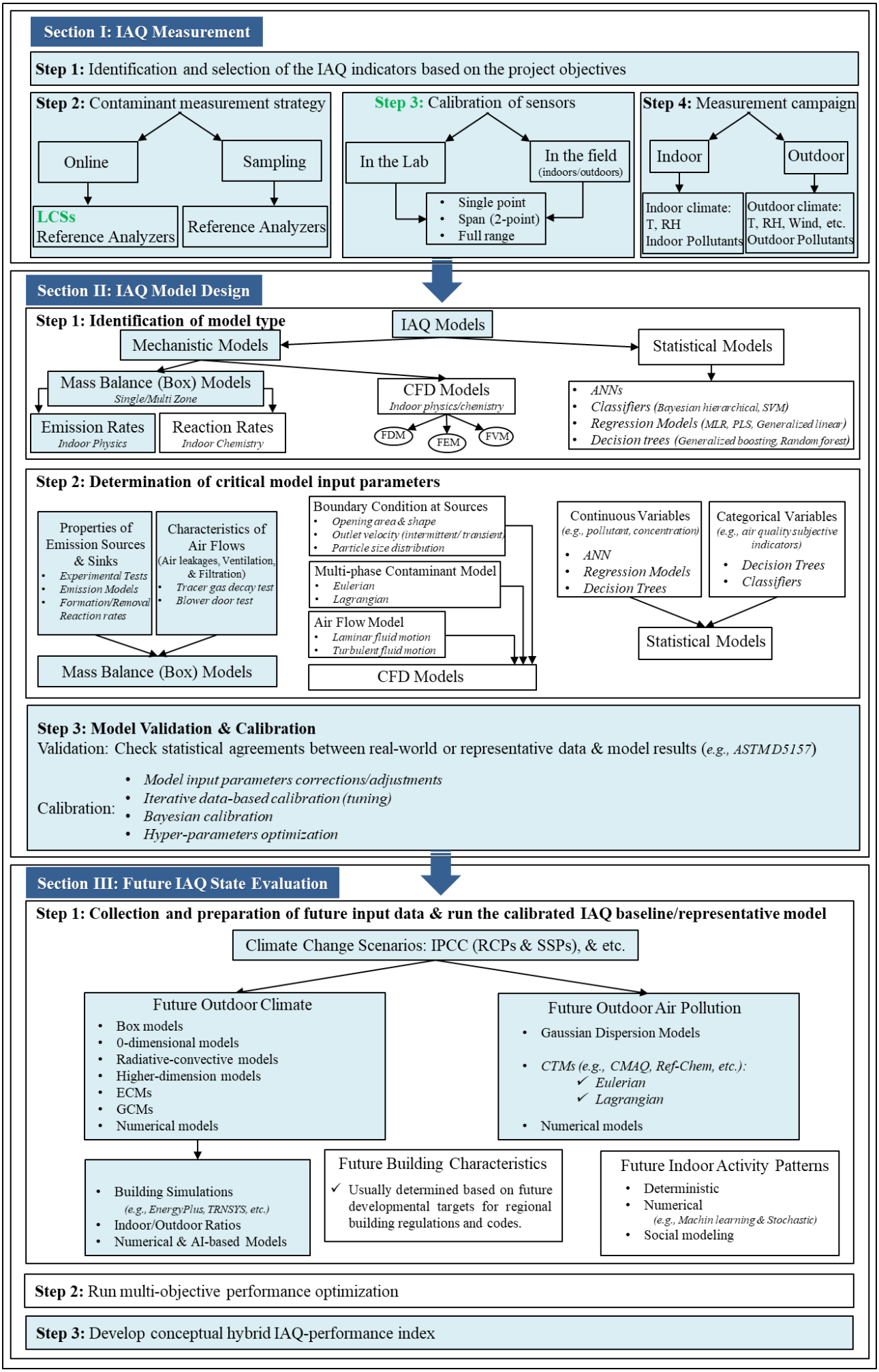

Fig 2.3. Systematic Framework for quantitative assessment of IAQ under future climate scenarios (the followed path in this PhD thesis is highlighted in light blue colour).

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3. APPLICATION OF LOW-COST AIR QUALITY SENSORS FOR IAQ EXPERIMENTS

3. Application Of Low-Cost Air Quality Sensors For IAQ Experiments

3.1. Introduction

IAQ measurements are essential for both assessing the presence (concentration) of pollutants in enclosed spaces, and also validation of IAQ model designs (model performance evaluation). Poor IAQ can have significant implications for human health, comfort, and productivity, making accurate measurement techniques crucial for identifying and mitigating indoor air pollution. This section provides an overview of IAQ measurements, including the importance of monitoring, common pollutants of concern, measurement techniques, and emerging trends in real time IAQ assessment. The content of this chapter is inspired by references (Pourkiaei et al, 2022), (Pourkiaei & Romain 2023) and (Pourkiaei et al. 2024) (Systematic framework for quantitative assessment of IAQ under future climate scenarios; 2100s projection of a Belgian case study). This chapter is an effort to answer the second research question (*RQ2*).

3.1.1. Importance Of Monitoring IAQ

Indoor air can contain a multitude of pollutants originating and influenced by various elements, including outdoor environment, building ventilation type and its activity patterns, building air tightness (infiltration/exfiltration), building materials, furniture, cleaning products, combustion processes, and human activities. Pollutants can accumulate indoors and pose health risks to occupants, leading to respiratory problems, allergies, asthma, and other adverse health effects. Additionally, poor IAQ can impact cognitive function, comfort, and overall well-being. Therefore, continuous monitoring of IAQ is essential for identifying potential risks, implementing effective mitigation strategies, and ensuring healthy indoor environments. IAQ measuring experiments play an essential role in obtaining the model required design parameters, input data, along with IAQ model performance evaluations which is commonly referred to as *validation of the IAQ models* (Section 3.1.5.). The main idea of implementing the experiments

step (development of monitoring devices and IAQ measurement campaigns) in the research framework of this thesis is to address the IAQ model validation objective.

3.1.2. Different IAQ Measurement Approaches

A variety of measurement techniques are employed to assess IAQ parameters and pollutant concentrations. These techniques enable comprehensive characterization of IAQ and identification of sources contributing to pollution. These techniques can be categorized into direct sampling methods, which involve the collection of air samples for laboratory analysis, and real-time monitoring methods, which provide continuous, on-site measurements. Direct sampling methods include grab sampling, passive sampling, and active sampling using devices such as pumps and sorbent tubes. Real-time monitoring methods on the other hand, utilize sensors and instruments to measure the target parameters in a continuous manner.

Although advanced measuring/analysis instruments (reference analyzers) allow the exact determination of indoor contaminant concentrations with the highest accuracy and precision, their cost and complicated operations make them unsuitable for various (high temporal & spatial) tasks. The main technologies of reference analyzers include but not limited to Gas Chromatography (GC), High-Performance Liquid Chromatography (HPLC), ion chromatography, Mass Spectrometry (MS), Fourier-transform infrared spectroscopy (FTIR), LED-based UV photometric detection, Flame Ionization Detection (FID), Non-Dispersive Infrared Gas detection (NDIR), Chemiluminescence Detection (CLD), Thermal Conductivity Detector (TCD), Electron Capture Detector (ECD), Cavity Attenuated Phase Shift spectroscopy (CAPS), UV fluorescence detection, and paramagnetic ionization detectors (Zhang Y et al. 2022, Eftekhari et al. 2023). The aforementioned techniques as well as their instrumentations are essentially designed for laboratory/stationary practices. Moreover, they need expert operators and long results time which make them unsuitable for prompt indoor air examinations (Abraham and Li 2014).

3.1.3. Emerging Trends In IAQ Measurement

Advancements in sensor technology, data analytics, and indoor environmental quality (IEQ) monitoring systems are driving innovation in IAQ assessment. Emerging trends in IAQ assessment are witnessing a significant shift towards the adoption of low-cost sensors (LCS), revolutionizing the landscape of IAQ monitoring.

The accuracy of low-cost air sensors varies significantly and is generally lower compared to high-end reference-grade instruments. These sensors can be influenced by environmental factors such as T, RH, and cross-sensitivity to other gases, which can affect their accuracy. Additionally, calibration drift over time can lead to further inaccuracies. Despite these limitations, with proper calibration and correction algorithms, low-cost sensors can provide reasonably reliable data for indicative monitoring and trend analysis. They are particularly valuable for large-scale deployments and citizen science projects where cost constraints prevent the use of more expensive equipment.

These sensors offer the advantages of affordability, portability, and real-time data collection, empowering individuals and building managers to monitor IAQ more comprehensively and efficiently. LCS monitoring devices provide dense temporal and spatial data measurement in a wider range of interior spaces. With the advances of LCSs in quality and operation, reliable devices with compact design and more affordable cost can be employed in holistic measurement/monitoring campaigns (Demanega et al. 2021).

LCS have various working principles including electrochemical sensors (Kumar et al. 2011), metal oxide (MOx) semiconductor sensors, Infrared radiation (IR) sensors, photoionization detectors (PID), and light scattering (Chojer 2020). However, it should be noted that the maintenance and reliability of air pollution LCS are crucial for ensuring accurate and dependable measurement of indoor and outdoor air quality. The following 2.1.4. subchapters are inspired from two recent review studies on the performance and performance evaluation of LCSs (Karagulian et al. 2019, Kang et al. 2022).

3.1.3.1. Calibration and Calibration Verification

Regular calibration of sensors against reference instruments or standard gas is essential to ensure accuracy. Additionally, calibration verification checks should be conducted periodically to confirm the stability and reliability of sensor readings over time.

3.1.3.2. Environmental Conditions

Sensors should be operated within specified environmental conditions (e.g., temperature, humidity) to maintain accuracy and reliability. Exposure to extreme temperatures, high humidity, or contaminants can affect sensor performance and longevity.

3.1.4.3. Sensor Stability and Drift

Monitoring sensor stability and drift over time is essential for detecting changes in performance and ensuring data reliability. Continuous monitoring and periodic recalibration can help mitigate sensor drift and maintain measurement accuracy.

3.1.3.4. Sensor Lifespan and Durability

Assessing the lifespan and durability of sensors is crucial for long-term monitoring applications. Factors such as sensor material, design, and manufacturing quality can influence lifespan and reliability. Regular maintenance, cleaning, and sensor replacement may be necessary to ensure continuous operation and reliable data collection.

3.1.4. Common Indoor Pollutants Of Interest

Several pollutants commonly found in indoor environments are of particular concern due to their adverse health effects. These include particulate matter (PM), volatile organic compounds (VOCs), carbon monoxide (CO), nitrogen dioxide (NO_2), formaldehyde (HCHO), ozone (O_3), radon (Rn), and biological contaminants such as mold, bacteria, and allergens. The sources of these pollutants vary, ranging from outdoor sources (e.g., vehicle emissions, industrial activities) to indoor sources (e.g., cooking, cleaning, smoking, etc.) and building materials (e.g., off-gassing of chemicals from furniture and flooring). With respect to the listed pollutants by the WHO guidelines for indoor air

pollutants (WHO 2010), and considering the project interests, and the availability and limitation factors (using the measurement tools available in the lab and that there were no extra budget for reference analyzers), seven target contaminants were chosen for this project as follows: $PM_{2.5}$, PM_{10}, NO, NO_2, O_3, CO, VOC.

Volatile organic compounds (VOCs) are organic compounds that have a high vapor pressure at room temperature. High vapor pressure correlates with a low boiling point, which relates to the number of the sample's molecules in the surrounding air, a trait known as volatility (Wikipedia 2024). On the other hand, Total Volatile Organic Compounds, or TVOCs, is a term used to describe a group of VOCs that are present in emissions or ambient air. The VOC sensor used in this research is actually a TVOC sensor for the group of Naphthalene, Benzene, Acetone, and Ethylene.

3.2. Material & Methods

3.2.1. LCS Monitoring Devices (OCT)

To provide measurement tools for this thesis project, there were two options of purchasing commercialized instruments (devices) from companies in which there are LCS made by other companies, or developing the instruments by our lab (SAM-ULiège) with commercial LCS (the same as those used in commercialized instruments). Following the second option, four IAQ monitoring devices based on commercial LCSs, were designed by SAM-ULiège for measurement of CO, NO, NO_2, O_3, $PM_{2.5}$, PM_{10}., VOCs, as well as Temperature (T), Pressure (P), and relative humidity (RH). Figure 3.1. shows the IAQ monitoring devices employing low-cost electrochemical, light scattering, and photoionization detector sensors. Since the development of these devices has been part of the OCCuPANt project they are named and referred as OCT in this study. Table 3.1. presents the OCT device sensors specifications. Further detailed specification and corresponding datasheets of sensors are hyperlinked in the Table 3.1.

Fig 3.1. Schematic of OCT IAQ measuring devices.

Table 3.1. LCSs in OCT devices.

Contaminant Sensor	Concentration Range	Sensor names & the providers
CO	2-1000 ppm (±2)	Alphasense Electrochemical B4
NO	2-20 ppm (±2)	Alphasense Electrochemical B4
NO_2	2-20 ppm (±2)	Alphasense Electrochemical B43F
O_3	1-20 ppm (±2)	Alphasense Electrochemical OX-B431
$PM_{2.5}$	0-1000 µg/m^3(±10)	Light scattering Sensirion SPS30
PM_{10}	0-1000 µg/m^3(±25)	Light scattering Sensirion SPS30
VOC	0.5 ppb - 2 ppm	Photoionization detector AMETEK MOCON (Blue)
T	-40 to 85 °C	Bosch BME280
RH	0 - 100%	Bosch BME280
P	300 – 1100 hPa	Bosch BME280

The Table 3.2. is presenting the principles, performances and limitations of each technology (category) used in OCT devices (Narayana 2022, Yatkin et al. 2022).

Table 3.2. Principles, performances and limitations of each technology (category) used in OCT devices.

Sensor Types	Principles, performances and limitations
Electrochemical	**Principle**: • Electrochemical sensors detect gases through a chemical reaction that occurs when the target gas interacts with an electrolyte solution inside the sensor. This reaction generates an electrical current that is proportional to the concentration of the gas. **Performance**: • **Accuracy**: Generally good, with precise measurements for specific gases. • **Response Time**: Fast response, typically within seconds. • **Selectivity**: High selectivity for specific gases. • **Sensitivity**: Can detect low concentrations of gases, often in (ppm) or even (ppb). **Limitations**: • **Lifetime**: Limited lifespan, typically ranging from 1 to 2 years, as the electrolyte can deplete over time. • **Environmental Sensitivity**: Performance can be affected by temperature and humidity variations. • **Cross-Sensitivity**: Potential interference from other gases, although usually designed to minimize this. • **Calibration**: Requires frequent calibration and maintenance to ensure accurate readings.
Light Scattering	**Principle**: • Light scattering sensors measure PM concentrations by detecting the scattering of light caused by particles suspended in the air. A light source (usually a laser or LED) illuminates the particles, and a photodetector measures the intensity of scattered light. **Performance**: • **Accuracy**: Varies depending on particle size and sensor calibration; generally good for relative concentration measurements. • **Response Time**: Rapid response, often within seconds. • **Selectivity**: Measures PM without distinguishing between different types of particles. • **Sensitivity**: Capable of detecting fine particles ($PM_{2.5}$ and PM_{10}), with some models able to measure ultrafine particles (PM_1). **Limitations**: • **Calibration**: Requires calibration to ensure accuracy, as scattering intensity depends on particle size and composition. • **Environmental Sensitivity**: Performance can be affected by high humidity and other environmental factors (Temperature, Acoustics, etc.) that influence light scattering. • **Particle Overloading**: High particle concentrations can lead to multiple scattering events, reducing measurement accuracy.
PID	**Principle**: • Photoionization detectors use ultraviolet (UV) light to ionize volatile organic compounds (VOCs) and other gases. The ions produced are collected by electrodes, generating a current proportional to the concentration of the ionized gases. **Performance**: • **Accuracy**: High accuracy for detecting a broad range of VOCs and some inorganic gases. • **Response Time**: Very fast response, typically within seconds. • **Selectivity**: Less selective, as it can ionize any gas with an ionization energy lower than the UV lamp's photon energy. • **Sensitivity**: High sensitivity, capable of detecting low concentrations of VOCs, often in ppb levels. **Limitations**: • **Calibration**: Requires frequent calibration and maintenance to ensure accurate readings. • **Environmental Sensitivity**: Performance can be affected by humidity, temperature, and the presence of other ionizable gases. • **Lamp Life**: The UV lamp has a limited operational life and may need periodic replacement. • **Cross-Sensitivity**: Can detect multiple compounds simultaneously, which may complicate the interpretation of results.

3.2.2 Calibration Of Lab Devices (OCTs For OCCuPANt)

Calibration of a sensor involves establishing a relationship between the electrical signal generated by the sensor and the quantity being measured, such as the concentration of a specific chemical in the air. In the context of air pollution sensors, calibration typically involves measuring a standard gas of known concentration and composition and correlating the resulting electrical signal from the sensor to the concentration of the target pollutant in the gas. This process is often achieved through a calibration curve, which is a mathematical model, often of the linear regression type, that relates the sensor's output signal to the concentration of the target pollutant. By comparing the sensor's response to known concentrations of the pollutant, a calibration curve can be generated, allowing for the conversion of electrical signals from the sensor into accurate measurements of pollutant concentrations in the air. Regular calibration ensures the accuracy and reliability of sensor measurements over time, accounting for factors such as sensor drift and environmental variations. One other approach for sensor calibration is using reference analyzers. Figure 3.2. illustrates mandates criteria of LCS calibrations. the The Table 3.3. summarizes processes, advantages, and disadvantages of these two approaches. Considering all, the approach of calibration with reference analyzers was chosen for this study.

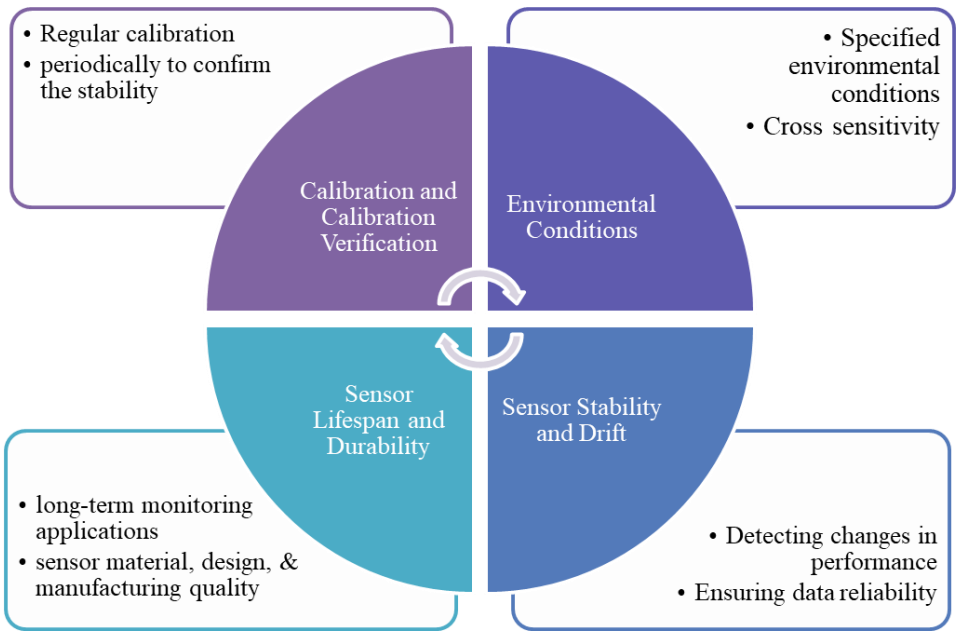

Fig 3.2. LCS calibration mandates.

Table 3.3. Processes, advantages, and disadvantages of sensor calibration with reference analyzers & gas.

Method	Processes, advantages, and disadvantages
Sensor Calibration with Reference Analyzers	**Process**: 1. **Co-Location**: Place the low-cost sensor and the reference analyzer in the same location to ensure they are exposed to the same environmental conditions and pollutant concentrations. 2. **Data Collection**: Collect data simultaneously from both the sensor and the reference analyzer over a defined period. 3. **Comparison and Adjustment**: Compare the sensor readings with the reference analyzer readings. Use statistical methods to develop calibration equations or correction factors to adjust the sensor data to match the reference analyzer data. **Advantages**: ✓ High accuracy: Ensures that the sensor readings are closely aligned with the established standard of the reference analyzer. ✓ Comprehensive: Takes into account real-world environmental conditions and potential interferences. **Disadvantages**: × Time-consuming: Requires extended periods of data collection for accurate calibration. × Costly: Involves the use of expensive reference analyzers and potentially additional personnel for data collection and analysis.
Sensor Calibration with Reference Gas	**Process**: 1. **Controlled Exposure**: Place the sensor in a chamber where it can be exposed to a reference gas at known concentrations. 2. **Data Collection**: Measure the sensor response to various concentrations of the reference gas. 3. **Calibration Curve**: Develop a calibration curve by plotting the sensor response against the known concentrations of the reference gas. Use this curve to adjust the sensor readings. **Advantages**: ✓ Precision: Provides a highly controlled and precise method for calibration. ✓ Efficiency: Can be quicker than co-location with reference analyzers, as it does not require extended field deployments. **Disadvantages**: × Limited Scope: Does not account for real-world environmental variables such as temperature, humidity, or interference from other pollutants. × Specificity: Calibration with one type of reference gas may not generalize well to other types of pollutants or different environmental conditions.
Summary of Differences	**Real-World Conditions vs. Controlled Environment**: ❖ **Reference Analyzers**: Calibration reflects real-world conditions, including environmental variables and potential interferences. ❖ **Reference Gas**: Calibration is conducted in a controlled environment, focusing solely on the target gas. **Accuracy and Comprehensive Calibration**: ❖ **Reference Analyzers**: Provides a more comprehensive calibration by considering the effects of environmental factors. ❖ **Reference Gas**: Offers precise calibration for the specific gas used but may not account for other environmental influences. **Time and Cost**: ❖ **Reference Analyzers**: Typically more time-consuming and costly due to the need for co-location and extended data collection periods. ❖ **Reference Gas**: Generally quicker and potentially less expensive, but may require access to certified reference gases and appropriate calibration chambers. **Application Suitability**: ❖ **Reference Analyzers**: Suitable for comprehensive calibration needed for regulatory or high-accuracy applications. ❖ **Reference Gas**: Suitable for initial calibration or when specific gas concentration responses are needed without environmental complexities.

Instruments and some commercial LCS often come with the calibration curve (implemented into the processor) as they already provide the concentration values (calibration by the sensor manufacturer). However, it is necessary to check (verify) if these calibration models are still sufficient by doing additional calibrations. Because sensors and instruments drift in time and have different performances in different environments.

The measurement accuracy of LCSs is highly correlated with factors such as Air Temperature and RH fluctuations, cross-sensitivity, interferences from other compounds, and electronic component tolerances (Pereira & Ramos 2022, Zhang & Srinivasan 2020). In this regard, uncertainties may stem from sensor calibration and synchronization errors. Uncertainties can also be among sensor data description and sampling, co-location experiments, sensor placement, aerosol concentration determination, and result interpretation (Zhang & Srinivasan 2020).

The idea of this verification is to compare the response given by the LCS instruments with the response of a reference instrument. The associations between the raw output of LCSs and measurements from the reference analyzers are then characterized by a calibration equation (Liang 2021, deSouza et. al 2022).

A sensor calibration measurement campaign had to be performed for the (re)calibration purpose of OCT devices. This was conducted from 2nd Oct 2020 at 8:30 local time, to 31st Oct 2020 at 23:30 at ISSeP (Institut Scientifique De Service Public) in Val-Benoît, Liège, Belgium (see Figures 3.3.a & 3.3.b) (ISSeP 2021). The sensors were located at the same place as the reference analyzers (both indoor and outdoor experiments) at the height of 2m. The meteorological data including the temperature, relative humidity, wind speed, and direction were recorded and employed to contextualize the data, to confirm that different conditions were characterized. The specification of ISSeP instruments are available at their website (ISSeP 2024). The key assumptions considered during this LCS calibration stage of the study are presented in the Table 3.4.

Table 3.4. Key assumptions for LCS calibration (with reference analyzers)

Assumptions	Description of assumptions versus the possibly in the reality
Calibration Consistency	✓ Sensors are calibrated correctly and consistently over time. × Calibration may drift, requiring regular maintenance and recalibration to ensure accuracy.
Environmental Stability	✓ Environmental factors such as temperature, humidity, and pressure have minimal impact on sensor performance. × These factors can significantly affect sensor readings, necessitating compensation algorithms or correction factors.
Specificity & Selectivity	✓ Sensors can specifically and selectively measure target pollutants without interference from other substances. × Cross-sensitivity to other gases and particles can lead to inaccurate readings.
Response Linearity	✓ The sensor's response to varying concentrations of pollutants is linear across the range of interest. × Sensor response may be non-linear, especially at high or low concentrations, requiring complex calibration curves.
Data Quality & Reliability	✓ The data generated by low-cost sensors are of high quality and reliable for analysis and decision-making. × Data quality may be compromised by sensor noise, drift, or malfunction, necessitating rigorous data validation and quality control procedures.
Lifetime & Durability	✓ Sensors will maintain their performance over an extended period. × Sensor lifespan can be limited, and performance may degrade over time due to environmental exposure and wear & tear.
Comparability to Reference Instruments	✓ Low-cost sensors provide results comparable to high-precision, regulatory-grade instruments. × While low-cost sensors offer valuable insights, their accuracy and precision typically do not match those of reference instruments, requiring careful comparison and validation.
Power Supply & Connectivity	✓ Sensors will operate continuously and transmit data reliably. × Power supply issues and connectivity problems can disrupt data collection, necessitating backup systems and robust network solutions.

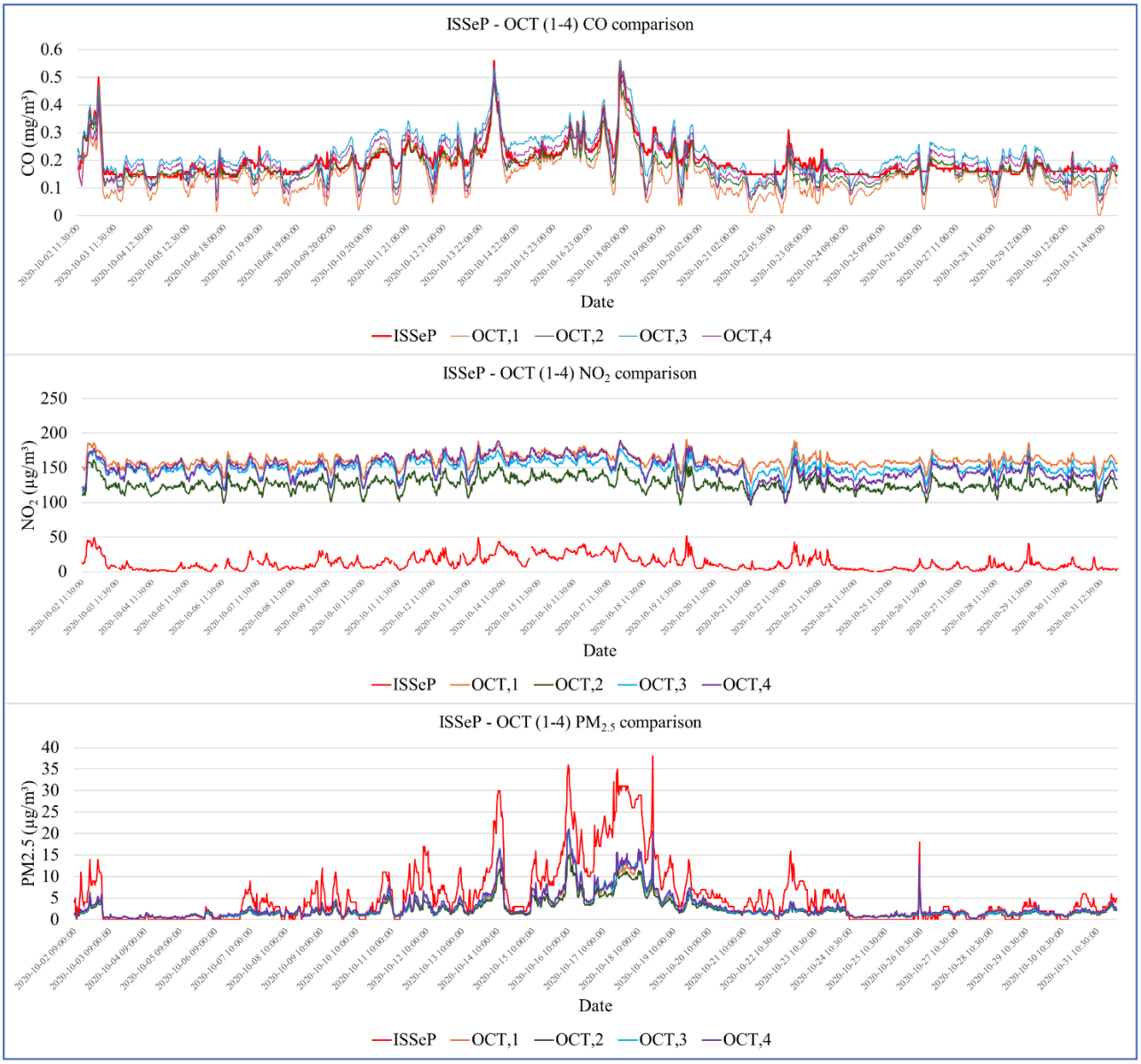

Fig 3.3.a OCT devices raw output vs. ISSeP reference analyzers results: CO, NO_2, $PM_{2.5}$.

Fig 3.3.b OCT devices raw output vs. ISSeP reference analyzers results: NO, O_3, PM_{10}

3.2.2.1. Sensor Calibration (Model Correction)

A final dataset of 1423 paired/concurrent measurements (LCS against analyzers concentration values) was recorded per sensors, for each of four devices, with the time acquisition of 30 minutes. The whole dataset included 48 382 datapoints (excluding VOC values by analyzers). The dataset population was divided with the ratio of 80 and 20% for calibration and validation datasets, respectively.

Data treatment is performed in MATLAB software. The K–S test (Kolmogorov–Smirnov examination) disapproved the hypothesis of normal distribution. Due to the synchronized real-time measurement process, a monotonic relationship is observed. Since Spearman's correlation (r_s) measures the strength and direction of monotonic association between variables, it was used to define the correlation between variables of paired dataset (OCT vs ISSeP).

Additionally, to compare the differences between each of the measurements among four different OCTs, the Kruskal–Wallis test, a nonparametric test, was applied to determine if there were statistically significant differences between them.

In the next step, corrections of the OCT outputs are applied after determination of calibration equations among analyzers concentration and OCT concentration (Y = analyzers concentrations and X = OCT sensors concentrations, 1138 paired data points for each sensor) by the orthogonal regression method (Späth 2014). Following, validation datasets (285 paired data) are used to evaluate the correctness of the sensors' outputs after applying calibration equations.

Derived values are then compared with those of the reference analyzers by the Bland–Altman method (Gerke 2020). The Bland-Altman (mean-difference and limits of agreement (LOA) plot) is applied to evaluate the difference between two measurements within 95% LOA (or 1.96 of the standard deviation Falzone et al. 2020; Moreno-Rangel et al. 2018.

3.3. Results

3.3.1 Low-Cost Sensors Calibration

Table 3.5. represents statistical analysis over primary OCTs' and reference ISSeP datasets. The analysis includes the correlation ranges of 4 OCT devices among each other (OCT Inter-variability), correlation ranges of 4 OCT devices and ISSeP results, the mean (average) and ranges of "average difference" between OCTs and ISSeP results, and the mean (average) and ranges of OCTs variances.

Table 3.5. Statistical analysis over OCT and ISSeP datasets.

OCT Inter-variability		**CO**(mg/m^3)	**NO**(µg/m^3)	**NO$_2$**(µg/m^3)	**O$_3$**(µg/m^3)	**PM$_{2.5}$**(µg/m^3)	**PM$_{10}$**(µg/m^3)
Correlations of OCT pairs (r_s, p<0.001)		0.96 - 0.98	0.96 - 0.98	0.90 - 0.96	–0.18 - 0.9	0.99	0.99
OCT-ISSeP variability		**CO**(mg/m^3)	**NO**(µg/m^3)	**NO$_2$**(µg/m^3)	**O$_3$**(µg/m^3)	**PM$_{2.5}$**(µg/m^3)	**PM$_{10}$**(µg/m^3)
Correlations of OCTs & ISSeP (r_s, p<0.001)		0.73 - 0.80	0.30 - 0.35	0.70- 0.83	0.22 - 0.67	0.93 - 0.95	0.86 - 0.88
Average difference of OCTs & ISSeP	**Mean(M)**	–0.016	+185.47	+134.66	+1.9	–3.2	–8.63
	Range	–0.05 - 0.01	171.17 – 199.4	114.57 - 149.21	–3.2 - 7.8	–2.76 - –2.47	–9.09 - –8.33
Variances of OCTs (σ^2)	**Mean(M)**	0.004	195.51	138.21	27.41	8.19	2.87
	Range	0.003 - 0.005	157.16 - 229.55	88.67 - 247.28	21.39 - 31.28	8.43 - 9.64	2.33 - 3.12

Table 3.6. presents the calibration equations (OCT vs ISSeP) and coefficient of determinations (R^2) for the best fit of each sensor among field and indoor experiments, using validation datasets.

Table 3.6. Calibration equations for the best fit using validation datasets, and R^2.

Contaminant	Best calibration equations	Best fit of validation datasets after applying regression equations to OCTs' values, (R^2)
CO(Field)	$0.033 + 0.96\ CO_{OCT}$	0.79
NO(Indoor)	$3.92 + 0.63\ NO_{OCT}$	0.80
NO_2(Indoor)	$-48.39 + 0.81\ NO_{2_{OCT}}$	0.78
O_3(Indoor)	$8.31 + 0.51\ O_{3_{OCT}}$	0.84
$PM_{2.5}$(Field)	$-1.57 + 3.08\ PM_{2.5_{OCT}}$	0.92
PM_{10}(Field)	$-2.12 + 4.77\ PM_{10_{OCT}}$	0.57

3.3.3.1. OCT Inter-Variability Analysis

CO.

Information of variability between OCTs is essential for the practical reliability of devices. Examination of the CO data from the four OCT devices presented a very high uniformity ($r_s = 0.96\ to\ 0.98,\ p < 0.001$) and low variability (avg $= 0.004\ mg/m^3$, from 0.003 to 0.005 mg/m³) among the CO measurements.

NO.

Investigation of the four OCTs revealed a very high uniformity ($r_s = 0.96\ to\ 0.98,\ p < 0.001$) and high difference regarding (avg $= 195.51\ \mu g/m^3$, from 157.16 to 229.55 µg/m³) of the NO reference data.

NO_2. Study of four OCT devices presented a very high uniformity ($r_s = 0.9\ to\ 0.96,\ p < 0.001$) and high variance (avg $= 138.21 \mu g/m^3$, from 88.67 to 247.28 µg/m³) between the different NO_2 sensors.

O_3. Investigation of the four OCT datasets presented a low but notable uniformity ($r_s = -0.18\ to\ 0.9,\ p < 001$) and a moderate variance (avg $= 27.41\ \mu g/m^3$, from 21.39 to 31.28 µg/m³) between the O_3 measurements.

$PM_{2.5}$. The examination of the four OCT monitors revealed a very high uniformity ($r_s = 0.99$, $p < 0.001$) and a small variance (avg $= 8.19 \mu g/m^3$, from 8.43 to 9.64 µg/m³) among $PM_{2.5}$ measurements.

PM_{10}. The study of four OCT datasets presented that there was a very high uniformity ($r_s = 0.99,\ p < 001$) and a small variance (avg $= 2.87\ \mu g/m^3$, from 2.33 to 3.12 µg/m³) between the different PM_{10} sensors.

3.3.1.2. ISSeP-OCT Comparison (OCT Calibration)

Figure 3.4. depicts the correlation between pollutant levels measured by ISSeP reference analyzers and calibrated OCT measurements. The calibrated OCT measurements are obtained after applying corrections using the corresponding best orthogonal regression models. The data of the four OCT devices were compared to those from the ISSeP**:**

CO.

The data analysis presented that the CO measurements were highly correlated ($r_s = 0.73\ to\ 0.8$, $p < 0.001$). As it is shown in Figure 3.3. (a), it was revealed that OCTs averagely underestimated CO concentration (avgerage (avg) $= -0.016$, 95% confidence interval from 0.05 to $-0.01\ mg/m^3$).

The best fit results in an R^2 of 0.79 and the CO equation generated by regression is:

$$CO(ISSeP) = 0.033 + 0.963\ CO(OCT) \quad (1)$$

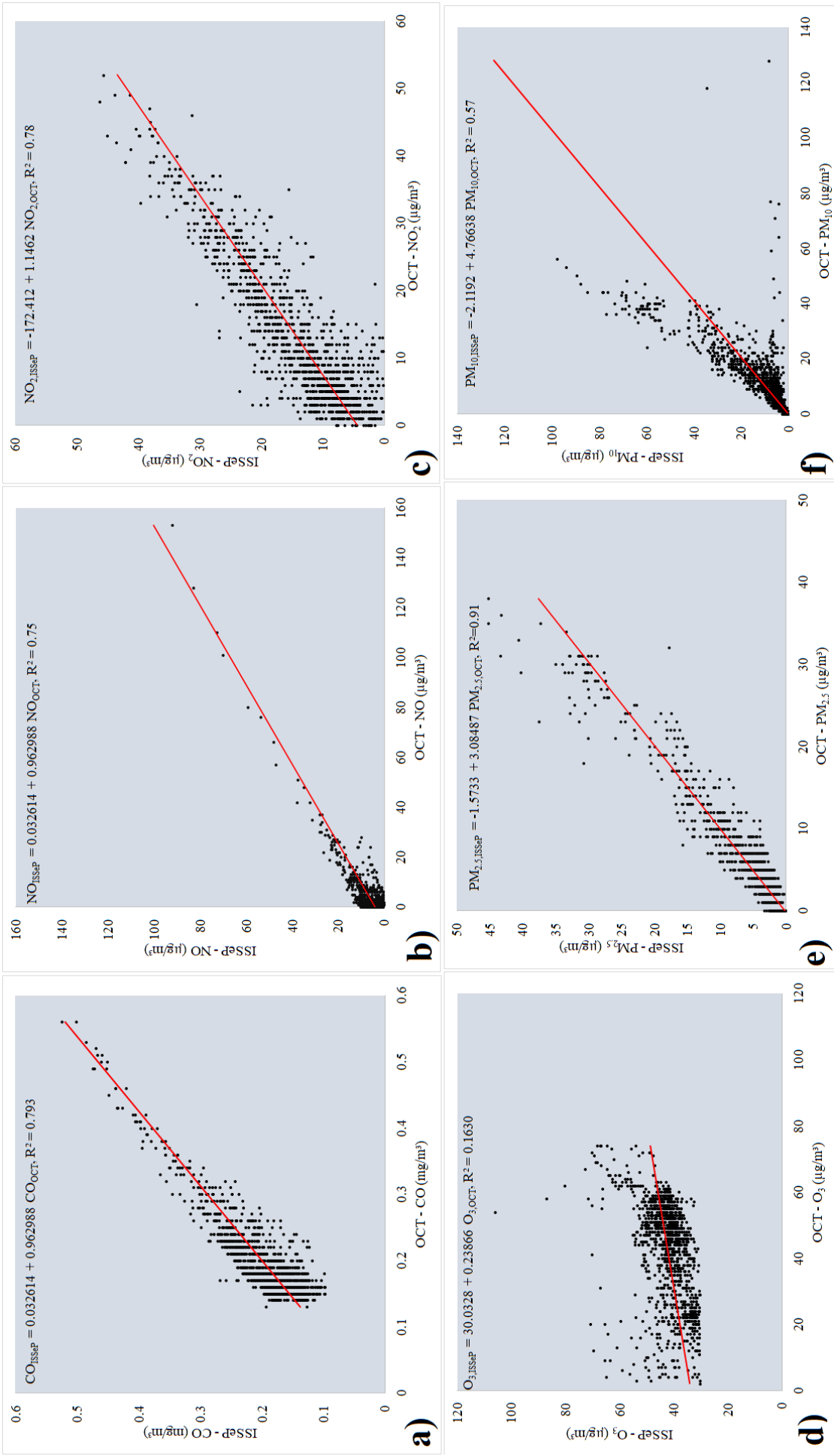

Fig 3.4. Comparison of calibrated OCTs with the ISSeP: (a) CO (b) NO (c) NO_2 (d) O_3 (e) $PM_{2.5}$ (f) PM_{10}

Figure 3.5. (a) presents the Bland–Altman analysis for the comparison of four calibrated sensor devices with the reference analyzer. It presents the mean difference between the ISSeP and the OCT CO calculated measurements (-2.34E-10 mg/m^3 with the LOA of –0.055 to 0.055 mg/m^3 at a 95% confidence interval). The number of 48 points (3.5 %) of the dataset were beyond of the LOA (42 higher than the upper LOA and 6 less than the lower LOA). This range is meaningfully far below the European Commission (EC) Exposure Limit Values (ELVs) for indoor CO which is about 10 mg/m^3 (Maximum daily, 8-hour mean, 2005).

NO. The data analysis presented that the NO measurements were weakly correlated ($r_s = 0.3\ to\ 0.39,\ p < 0.001$) by the four OCT and the ISSeP monitors. As it is shown Figure 3.3. (b) a shift of the values was detected between OCT and ISSeP measurements, as long as the OCT overestimated the NO levels by an average of 185.47 µg/m³, from 171.17 to 199.42 µg/m³. Figure 3.4. (b) illustrates the relationship between the ISSeP and OCT calibrated NO levels determined by the Orthogonal regression model. The best fit results in an R^2 of 0.75 and the NO regression output modeled is:

NO(ISSeP) = 0.033 + 0.963 NO(OCT) (2)

Figure 3.5. (b) depicts the Bland–Altman analysis for the ISSeP NO measurements by the corresponding best fit determined by the Orthogonal regression for the validation dataset from the four OCT measurement devices. It presents the mean difference between the ISSeP and the OCT NO calculated measurements (-2.19 µg/m³ with the LOA of -12.14 to 8.03 µg/m³ at a 95% confidence interval). The number of 28 points (2.8 %) of the dataset were beyond of the LOA (28 higher than the upper LOA).

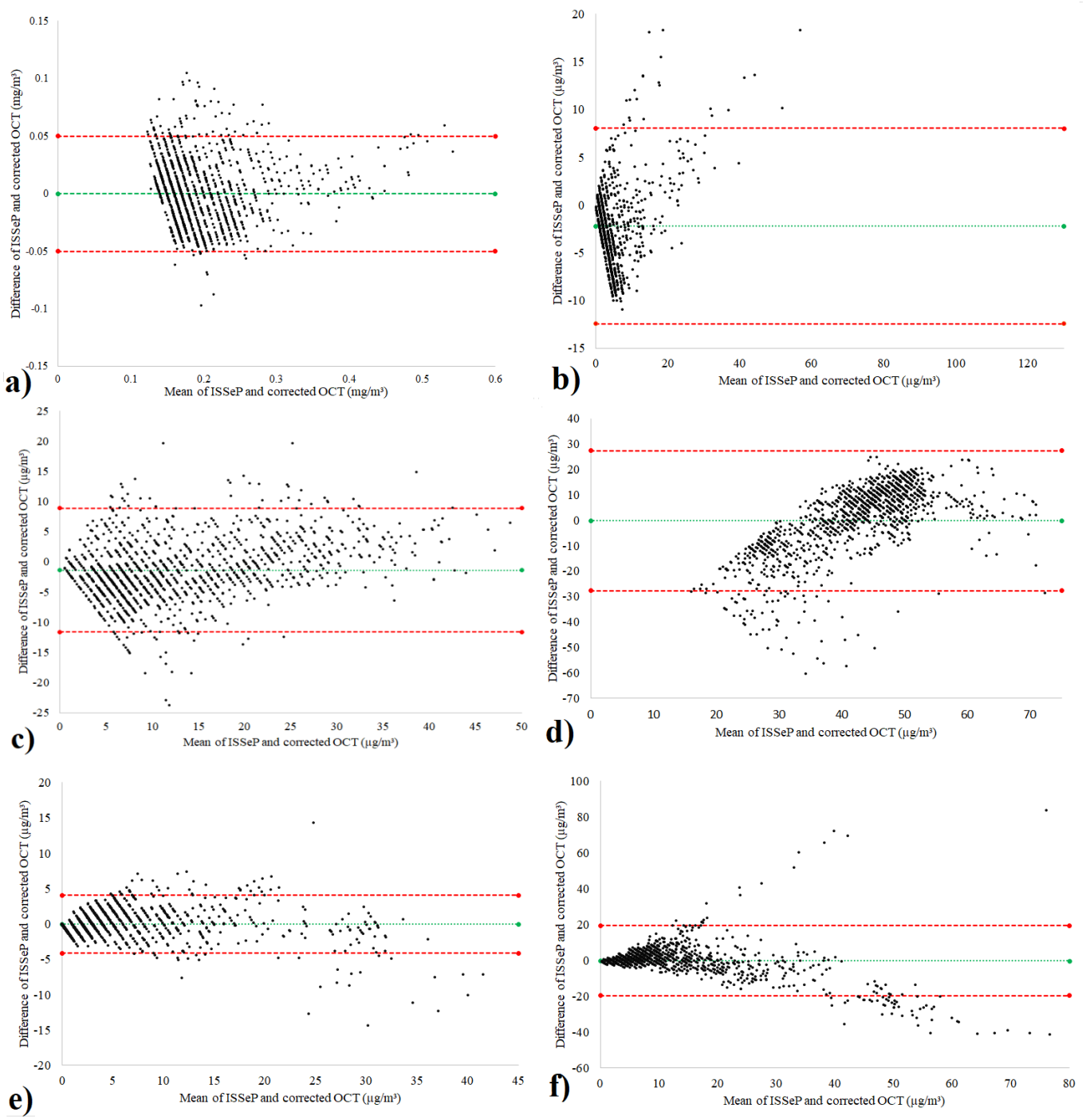

Fig 3.5. Bland–Altman plot for validation datasets: (a) CO (b) NO (c) NO_2 (d) O_3 (e) $PM_{2.5}$ (f) PM_{10}

NO_2. The statistical analysis showed that the NO_2 measurements from the four OCT devices and the ISSeP NO_2 showed a good correlation ($r_s = -0.706\ to - 0.824,\ p < 0.001$). As it is depicted in Figure 3.3. (a) very high variability was detected between OCT and ISSeP measurements, as long as the OCT overestimated the NO_2 levels by average of 134.66 µg/m³, from

114.57 to 149.21 μg/m³. Study of four OCT devices presented a very high uniformity ($r_s = 0.9\ to\ 0.96,\ p < 0.001$) and high variance (avg $= 138.21 \mu g/m^3$, from 88.67 to 247.28 μg/m³) between the different NO_2 sensors. Figure 3.4. (c) illustrates the relationship between the ISSeP and OCT calibrated NO_2 levels by the Orthogonal regression model. The best fit results in an R^2 of 0.78 and the NO_2 regression equation is:

$NO_2(ISSeP) = -172.41 + 1.14\ NO_2(OCT)$ (3)

Where NO_2 is the concentration (μg/m^3). Figure 3.5. (c) depicts the Bland–Altman analysis for the ISSeP NO_2 measurements by the corresponding best fit determined by the Orthogonal regression for the validation dataset from the four OCT measurement devices. It presents the mean difference between the ISSeP and the OCT NO_2 calculated measurements (-1.39 μg/m³ with the LOA of -11.64 to 8.85 μg/m³ at a 95% confidence interval). The number of 75 points (5.7 %) of the dataset were beyond the LOA (40 higher than the upper LOA and 35 less than the lower LOA). This range is much less than the EC defined indoor ELV for NO_2 equal to 200 μg/m^3 (1-hour mean, 2010).

O_3. Investigation of the O_3 measurement by the OCT devices and the ISSeP reference data revealed that the OCT O_3 concentrations varied from those of ISSeP. Figure 3.3. (b) presents a low correlation ($r_s = 0.22\ to\ 0.67,\ p < 0.001$) was identified. The OCTs overrated the O_3 levels (avg $= 1.9 \mu g/m^3$, from -3.2 to 7.8 μg/m³). Investigation of the four OCT datasets presented a low but notable uniformity ($r_s = -0.18\ to\ 0.9,\ p < 001$) and a moderate variance (avg $= 27.41\ \mu g/m^3$, from 21.39 to 31.28 μg/m³) between the O_3 measurements. Figure 3.4. (d) illustrates the relationship between the ISSeP and OCT calibrated O_3 levels from the Orthogonal regression model. The best fit results in an R^2 of 0.16 and the regression formulation of O_3 is:

$O_3(ISSeP) = 30.0328 + 0.23866\ O_3(OCT)$ (4)

Where O_3 is the concentration (μg/m^3). Figure 3.5. (d) depicts the Bland–Altman analysis for the

ISSeP O_3 measurements by the corresponding best fit determined by the Orthogonal regression for the validation dataset from the four OCT measurement devices. It presents the mean difference between the ISSeP and the OCT O_3 calculated measurements (-0.188 µg/m³ with the LOA of -27.78 to 27.4 µg/m³ at a 95% confidence interval). The number of 65 points (5.2 %) of the dataset were beyond of the LOA (65 less than the lower LOA). This range is remarkably less than the defined EC indoor ELV for O_3 equal to 120 µg/m^3 (Maximum daily, 8-hour mean, 2010).

$PM_{2.5}$. $PM_{2.5}$ measurements from the four OCT devices and the ISSeP were very highly correlated ($r_s = 0.93\ to\ 0.95,\ p < 0.001$) to each other. As it is shown by Figure 3.3. (a) the OCT underestimate $PM_{2.5}$ values (avg $= -3.2\ \mu g/m^3$, from -2.76 to -2.47 µg/m³). The examination of the four OCT monitors revealed a very high uniformity ($r_s = 0.99,\ p < 001$) and a small variance (avg $= 8.19 \mu g/m^3$, from 8.43 to 9.64 µg/m³) among $PM_{2.5}$ measurements. Figure 3.4. (e) illustrates the relationship between the ISSeP and OCT calibrated $PM_{2.5}$ levels from the Orthogonal regression model. The best fit results in an R^2 of 0.91 and the $PM_{2.5}$ regression equation is:

$PM_{2.5}$(ISSeP) = -1.57 + 3.08 $PM_{2.5}$(OCT) (5)

Where $PM_{2.5}$ is the concentration (µg/m^3). Figure 3.5. (e) depicts the Bland–Altman analysis for the ISSeP $PM_{2.5}$ measurements by the corresponding best fit determined by the Orthogonal regression for the validation dataset from the four OCT measurement devices. It presents the mean difference between the ISSeP and the OCT $PM_{2.5}$ calculated measurements (-0.017 µg/m³ with the LOA of -4.1 to 4.07 µg/m³ at a 95% confidence interval). The number of 69 points (5.3 %) of the dataset was beyond of the LOA (40 higher than the upper LOA 29 less than the lower LOA). This range is much less than the defined EC indoor ELV for $PM_{2.5}$ which is 25 µg/m^3 (yearly, 2010).

PM_{10}. It should be mentioned that the sensor does not measure PM10 but a correction factor is applied by the producer on the PM2.5 measurements.

The statistical analysis showed that the PM_{10} measurements from the four OCT monitors and the ISSeP were highly correlated ($r_s = 0.86\ to\ 0.88,\ p < 0.001$) to each other. As it is depicted by Figure 3.3. (b) the analysis of the measurements showed that the OCT underestimated PM_{10} concentrations (avg $= -8.63\ \mu g/m^3$, from -9.09 to -8.33 µg/m³). The study of four OCT datasets presented that there was a very high uniformity ($r_s = 0.99,\ p < 001$) and a small variance (avg $= 2.87\ \mu g/m^3$, from 2.33 to 3.12 µg/m³) between the different PM_{10} sensors. Figure 3.4. (f) illustrates the relationship between the ISSeP and OCT calibrated PM_{10} levels by the Orthogonal regression model. The best fit results in an R^2 of 0.57 and the regression model of PM_{10} is:

PM_{10}(ISSeP) = -2.12 + 4.77 PM_{10}(OCT) (6)

Where PM_{10} is the concentration (µg/m^3). Figure 3.5. (f) depicts the Bland–Altman analysis for the ISSeP PM_{10} measurements by the corresponding best fit determined by the Orthogonal regression for the validation dataset from the four OCT measurement devices. It presents the mean difference between the ISSeP and the OCT $PM_{2.5}$ calculated measurements (-0.06 µg/m³ with the LOA of -19.63 to 19.5 µg/m³ at a 95% confidence interval). The number of 69 points (5.3 %) of the dataset were out of the LOA (51 higher than the upper LOA 18 less than the lower LOA).

This range is almost equal to the EC indoor ELV for PM_{10} which is 50 µg/m^3 (24 hours, 2005). The number of data points on which the PM_{10} levels surpassed 50 µg/m^3 is about an average of 0.38%. At last, the correlation between the calibration and validation datasets were favorably accredited. Both presented a sufficient agreement on the PM_{10} levels higher than 50 µg/m^3.

3.4. Discussions

In this very first step, the accuracy of lab-made devices for measurement of pollutants (CO, NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) during a campaign of one-month is evaluated. Calibration was not performed in the lab by using synthetic gases but by comparison with reference analyzers (from

Scientific Institute of Public Service of Wallonia, environmental institute of Wallonia, ISSeP). To achieve best results, specific calibration equations should be derived for each device. The validation outcomes presented that there was correct agreement between the reference analyzer data and those of the OCT devices for some pollutants, when using the regression equations.

However, regarding the O_3 (Alphasense O_X-B431) sensor it should be noted that O_3 values are derived by the following Equation:

$O_3 = OX - NO_2$

Considering the fact that the calibration of NO_2 is not sufficient and the performance of OX sensor still remains uncalibrated, a secondary (auxiliary) calibration between O_3 values of reference analyzer and the O_3 values obtained from ((OX) – (Calibrated NO_2)) was performed. The Figure 3.6. illustrates the post-calibration improvement of O_3 (auxiliary) calibration against reference values (also see Fig 3.2.b for comparison the improvement).

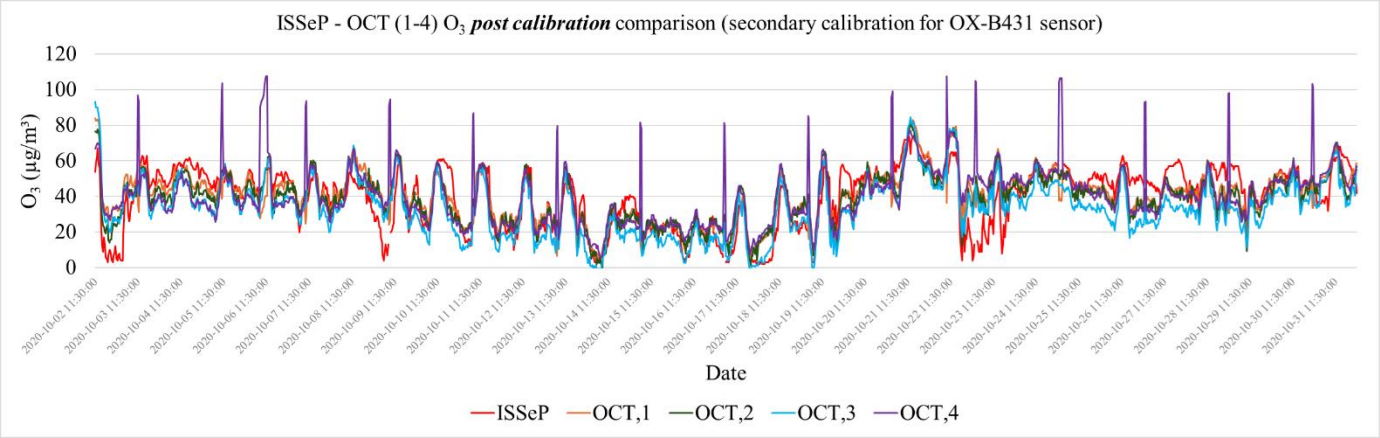

Fig 3.6. Improvement of O_3 auxiliary calibration (O_3: OX-NO_2).

The OCT devices presented a very good agreement with the ISSeP analyzers, for CO (r_s = 0.73 *to* 0.8), NO_2 (r_s = -0.70 to-0.82), $PM_{2.5}$ (r_s = 0.93 *to* 0.95) and PM_{10} (r_s = 0.86 *to* 0.88) data. The NO concentration was overestimated by an average of 185.47 µg/m³. The generated regression fits for CO, NO, NO_2 and $PM_{2.5}$ decreased the variance among the measurements sufficiently and enhanced their performances in comparison with ISSeP which led to R^2 values equal to 0.79, 0.75, 0.78 and 0.91, respectively. The absence of an exact O_3 detector

resulted in two calibration stage for the O_3. Nevertheless, outcomes indicated that it has not influenced the performance of the other detectors.

The results revealed that OCT devices based on LCSs, can detect ELV exceedance by high contaminant picks. It is noteworthy to be mentioned that Wi-Fi communication with a physical as well as a cloud storage, make the OCT a user-friendly device to assess the IAQ in wider temporal and spatial dimension, in comparison with typical methods. Implementation of several devices in a measurement campaign and applying calibration modifications increase the accuracy and precision of the measurements. According to the OCT calibration results, it was revealed that less than 5% of the CO, NO, NO_2, O_3, $PM_{2.5}$, and PM_{10} values were beyond the LOA range when the range was set to ±1.96 SD of the difference. Variability of the fraction of concentrations higher than ELVs was mostly insignificant and was considered to be improbable to make drastic alteration in the IAQ evaluation.

With the use of calibrated LCS monitoring devices, an IAQ measurement campaign was carried out to obtain IAQ experimental datasets. The naturally ventilated residential case-study house was located in the Wallonia region, Arlon, Belgium. The measurements were carried out in the summer 2021, concurrently. The recorded parameters included 7 contaminates, T, P, and RH (both indoors and outdoors), as well as the outdoor weather data. The experimental datasets provided during this campaign are being used for the IAQ model validation and development in the next chapter (Chapter 3).

3.5. Conclusion

The results indicates that the OCTs can satisfy the minimum requirements for the IAQ case study experiments. It is important to evaluate the accuracy of LCS to study their reliability and correctness. The OCT monitoring devices based on LCSs, will provide essential data for IAQ model design, validation, and development (Chapter 5). In the next chapter (Chapter 4), the results of the IAQ experiments conducted with calibrated OCTs will be presented.

Correlated publishment of this chapter:

Pourkiaei, et al. (2022). Exploring the Indoor Air Quality in the Context of Changing Climate in Residential Buildings-Part A: Developed Measurement Devices of Low-Cost Sensors. In *ASHRAE Topical Conference Proceedings* (pp. 1-9). American Society of Heating, Refrigeration and Air Conditioning Engineers, Inc. https://www.aivc.org/resource/exploring-indoor-air-quality-context-changing-climate-residential-buildings-part-developed

Pourkiaei, et al. (2024). Systematic Framework for Quantitative Assessment of Indoor Air Quality Under Future Climate Scenarios; 2100s Projection of a Belgian Case Study. *Journal of Building Engineering*, 109611, https://doi.org/10.1016/j.jobe.2024.109611

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4. INDOOR AIR QUALITY MEASUREMENTS FOR IAQ MODEL DESIGN & CALIBRATION

4. Indoor Air Quality Measurements *For IAQ Model Design & Calibration*

4.1. IAQ Measurement Campaign

This chapter is an continued effort (of chapter 3) to answer the second research question (*RQ2*).After calibrating Lab devices in the previous section, an IAQ measurement campaign was conducted. Detailed results of sensors performance validation (post-calibration) are presented in the section 3.3.1. of the previous chapter. The aim of the IAQ measuring campaign is to obtain the IAQ model required design inputs, and performing the IAQ model validation and calibration procedures.

With the aim of performing an IAQ measurement for basis year IAQ model development, a case-study house was chosen in the Wallonia region, Arlon, Belgium. Considering the focus of the project on the summer times, measurements were carried out from 20th June to 31st August 2021, both indoors and outdoors, concurrently. The sensors were located in the kitchen (shared area) at the height of 1.5m, in the optimum distance from the doors and the stove/cooktop. No recalibration of monitoring devices was considered during the campaign (over 73 days). The case-study house was located at the first floor of a naturally ventilated residential building of 4 floors.

Also, a comprehensive questionnaire (hourly checklist) was designed to log the occupancy pattern (3 adult inhabitants), indoor activities incidences (sleeping, cooking, cleaning, showering, smoking), natural ventilation behavior (opening of windows), and 2 exhaust fans operations. Table 4.1. presents the questionnaire table developed for the IAQ measurement campaign. The recorded parameters by OCTs were CO, NO, NO_2, O_3, $PM_{2.5}$, PM_{10}, VOCs, as well as the T, P, and RH. The data logging interval was set to 10 seconds. Additional outdoor weather data (wind speed, wind direction, and solar radiation) were collected from the IRM's website (Royal Meteorological Institute of Belgium). Additional to the performed measurements in 2021 (Arlon case study - Basis year & case study selected for the IAQ model development in the next chapter), there have been other IAQ measurements conducted in another naturally ventilated house in the city of Habay (without a completed questionnaire).

Table 4.1. The questionnaire table developed for the IAQ measurement campaign.

Daily activities table (Date: __/__/2021)

Time	Occupancy number	Cooking	Windows opening (Number and %)		Cleaning	Shower	Smoke, candle, incense
00:00-01:00							
01:00-02:00							
02:00-03:00							

These measurements were also repeated for the next summer (2022) without questionnaire.

4.2. Results And Discussions

The findings presented in this section mainly stem from a comprehensive IAQ measurement campaign conducted at the case-study house in Arlon, over 73 days (1752 hours) of summer 2021. This campaign sought to assess the quality of indoor air within various real life settings, as a base-line for IAQ model development. The measurement campaign employed LCS and monitoring equipment to collect real-time data on key air quality parameters such as CO, NO, NO_2, O_3, $PM_{2.5}$, PM_{10}, VOCs, as well as the T, P, and RH. By measuring indoor air across zones and occupancy conditions, this measurement aims to provide a base-line perspective into IAQ trends (of a single case-study), identify potential sources of indoor pollutants (obtaining the affordable emissions information), and evaluate the long-term average indoor pollutants levels. Figure 4.1. shows examples of indoor air concentration level variation in accordance to logged occupant's questionnaire. Additionally, indoor and outdoor measurements (without questionnaires) for another naturally ventilated case study house in Habay (summers of 2021 and 2022), as well as the Arlon case study in the summer 2022, are presented. The results of Arlon-2021 presented herein serve as a foundation for validation and development of an IAQ model which is the main focus of the next chapter (Chapter 5). Figure 4.2. presents the Box & Whisker plot of indoor and outdoor recorded T, in Arlon and Habay naturally ventilated houses, during the summers of 2021 and 2022 (73 days: 17 June – 31 August). Figures 4.3. and 4.4. illustrate the hourly comparative presentations of indoor and outdoor recorded T during the summers of 2021 and 2022 (73 days: 17 June – 31 August), for Arlon and Habay case studies, respectively.

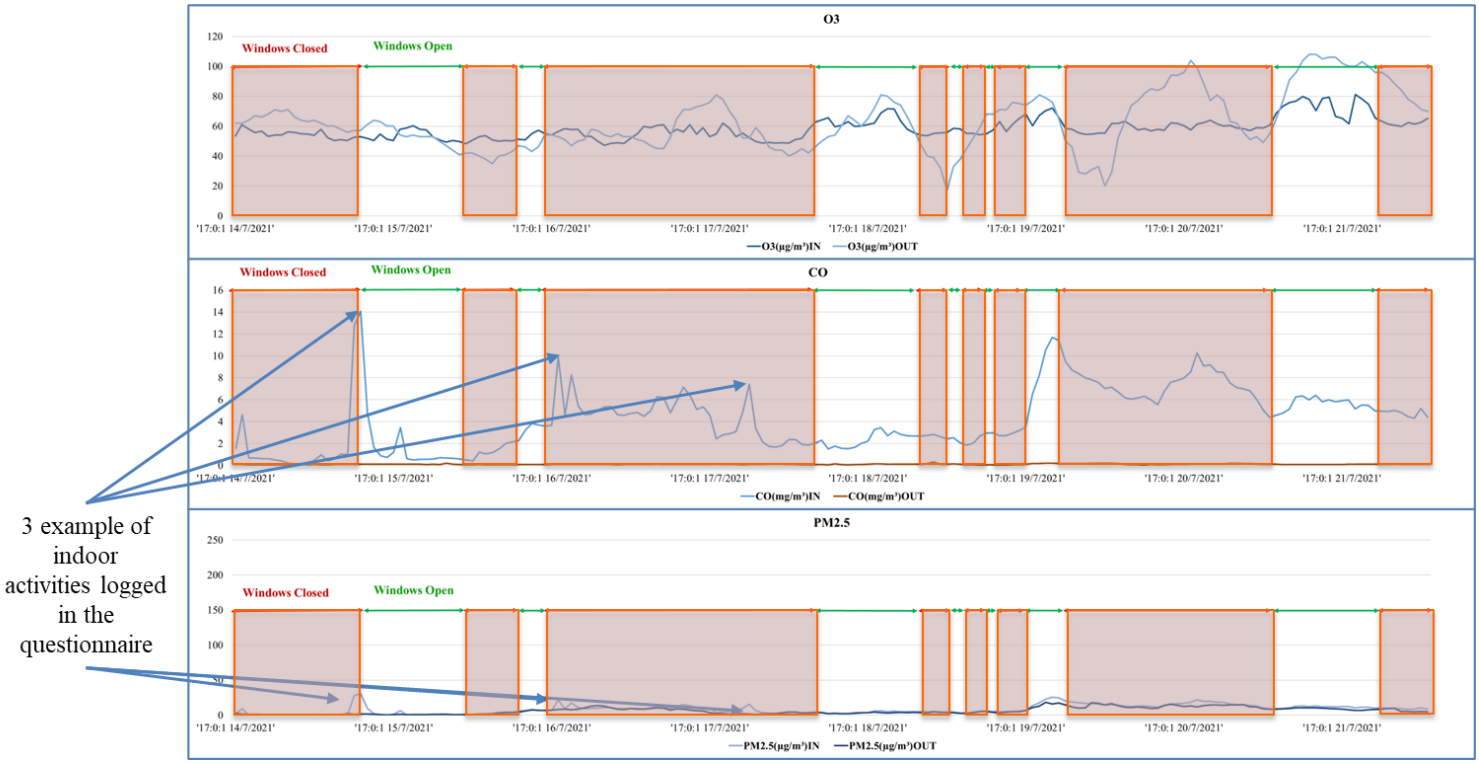

Figure 4.1. Presentation of indoor concentration levels in accordance with sample cooking activities and natural ventilation performance.

Although there may have been instances of missing data in the raw dataset (recorded at 10-second intervals), any interruptions were brief, not exceeding one hour. This is confirmed by the fact that no hourly averages were missing. Figure 4.5. presents the Box & Whisker plot of indoor and outdoor recorded pollutant concentrations, in Arlon and Habay naturally ventilated houses, during the summers of 2021 and 2022 (73 days: 17 June – 31 August). Figures 4.6. and 4.7. illustrate the hourly presentations of indoor and outdoor recorded pollutant concentrations in the Arlon naturally ventilated case study house during the summers (73 days: 17 June – 31 August) of 2021 and 2022, respectively. Figures 4.8. and 4.9. illustrate the hourly indoor and outdoor recorded pollutant concentrations in the Habay naturally ventilated case study house during the summers (73 days: 17 June – 31 August) of 2021 and 2022, respectively. Outdoor VOCs were not measured during the measurements.

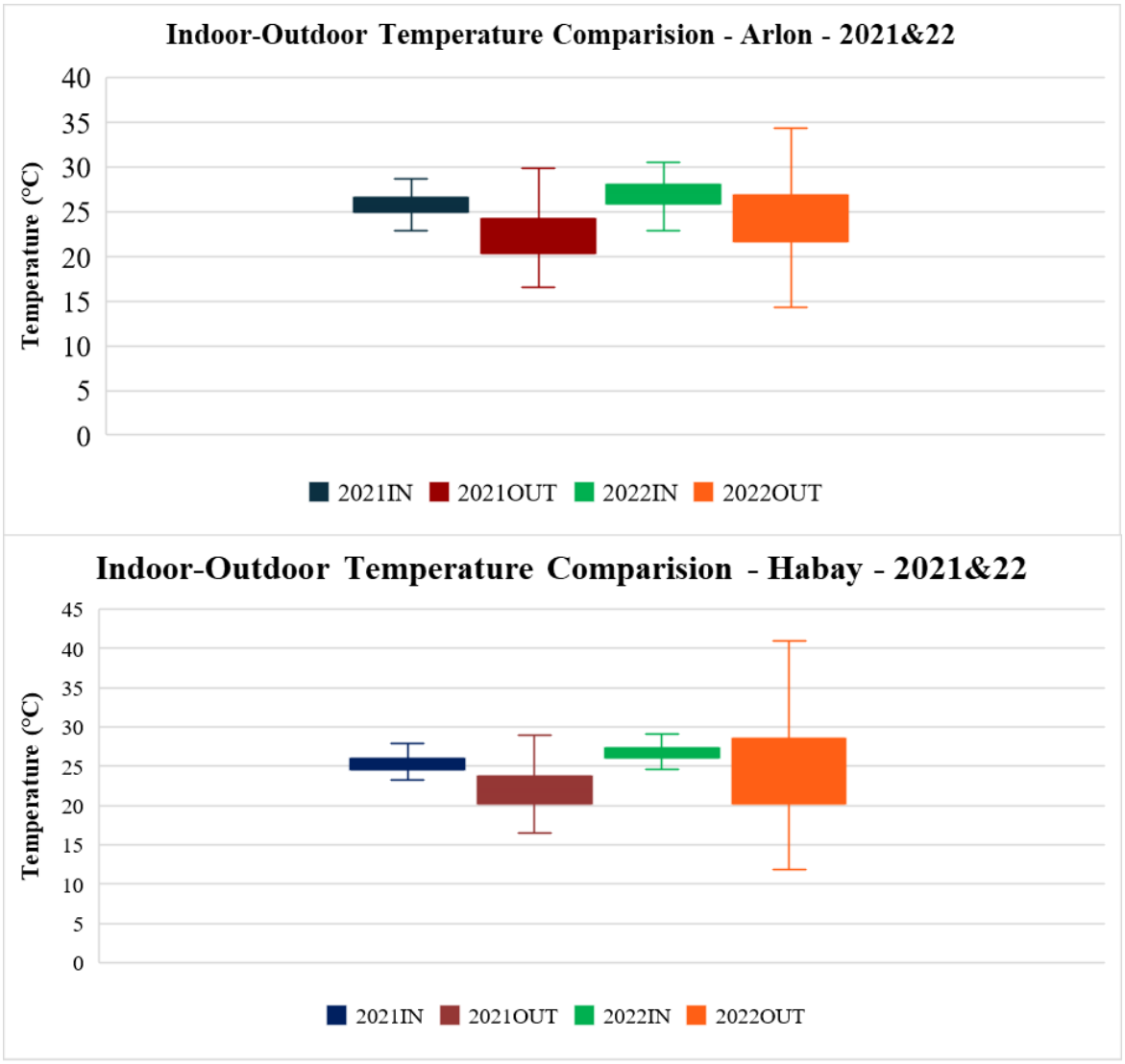

Fig 4.2. Indoor and outdoor Temperatures in Arlon and Habay case study houses, summers (73 days) 2021&22.

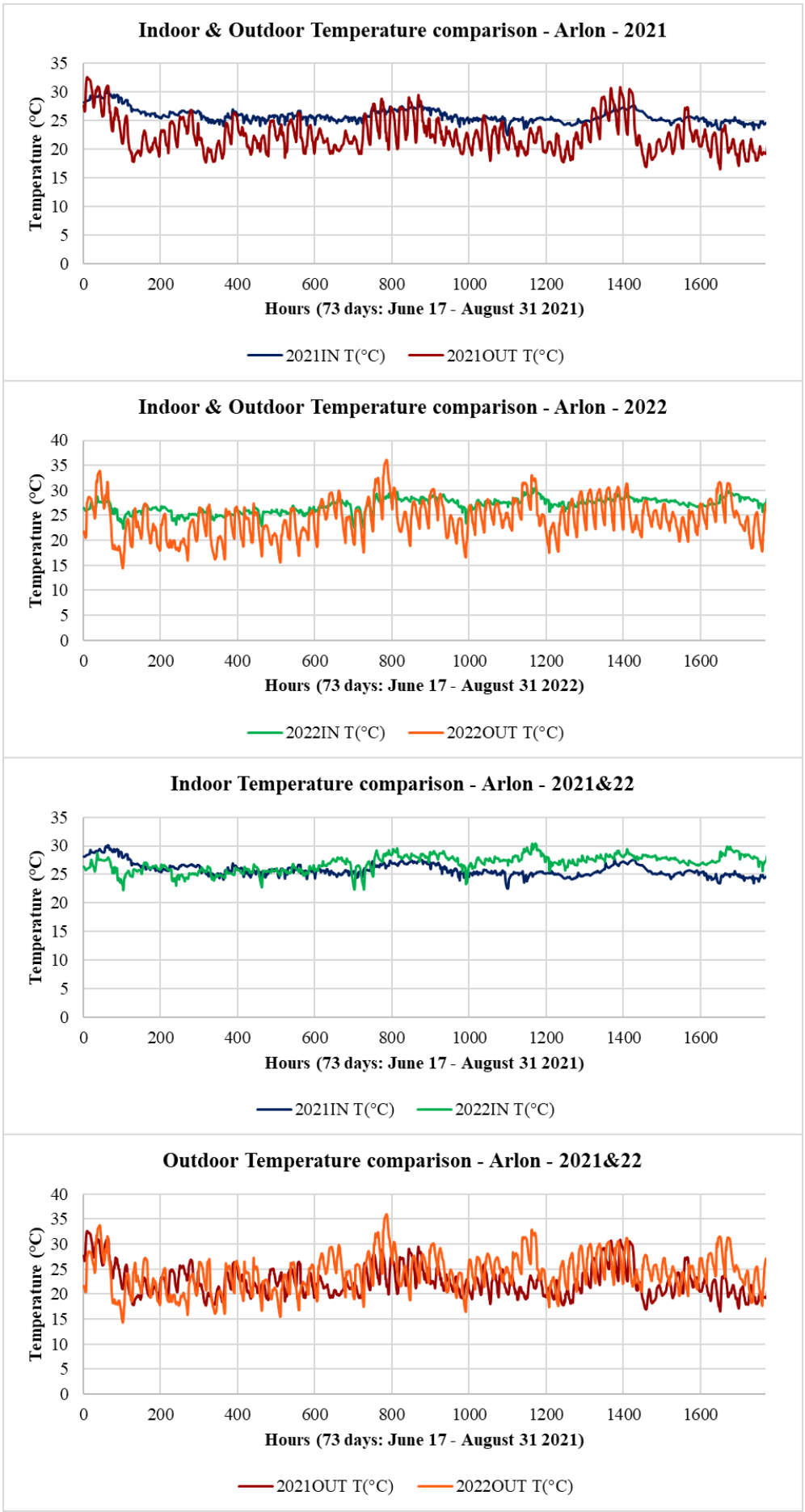

Fig 4.3. Hourly indoor and outdoor Temperatures in summer 2021&22 – Case study house in Arlon.

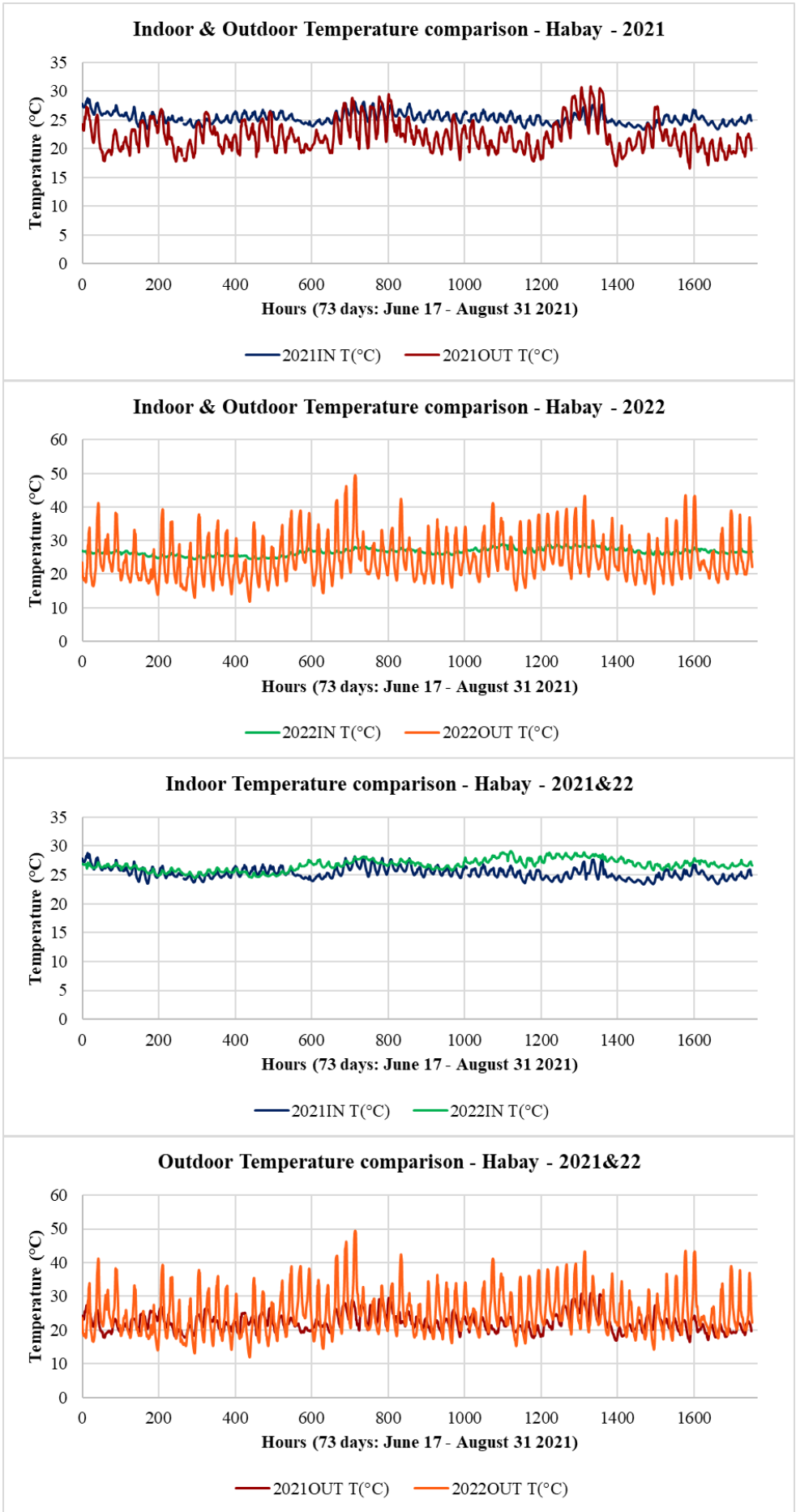

Fig 4.4. Hourly indoor and outdoor Temperatures in summer 2021&22 – Case study house in Habay.

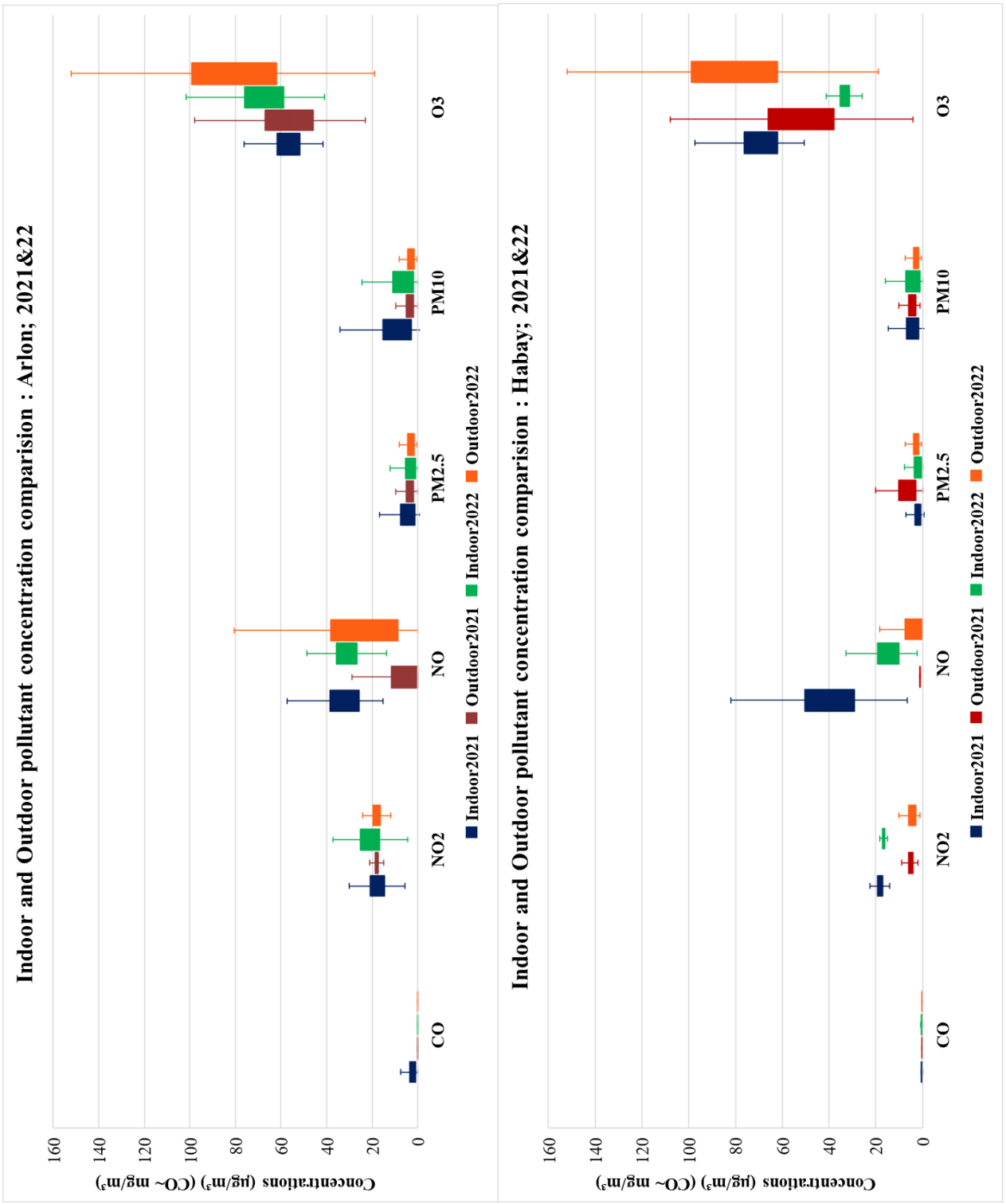

Fig 4.5. Indoor and outdoor Temperatures in Arlon and Habay case study houses, summer (June 17th- August 31st; 73 days) 2021&22.

**The corresponding ELVs are presented in the Table 7.1.*

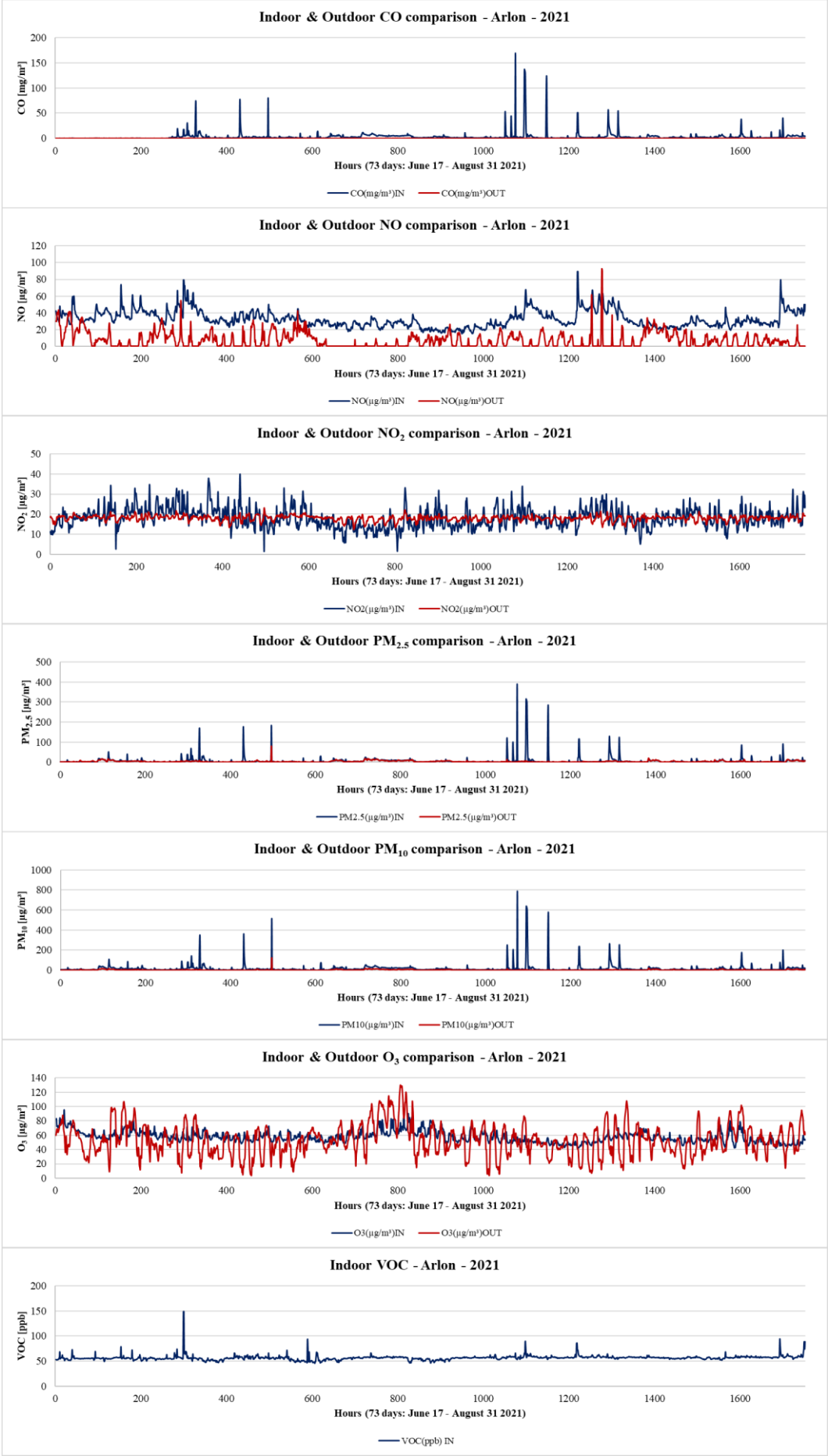

Fig 4.6. Hourly indoor & outdoor pollutant concentrations - summer 2021 - Case study house in Arlon.

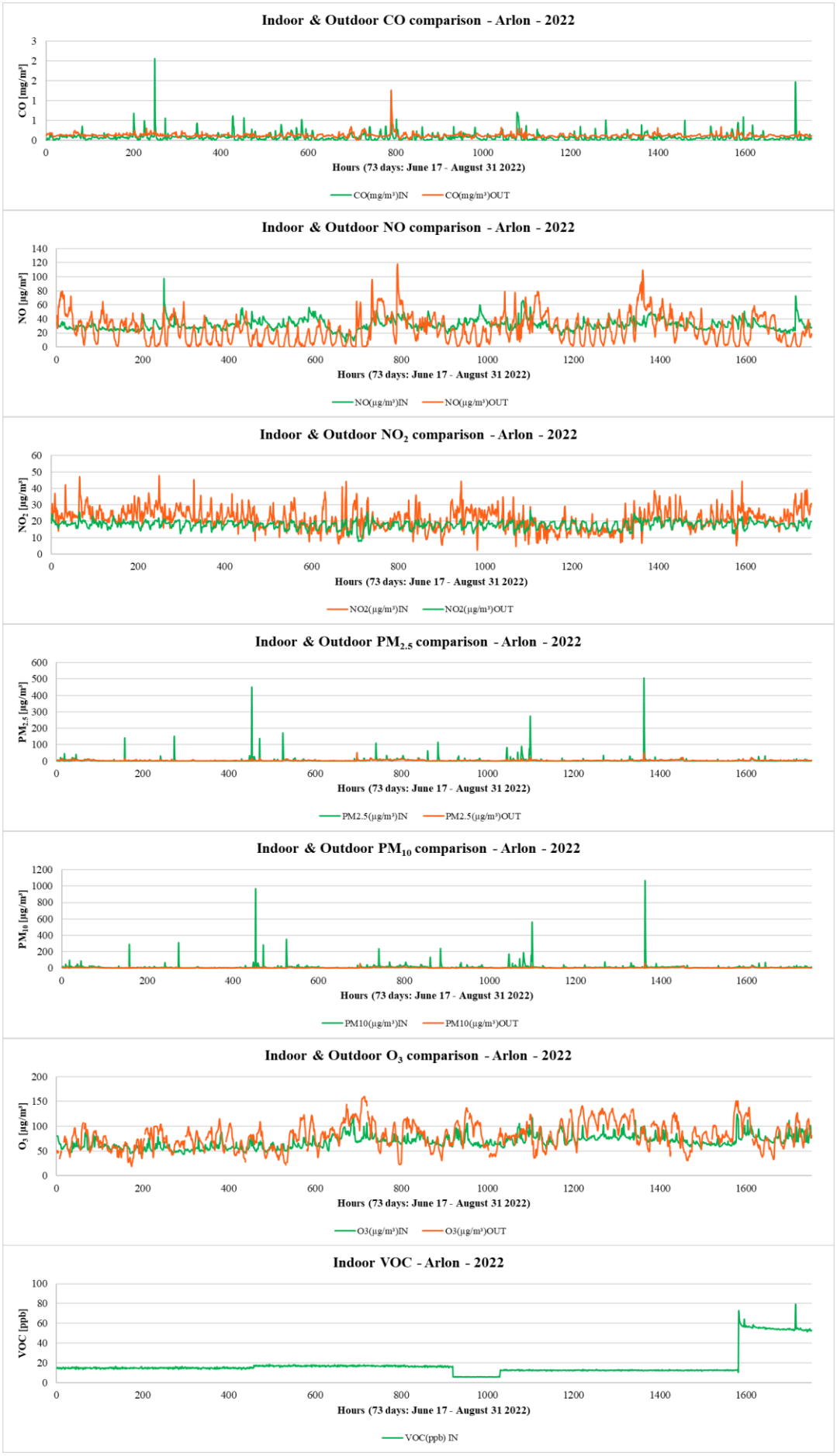

Fig 4.7. Hourly indoor & outdoor pollutant concentrations - summer 2022 - Case study house in Arlon.

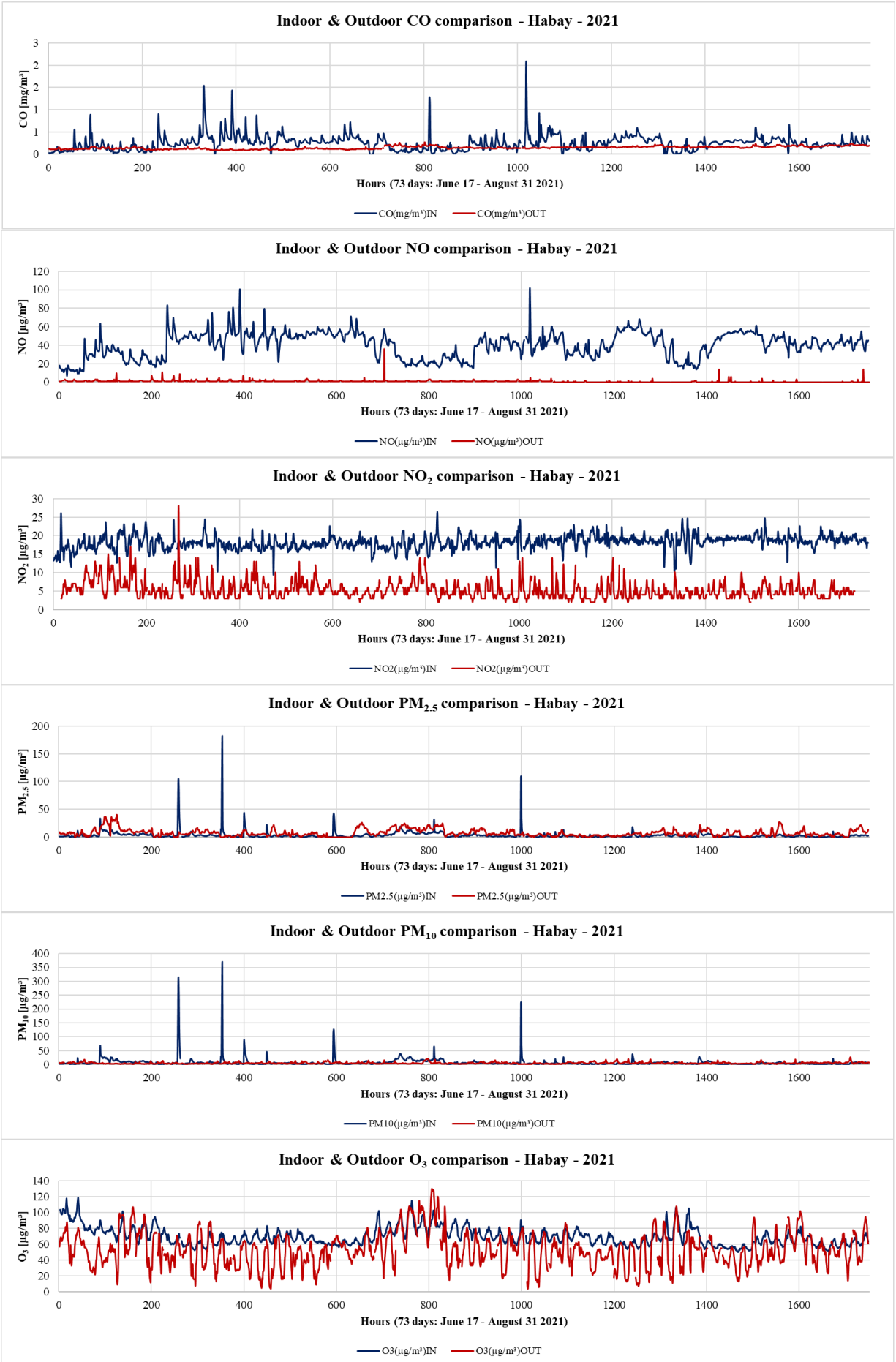

Fig 4.8. Hourly indoor & outdoor pollutant concentrations - summer 2021 - Case study house in Habay.

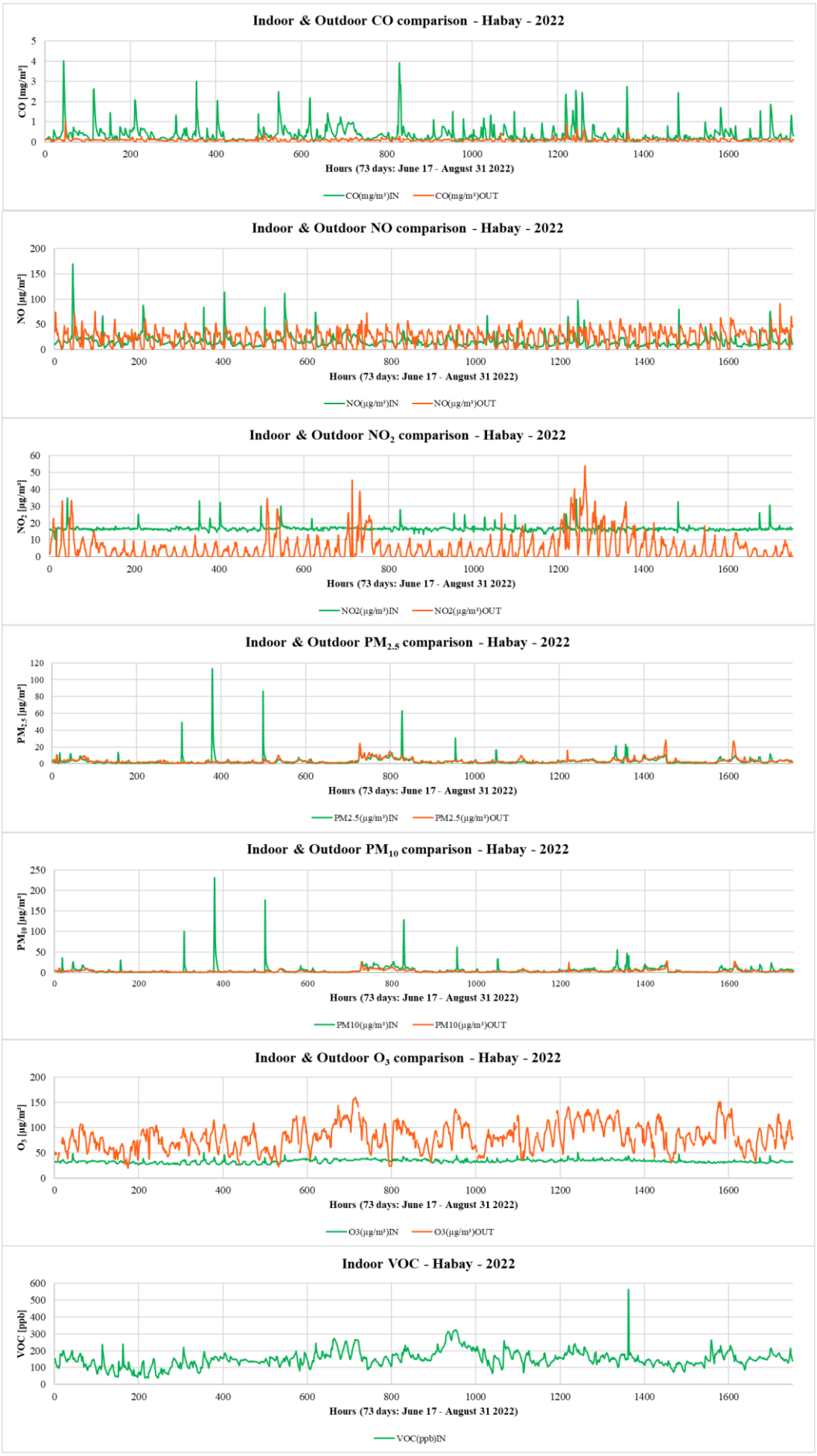

Fig 4.9. Hourly indoor & outdoor pollutant concentrations - summer 2022 - Case study house in Habay.

4.2.1. Straightforward Indoor and Outdoor Pollutant Concentration Analysis (Arlon 2021&22)

The quality of indoor air is linked (but not limited) to the indoor emission sources, outdoor weather, and outdoor air quality, particularly in naturally ventilated buildings where the exchange of air is largely uncontrolled. This analysis presents an investigation of pollutant concentration peaks for O_3, $PM_{2.5}$, PM_{10}, CO, NO, and NO_2, focusing on the interaction between indoor and outdoor environments with a macroscopic point of view. The objective is to understand the dynamics of pollutant peaks and their correlation between indoor and outdoor settings.

This analysis examines indoor and outdoor pollutant concentrations in the naturally ventilated case study house in Arlon during the summers of 2021 and 2022. The aim is to understand the pollutant dynamics between indoor and outdoor environments and assess the correlation of their levels over two consecutive years. All the hourly data spans a period of 73 days for each year, from June 17th to August 31st. (The time range in 2022 is considered identical to that of 2021 for a synchronized comparison.)

4.2.1.1. O_3 Data Overview

Observations Year 2021

Outdoor Ozone Levels:

- ✓ **Range**: The outdoor O_3 levels varied from approximately 20 µg/m³ to 100 µg/m³.
- ✓ **Peaks**: Several significant peaks were observed, typically during the daytime.
- ✓ **Trends**: The diurnal pattern is prominent, with peaks occurring in the afternoon and lower concentrations at night.

Indoor O_3 Levels:

- ✓ **Range**: Indoor O_3 levels ranged from about 40 µg/m³ to 80 µg/m³.
- ✓ **Peaks**: Indoor peaks generally followed the outdoor peaks but were less pronounced.
- ✓ **Trends**: Indoor O_3 showed a similar diurnal trend but with reduced amplitude compared to outdoor levels.

Observations Year 2022

Outdoor O_3 Levels:

- ✓ **Range**: The outdoor O_3 levels ranged from around 20 µg/m³ to 150 µg/m³.
- ✓ **Peaks**: Peaks were frequent, especially in the afternoons.
- ✓ **Trends**: The diurnal pattern remained consistent, with higher concentrations during daylight hours.

Indoor O_3 Levels:

- ✓ **Range**: Indoor O_3 levels were between 40 µg/m³ and 100 µg/m³.
- ✓ **Peaks**: Indoor peaks were less intense than outdoor peaks but followed a similar pattern.
- ✓ **Trends**: Indoor levels exhibited a dampened diurnal pattern similar to the outdoor levels.

Correlation Analysis

Indoor vs. Outdoor (2021):

- **Correlation Coefficient**: 0.65
- **Interpretation**: Moderate positive correlation indicates that while outdoor O_3 levels influence indoor levels, the indoors consistently has a lower range due to the building's inactive natural ventilation performance periods.

Indoor vs. Outdoor (2022):

- **Correlation Coefficient**: 0.70
- **Interpretation**: A slightly higher correlation than in 2021, suggesting a stronger influence of outdoor O_3 on indoor levels in 2022 by penetration and active natural ventilation performances.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor O_3 Comparison:

- **Average Concentration**:

  2021: ~55 µg/m³

  2022: ~80 µg/m³

- **Interpretation**: Higher average outdoor O_3 levels in 2022 is highly linked to varying meteorological conditions (Temperature increase) or changes in local pollution sources.

Indoor O_3 Comparison:

- **Average Concentration**:

  2021: ~55 µg/m³

  2022: ~70 µg/m³

- **Interpretation**: Lower average indoor O_3 levels in 2022 despite higher outdoor levels suggest improved filtering efficiency (promoted by less active natural ventilation

performance for protection against high outdoor temperatures), or possibly increased indoor activities contributing to O_3 decay.

4.2.1.2. $PM_{2.5}$ Data Overview

Observations Year 2021

Outdoor $PM_{2.5}$ Levels:

- ✓ **Range**: Outdoor $PM_{2.5}$ levels remained relatively low, generally under 10 µg/m³.
- ✓ **Peaks**: Few peaks were observed, with levels occasionally between 10-20 µg/m³.
- ✓ **Trends**: The outdoor $PM_{2.5}$ levels were relatively stable with minor fluctuations.

Indoor $PM_{2.5}$ Levels:

- ✓ **Range**: Indoor $PM_{2.5}$ levels exhibited significant peaks, however the baseline was 5 µg/m³.
- ✓ **Peaks**: Significant sharp peaks were observed, ranging from 10 to 400 µg/m³, indicating indoor activities or events.
- ✓ **Trends**: Indoor $PM_{2.5}$ levels showed high variability with numerous spikes (indoor activities).

Observations Year 2022

Outdoor $PM_{2.5}$ Levels:

- ✓ **Range**: Outdoor $PM_{2.5}$ levels remained low, generally under 5 µg/m³, similar to 2021.
- ✓ **Peaks**: Few peaks were observed, occasionally rising above 20 µg/m³.
- ✓ **Trends**: The outdoor $PM_{2.5}$ levels more fluctuations compared to 2021 (might be due to higher outdoor temperatures).

Indoor $PM_{2.5}$ Levels:

- ✓ **Range**: Indoor $PM_{2.5}$ levels exhibited full fluctuational pattern, ranging from 0 to 500 µg/m³.
- ✓ **Peaks**: Several significant peaks (~20 times) were observed, majorly due to indoor activities and fewer due to outdoor peaks (indoor peaks originated by outdoor peaks only taken place in active natural ventilation periods).
- ✓ **Trends**: Indoor $PM_{2.5}$ levels showed variability with notable spikes.

Correlation Analysis

Indoor vs. Outdoor (2021):

- ➢ **Correlation Coefficient**: 0.30
- ➢ **Interpretation**: Low positive correlation indicating that indoor $PM_{2.5}$ levels are influenced by indoor sources more than outdoor levels.

Indoor vs. Outdoor (2022):

- ➢ **Correlation Coefficient**: 0.25
- ➢ **Interpretation**: Slightly lower correlation than in 2021, reinforcing the influence of indoor activities on $PM_{2.5}$ levels.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor $PM_{2.5}$ Comparison:

- ❖ **Average Concentration**:

  2021: ~4 µg/m³

  2022: ~4 µg/m³

- ❖ **Interpretation**: Outdoor $PM_{2.5}$ levels were almost identical in both years, (potentially due to the fact that combustion of gasoline, oil, diesel fuel or wood produce much of the $PM_{2.5}$ pollution found in outdoor air – not our case).

Indoor $PM_{2.5}$ Comparison:

- **Average Concentration**:

  2021: ~50 µg/m³

  2022: ~55 µg/m³

- **Interpretation**: Indoor $PM_{2.5}$ levels were higher in 2021, indicating more frequent or intense indoor activities contributing to $PM_{2.5}$ levels.

4.2.1.3. PM_{10} Data Overview

Observations Year 2021

Outdoor PM_{10} Levels:

- ✓ **Range**: Outdoor PM_{10} levels remained relatively low, generally under 10 µg/m³.
- ✓ **Peaks**: Few peaks were observed, occasionally between 10-20 µg/m³.
- ✓ **Trends**: The outdoor PM_{10} levels were relatively stable with minor fluctuations.

Indoor PM_{10} Levels:

- ✓ **Range**: Indoor PM_{10} levels exhibited significant peaks, ranging from 0 to 400 µg/m³.
- ✓ **Peaks**: Numerous sharp peaks were observed, indicating potential indoor burning category activities or events.
- ✓ **Trends**: Indoor PM_{10} levels showed high variability with numerous spikes.

Observations Year 2022

Outdoor PM_{10} Levels:

- ✓ **Range**: Outdoor PM_{10} levels remained low, generally under 10 µg/m³.
- ✓ **Peaks**: couple of peak spikes were observed, occasionally between 10-25 µg/m³. Also, several (~5) peak long range periods were observed higher than 20 and up to 60 µg/m³.
- ✓ **Trends**: The outdoor PM_{10} levels showed considerable fluctuations, however mostly below 20 µg/m³.

Indoor PM_{10} Levels:

- ✓ **Range**: Indoor PM_{10} levels exhibited significant peaks, ranging from 0 to 1000 µg/m³.
- ✓ **Peaks**: Numerous peaks were observed, mainly due to indoor activities and also contributions to outdoor originated peaks with concurrent active natural ventilation performances.
- ✓ **Trends**: Indoor PM_{10} levels showed high variability with notable spikes.

Correlation Analysis

Indoor vs. Outdoor (2021):

- ➢ **Correlation Coefficient**: 0.30
- ➢ **Interpretation**: Low positive correlation indicating that indoor PM_{10} levels are influenced by indoor sources more than outdoor levels.

Indoor vs. Outdoor (2022):

- ➢ **Correlation Coefficient**: 0.25
- ➢ **Interpretation**: Slightly lower correlation than in 2021, reinforcing the influence of indoor activities on PM_{10} levels, or decreased (impacts by outdoor sources through) active natural ventilation durations.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor PM_{10} Comparison:

- ❖ **Average Concentration**:

  2021: ~4 µg/m³

  2022: ~4 µg/m³

- ❖ **Interpretation**: Outdoor PM_{10} levels were almost identical among 2021 and 2022, but showed more peaks and fluctuations in the year 2022, likely due to increased outdoor temperatures.

Indoor PM_{10} Comparison:

- **Average Concentration**:

  2021: ~15 µg/m³

  2022: ~12 µg/m³

- **Interpretation**: Indoor PM_{10} levels were higher in 2021, indicating more impacts by active natural ventilation performance periods in 2021, relatively. Frequent or intense indoor activities contributing to PM_{10} levels are less likely.

4.2.1.4. CO Data Overview

Observations Year 2021

Outdoor CO Levels:

- ✓ **Range**: Outdoor CO levels remained very low, consistently under 1 mg/m³.
- ✓ **Peaks**: No significant peaks were observed in outdoor CO levels.
- ✓ **Trends**: Outdoor CO levels were stable with minimal variation.

Indoor CO Levels:

- ✓ **Range**: Indoor CO levels exhibited several peaks, ranging from 0 to about 150 mg/m³. However this values are unexpectedly high.
- ✓ **Peaks**: Multiple significant peaks were observed, indicating potential indoor sources or activities.
- ✓ **Trends**: Indoor CO levels showed high variability with numerous spikes. This is potentially due to burning category indoor activities (Stove, smoking, wall-mounted hot water boiler, etc.)

Observations Year 2022

Outdoor CO Levels:

- ✓ **Range**: Outdoor CO levels remained very low, generally under 1 mg/m³, similar to 2021.
- ✓ **Peaks**: A few minor peaks were observed, with levels occasionally rising above 1 mg/m³.
- ✓ **Trends**: Outdoor CO levels were stable with minor fluctuations.

Indoor CO Levels:

- ✓ **Range**: Indoor CO levels exhibited several peaks, ranging from 0 to 3 mg/m³.
- ✓ **Peaks**: Several significant peaks were observed, potentially due to indoor activities or events.
- ✓ **Trends**: Indoor CO levels showed variability with notable spikes.

Correlation Analysis

Indoor vs. Outdoor (2021):

- ➢ **Correlation Coefficient**: 0.10
- ➢ **Interpretation**: Very low positive correlation indicating that indoor CO levels are influenced by indoor sources only.

Indoor vs. Outdoor (2022):

- ➢ **Correlation Coefficient**: 0.15
- ➢ **Interpretation**: Slightly higher correlation than in 2021, but still very low, reinforcing the influence of indoor activities on CO levels.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor CO Comparison:

- ❖ **Average Concentration**:

  2021: ~0.1 mg/m³

  2022: ~0.1 mg/m³

- **Interpretation**: Outdoor CO levels were identical at very low levels. This represents consistency in emission sources and no significant new sources.

Indoor CO Comparison:

- **Average Concentration**:

  2021: ~3 mg/m³

  2022: ~0.1 mg/m³

- **Interpretation**: Indoor CO levels were significantly lower in 2022, indicating fewer indoor activities contributing to CO levels, and not due to improved natural ventilation performance which was not the case.

4.2.1.5. NO Data Overview

Observations Year 2021

Outdoor NO Levels:

- ✓ **Range**: Outdoor NO levels ranged from approximately 0 to 80 µg/m³.
- ✓ **Peaks**: Periodic peak patterns were observed, typically during rush hours, indicating traffic as a primary source.
- ✓ **Trends**: The diurnal pattern is noticeable, with peaks occurring during the day and lower concentrations at night.

Indoor NO Levels:

- ✓ **Range**: Indoor NO levels ranged from around 20 to 100 µg/m³.
- ✓ **Peaks**: Indoor peaks were more frequent and higher than outdoor peaks, indicating significant indoor sources or activities or strong infiltration through leaky airflow paths.
- ✓ **Trends**: Indoor NO levels showed more variability with higher average concentrations than outdoor levels.

Observations Year 2022

Outdoor NO Levels:

- ✓ **Range**: Outdoor NO levels ranged from about 0 to 120 µg/m³.
- ✓ **Peaks**: Peaks were observed during daytime hours, suggesting traffic and other outdoor sources.
- ✓ **Trends**: The diurnal pattern remained consistent, with higher concentrations during the day.

Indoor NO Levels:

- ✓ **Range**: Indoor NO levels ranged from 5 to 100 µg/m³.
- ✓ **Peaks**: Indoor peaks corresponded with outdoor peaks but were generally higher, suggesting possible indoor contributions or strong infiltration through leaky airflow paths.
- ✓ **Trends**: Indoor levels showed significant variability, reflecting both indoor and outdoor influences.

Correlation Analysis

Indoor vs. Outdoor (2021):

- ➢ **Correlation Coefficient**: 0.55
- ➢ **Interpretation**: Moderate positive correlation indicates that outdoor NO levels influence indoor levels, but indoor sources also significantly contribute.

Indoor vs. Outdoor (2022):

- ➢ **Correlation Coefficient**: 0.60
- ➢ **Interpretation**: A slightly higher correlation than in 2021, suggesting a stronger influence of outdoor NO on indoor levels, along with consistent indoor sources.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor NO Comparison:

- ❖ **Average Concentration**:

2021: ~7 µg/m³

2022: ~25 µg/m³

- **Interpretation**: Higher average outdoor NO levels in 2022 may be due to increased traffic or other outdoor sources or the climate and higher temperature levels.

Indoor NO Comparison:

- **Average Concentration**:

2021: ~33 µg/m³

2022: ~32 µg/m³

- **Interpretation**: Slightly lower average indoor NO levels in 2022 despite higher outdoor levels suggest improved indoor air management, or less active natural ventilation on outdoor peaks, relatively.

4.2.1.4. NO_2 Data Overview

Observations Year 2021

Outdoor NO_2 Levels:

- ✓ **Range**: Outdoor NO_2 levels ranged from approximately 10 to 30 µg/m³.
- ✓ **Peaks**: Periodic peaks were observed, typically during rush hours, indicating traffic as a primary source.
- ✓ **Trends**: The diurnal pattern is noticeable, with peaks occurring during the day and lower concentrations at night.

Indoor NO_2 Levels:

- ✓ **Range**: Indoor NO_2 levels ranged from around 10 to 40 µg/m³.
- ✓ **Peaks**: Indoor peaks were more frequent and slightly higher than outdoor peaks, indicating significant indoor sources or activities, or strong infiltration through leaky airflow paths.

- ✓ **Trends**: Indoor NO_2 levels showed more variability with higher average concentrations than outdoor levels.

Observations Year 2022

Outdoor NO_2 Levels:

- ✓ **Range**: Outdoor NO_2 levels ranged from about 10 to 25 µg/m³.
- ✓ **Peaks**: Peaks were observed during daytime hours, suggesting traffic and other outdoor sources.
- ✓ **Trends**: The diurnal pattern remained consistent, with higher concentrations during the day.

Indoor NO_2 Levels:

- ✓ **Range**: Indoor NO_2 levels ranged from 10 to 45 µg/m³.
- ✓ **Peaks**: Indoor peaks corresponded with outdoor peaks but were generally higher, suggesting indoor contributions or strong infiltration through leaky airflow paths.
- ✓ **Trends**: Indoor levels showed significant variability, reflecting both indoor and outdoor influences.

Correlation Analysis

Indoor vs. Outdoor (2021):

- ➢ **Correlation Coefficient**: 0.65
- ➢ **Interpretation**: Moderate positive correlation indicates that outdoor NO_2 levels influence indoor levels, but indoor sources also significantly contribute.

Indoor vs. Outdoor (2022):

- ➢ **Correlation Coefficient**: 0.70
- ➢ **Interpretation**: A slightly higher correlation than in 2021, suggesting a stronger influence of outdoor NO_2 on indoor levels, along with consistent indoor sources.

Year-on-Year Analysis (2021 vs. 2022)

Outdoor NO_2 Comparison:

- **Average Concentration**:

  2021: ~18 µg/m³

  2022: ~18 µg/m³

- **Interpretation**: Identical outdoor NO_2 levels represents consistency in emission sources and no significant new sources.

Indoor NO_2 Comparison:

- **Average Concentration**:

  2021: ~18 µg/m³

  2022: ~21 µg/m³

- **Interpretation**: Slightly higher average indoor NO_2 levels in 2022 despite identical outdoor levels suggest slight increased indoor sources.

4.3. Conclusions

The analysis revealed that outdoor O_3 levels significantly impacted indoor O_3 concentrations in naturally ventilated houses, with a clear correlation between the two. The building structure and active ventilation patterns play crucial roles in varying indoor O_3 levels. In 2022, the correlation between indoor and outdoor O_3 was slightly stronger than in 2021, possibly due to increased outdoor O_3 levels and varying weather conditions. Despite the naturally ventilated state of the house, indoor O_3 levels were consistently higher than outdoor levels, indicating ineffective active natural ventilation periods. However, the peaks in indoor O_3 levels still suggest potential exposure risks, particularly during periods of high outdoor O_3. The analysis highlights the importance of continuous monitoring and implementing strategies to manage O_3, especially in naturally ventilated buildings. Future work should focus on exploring more effective ventilation strategies and air purification methods to further reduce indoor O_3 exposure.

The analysis demonstrated that indoor $PM_{2.5}$ levels in the case study house in Arlon were influenced more by indoor sources and activities than by outdoor $PM_{2.5}$ levels. The low correlation between indoor and outdoor $PM_{2.5}$ levels supports this observation. Significant peaks in indoor $PM_{2.5}$ levels suggest that indoor activities (cooking and cleaning), or other events are primary contributors. Despite stable and low outdoor $PM_{2.5}$ levels in both years, the indoor environment exhibited notable variability and spikes, indicating the necessity for effective/cautious natural ventilation control corresponding to them. Reducing indoor sources of $PM_{2.5}$, improving exhaust ventilation performance by regular maintenance, and using air purifiers could help mitigate indoor $PM_{2.5}$ levels and enhance IAQ.

The analysis also demonstrated that indoor PM_{10} levels in the case study house in Arlon were influenced partially by indoor sources and activities and by outdoor PM_{10} levels. However, the low correlation between indoor and outdoor PM_{10} levels supports the higher impacts of outdoor sources only when natural ventilation is in active performance concurrently with outdoor peaks. Significant peaks in indoor PM_{10} levels when there is no outdoor peaks, suggest that still indoor activities could be primary contributors, while PM_{10} emissions are generally originated outdoors. Despite stable and outdoor PM_{10} levels with less relative fluctuations in both years, the indoor environment exhibited notable variability and spikes, indicating the necessity for effective IAQ management strategies including cautious natural ventilation performance in accordance to outdoor air quality state. Reducing indoor sources of PM_{10}, implementing filtered mechanical ventilation systems, and using air purifiers could help mitigate indoor PM_{10} levels and enhance IAQ.

The analysis demonstrated that indoor CO levels in the Arlon case study house are influenced more by indoor sources and activities than by outdoor CO levels. The very low correlation between indoor and outdoor CO levels supports this observation. Significant peaks in indoor CO levels suggest that indoor activities mainly cooking, use of wall-mounted water boiler, or other events are primary contributors. Despite stable and low outdoor CO levels in both years, the indoor environment

exhibited notable variability and spikes in 2021, indicating the necessity for effective natural ventilation control, or enhanced ventilation strategies. Reducing indoor sources of CO, improving ventilation, and using CO detectors could help mitigate indoor CO levels and enhance IAQ.

The analysis demonstrated that indoor NO levels in the naturally ventilated house in Arlon are influenced by both indoor and outdoor sources. The moderate correlation between indoor and outdoor NO levels indicates that while outdoor sources such as traffic significantly impact indoor NO concentrations, indoor activities also could contribute to the observed levels mainly by incomplete burning processes. Higher indoor NO peaks and variability suggest that indoor activities such as cooking or use of heating appliances (wall-mounted hot water boiler) are major contributors. The slightly higher correlation in 2022 compared to 2021 in the case study indicates a consistent influence of outdoor NO on indoor levels primarily derived by infiltration through leaky airflow paths in a relatively less active natural ventilation performances in 2022. To mitigate indoor NO levels, it is essential to primarily reduce burning based indoor activities of all kind, and have cautious natural ventilation control in rush hours.

The analysis also demonstrates that indoor NO_2 levels in the naturally ventilated house in Arlon are influenced by both indoor and outdoor sources. The moderate correlation between indoor and outdoor NO_2 levels indicates that while outdoor sources such as traffic significantly impact indoor NO_2 concentrations, indoor activities also contribute to the observed levels. Higher indoor NO_2 peaks and variability suggest that indoor activities such as cooking or use of heating appliances (wall-mounted hot water boiler) are major contributors. The slightly higher correlation in 2022 compared to 2021 indicates a consistent influence of outdoor NO2 on indoor levels via infiltrations through leaky airflows. To mitigate indoor NO_2 levels, it is essential to primarily reduce burning based indoor activities of all kind, and have cautious natural ventilation control in rush hours.

5. INDOOR AIR QUALITY MODEL

5. Indoor Air Quality Model

5.1 Introduction

This chapter is inspired by references (Pourkiaei & Romain 2022) and Pourkiaei et al. 2024 (Systematic framework for quantitative assessment of Indoor Air Quality under future climate scenarios; 2100s projection of a Belgian case study). This chapter is an effort to answer the fourth research question (*RQ4*).

IAQ models establish a path to link data of sources, sinks, building elements, and ambient to predict indoor pollutant levels. Various models have been advanced for IAQ applications (Haghighat 1989, Jamriska 2003, Pepper 2009, Wei et al. 2019). The choice of model depends on the aimed objectives. The prime applications of IAQ models are:

- Predicting occupant exposures to different indoor contaminants
- Evaluating the influence of specific sources on pollutant levels
- Assessing the effect of particular sources and IAQ control strategies on personal exposure

The intended application of an IAQ model shapes its inherent characteristics and composition. Considering the diverse applications of IAQ models and the range of methodologies employed in their development they can be categorized into three main groups:

1. Mass balance models (Mechanistic approach: indoor physics & chemistry)
2. Computational Fluid Dynamic models (CFD) (Mechanistic approach: indoor physics & chemistry)
3. Statistical models (Numerical approach)

In this chapter, detailed information concerning the IAQ model descriptions, their general principles, their involved elements and parameters, their strengths and drawbacks, as well as their validation and calibration procedures are presented.

5.1.1. Mass Balance Models

Mass balance models are formulated to enable the estimation of pollutant concentrations and the influence of sources, sinks, and IAQ control strategies on contaminant levels. These models are rooted in the conservation of mass principle (Nazaroff & Cass 1989). They can be defined over either a single zone (compartment/room) or multi-zone ordonnances. In a single-zone model, the entire building is characterized as a shoe box model. On the other hand, multi-zone models characterize a building through interconnected spaces. The general mass balance equation for a well-mixed single zone is expressed as follows (Spengler et al. 2001,):

$$V_i \frac{dC_i}{dt} = C_a Pt_a Q_{a,i} + C_h Q_{h,i} + \sum_{i=1,j\neq N}^{N} C_j Q_{j,i} - C_i Q_{i,a} - C_i Q_{i,h} - \sum_{i=1,j\neq N}^{N} C_i Q_{i,j} + E_i - S_i \quad (1)$$

in which V_i denotes the zone volume, C_i denotes the indoor pollutant concentration in zone i, C_a denotes the outdoor concentration, Pt_a is the penetration factor for outdoor pollutants entering the indoors, $Q_{a,i}$ is the airflow from the outdoors into zone i, C_h is the concentration in the HVAC system, $Q_{h,i}$ is the airflow from the HVAC system into zone i, C_j is the concentration in zone j, $Q_{j,i}$ is the airflow from zone j into zone i, $Q_{i,a}$ is the airflow from zone i to the outdoors, $Q_{i,h}$ is the airflow from zone i into the HVAC system, $Q_{i,j}$ is the airflow from zone i into zone j, E_i denotes the emission source term, S_i denotes the pollutant removal term (e.g., air cleaners and sinks, etc.).

It is important to recognize that the emission source and sink terms, might involve extra differential equations that define their characteristics.

A key assumption in various mass balance models is the assumption of well-mixed zones. This assumption is held under the following circumstances (Drescher et al. 1995, Spengler et al. 2001):

- When time scales are several minutes or longer.
- When concentrations near significant sources are not of concern.

- When there are no local flow disruptions near the target zone.

The intrazonal airflows (airflows among zones themselves, and between zones and the ambient) can be influenced by the mechanical and (less) natural ventilation. Some IAQ models (such as CONTAM) are capable of calculating various airflows, contingent on adequate data regarding door and window openings, temperature differentials, HVAC characteristics, and similar factors. In contrast, other models may necessitate the parameterization of input airflow as data.

Mass balance models are formulated to estimate the average indoor pollutant concentrations. In numerous scenarios, this average concentration serves as the focal point. Nonetheless, there are instances where the average concentration is not the primary focus. For instance, if the concern is the exposure of an individual utilizing a potent emitting product the mean indoor concentration falls short. In such cases, mass balance models may prove insufficient (Norbeck et al. 2022, Sedighi et al. 2023).

5.1.2. CFD Models

Certain scenarios in IAQ modeling require to prediction of punctual (local) concentrations rather than average zonal concentrations. In these cases, the mass balance models fail to achieve targeted objectives. In such situations, objectives can be better addressed by CFD models. CFD models have two significant differences with mass balance models. First, CFD models estimate air velocity and contaminant concentration at discrete points within a zone. Secondly, CFD models tackle a set of partial differential equations as opposed to the ordinary differential equations targeted by mass balance models (Sajjadi et al. 2016, Xu et al. 2023). As a consequence, CFD models are computationally more expensive compared to mass balance models.

CFD models prove particularly valuable for examining airflows and distribution within zones (Cao et al. 2023). Additionally, emission source and sink models play a crucial role in estimating pollutant concentrations using CFD models. If the characterization of the emission source and sink is insufficient, concentration estimation will be inaccurate, despite accurate airflow

calculations (Liu & Zhai 2007, Zhang & Chen 2007). The partial differential equations governing fluid flow and concentration are rooted in the principles of mass, momentum, and contaminant concentration conservation. The variables of interest include velocity components, concentration, and certain turbulence parameters that consider turbulent flow effects (Sedighi et al. 2023). These fundamental equations are typically expressed in the following manner (Pepper 2009):

Conservation of mass:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x}+\frac{\partial \rho v}{\partial y}+\frac{\partial \rho w}{\partial z}=0 \tag{2}$$

Conservation of momentum (x-direction):

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial p}{\partial x}+\frac{\partial \sigma_{xx}}{\partial x}+\frac{\partial \sigma_{xy}}{\partial y}+\frac{\partial \sigma_{xz}}{\partial z}+f_{xx} \tag{3}$$

where u, v, and w are horizontal, lateral and vertical velocities, respectively, ρ is density, p is pressure, f_x is velocity body force terms, σ_{xx} is normal viscous stress, σ_{xy}, σ_{xz} are tangential (shear) viscous stress terms. The CFD concentration formulation is presented in section 3.1.4.2.

There are three fundamental CFD approaches typically employed for simulating flow and contaminants transport within zones: Finite Difference Method (FDM), Finite Volume Method (FVM), and the Finite Element Method (FEM) (Pepper 2009). CFD solvers can run structured, unstructured, or hybrid meshing with 2D (triangle, quadrilateral) or 3D (tetrahedral, hexahedron, etc.) forms with varying densities. Over the past decades, various other methods have emerged in scholarly literature, including the Boundary Element Method (BEM), the Lagrangian Particle Transport technique (LPT), the Particle-in-Cell method (PIC), and the Meshless method (MM) (Sommerfeld & Schmalfuß 2019, McLoone & Quinlan 2020, Shree et al. 2019, Kim et al. 2020, Ranganathan et al. 2022).

5.1.3. Statistical Models

Projection of IAQ through mechanistic methods is based on comprehension of the fundamental mechanisms governing the displacement and transport of indoor air contaminants. As

mechanistic models demand intricate inputs, securing sufficient information for their operation becomes challenging. This becomes even more critical in scenarios such as the study of building stocks, and real-world conditions where occupants interact with indoor settings. In such instances, statistical (also called numerical or mathematical) models based on mathematical approaches and Artificial intelligence (AI) offer an alternative pathway for IAQ prediction.

Machine learning and statistical models have gained substantial traction in outdoor settings for estimating atmospheric pollutant concentrations (Cabaneros et al. 2019, Masood & Ahmad 2021, Balogun et al. 2021) and in indoor settings for predicting thermal comfort and building energy efficiency (Fard et al. 2022, Zhang et al. 2022, Lala & Hagishima 2022). Although many statistical models have been applied to predict IAQ, research regarding the depth and scope of their applications is relatively new (Kotzias et al. 2009, Symonds et al. 2016, Sharma et al. 2021, Ma et al. 2021, Tien et al. 2022, Dong et al. 2023).

Statistical models offer the capacity to estimate IAQ through the utilization of questionnaires and/or measurements. Important statistical models employed for IAQ predictions include Artificial Neural Networks (ANNs), Regression models, and Decision Trees (Wei et al. 2019).

As a popular method in this category, ANNs operate on a network of interconnected nodes or neurons (Li et al. 2022, Sun et al. 2021). They employ an intuitive learning and prediction process making it particularly effective for solving non-linear problems. ANNs employ multicomplex combinations of weights and functions to transform input variables into predicted outputs, eliminating the need for predefined assumptions regarding variable relationships (black box modeling) (Wei et al. 2019, Dong et al. 2023).

Alternatively, Regression models such as Multiple Linear Regression (MLR), Kernel regression, and Partial Least Squares (PLS), approximate the relationships between variables. Among them, MLR is the main and extensively adopted model to assess the linear links between an output

(dependent variable) and various inputs (explanatory variables). The MLR model basis can be formulated as (Elbayoumi et al. 2015, Wei et al. 2019):

$$y = b_0 + b_1 x_1 + b_2 x_2 + ... + b_k x_k + \varepsilon \quad (4)$$

in which for k observations; y denotes the output, x_i denotes inputs, b_0 denotes the y-intercept (constant term), b_k represents the regression (slope) coefficients for each input, and ε denotes the stochastic error (residuals).

In addition to MLR, alternative regression models such as the Least Absolute Shrinkage and Selection Operator (LASSO) regression and stepwise regression might offer more advanced exploration and selection of input variables (Wei et al. 2020).

On the other hand, decision trees employ a tree-like structure to model decisions and their potential outcomes for data classification or regression. It serves for both classification (classification tree) and prediction (regression tree). An ensemble of regression trees (aggregation of multiple regression trees) is called Random Forest Regression (RFR). While a solitary regression tree may struggle with complex problems and lack of robustness, an RFR stands as the most frequently employed decision tree-oriented model (Yuchi et al. 2019).

Overall, mechanistic models may project a sense of reliability while statistical models offer a significant utility of black box (or gray box) understanding. In situations where the specific mechanisms or their dynamic variations lack well-established foundations and extensive datasets are available, statistical models are more favorable.

5.1.4. Indoor Air Chemistry Models

The field of Indoor Air Chemistry (IAC) aims to comprehend the elements influencing exposure by investigating the chemical processes that take place in the air, aerosol particles, and surface reservoirs within indoor settings. Within this field, primary chemical sources include emissions originating indoors, or infiltrating from the outdoors. Contrarily, secondary sources are related to those by reactive chemistry happening indoors. These sources may be involved with

permanent (sustained; i.e. from building materials), periodic (episodic; i.e. human activities), or transient characteristics. There are five major domains of indoor environments influencing indoor chemistry as follows (Abbatt & Wang 2020):

1. Indoor airflow features. Especially those linked to the building structure and interior characteristics, including AERs and mixing time (inter/intra-zonal).
2. Extremely high Surface-Area-to-Volume ratio (SA/V) of indoor spaces. This ratio is approximately around 3 m^{-1} when considering only macroscopic surface areas. This value serves as a conservative estimate, acknowledging that at the microscopic scale, surfaces may possess porosity or roughness. Additionally, building materials, furnishings, and paintings may feature low viscosity or high porosity, facilitating molecular diffusion into them. These surface reservoirs are pivotal in influencing nonreactive partitioning processes and reactive chemistry.
3. Indoor photon fluxes. Particularly in the ultraviolet light range. These fluxes are notably lower compared to outdoor conditions. The intensity and spectral composition of light indoors are highly influenced by factors such as the efficiency of sunlight transmission through the glass, cleanliness of the glass, time of day, type and number of windows, distance from the window, ambient cloudiness, and the types of indoor lighting.
4. Indoor T and RH. In contrast to outdoor environments, indoor T and RH are frequently controlled, preventing the wet deposition process (less for kitchen and bathroom while using). Even in the absence of HVACs, indoor T and RH variations are relatively lower than those experienced outdoors.
5. The human presence indoors. Occupants' activities, including cooking and cleaning, play a crucial role, but humans also cause direct effects through emissions and multiphase chemistry, via their clothing and skin. These impacts can be significant in densely populated environments.

Indoor settings are characterized by low light levels, relatively low concentrations of gas-phase oxidants, and limited durations for the reactive processing of gaseous and particulate components, owing to air exchange. Nonetheless, significant gas-surface partitioning and reactive multiphase chemistry take place within the extensive surface reservoirs present in all indoor environments. These interactions are crucial in shaping the composition of indoor surfaces as well as the surrounding gases and aerosol particles, thereby influencing human chemical exposure.

Although gas-phase chemistry typically doesn't play a dominant role in determining the fate of most VOCs, it still involves substantial radical cycling and organic nitrate formation (Carslaw 2007, Abbatt & Wang 2020). Additionally, the formation of Secondary Organic Aerosol (SOA) can occur through gas-phase oxidation of various precursors, including monoterpenes, unsaturated compounds from skin and cooking oils, and cigarette smoke (Abbatt & Wang 2020). While indoor SOA is not usually the primary component of indoor aerosols, its significance increases under specific conditions, such as elevated O_3 levels and low AERs. Episodic events with high precursor concentrations, like using a terpene-based cleaner or cigarette smoking, can also contribute to the formation of ultrafine particles (Sarwar et al. 2003, Waring 2014, Abbatt & Wang 2020). Further detailed information about gas-phase and multi-phase chemistry (gas-phase autoxidation mechanisms, gas-phase and condensed-phase photochemistry, multiphase thermodynamic partitioning, aerosol partitioning, equilibrium partitioning models, surface chemistry, and chemical reactions) are available in two valuable recent references of indoor chemistry (Abbatt & Wang 2020, Zhang Y et al. 2022).

Various techniques can model indoor chemical processes. Central to many models for indoor chemical processes, is the utilization of mass or concentration balances. These balances can be applied in both single- or multizonal well-mixed models to forecast the dynamic changes in gas- and particle-phase species over time. The 2 main approaches for indoor chemistry models are Box models and CFD models. The box model is the most commonly used for indoor chemistry

studies since, in essence, a modeler should select between modeling chemical complexity with a box model or spatial complexity with other methods. Recently, CFD has been applied to simulate certain simple chemical situations that present spatial variation (Waring & Shiraiwa 2022). Neither model can fully represent the complexities of indoor chemistry, while each seeks to address a unique gap in knowledge. The user must define the models' parameters accurately to acquire the most efficient understanding of the indoor processes (Shaw et al. 2023).

5.1.4.1. Box Models

To model the fate of a generic molecule F, the generation and removal reactions R1 and R2 are assumed as follows, respectively:

$$G + H \rightarrow y_F F + \ldots \quad \text{(R1)}$$

$$F + J \rightarrow \ldots \quad \text{(R2)}$$

The reaction between molecules G and H yields molecule F, with the molar yield of y_F. Additionally, F can be removed from the indoor air by reaction with another molecule J. With respect to R1 and R2, the concentration balance is as follows (Nazaroff & Cass 1986, Waring & Shiraiwa 2022):

$$\frac{dC_F}{d_t} = P_F + \lambda C_{F,out} + E_F - r_F C_F - \lambda C_F - v_{d,F}\frac{A}{V}C_F \quad (5)$$

In which C_i is the concentration (ppb) of species i, t is time (h), P_F (ppb/h) is the formation rate of F due to gas-phase reactions (in R1), r_F (h^{-1}) is the loss rate of F (in R2), $C_{F,out}$ (ppb) is the outdoor concentration of F; λ (h^{-1}) is the AER, E_F (ppb/h) is emission rate of F, $v_{d,F}$ (m/h) is the deposition velocity of F to indoor surfaces; and A (m^2) is the surface area indoors. The gas-phase chemistry formation and loss rate of F in Eq.5 are defined as follows:

$$P_F = y_F k_{G\text{-}H} C_G C_H \quad (6)$$

$$r_F = k_{F\text{-}J} C_J \quad (7)$$

In which $k_{G\text{-}H}$ and $k_{F\text{-}J}$ ($ppb^{-1}.h^{-1}$) are the biomolecular reaction rate constant between "G and H", and "F and J". Additional subset models of indoor SOA, inorganic aerosol, and surface chemistry are available in the reference of (Waring & Shiraiwa 2022). The developed box model INCHEM-Py v1.2, supports complex chemical mechanisms (> 6000 species, > 19000 reactions) (Shaw et al. 2023)

5.1.4.2. CFD Models

The fundamental equations of the indoor chemistry CFD model are typically expressed in the following manner (Pepper 2009):

Species concentration:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy}\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_{zz}\frac{\partial C}{\partial z}\right) + S \quad (8)$$

where S denotes source/sink terms, and D_{xx}, D_{yy}, and D_{zz} are the species concentration diffusion coefficients.

5.1.5. IAQ Model Validation & Calibration

Answering the question "How accurate is the model prediction?" depends on the model objectives and the type of data available for model inputs. The degree of agreement between model outputs and actual measurements is primarily influenced by the quality of the emission source and sink models. In situations where comprehension of the emission sources, sinks, and indoor-outdoor AER is robust, the disagreement between estimated and observed pollutant concentrations is rooted in measurement errors. Accordingly, for scenarios that require the assessment of a specific source using adequate source and sink models, predicted concentrations in a range of ±100% of measured values are expected (Spengler et al. 2001).

Error in indoor-outdoor AERs are less crucial compared to those present in the emission source and sink models. Notably, predictions made by the IAQ model are minimally affected by natural interzonal airflows (Spengler et al. 2001, McGrath et al. 2014).

5.1.5.1. IAQ Models Validation

Concerning the mass-balance model validation, Sparks et al. proposed a range of quantitative criteria for evaluating the overall agreement between model outputs and experimental data (Sparks et al. 1996). Many of those criteria are from the ASTM D5157. The initial criteria involve calculating the absolute value of the average fractional residual between the predicted concentration and the measured or observed concentration. Additional quantitative measures for gauging the alignment between model predictions and measurements are r (correlation), M (regression slope), b (regression intercept), NMSE (normalized mean square error), FB (fractional bias), and FS (fractional bias based on variance). A model may meet one or more criteria and still be inadequate, or conversely, a model may not satisfy one or more criteria and remain adequate for a given task (Sparks et al. 1996, Spengler et al. 2001, ASTM 2019).

For the validation of CFD models, in addition to the application of Mean Absolute Error (MAE), there are two valuable references in which descriptive information about the model validation can be found (Sørensen & Nielsen 2003, Li & Nielsen 2011), however simple comparison between CFD and experimental results is very common in the literature (Zhang et al. 2019).

On the other hand, the evaluation of statistical models' accuracy typically involves assessing the measured and predicted outputs via various performance metrics and approaches, including but not limited to Cross-validation (rotation estimation), Accuracy & Predictive Ability (PA), Root Mean Square Error (RMSE), Pearson correlation coefficient (r), coefficient of determination (R^2), Mean Absolute Percent Error (MAPE), Bayesian Information Criterion (BIC), Akaike Information Criterion (AIC), MAE, and Normalized Mean Absolute Error (NMAE) (Wei et al. 2019).

Regarding the validation of indoor chemistry models, due to the enormous heterogeneity of indoor spaces, they have to be tested against measurements in a wide range of environments. This validation step is required to ensure that model predictions are quantitatively accurate and transferable (Weschler & Carslaw 2018, Abbatt & Wang 2020)

5.1.5.2. IAQ Models Calibration

Regarding the IAQ model calibration (particularly mass balance and CFD models), this process is simply defined as the adjustment of statistical or physical modeling elements to improve the agreement of results with experimental data (CFD committee 1998, Zhao et al. 2021). Accordingly, one typical calibration approach is the Bayesian calibration using the Markov Chain Monte Carlo (MCMC) technique. Bayesian calibration involves an iterative procedure wherein uncertainty distributions related to the IAQ model parameters are revised in a manner that is consistent with the observed data (Johnston et al. 2014, Muehleisen & Bergerson 2016).

Concerning the calibration of statistical models based on machine learning, a typical model needs various constraints, weights, or learning rates to effectively assist various data patterns. These attributes are termed hyperparameters, and their calibration is essential to enable the model to proficiently address the machine learning task (Claesen & De Moor 2015). The process of hyperparameter optimization identifies a combination of hyperparameters that results in an optimal model, minimizing a predetermined loss function on provided independent data. Cross-validation is frequently employed to determine this generalization performance. Other popular approaches are Grid search, Random search, Bayesian optimization, Gradient-based optimization, Evolutionary optimization (e.g., Genetic Algorithm (GA), etc.), Population Based Training (PBT), Early stopping-based, Radial Basis Function (RBF), Spectral methods, and Adaptive Moment Estimation (ADAM) optimization (Yang & Shami 2020, Yu & Zhu 2020, Martínez-Comesaña et al. 2022).

Mostly inspired by the EU Commission's proposal to cut greenhouse gas (GHG) emissions by at least 55% by 2030, European countries are being set on a responsible track to becoming climate neutral by 2050 (EC, 2019). In Belgium, the Climate Change Department of the FPS (Federal Public Service Health) launched an initiative entitled "A low-carbon Belgium by 2050" in 2012. The built environment is one of the main energy-consuming sectors in Belgium, with about 34% of the overall final energy consumption in 2010 (CLIMAT: Cornet et al, 2013). GHG emissions in the built environment increased significantly by 18% over the period 1990-2010 which was mainly caused by the +13% growth in the number of households and +35% output growth of the services sector (CLIMAT: Cornet et al. 2013). Hence, the current dwellings, mainly naturally ventilated, are projected to account for approximately more than 80% of the housing stock by 2050. To reach 2050 climate-neutral targets, current policies propose existing dwellings must undergo extensive retrofitting, with the implementation of insulation and more efficient HVAC systems combined with an increase in air tightness (Wilkinson et al., 2009). However, such measures to air tightness and ventilation systems are expected to result in variations of IAQ and personal exposure to airborne pollutants which will have a direct influence on population health. Concentrations of chemical contaminants and airborne pollutants in residential buildings are related to the infiltration of outdoor compounds, emissions from indoor sources (activities, building materials, ventilation systems, etc.) and the removal from the internal air by deposition, filtration and exfiltration, though some re-suspension also occurs largely related to domestic activities. Indoor emissions include transient emissions from internal sources such as building materials, fixtures and appliances, as well as intermittent emissions such as burning fuel and candles, smoking, cooking, heating and human household activities. (Shrubsole et al., 2012). This study investigates the validation of a "Poly-contaminant CONTAM model" of a naturally ventilated studio house as part of the "OCCuPANt" project which aims at the assessment climate change effects on IAQ. The contaminants include CO, $PM_{2.5}$, PM_{10}, VOCs, NO, NO_2 and O_3.

This research is the first model validation of a design in CONTAM for IAQ assessment from the point of contaminants number, and time duration (7 contaminants for 73 days).

5.2. Material & Methods

5.2.1. CONTAM Description

To provide the baseline IAQ model of the case study, an IAQ "poly-contaminant" design of the test house was developed in CONTAM. The multizone IAQ and ventilation analysis computer program CONTAM, developed by NIST (National Institute of Standards and Technology), has been widely used to study various IAQ problems (Emmerich & Persily 1996, Paralovo et al. 2021). CONTAM enables indoor air multizone modelling, in which the building design is represented as a network of zones defined by the airflow paths over various zones (i.e., doors, windows, leakages, cracks, HVAC, etc.). The network nodes describe the zones concerning variant hydrostatic pressure, continuous temperature, and pollutant concentration. CONTAM is able to simulate the natural ventilation processes by applying the wind pressures acting on the exterior of the building, and buoyancy effects induced by temperature differences between zones, including the outdoors.

5.2.1.1. Essential Application For This Study

Since our case study involved a naturally ventilated house and no AER experiments were considered, the application of CONTAM in this study extends beyond a simple modular mass-balance multi-zone simulation. Recognizing that the evaluation of future IAQ states (Chapters 6 and 7) also requires future AER values, CONTAM ensures this consideration is accounted for.

5.2.1.2. Literature Background

In the following, correlated studies with CONTAM application in IAQ model design are presented, briefly. CONTAM has been dynamically linked with energy analysis software such as EnergyPlus and TRNSYS (Alonso et al. 2022, Tognon et al. 2023). Temenos et al. investigated the IAQ of Greek apartments, using CONTAM model (Temenos et al. 2015). Their study showed that

the variation of the baseline levels of the CONTAM inputs affects the output results and the modeled health effects. Silva et al., evaluated different scenarios of natural ventilation operation and the IAQ at a classroom in Portugal, using CONTAM. They performed the validation with the aid of a 24-hour experimental dataset (Silva et al. 2017). Fine & Touchie, investigated the ventilation system retrofits of high-rise residential buildings in Canada using a CONTAM model (Fine & Touchie 2021). Yang et al. suggested integrating the IAQ model into healthy building design by developing a simulation toolbox, named i-IAQ, via MATLAB®. For the implementation of the airflow module, they principally followed the simulation setup of CONTAM. They carried out an experimental validation period of one week (Yang et al. 2022). Na et al., optimized the IAQ and acoustic levels in old school classrooms with air purifiers and heat recovery ventilation systems, in South Korea (Na et al. 2023). Alonso et al., presented a methodology for the improvement of demand-controlled ventilation using measurements of IAQ parameters with Low-Cost Sensors (LCSs), correlation analysis, and co-simulation EnergyPlus/CONTAM, in Norway (Alonso et al. 2023). Sung et al. investigated the building retrofit, ventilation, and filtration measures for IAQ in a school in South Korea (Sung et al. 2023). Their CONTAM-based models were calibrated with the measured airflow and contaminant transport variables via ASTM D5157.

5.2.2. Model Design In CONTAM

Regarding our case study (see section 2.2.3.), the floor plan properties were introduced to the software concerning the test house characteristics (area: 100m^2, volume: 320m^3, ceiling height: 3.2m). The envelope effective leakage area is defined at a pressure of 4 Pa, exponent of 0.65, and discharge coefficient of 1 (default values settings).

Two exhaust fans with on-off operating modes, one in the bathroom and one in the kitchen, were considered in the design by flow rates of 24 $L.s^{-1}$. In total, 8 zones with 34 airflow paths (doors, windows, cracks and leakages, and exhausts) were implemented in the model based on the case study geometry.

The simulations ran with the use of Outdoor Contaminant files (.CTM), Outdoor Weather files (.WTH), and Continuous Value Files (.CVF) for continuous indoor temperature, indoor emission rates, natural ventilation activity, and occupancy pattern (Dols & Polidoro 2020). The aforementioned CONTAM file extensions are created with text (.txt) editor software and transporting the corresponding datasets into them (via CONTAM defined template). Figure 5.1. illustrate the corresponding CONTAM sketchpad of the first floor.

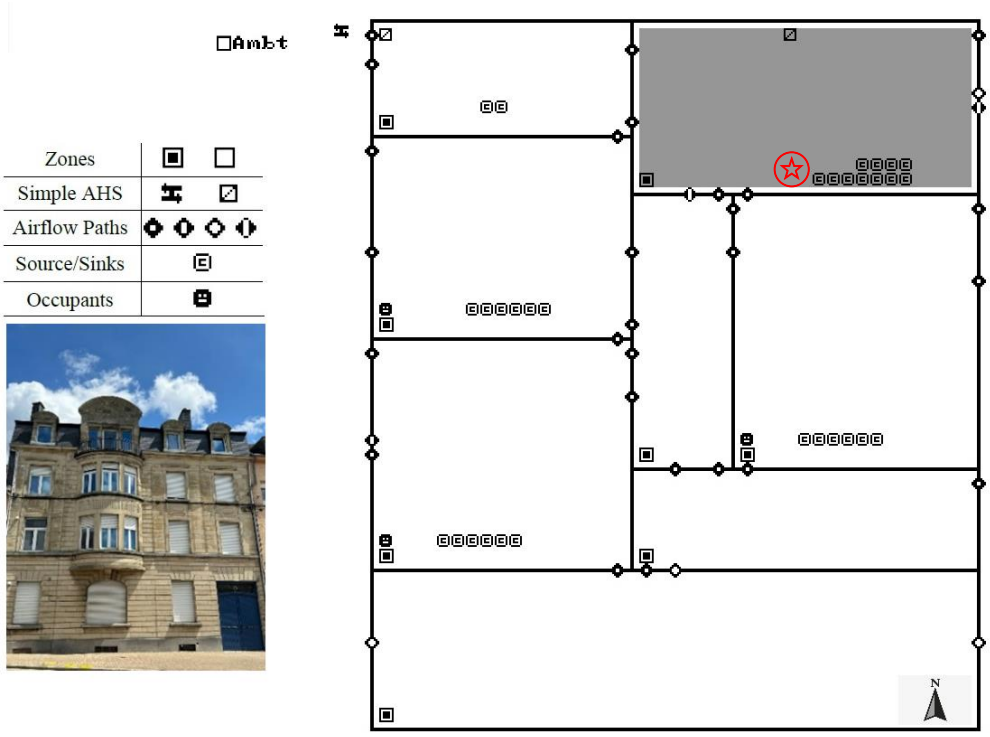

Fig 5.1. The test house in Arlon, and the corresponding CONTAM sketchpad of the first floor. Zones icons represent indoor and ambient zones, AHS icons represent Air Handling Systems (exhaust fans), Air flow paths represent doors, windows, and air leakage areas, Source/sink icons represent the generation rate of pollutants, Occupants icon is representing the inhabitants, and the star mark displays the sensors location in the grey zone (kitchen zone).

Table 5.1. shows the specified air flow paths in the model. The model parameters of different flow path elements were extracted from ASHRAE 2015 Handbook (ASHRAE 2015). In the 2021 indoor measurement campaign, given that zones other than the measured one (kitchen) did not have significant indoor emissions, due to the absence of sources and cross-sectional air exchange or ventilation, the design is considered highly reliable thanks to the inclusion of airflow paths for the entire multizone system.

Table 5.1. Properties of airflow paths in the IAQ model.

Element	Model Summary	Formula	Model Parameter
Exterior wall leakage	One-way flow using power law	Leakage area per unit length	15 cm^2/m
Interior wall leakage	One-way flow using power law	Leakage area per unit length	20 cm^2/m
Windows Close	One-way flow using power law	Leakage area per item	2 cm^2
Doors Closed (old)	One-way flow using power law	Leakage area per item	150 cm^2
Windows Open	Two-way flow	One opening	Cross section area
Doors Open	Two-way flow	One opening	Cross section area

5.2.2.1. Indoor Emission Rates

Regarding the indoor emission rates, two approaches were carried out. In the first approach, the average indoor emission rates were extracted from the literature and introduced into CONTAM to model a random 7-day period among the whole measurement period. In the second approach, calculated continuous emission rates (by experimental data and mass balance calculations) were introduced to CONTAM for modelling a period of about 3 summer months (73 days). These 2 approaches are described in the following.

Averaged Indoor Emission Rates from Literature

In this approach, we employed reported indoor emission rates available in the literature and introduced them to the software based on the questionnaire and activity pattern of the occupants for one week (18-24 July 2021). Our motive was to obtain acceptable approximates of typical indoor emission rates of the activities in our case study. For the VOCs, even though source strengths and activity patterns will vary from case to case, an approximate volumetric steady-state indoor emission rate of 40 $\mu g/m^3.h$ was considered (Holøs et al. 2018, Fazli & Stephens 2018). For the $PM_{2.5}$, PM_{10}, NO_2, and CO, indoor emission rates were considered following the most common source (cooking activity) from comprehensive studies. Regarding the different values reported in the literature, the median values among them have been considered, due to the variety of cooking utilities and activities (boiling, frying, grilling, toasting, and microwaving), and food ingredients. Correspondingly, the estimated $PM_{2.5}$, PM_{10}, NO_2, and CO emission rates were determined to be 1.6, 4.1, 3.1, and 5.3 mg/min, respectively (He et al. 2004, Dimitroulopoulou et al. 2006, Buonanno et al. 2009, Kim et al. 2011, Zhou et al. 2018, Kang et al. 2019). The aforementioned values in this section were reported

according to their units in the corresponding references. The unit conversions were taken into account with the CONTAM auto scale-convertor.

Continuous Emission Rates by Mass-Balance Approach (Calibration)

The continuous calculation of emission rates inherently accounts for the impact of occupant activities' emission sources and also from the materials. In other words, the influence of occupant activities has been fully integrated into the analysis. This is a fundamental aspect of continuous emission rate calculations. Rather than correlating fluctuations in concentration directly with specific indoor activities, this method streamlines the process by considering indoor and outdoor concentrations, ventilation performance, and air exchange rates. As a result, emission rates have been calculated with a resolution of one hour, ensuring a comprehensive reflection of all contributing factors. To calculate continuous emission rates, the method based on the widely used mass balance model was employed (Hussein et al. 2005, Olson & Burke 2006, Ott et al. 2006, Dacunto et al. 2013):

$$C(t)=C_b+\frac{\lambda}{(\lambda+k)V}+\left(C(0)+C_b+\frac{G}{(\lambda+k)V}\right)e^{-(\lambda+k)t} \quad (9)$$

In the Equation (9), $C(t)$ is the concentration at time t, C_b is the background concentration, $C(0)$ is the initial concentration, G is the emission rate (mass per time), V is the mixing volume, and $(\lambda+k)$ is the total decay rate due to ventilation, deposition, and coagulation (λ is the ventilation rate and k is the deposition rate). With the assumption of a well-mixed decay period and to obtain the emission rates over an emission period T, Equation (9) could be simplified to Equation (10) (O'Leary & Jones 2017):

$$G=(\lambda+k)V\left(\frac{(C_p-C_b)-(C(0)-C_b)e^{-(\lambda+k)T}}{1-e^{-(\lambda+k)T}}\right) \quad (10)$$

In which, C_p is the peak concentration at the time t_p. Nonetheless, the substantial fluctuations in daily indoor-generated pollutant source intensities contradict the presumption of a singular total decay rate, applicable to all days. The continuous total decay rate can be quantified as the negative slope in the logarithm of the indoor concentration as a function of time approximately (Zhao et al. 2021):

$$(\lambda+k)=\frac{1}{t_2-t_1}\ln\frac{C_{t1}}{C_{t2}} \quad (11)$$

Regarding the deposition of PM, negative calculated values of G represent the sinks. To calculate the emission rates of gases, and with the assumption of $t \ll \tau$ (τ is the residence time), the "peak estimation approach" presented by Ott et al., was applied (Ott et al. 2006):

$$G \cong \frac{VC_{\max}}{t} \quad (12)$$

In which, $C_{\max}$ is the maximum concentration during the residence time (see 18.8 ref Ott et al. 2006). Finally, calculated indoor emission rates (solving the equations 10 & 11 simultaneously) were fed to the CONTAM by .CVF input files. We also labeled this procedure in our study as "IAQ model calibration" or "emission rates calibration". The approach has also been cited in the literature as *Adjustment*, *Tuning*, and so forth. Table 5.2. presents the Standard Deviation (SD), average, and maximum values of calculated indoor emission rates for CO, NO_2, $PM_{2.5}$, and PM_{10}. No periodic indoor emission sources for O_3 and NO were considered.

Table 5.2. Calculated indoor emission rates by mass-balance approach, SD, Average, and the Maximum.

Emission Rates (mg/min)	CO	NO_2	$PM_{2.5}$	PM_{10}
Standard Deviation	6.87	2.11	15.28	31.81
Average	2.40	1.26	2.96	8.32
Maximum	121.80	13.92	278.82	565.90

Following the instructions provided by the research frameworks (see Figures 2.2. & 2.3.), this section is dedicated to presenting the outcomes of total 21 simulation cases. These cases are the combinations of 3 simulation series, 7 contaminants each:

1. 7 days - averaged indoor emission rates from literature
2. 7 days - continuous emission rates by mass-balance approach (more accurate, final approach)
3. 73 days - continuous emission rates by mass-balance approach

5.2.3. IAQ Model Validation

With the aim of "IAQ model validation" as one of the requirements, the Standard Guide for Statistical Evaluation of IAQ Models: ASTM D5157-19 was considered (ASTM 2019). This

standard guid is developed by "ASTM International", an international standards organization formerly known as American Society for Testing and Materials. It is noteworthy to mention that ASTM D5157 is the only available official guideline mandating criteria (quantitative) for the IAQ model evaluation, since 1993 to date. Table 5.3. represents the evaluation parameters of D5157 along with their definition and corresponding acceptable ranges.

Table 5.3. ASTM D5157 criteria for IAQ model evaluation.

Evaluation Parameter	Parameter Definition	D5157 Acceptable Values
Correlation Coefficient	$r = \frac{\sum(M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum(M_i - \bar{M})^2 \sum(O_i - \bar{O})^2}}$	$r \geq 0.9$
Regression Slope	M	$0.75 \leq M \leq 1.25$
Regression Intercept	b	$\|b\| \leq 0.25\bar{O}$
NMSE	$NMSE = \frac{\overline{(C_p - C_o)^2}}{(\overline{C_p}.\overline{C_o})}$	$NSME \leq 0.25$
FB	$FB = \frac{2(\bar{M} - \bar{O})}{(\bar{M} + \bar{O})}$	$FB \leq 0.25$
FS	$FS = \frac{2(\sum(M_i - \bar{M})^2 - \sum(O_i - \bar{O})^2)}{\sum(M_i - \bar{M})^2 + \sum(O_i - \bar{O})^2}$	$FS \leq 0.5$

*The *M* and *O* stands for predicted and observed concentrations

5.3. Results

Figure 5.2. shows the hourly indoor, and outdoor measured concentrations and indoor concentrations results by CONTAM for the kitchen zone (most complex zone) of the test-house, during 168 hours (7 days, 18-24 July 2021).

Figure 5.2.a presents the CONTAM results while it is fed by average event emission rates from the literature, and Figure 5.2.b presents the CONTAM results when it is fed by calibrated continuous emission rates derived by the mass-balance approach.

Figure 5.3. presents the same parameters as Figure 5.2. but for 1752 hours (73 days, 20 June-31 August 2021) with calibrated emission rates. For better presentation purposes in Figure 5.3., the upper concentration range is kept limited for CO, $PM_{2.5}$, and PM_{10}. However maximum records of CO: 150 mg/m^3, $PM_{2.5}$: 400, and PM_{10}: 800 µg/m^3 were recorded during the measurement campaign.

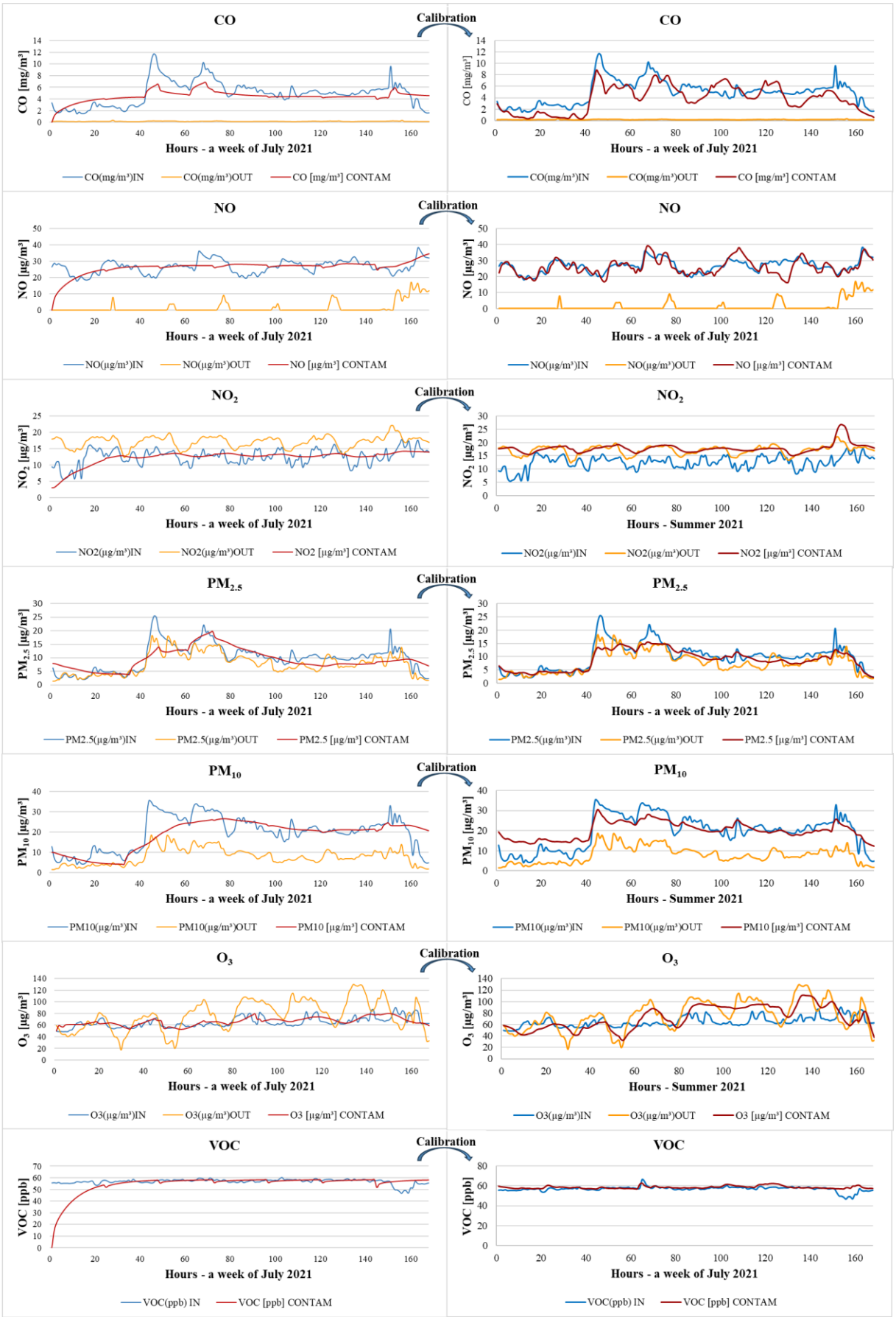

Fig 5.2. Hourly concentration of indoor and outdoor measurements and indoor results by CONTAM (168 hours = 7 days; 18-24 July 2021) – Case study house, a) Average emission rates b) Calibrated emission rates.

Fig 5.3. Hourly concentration of indoor and outdoor measurements and results by CONTAM (1752 hours = 73 days; 20 June - 31 August 2021) – Case study house, Calibrated emission rates. The green shaded area shows the equivalent time range of Fig 5.2.

The equivalent time range of Figure 5.2. is highlighted by a green shading in Figure 5.3. Also, the initial concentrations of pollutants were introduced to CONTAM based on the mean outdoor concentration of contaminants during the IAQ measurement campaign. As it is recognizable from Figure 5.3., CONTAM simulation results are in high harmony with the measured values over the 73 days. To statistically examine the model performance and the agreement between model results and indoor measurement (see Figure 5.3.), ASTM D5157-19 was employed (ASTM 2019). Data characteristics were sufficient to evaluate CONTAM estimates of different zone pollutant levels. We calculated the NMSE parameter based on the definition presented by an exclusive EPA (U.S. Environmental Protection Agency) chapter of the McGraw-Hill IAQ Handbook (Spengler et al. 2001). The aforementioned definition is as follows:

$$NMSE = \frac{\overline{(C_p - C_o)^2}}{(\overline{C_p}.\overline{C_o})} \tag{13}$$

in which C_o represents the measured or observed concentration and C_p represents the predicted or modelled concentration. The bar accent denotes averaged values.

Table 5.4. presents the results of D5157 evaluation criteria for the model output and observed (measured) datasets, both for average emission rates of the literature and calculated continuous emission rates. The results falling in the D5157 expected ranges are remarked in green cells. Also, corresponding scatter plots are presented in Figure 5.4.

Table 5.4. Results of D5157 evaluation criteria over the modelled and measured datasets.

7 days (18-24 July 2021), CONTAM average emission rates								
Acceptable range	**Measure**	**CO**	**NO**	**NO_2**	**$PM_{2.5}$**	**PM_{10}**	**VOC**	**O_3**
$r \geq 0.9$	***r***	0.39	0.48	0.46	0.74	0.8	0.35	0.62
$0.75 \leq M \leq 1.25$	**M**	**1.90**	**0.79**	**0.76**	**0.96**	**0.9**	0.13	**0.81**
b≤0.25(observations)	**b**	3.9≥1.2	**5.32≤6.6**	**3.06≤3.1**	**0.79≤2.5**	**3.22≤4.9**	50.23≥14.22	**10.87≤16.2**
NMSE ≤ 0.25	**NMSE**	**0.09**	**0.01**	**0.02**	**0.11**	**0.09**	**0**	**0.01**
FB ≤ 0.25	**FB**	**-0.09**	**0.01**	**0.00**	**-0.04**	**0.04**	**-0.01**	**0.02**
FS ≤ 0.5	**FS**	-1.44	1.06	-0.84	-0.52	**-0.31**	0.62	0.62
73 days (20June-31August 2021), CONTAM calibrated emission rates								
$r \geq 0.9$	***r***	0.74	**0.92**	0.72	0.75	0.74	0.65	0.55
$0.75 \leq M \leq 1.25$	**M**	**0.82**	**0.99**	0.41	0.38	0.37	0.6	**1.04**
b≤0.25(observations)	**b**	**1.04≤1.14**	**0≤8.13**	12.68≥5.03	4.88≥1.93	6.2≥2.97	25.16≥14.22	**0.26≤14.97**
NMSE ≤ 0.25	**NMSE**	**0.11**	**0.01**	**0.04**	**0.22**	**0.13**	**0**	**0.04**
FB ≤ 0.25	**FB**	**0.2**	**–0.01**	**0.11**	**0.03**	**0.25**	**0.04**	**0.04**
FS ≤ 0.5	**FS**	**0.33**	**0.15**	–1.1	–1.18	–1.2	**–0.15**	1.12

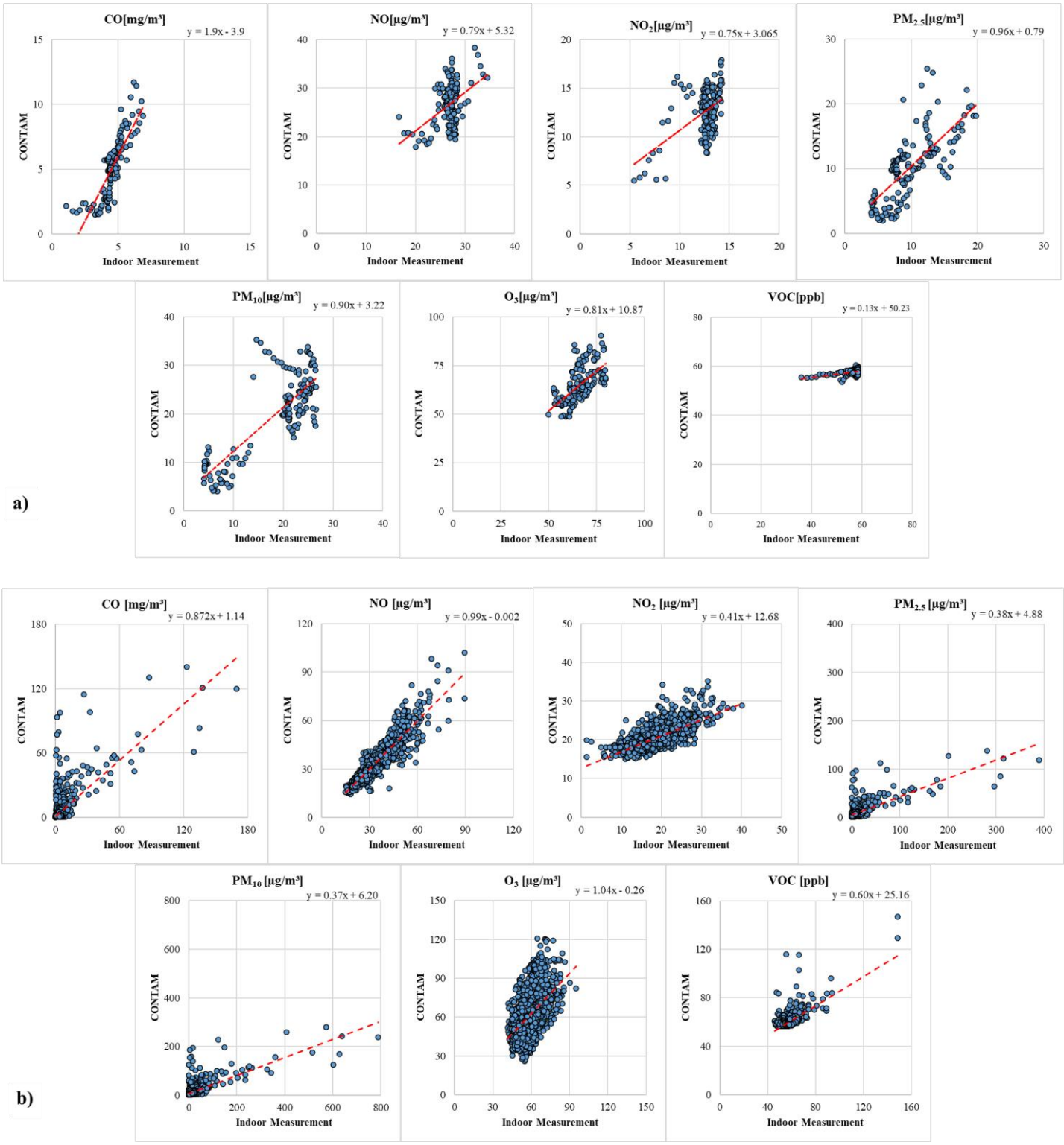

Fig 5.4. Scatter plots of the model concentration vs. measured values a) 7 days, 18-24 July 2021 (CONTAM averaged emission rates), b) 73 days, 20 June-31 August 2021 (CONTAM calibrated emission rates)

5.4. Discussions

As presented, after confirming the performance of LCSs in the "sensor calibration study", and subsequently conducting tests in the "IAQ measurement campaign", the performance of the designed IAQ model in CONTAM was explored.

As shown in Figure 5.3., the continuous emission rates which were calculated based on the mass-balance approach led to more realistic continuum results indicating improved model performance (compared to literature-extracted emission rates). Regarding the IAQ model validation (performance evaluation), as can be seen in Table 5.3., statistical compliance with ASTM-D5157 (ASTM 2019) criteria varies among different pollutants. The results based on the continuous emission rates approach are better to some extent, specifically with improved overall mean *r* (average *r* of all contaminants) from 0.54 to 0.72.

The interpretation of scatter plots of the CONTAM results against measured values (see Fig 5.4.) suggests that: I) there is a positive correlation among all estimated and measured values, for both emission rate approaches, II) in the second approach (see Figure 5.4.b.) the correlation between CONTAM results and measured values demonstrates a significant improvement (stronger relationship) even in a longer period, but not for PM and O_3. This could be due to the strong relatively outdoor sources of these contaminants, outside of the indoor emission episodes, and the uncertainties in the questionnaire completion (accurate record of natural ventilation and exhaust fans operation).

It should be mentioned that although some criteria do not met the high expectations of D5157, considering the long-term comprehensive experiment duration and involved uncertainties (e.g., sensors performance, questionnaire, model parameters, etc.), still the model performance is reasonable.

Figure 5.5. illustrates the comparison of pollutant concentration box plots of CONTAM results against measured values of the case study, for both emission rate approaches. The CONTAM results are well within the magnitudes and ranges of those by real measurements in both emission rate approaches. As presented in Figure 5.5.b, the levels of the modeled and observed average concentrations for VOCs: (59.37 and 56.78 ppb), and O_3: (59.88 and 57.52 µg/m³), demonstrate a very close agreement from the average perspective (same pattern for the Figure 5.5.a). Strictly speaking, while the D5157 statistical criteria can support understanding the advantages/disadvantages of a designed IAQ model, one additional general assessment can be the comparison of whole datasets in terms of average values. This inclusive assessment confirms that the model's strength to estimate the relative outputs (when different variables are varied), has a consistent agreement (e.g., exhaust fans and natural ventilation performances or existence of emission sources based on occupant activities). Concerning the satisfactory model performance with calculated emission rates by the mass-balance approach, the overall mean FB value (average FB of all contaminants) of 0.11, indicates a minimum systematic error.

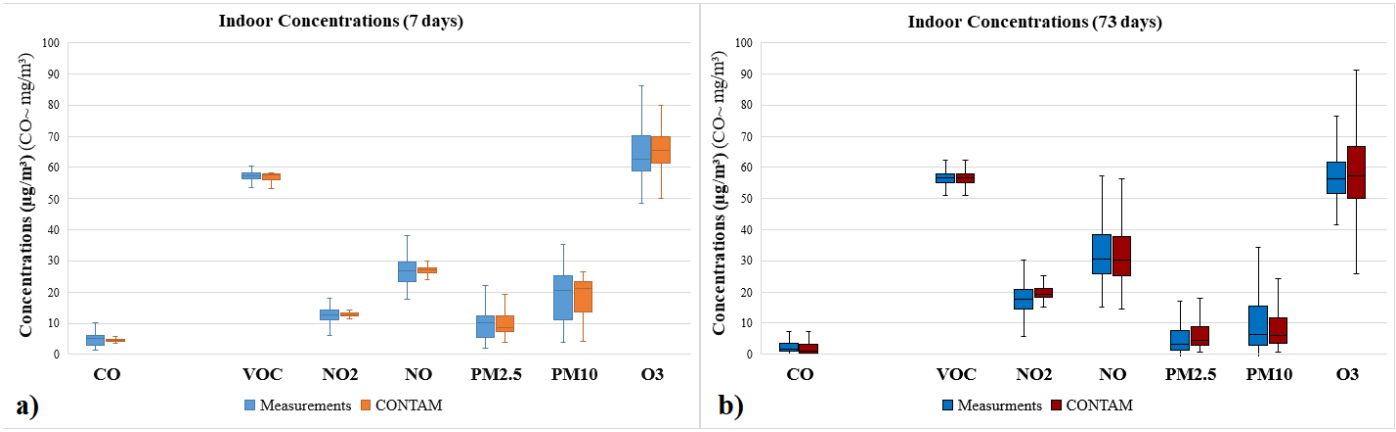

Fig 5.5. CONTAM results vs. indoor measurements of the case study, a) 7 days, 18-24 July 2021, average emission rates, and b) 73 days, 20 June - 31 August 2021, mass-balance approach emission rates.

To summarize the significant recommendations for IAQ modelling, it is recommended to:

- It is recommended to use calibrated LCSs for IAQ experiments due to their simple application in concurrent multi-zone measurements. Considering, the usual drift of the sensors, re-calibration must be managed each year for PM sensors (auto-calibrated, if drift data show no need to recalibrate before 12 months) and each 6 months for the others.
- use CONTAM IAQ model due to its prominent design and coupling capabilities, as well as being time and cost-efficient.
- to perform the emission rate determination tests under highly controlled conditions, due to the sensitive impact it has on the results.

5.5. Conclusions

A series of experiments to characterize the temporal profiles of poly-contaminants concentrations from a test residential house was carried in the summer of 2021 in Belgium to support the validation process of a designed model in the IAQ simulation software, CONTAM. Seven contaminants CO, $PM_{2.5}$, PM_{10}, VOCs, NO, NO_2 and O_3 are considered.

Initially, the IAQ design with literature-based values of indoor emission rates was validated. Afterwards, with support of the experimental IAQ data and mass-balance approach, the indoor emission rates were tunned/adjusted in a continuous form (model calibration). The outdoor weather data was used to create CONTAM .CTM files. The long-term period of the designed model is 73 days of 3 summer months (20 Jun – 31 Aug 2021).

Absolute validation of a complex model, such as CONTAM, is impossible as there are countless possible designs that can be developed by a user for a single case of study. Nonetheless, for the simulation performed by the designed model in this study, no substantial errors in the CONTAM performance were detected, specially from the average point of view of concentrations in the examination time range. The agreement between the measurements and predictions of the CO,

NOx and PMs concentrations in the kitchen zone was very good. Between one to four of the calculated statistical values met the ASTM D5157 criteria for each contaminant. The average values of simulated and measured concentrations for each contaminant in the whole summer time were identical at the level of 83% for CO, 77% for PM_{10} and +90% for other contaminants.

The following chapter (Chapter 6) will focus on acquiring future inputs for the CONTAM IAQ basis model (year 2021), considering the climate change.

Correlated publishment of this chapter:

Pourkiaei, M., & Romain, A. C. (2022, June). Exploring the Indoor Air Quality in the context of changing climate in a naturally ventilated residential Building using CONTAM. In *Indoor Air 2022*, https://hdl.handle.net/2268/292660

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6.FUTURE CLIMATE SCENARIOS
&
FUTURE IAQ MODEL INPUTS

6. Future Climate Scenarios & Future IAQ Model Inputs

6.1. Introduction

This chapter is mainly drafted from reference Pourkiaei et al. 2024 (Systematic framework for quantitative assessment of IAQ under future climate scenarios; 2100s projection of a Belgian case study). This chapter is an effort to answer the third research question (*RQ3*).

To quantitatively evaluate the IAQ in its future state, all or main influential elements must be acquired/determined within the pre-defined scenarios. This is vital to assemble a comprehensive, and future-representative input dataset for the designated IAQ model. In this regard, the following five questions should be addressed:

1. How would the climate trends (meteorological conditions) vary in future scenarios?
2. How would the "outdoor Air Pollution (AP)" levels evolve in future scenarios?
3. How would the "indoor climate" change in the future scenarios?
4. How may building characteristics and retrofit plans advance in future scenarios to address mitigation and adaptation plans?
5. How may human behavior evolve in the context of changing climate?

In the following, it has been tried to study the available solutions (see 6.1.1. – 6.1.5.) and present selected solutions (see 6.2.) related to each question, respectively.

6.1.1. Future Climate (Meteorology)

Numerical climate models utilize quantitative techniques to replicate the complicated interactions among pivotal climate drivers (i.e., atmosphere, oceans, land surface, and ice). These models are being employed across a spectrum, ranging from probing the dynamics of the climate system to projecting future climatic scenarios. Not being limited to exclusively numerical formation, climate models can also assume qualitative frameworks and narratives that mainly involve descriptive scenarios for potential futures (IPCC 2014, Gjerstad & Fløttum 2022).

Climate models can be classified into the following six main categories (Wikipedia: Climate Model):

- Box models
- Energy Balance Models (EBMs)
    - Zero-dimensional models
        - Model with combined surface and atmosphere
        - Models with separated surface and atmospheric layers
- Higher-dimension models
- Radiative-convective models
- Earth System Models (ECMs)
    - Global Climate Models or General Circulation Models (GCMs)
- Numerical models (AI-based models)

While simpler models have also been used to provide globally- or regionally-averaged estimates of the climate response, only GCMs are introduced in this section, as a result of their superior capabilities (Edwards 2011).

GCMs demonstrating physical processes in the environment, are the most advanced tools available today for analyzing the reaction of the climate system to the increasing levels of greenhouse gases. Only GCMs in combination with nested grid regional models have the potential to provide geographically and physically consistent estimates. GCMs characterize the climate by a global 3D grid, usually with a horizontal resolution of 250-600 km, and 10-20 vertical layers in the atmosphere (IPCC 2023).

Furthermore, numerous physical phenomena, including those linked with clouds take place on smaller magnitudes and are challenging to be accurately simulated (source of uncertainty). Instead, their recognized attributes need to be averaged across broader scales, within a method referred to as parametrization (Wikipedia: parametrization). Additional uncertainties are caused

by the different responses to the same forcing and representation of diverse feedback mechanisms. Distinct responses to the same forcing are caused by the variances in how particular processes and feedback loops are defined. On the other hand, diverse feedback mechanisms include water vapor, temperature rise, clouds and radiation, future atmospheric composition, etc. (Adachi & Tomita 2020, Tapiador et al. 2022).

“Climate change projections with climate models require information about future emissions or concentrations of greenhouse gases, aerosols, ozone-depleting substances, and land use over time (Figure 6.1.). This information can be provided by scenarios, which are internally consistent projections of these quantities based on assumptions of how socio-economic systems could evolve over the 21st century.” (Arias et al. 2021)

Intergovernmental Panel on Climate Change (IPCC) is an internationally accredited organization on climate change and is well-known due to carrying a leading role in climate scientists, as well as governments. The panel gathers objective and inclusive scientific data on anthropogenic climate variations. In 2014, the IPCC fifth Assessment Report (AR5) presented four scenarios entitled, Representative Concentration Pathways (RCPs). RCPs were GHG concentration (not emissions) trajectories approved by IPCC (O’Neill et al. 2014). In 2019, the IPCC AR6 presented five climate scenarios entitled, Shared Socioeconomic Pathways (SSPs) which are scenarios of projected socioeconomic worldwide variations till 2100. These five central states, namely SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5, represent increasing temperature till 2100. They are employed to originate GHG emissions scenarios by various climate policies (Riahi et al. 2017, Rogelj et al. 2018).

The likelihoods of these scenarios were not assessed in the AR5. However, a study from 2020 characterized the SSP5-8.5 as “highly unlikely”, SSP3-7.0 as “unlikely”, and SSP2-4.5 as “likely”

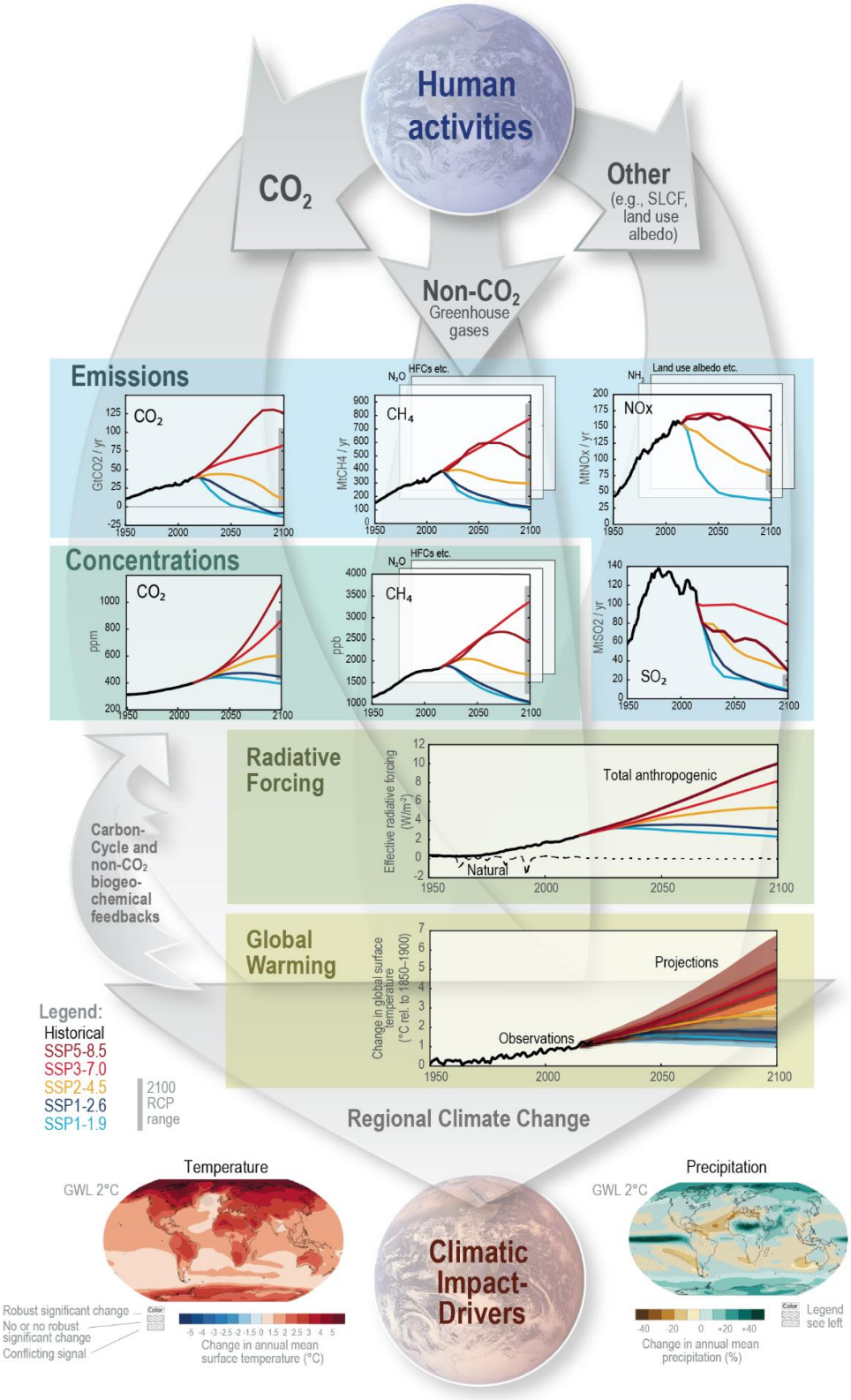


Fig 6.1. Exact Figure TS.4 from Ref. (Arias et al. 2021) | The climate change cause–effect chain: The intent of this figure is to illustrate the process chain starting from anthropogenic emissions, to changes in atmospheric concentration, to changes in Earth's energy balance ('forcing'), to changes in global climate and ultimately regional climate and climatic impact-drivers. Shown is the core set of five Shared Socio-economic Pathway (SSP) scenarios as well as emissions and concentration ranges for the previous Representative Concentration Pathway (RCP) scenarios in year 2100; carbon dioxide (CO_2) emissions ($GtCO_2yr^{-1}$), panel top left; methane (CH_4) emissions (middle) and sulphur dioxide (SO_2), nitrogen oxide (NOx) emissions (all in Mt yr^{-1}), top right; concentrations of atmospheric CO_2(ppm) and CH_4 (ppb), second row left and right; effective radiative forcing for both anthropogenic and natural forcings ($W.m^{-2}$), third row; changes in global surface air temperature (°C) relative to 1850–1900, fourth row; maps of projected temperature change (°C) (left) and changes in annual-mean precipitation (%) (right) at a global warming level (GWL) of 2°C relative to 1850–1900 (see also Figure TS.5), bottom row. Carbon cycle and non-CO_2 biogeochemical feedbacks will also influence the ultimate response to anthropogenic emissions (arrows on the left).

(Hausfather & Peters 2020). On the other hand, a report referring to the aforementioned reference; described that the RCP8.5 scenario is most closely with cumulative emissions from 2005 to 2020 (Schwalm et al. 2020).

6.1.2. Future Outdoor Air Pollution

Climate change can impact air contaminant levels by influencing weather, anthropogenic emissions (caused by human activities e.g., burning of fossil fuels, deforestation, land use and land-use changes (LULUC), livestock production, fertilization, waste management and industrial processes), biogenic emissions, and altering the distribution and characterization of airborne allergens. The local climate impacts atmospheric chemical reactions and the interactions that take place among micro-scale and global-scale environments. By assuming variations of the climate via higher temperatures, atmospheric dispersion is going to be potentially influenced. Yet, the particular magnitude of change (including micro, meso, synoptic, and global), the tendency of alterations in a specific location, and the intensity of variations in air quality remain points of concern. Figure 6.2. presents the general assumptions concerning climate change and its attributions to the atmospheric contaminant levels. Taking into account the uncertainties of the general scheme and its elements, it is beneficial to aim at climate change and air pollution simultaneously (Bernard et al. 2001).

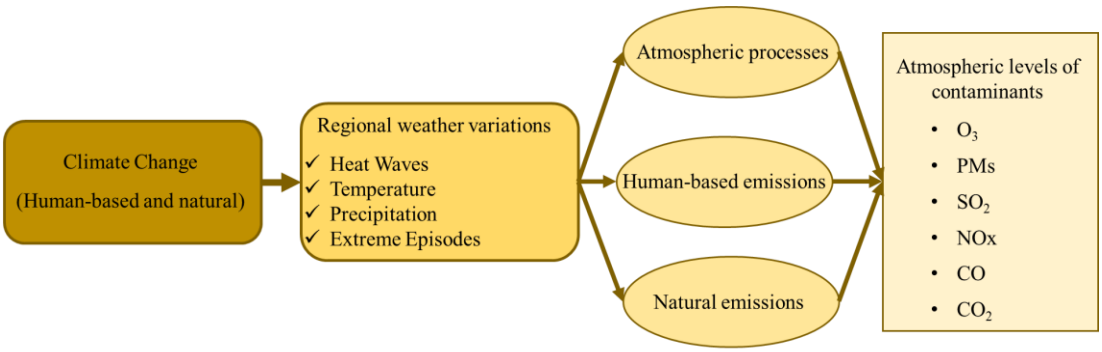


Figure 6.2. Framework of climate change and its attributions to pollutant concentrations, Re-illustration from (Bernard et al. 2001).

Atmospheric dispersion models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants as they disperse and react in the

atmosphere. Figure 6.3. presents a general hierarchy of data flow to obtain an atmospheric dispersion model.

Atmospheric dispersion models apply mathematical equations to estimate the transport (by the wind), the diffusion transfer (by atmospheric turbulence), and the dissemination of pollutants within the atmosphere. They find utility in examining an array of pollutants and are frequently deployed to examine the outcomes of emissions from industrial origins or to evaluate potential exposure associated with hazardous substances. General categories of atmospheric dispersion models include (Watson et al. 1988, Snoun et al. 2023):

- Gaussian dispersion models
- Chemical Transport Models (CTMs) (Lagrangian & Eulerian)
- Numerical models

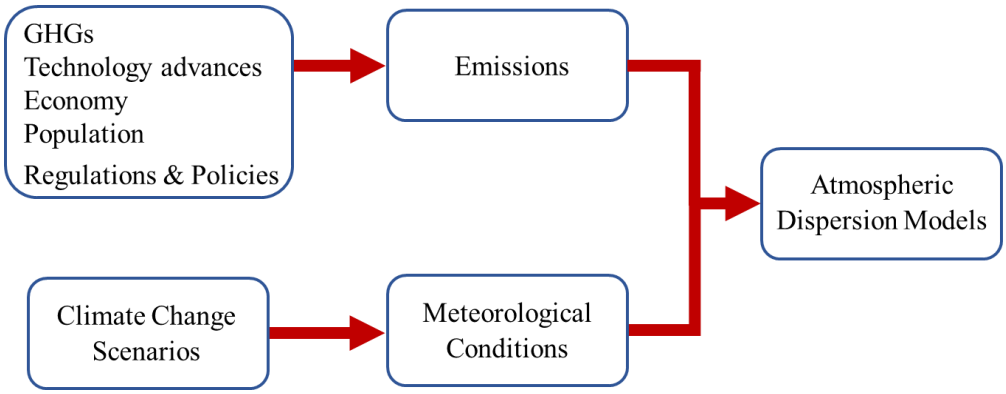


Fig 6.3. General data-flow hierarchy for obtaining an atmospheric dispersion model.

Gaussian dispersion models (also referred to as plume or stationary models) operate on the assumption that the pollutant concentration at any given point is established on factors such as emission rate, meteorological conditions, and distance from the source. They are usually employed due to their relatively straightforward implementation and their ability to estimate concentrations across a local scale distances from the source (in the first tens of kilometers around a source) (Fernandes et al. 2021, Snoun et al. 2023).

Lagrangian models are defined as the generation and transport of parcels of air "*puffs*" over time. These models trace the transport of pollutants by following a collection of particles representing the pollutants as they move through the atmosphere. They are used for pollutant dispersion over limited distances and in assessing the influence of complex terrain on pollutant transfer (Mensink & Matthias 2021).

Eulerian models are defined as "*grids* or *boxes*" within which fluxes take. They utilize a fixed cell system to calculate the transport of pollutants throughout the atmosphere. They prove particularly valuable for examining the distant (long-range) movement of pollutants and for evaluating the effects of emissions by numerous sources. Eulerian grid models are the most complex, but potentially the most powerful atmospheric dispersion models involving the least-restrictive assumptions (Khan & Hasan 2020).

CTMs, such as CMAQ, WRF-Chem, and CHIMERE are some of well-known developed software and models for urban air quality prediction.

Along with the 4th industrial revolution, newly valuable literature reviews have been carried out to provide detailed insights into the performance analysis of AI, machine learning, and ANNs in terms of a numerical modeling approach for future outdoor air pollution prediction (Cabaneros et al. 2019, Balogun et al. 2021, Masood & Ahmad 2021). Deep Learning (DL) networks such as Convolutional Neural Networks, Recurrent Neural Networks (RNN) and Long Short-Term Memory recurrent networks (LSTM), as well as hybrid architectures, have been employed to estimate air pollution with high efficiency competently (Cabaneros et al. 2019, Feng et al. 2019, Li et al. 2020, Wang et al. 2020, Balogun et al. 2021, Masood et al. 2021). Recent studies carrying out comparisons between the accuracy performance of CTMs and AI techniques for outdoor Air Pollution (AP) prediction, also show a better performance of ML and DL in terms of prediction accuracy (Fang et al. 2023).

Reminder: Deep Learning (DL) approach is a subdivision of Machine Learning (ML). Generally, it is a neural network with a more complex design structure. It is best to utilize multi-dimensional data efficiently due to its powerful learning ability, strong generalization, and flexible model structure. Due to its strong learning capability, powerful generalization, and adjustable architecture, it is efficient to be utilized for data with high dimensions(LeCun et al. 2015).

6.1.2.1. Atmospheric Chemistry and Outdoor Air Pollution: Mechanisms and Climate Change

Atmospheric chemistry is a critical field of study that focuses on the chemical composition of the Earth's atmosphere and the reactions that occur within it. This discipline is essential for understanding outdoor air pollution and its intricate relationship with climate change. This section discuss the general mechanisms that affect outdoor air pollution levels and explores how these processes are intertwined with climate change (Romain 2022, a, b, c).

Mechanisms Affecting Outdoor Air Pollution

Outdoor air pollution is influenced by a variety of sources and processes, both natural and anthropogenic. Key pollutants include particulate matter (PM), nitrogen oxides (NOx), sulfur dioxide (SO_2), carbon monoxide (CO), volatile organic compounds (VOCs), and ozone (O_3) (ground level ozone → secondary pollutant). The concentration and distribution of these pollutants are determined by several mechanisms. Main influential elements are chemical reactions, meteorological factors, and physical processes.

(i) Chemical Reactions

In terms of anthropogenic emission sources, major contributors include vehicle emissions, industrial activities, power plants, and residential heating. These sources emit significant amounts of NOx, SO_2, CO, PM (primary ones) and VOCs, which are precursors to secondary pollutants like ozone and particulate matter. On the other hand, natural emission sources include but not limited to volcanic eruptions, forest fires, and biogenic emissions from plants also contribute to atmospheric pollutants. Natural sources can release large quantities of PM and

VOCs, influencing air quality over high spatial ranges (Finlayson-Pitts & Pitts 1999, Seinfeld & Pandis 2016).

Main atmospheric chemical reactions are photochemical and oxidation processes. Considering the photochemical reactions, sunlight drives many atmospheric reactions, particularly the formation of ozone. NOx and VOCs react in the presence of sunlight to produce ground-level ozone, a major component of smog. In terms of the oxidation reactions, reactive oxygen species, such as hydroxyl radicals ($OH^{\bullet}$), play a crucial role in the oxidation of pollutants, transforming them into secondary pollutants or aiding in their removal from the atmosphere (Jacob 1999, Atkinson 2000).

(ii) Meteorological Factors

The main influential meteorological factors on the atmospheric chemistry in order of their impacts are; wind speed and direction, temperature, atmospheric stability, solar radiation, precipitation, humidity, mixing height, and pressure systems (Jacob 1999, Finlayson-Pitts & Pitts 1999, Holton 2013, Seinfeld 2016). Higher temperatures and intense solar radiation (UV) enhance photochemical reactions, leading to increased ozone formation. Wind disperses pollutants, affecting their concentration and distribution. Atmospheric stability (refers to the tendency of the atmosphere to resist vertical motion, lack of strong winds or sufficient precipitation) can lead to the accumulation of pollutants. Rain can remove pollutants from the atmosphere through wet deposition, effectively cleaning the air. Conversely, dry periods can lead to the buildup of pollutants (Stull 1988, Holton 2013).

(iii)Physical Processes

The key physical processes involved in the outdoor air pollution are the deposition and transport. In the deposition process, pollutants can settle out of the atmosphere via dry deposition (settling on surfaces) and wet deposition (rainout or washout). These processes help to remove pollutants from the air. On the other hand, the transport process incorporates the long-range transport

(spread) of pollutants across regions and even continents, influencing air quality far from the original source (Stull 1988, Holton 2013).

Air Pollution Relationship with Climate Change

The interplay between air pollution and climate change is complex, with each influencing the other through various feedback mechanisms:

(i) Greenhouse Gases and Pollutants

In the literature, the CO_2 and Methane (CH_4), are discussed to contribute to climate change by trapping heat in the atmosphere. Increased temperatures can, in turn, exacerbate air pollution by enhancing photochemical reactions (Forster et al. 2007, Bond et al. 2013). Rising temperatures and intense solar radiation can enhance the formation of ground-level ozone and secondary organic aerosols. Warmer conditions also increase the frequency and intensity of wildfires, which emit large quantities of PM and VOCs (Fiore et al. 2015). Also, it is discussed that PM, particularly black carbon, absorbs sunlight and warms the atmosphere. Conversely, sulfate aerosols reflect sunlight, leading to a cooling effect. The net impact of aerosols on climate is a balance between these warming and cooling effects (Forster et al. 2007, Bond et al. 2013). Climate change can alter wind patterns, precipitation rates, and atmospheric stability, all of which affect the dispersion and deposition of pollutants. For example, more frequent and intense heatwaves can lead to stagnant air conditions, trapping pollutants and worsening air quality (Jacob & Winner 2009).

Feedback Mechanisms

(i) Pollutant Effects on Climate

Air pollutants like ozone and aerosols directly influence the Earth's radiative balance. Ozone in the troposphere (ground level ozone – secondary polluatnt) acts as a greenhouse gas, contributing

to warming. Aerosols, depending on their composition, can either cool the atmosphere by reflecting sunlight or warm it by absorbing heat (Jacob & Winner 2009, Fiore et al. 2015).

(ii) Climate-Driven Emissions

Changes in climate can influence natural emissions of pollutants. For instance, higher temperatures can increase the emission of biogenic VOCs from plants, which are precursors to ozone and secondary organic aerosols (Jacob & Winner 2009, Fiore et al. 2015).

6.1.3. Future Indoor Climate

There are several approaches available to predict future indoor climate. The future indoor climate of buildings can be estimated by building simulations fed with input data from global climate models. Building simulations to obtain future indoor climate can be carried out by well-known software such as EnergyPluse, TRANSYS, MATLAB, CFD-based models, etc. One additional approach is implementing the indoor-to-outdoor (I/O) temperature ratios (Ilacqua et al . 2017, Fazli et al. 2021). The other methods are applying machine learning predictive models to predict future indoor climate. In this approach, the common choice for indoor climate prediction is the ANN, particularly the RNN variants like Long Short-Term Memory (LSTM) network and Gated Recurrent Units (GRU) (Setiawan et al. 2022).

6.1.4. Future Building Characteristics

Warmer seasons under climate change conditions may lead to increased operation of natural ventilation, while the application of cooling systems during extreme heat events may reduce natural ventilation use. The strategies for building adaptation comprise strengthening the insulations (more air tightened and less natural AERs), implementing new materials, and intelligent building technologies, and potentially adopting extended utilization of air conditioning systems during summers as compared to the present practices (Mansouri et al. 2022).

The main motivation for the development of future building retrofit scenarios in terms of climate mitigation and adaptations, is improving the Indoor Environmental Quality (IEQ) and building energy performance (Suppa & Ballarini 2023, Grassie et al. 2023). Generally, the building retrofit action plans impact the IAQ in three fashions, as follows:

1. Transition from fossil fuel-consuming heating (& cooking) systems to electric and renewable- or sustainable-based systems, that enhance the IAQ by eliminating pollutant emission sources.
2. Advancement of HVAC control strategies based on optimal indoor thermal comfort which potentially reduces the IAQ due to relatively reduced AERs (Laverge et al. 2011, Guyot et al. 2018, Guyot et al. 2019). Similarly, reduced use of mechanical ventilation or shift to natural ventilation (in summers), which can potentially reduce the minimum acceptable indoor airflow rates, are settled in this category.
3. Increased air tightness and reduced infiltration/exfiltration rates of buildings to conserve indoor air thermal capacity and prevent heat losses, which leads to reduced IAQ levels.

Commonly, the abovementioned scenarios are defined and aimed by regional building codes and energy sectors, applicable as input data for IAQ and whole building simulations.

6.1.5. Future Occupants' Behavior

Within the multidisciplinary fields of indoor chemistry and building physics, there is increasing attention to occupants' behavior due to its significance in IAQ and building energy performance (Andersen et al. 2009, Palani et al. 2023). The study of occupant behavior involves disciplines ranging from building physics to human biology, to evaluate IEQ (Tijani et al. 2016, Han et al. 2019). Three distinct approaches to this end are as follows:

1. Deterministic methods via established scenarios and behavioral rules (including but not limited to occupancy degree, indoor activity type/schedule, and airflow rate gain by ventilation patterns)

2. Numerical methods based on experimental observations (e.g., surveys, automated mechanical and natural ventilation loggers, etc.)
3. Social modeling methods that address cognitive and deliberative behaviors
4. In the context of climate change, future occupants' behavior scenarios are practically defined in terms of variant ventilation processes and operations types/periods, variant residence time, and cooking emissions.

6.2. Material & Methods

6.2.1. Future Weather Data (Meteorology Conditions)

The OCCuPANt project partner has provided a historical and forthcoming weather database for dynamic building modeling in Belgium via the regional climate model "MAR" (Modèle Atmosphérique Régional) version 3.11.4 (Doutreloup & Fettweis 2021, Doutreloup et al. 2022). The database provides 13 weather variables including dry bulb temperature at 2m, RH at 2m, global horizontal radiation, diffuse solar radiation, direct normal radiation, wind speed at 10m, wind direction, dew point at 2m, atmospheric pressure, cloudiness, sky temperature, specific humidity at 2m, and precipitation. MAR is a 3D atmospheric model coupled to a one-dimensional (1D) transfer scheme between the surface, vegetation, and atmosphere. The spatial resolution of MAR is 5km atop an integration domain (120 x 90 grid cells) centered above Belgium as depicted in Figure 6.4. to derive hourly results. The central role of MAR is to downscale a global model or reanalysis to obtain weather data at a higher resolution of time (temporal) and space (spatial). This regional model simulates the past climate (1980-2020) and also provides various future forecasts and associated uncertainties for different scenarios based on SSP5-8.5.

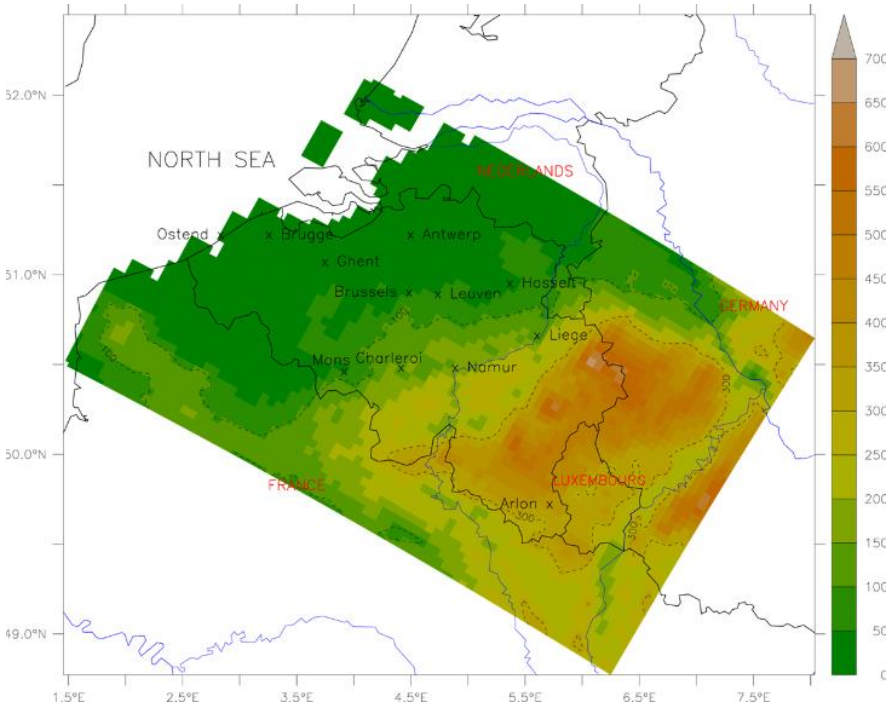


Fig 6.4. MAR model topography (forms and features of land surfaces).

6.2.2. Future Outdoor Air Pollution

Applying representative CTM methods, such as CMAQ and WRF-Chem, are typical methods for urban air quality prediction. However, because of unreliable pollutant emission rates, complex underlying surface states, and inadequate theoretical groundwork, the calculated results lack estimation accuracy (Vautard et al. 2007, Stern et al. 2008, Li et al. 2016). Although these approaches are helpful analysis of atmospheric dispersion, turbulent diffusion, wet and dry deposition, and decay; severe barriers to models' accuracy are still present (Sharma et al. 2017, Leelőssy et al. 2018, Mirzaei 2021). The origin of error in a CTM is the unreliability of temporal variations of emission rates, though the sites of emission sources are normally detected. Mesoscale atmospheric interactions (e.g., convection, inversion) and the indeterminate wet deposition processes are significant origins of error as well. Also, the functionality of CTMs to calculate complex atmospheric photochemical reactions is partial, due to a couple of issues; such as unreliability in emission descriptions. Almost all researches carried out by CTMs rely on hypothesizes or main variables like emission rates, mixing heights, and cloudiness (Bernard et

al. 2001, Vautard et al. 2007, Stern et al. 2008, Li et al. 2016, Sharma et al. 2017, Leelőssy et al. 2018, Mirzaei 2021).

6.2.2.1. Deep Air-Quality Forecasting

Air quality data are high dimensional (with strong nonlinearities). In the context of air pollution, high nonlinearity refers to complex relationships between various factors that influence the dispersion, transformation, and concentration of pollutants in the atmosphere. Air pollution is influenced by numerous nonlinear processes and interactions, including atmospheric chemistry, meteorological conditions, emissions from multiple sources, and the physical characteristics of pollutants. Subsequently, air quality prediction is an arduous task because of rapid weather variations, pollutant emission phenomena, and the presence of numerous influential elements. Additionally, the involved parameters in atmospheric dispersion are nonlinear and dynamic; including but not limited to wind speed and direction, solar radiation, air temperature, air humidity, as well as the pollutant concentrations themselves. All in all, air quality prediction in a complex and highly non-linear context is a challenging goal to be spatially and temporally precise. Since these elements are inherently interdependent, dealing with interdependencies and utilizing them for prediction from multivariable time series data is not easy. To overcome these challenges, a hybrid deep learner algorithm consisting of multiplex 1D Convolutional Neural Networks and a Bi-directional Long Short-Term Memory recurrent network is developed based on the Deep Air Quality Forecasting Framework; DAQFF, in MATLAB software (Du et al. 2019). The CNN-LSTM deep network considers both spatial and temporal dependencies of air quality-related time series data and is explained more in detail in the following part (Du et al. 2019, Qin et al. 2019, Wang et al. 2020, Li et al. 2020).

Convolutional Neural Network (CNN) Design

A representative CNN consists of 3 layers (see Figure 6.5): convolutional, activation, and pooling layer. Dissimilar to the traditional convolutional network (classic 2D with application for

images), multiples 1D filters convolved over all time steps of air quality time series data (1D-CNNs), are implemented. As a part of the CNN design, the *ReLU* is set as the activation function. The *ReLU* is expressed as follows:

$$ReLU \Rightarrow \quad y(x) = \max(x, 0)$$

To learn the spatial pattern features, 3 convolution layers are applied as a part of the CNN design,. After functioning 3 convolution layers, to alter the high-level expression to a feature vector, and employ a fully connected layer to decrease the final output vector dimension, a flattened layer is utilized. At this point, a concatenated layer delivers the final output. This enables receiving the spatial pattern features of single station time series data (as the 1D filter is employed in each convolutional layer, the variation of spatial pattern features, over time series can be apprehended), as well as integration of the probable spatial association features of multiple stations. Besides, the spatial comprehension and weighted sharing features of the 1D convolutional network decrease the parameters for operating with multiplex time series data and lead to higher learning performance. Accordingly, with the aid of this approach, the learning takes place for more deep representation features of air quality data.

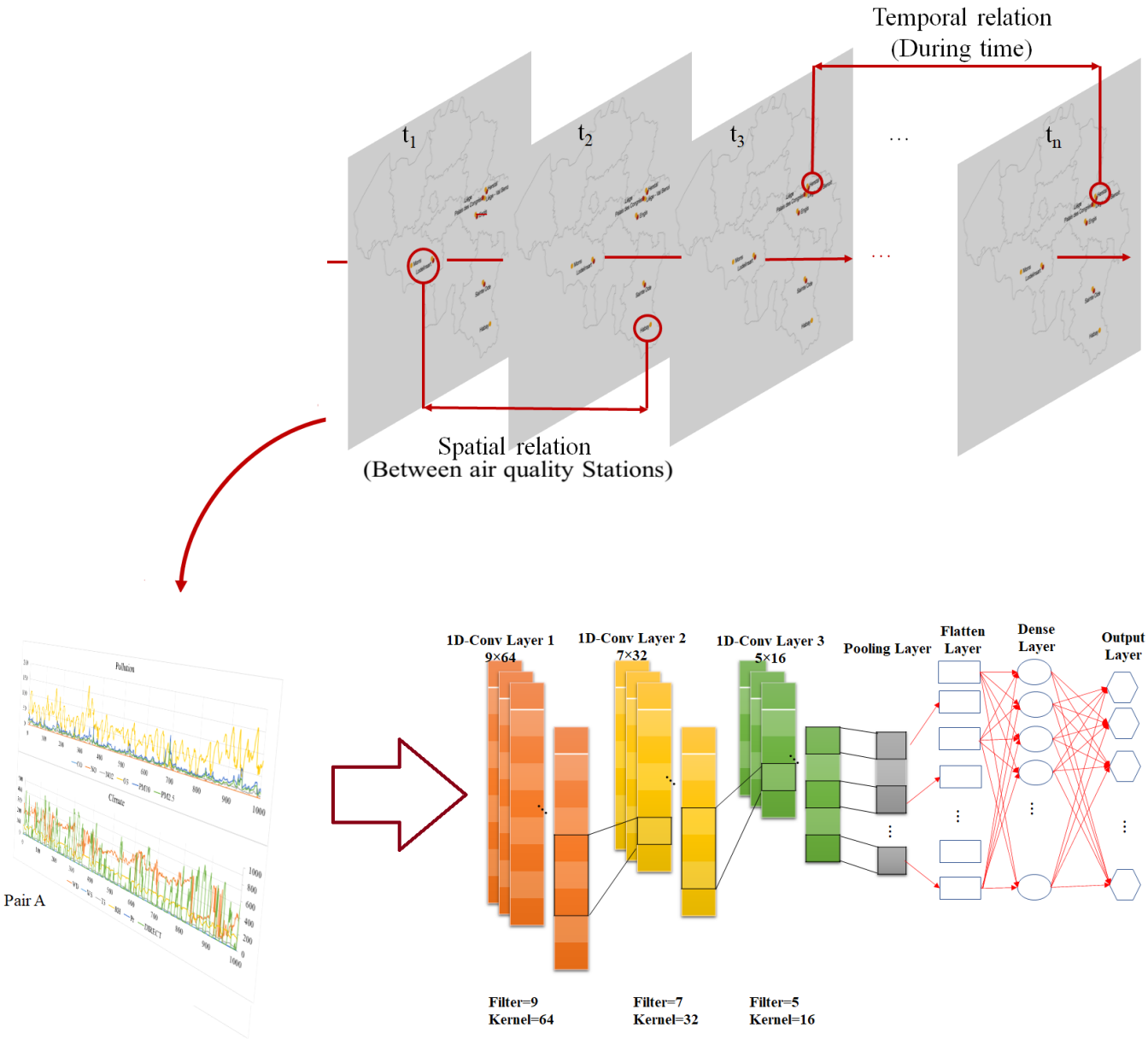


Fig 6.5. 1D-CNN design configuration for the current study with 3 Coevolution, 1 Flatten, and 1 Dense layer.

Bi-Directional Long Short-Term Memory Recurrent Network (Bi-LSTM) Design

A general LSTM segment consists of a cell with 3 gates (see Figure 6.6); input, output, and forget. The cell recalls values upon optional time intermissions, and the 3 gates control the input and output flow of data. Because of this specific memory cell architecture, the LSTM arrangement can consider long-term associations of time series data, and prevail over the disadvantages of typical recurrent networks (particularly the issue of gradient loss and burst). A chain of repeating cells forms the LSTM layer. Also, the *tanh* can be set for the activation function. With the aid of

2 independent hidden layers, a Bi-LSTM network can operate through 2 directions with time series data, at the same time. These data are concatenated and fed forward to the output layer. Simply put, Bi-LSTM networks are repeatedly functional with time series data in 2 directions.

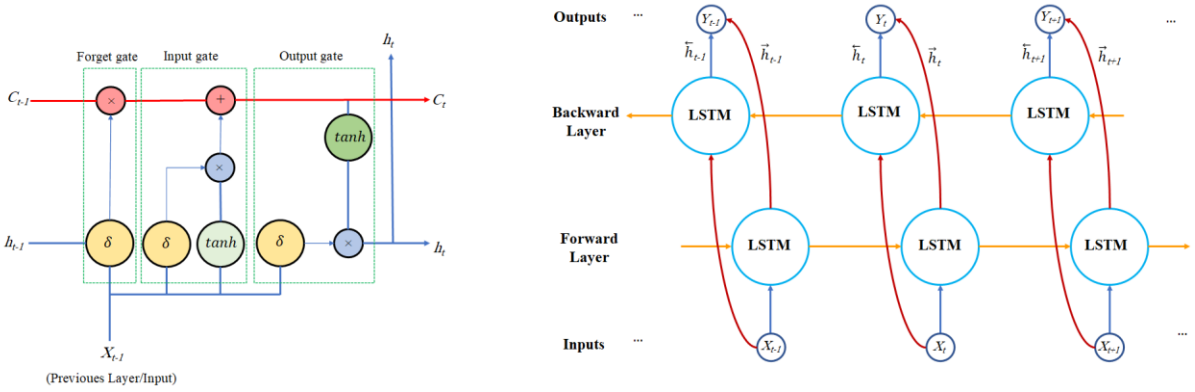


Fig 6.6. Bi-LSTM cell and network configuration.

6.2.2.2. Data Preparation and Deep-Learner Network Setup

The hourly recorded air pollution data of the past 15 years (2006-2021) for the CO, NO_2, NO, $PM_{2.5}$, PM_{10}, and O_3, from 5 air quality stations in Belgium were collected (ISSeP, 2021). VOCs were not considered during this study due to the lack of outdoor data. Accordingly, hourly weather data for the past 14 years (2008-2021) for the T, P, RH, wind speed (WS) and direction (WD), solar irradiance (IR), and precipitation (PR), were gathered (ISSeP, 2021). The geographical (spatial) locations of the air quality stations (yellow) and weather stations (red) are illustrated in Figure 6.7. Information on the weather and air quality stations and their corresponding datasets are presented in Table 6.1. The primary data were randomly divided into calibration (80%), validation (10%), and test (10%) datasets. Also, the data of a whole month in the summer 2020 was kept blind for presenting the deep-learner network performance.

Fig 6.7. Locations of air quality (yellow) and weather stations (red) in Belgium which their corresponding data were employed for DL network training.

Table 6.1. Pairs of weather and air quality monitoring stations and their corresponding datasets information.

Air Pollution stations	**Pairs for weather and air quality stations**	**Weather stations** T, P, RH, WS, WD, IR, PR
Sainte-Ode (NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) [07/04/2011– 18/02/2022] ***Habay (Arlon)*** (CO)* [07/02/2008 – 18/02/2022]	Pair A	***Sainte-Ode (Arlon)*** [07/02/2008 – 18/02/2022]
Herstal (NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) [03/01/2013 – 01/01/2020] ***Liege-Val Benoit*** (CO)* [10/05/2011 – 01/01/2020]	Pair B	***Herstal*** [03/01/2013 – 01/01/2020]
Liège -Val Benoit (CO, NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) [10/05/2011 – 01/01/2020]	Pair C	***Palais des congrès de Liège*** [10/05/2011 - 01/01/2020]
Engis (NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) [11/02/2008 – 01/01/2020] ***Liege-Val Benoit*** (CO)* [10/05/2011 – 01/01/2020]	Pair D	***Engis*** [11/02/2008 – 01/01/2020]
Lodelinsart (NO, NO_2, O_3, $PM_{2.5}$, PM_{10}) [06/02/2008 - 01/01/2020]	Pair E	***Lodelinsart*** [06/02/2008 - 01/01/2020]

**The "Sainte-Ode", "Herstal", and "Engisstations" air quality stations don't record CO data. Hence, complementary CO records are employed from the nearest available stations, correspondingly.*

- The common historical time ranges per contaminant, per pairs, were applied for the initial learning steps. For the final overall learning run among all contaminants and stations, the tiem range of [03/01/2013 – 01/01/2020] is used.

Also, to expedite the convergence of the DL network, and decrease the effect of outliers, a features' normalization step is performed for the raw data, to the range of [0,1] (by max-min function). As part of the Deep-Learner Network design, to prevent the over-fitting issue, several methods were employed; including a dropout policy with a probability of 0.3, which is utilized broadly among layers. Selecting an appropriate dropout rate is critical for the model's learning balance, some common dropout rates range from 0.2 to 0.5; however, the optimal rate varies depending on the specific architecture and problem domain (Lim 2020). Moreover, the early stopping approach is applied for high-performance learning, in which a training procedure can be interrupted when the validation loss is reduced no more. Correspondingly, mean square error (MSE) was employed as the algorithm loss function representative. The hyper-parameters were initially regulated by the model performance over the validation dataset, and next, the Adam optimizer was applied. The designed CNN-BiLSTM employs singular hidden layers as default, consisting of 64 neurons. For spatial and temporal trend feature learning, 3 convolution layers, and Bi-LSTM structure with 128 hidden neurons, were applied respectively. The activation operator of the output layer is linear and is correspondingly employed for the final prediction. Missing features of experimental data are completed by the linear interpolation for single missing data points and the average value of the column in which they are placed for the remaining missing data points. Convolutional networks are capable of both recursive or direct forecast tactics; where the network proceeds one-step estimation and outputs are being fed as inputs for following estimations, and where one model is established for each time-step to be estimated. Consecutively, Convolutional networks can be employed to estimate the whole output sequence, as a one-step estimation of the whole vector. This is a universal advantage of feed-forward ANN. Computational tasks were conducted on a PC server, with the AMD Ryzen 5 3500U with Radeon Vega Mobile Gfx 2.10 GHz processor, and 16GB of memory.

6.2.3. Future Indoor Climate

For obtaining the future indoor climate; mainly the T and RH, we applied the Input-Output (I/O) ratios recorded in the case study summer measurement campaign of 2021. To put it simply, it is calculated as the ratio between indoor and outdoor values. These ratios are applied to the future outdoor T and RH of the selected Typical Meteorological Years (TMYs) to obtain the corresponding indoor values.

6.2.4. Future Building Characteristics & Occupants Behavior

Owed to the focus of our study on ambient conditions in the context of climate change, the building characteristics and occupants' behavior patterns were assumed to be fixed. However, it is noteworthy to mention that, there is a simple possibility to modify (reduce based on defined scenarios) the air tightness and leakage information of the building in CONTAM.

6.3. Result & Discussions (*Future AP*)

Several statistical indexes, such as MAE, RMSE, and *r* were applied to evaluate the performance of the proposed model (Wei et al. 2019). Table 6.2. represents the test error analysis of CNN-BiLSTM model for the single-step prediction at each paired weather and air quality stations (A-E in Table 6.1.).

Concerning the single-step prediction efficiency of the designed CNN-BiLSTM model, the prediction of contaminants over one blind month with untrained inputs was carried out. Figure 6.8. illustrates the hourly prediction performance of CNN-BiLSTM for 31 consecutive blind days of summer 2020 (no missing data completion) in the target city of Arlon for 5 contaminants (NO, NO_2, O_3, $PM_{2.5}$, PM_{10}, CO(*Habay station*)). The Figure 6.8. demonstrates the recognized agreement level of measured and predicted values, graphically. Excluding sharp fluctuations and incidental peaks, the agreement level is satisfactorily acceptable.

Table 6.2. The Error analysis of CNN-BiLSTM model for the single-step prediction among paired weather and air quality stations (A-E). Test dataset (untrained).

CNN-BiLSTM	CO			NO			NO2			O_3			$PM_{2.5}$			PM_{10}		
	RMSE	*MAE*	*r*	*RMSE*	*MAE*	*r*	*RMSE*	*MAE*	*r*	*RMSE*	*MAE*	*r*	*RMSE*	*MAE*	*r*	*RMSE*	*MAE*	*r*
Pair A	0.86	0.05	0.57	17.43	0.42	0.64	80.82	1.94	0.67	443.7	12.9	0.87	148.4	4.65	0.63	251.7	5.94	0.61
Pair B	0.79	0.01	0.59	16.38	0.38	0.64	79.98	1.88	0.68	435.7	10.2	0.88	132.4	3.12	0.64	249.6	5.88	0.62
Pair C	0.93	0.06	0.54	19.3	0.56	0.63	82.9	2.18	0.64	466.4	14.9	0.81	152.6	3.19	0.6	263.7	6.17	0.61
Pair D	0.89	0.15	0.57	21.45	0.52	0.61	86.7	2.09	0.64	491.3	16.1	0.79	166.5	5.3	0.61	286.4	9.36	0.59
Pair E	0.96	0.17	0.55	23.1	0.62	0.6	92.06	2.18	0.62	501.6	15.7	0.76	184.4	7.04	0.59	311.5	12.1	0.57

Six future Typical Meteorological Years weather files were selected among our database (Doutreloup & Fettweis, 2021), to represent the temporal effects of climate change with 3 different SSP scenarios in Arlon. Additionally, for a better comparison with the past, the modeled average TMY of 2001-2020 period was taken into account, as well. The seven selected TMY weather files are as follows:

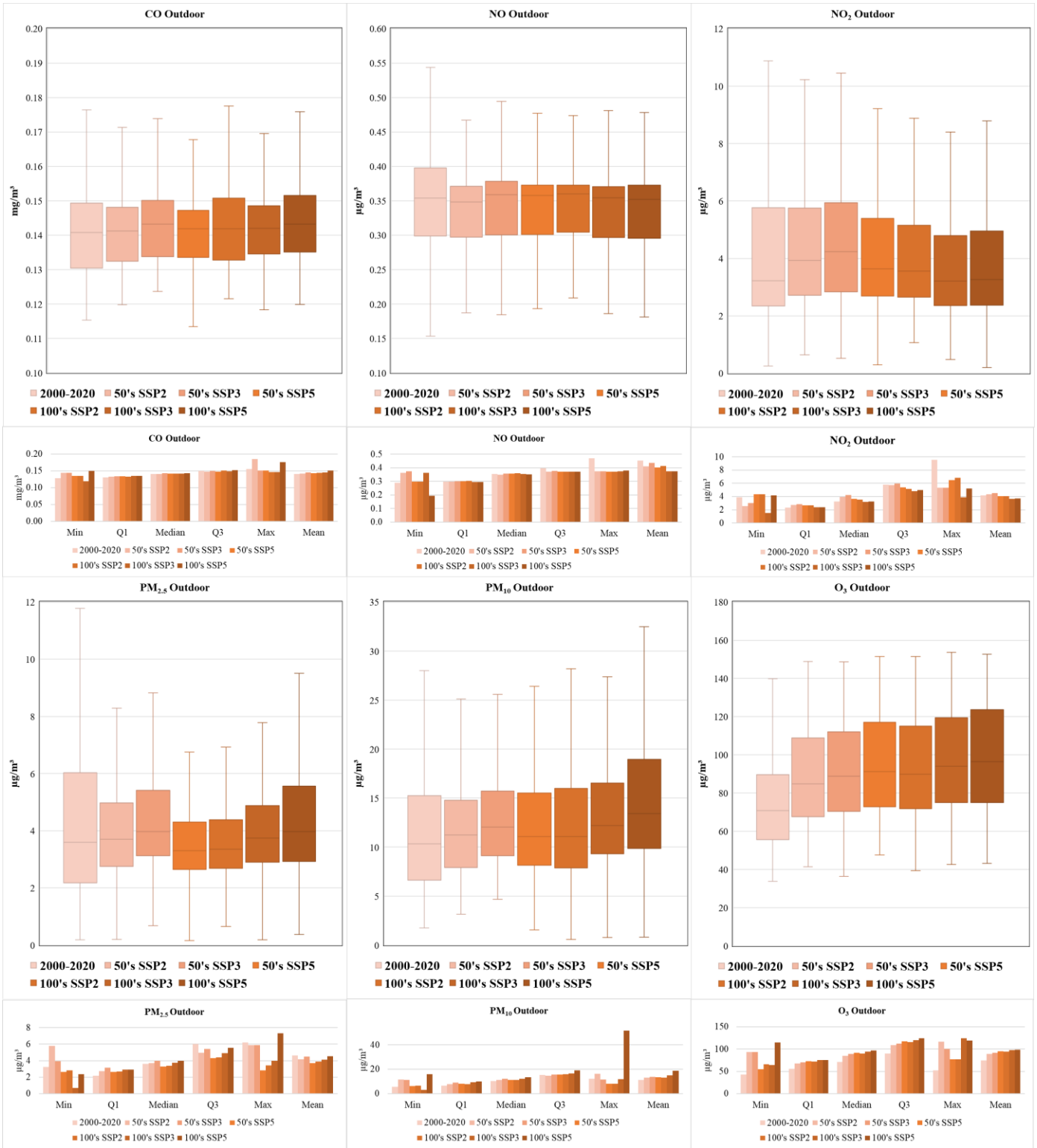
- Arlon TMY2001-2020_MAR
- Arlon TMY2041-2060_SSP2_MAR-BCC
- Arlon TMY2041-2060_SSP3_MAR-BCC
- Arlon TMY2041-2060_SSP5_MAR-BCC
- Arlon TMY2081-2100_SSP2_MAR-BCC
- Arlon TMY2081-2100_SSP3_MAR-BCC
- Arlon TMY2081-2100_SSP5_MAR-BCC

Figure 6.9, illustrates the box plots of the hourly predictions of outdoor air concentrations, derived from deep-learner model, for the city of Arlon, in “2000-2020”, “2050s”, and “2100s” : SSPs 2-4.5, 3-7.0, and 5-8.5.

Concerning outdoor air pollution, although, the emissions of key pollutants in Europe have almost decreased in the past decade, it is still an important concern. This is because of the complexities of the processes related to emissions and air quality, especially interactions with meteorology, in which spatial decrease of emissions, do not necessarily reduce atmospheric pollutant levels (Doherty et al. 2017, Defra 2022). The outdoor concentration of major of contaminants (with outdoor sources) is estimated to reduce in the future by the 2050s and 2100s, but PM_{10} and O_3. Two remarkable exceptions are O_3 and PM_{10}, which are expected to elevate in the future climate trends, thus leading to an increase in their levels which infiltrate and remain in buildings (Orru et al. 2013).

Because of well-controlled emissions of CO, it is considered a pollutant with persistent indoor sources. However, CO had presented the lowest correlation with outdoor weather among all pollutants within our indoor measurement campaigns which led to the lowest "future outdoor CO" prediction performance by the deep learner model among all stations (Table 6.2.). In other words, the outdoor CO levels, has the minimal varying pattern to learn for the DL (in comparison to other contaminants) since it had a robust constant average during past years. On the whole, average outdoor CO is predicted to remain constant (or so) by the 2050s and 2100s and the increase. For the PM_{10}, the average outdoor concentrations decrease slightly till 2050s, and then increase to some extent till 2100s. The prediction of future outdoor PM highly relies on the key assumptions (existing a black box-based relationship among outdoor PM concentration and weather conditions) in the prediction approach. There have been reported several different and contradictory results in terms of future outdoor PM concentration predictions over different regions (Deutsch et al. 2010, Ridder et al. 2020). The increase in PM_{10} outdoor concentration (relatively SSP5>3>2) can be explained by the greater impacts of higher temperatures on PM_{10} emission and water evaporation rates. According to the key findings of a study conducted in collaboration with the Belgian Interregional Environment Agency (IRCEL - CELINE) in 2010, among various elements; climate change is capable of moderately or fully undoing the valuable impacts of expected contaminant emission reductions due to higher temperatures (increased kinetic of atmospheric chemistry) and the incidence of droughts (lack of sufficient precipitation) (Deutsch et al. 2010, Jacob & Winner 2009, Sá et al. 2016).

Fig 6.8. Hourly prediction of CNN-BiLSTM for 31 test days of summer 2020 (untrained input), Arlon.



Fige 6.9. Outdoor pollutant concentrations of Arlon (AI) for TMYs: "2000-2020" and "2040-2060, 2080-2100: SSPs 2-4.5, 3-7.0, and 5-8.5", and corresponding statistics.

6.4. Conclusion

In this chapter providing the required future inputs of the designed IAQ model in CONTAM, was presented. The regional future outdoor climate data were obtained by the Belgian database for the future climate till 2100 (SSP2,3,5). Future ambient air pollution concentrations were obtained by a hybrid deep learner network. The structure of the network was "1D CNN-BiLSTM RNN" and the learning dataset contained up to past 15 years of hourly outdoor weather and air pollution data in 5 different location in Belgium. The occupants activity patterns and building characteristics kept constant, while future AER modeling is considered by CONTAM model. Each input may arise uncertainties to a certain degree which were not considered during this study.

Correlated publishment of this chapter:

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7. FUTURE IAQ STATE IN THE CONTEXT OF CHANGING CLIMATE & INTRODUCTION OF CLIMATE CHANGE-INDOOR AIR QUALITY INDEX (*CAPI*)

7. Future IAQ State In The Context Of Changing Climate & Introduction Of Climate Change-Indoor Air Quality Index (*CAPI*)

7.1. Quantitative Analysis Of Future IAQ Under Climate Change Scenarios, Till 2100

This section (7.1) has been drafted from reference Pourkiaei et al. 2024 (Systematic framework for quantitative assessment of Indoor Air Quality under future climate scenarios; 2100s projection of a Belgian case study). This chapter is an continued effort (to chapter 5) to answer the fourth research question (*RQ4*).

After obtaining all the IAQ model inputs with their future values, the simulations to predict the future IAQ state of the case study house in CONTAM (basis year 2021) were carried out. Figure 7.1., shows the CONTAM hourly indoor pollutant concentration estimates for CO, NO_2, NO, $PM_{2.5}$, PM_{10}, and O_3, in "2000-2020", "2050s", and "2100s": SSPs 2-4.5, 3-7.0, and 5-8.5. The estimated indoor pollutant concentrations by CONTAM, are derived from an internal integrated process of mass balance equations in which, different contributions of indoor and outdoor origins are taken into account.

Considering long-term IAQ measurement campaigns with the help of low-cost sensors and establishing IAQ databases are crucial for better insight and future studies. The proposed hybrid deep-learner algorithm is capable of drawing out and learning the high-dimensional spatial and temporal features of air quality data time series in different regions. Our model performance is satisfactory since it can adopt regional pattern features by 1D-CNN, and long-term reliance features by Bi-LSTM.

The predicted reduction in outdoor pollution concentration combined with the natural ventilation system will, on average, contribute to the reduction of indoor pollutant concentrations, which are infiltrated from outdoors. Outdoor O_3 and PM_{10}, which are expected to elevate in the future climate trends (see Figure 6.9), thus leading to an increase in their levels which infiltrate and remain in buildings.

Since the average outdoor CO is predicted to remain constant the increase in the indoor levels is only due to the contribution of indoor sources of the Arlon case-study basis model. For contaminants with primarily periodic indoor sources such as $PM_{2.5}$, $PM_{10,}$ and NO, the main contributions are from indoor sources. $PM_{2.5}$ and NO mean indoor levels are marginally decreased in future climate trends. This reduction is due the natural ventilation and a slight decrease in average outdoor $PM_{2.5}$ and NO levels.

For the PM_{10}, the average indoor concentrations decrease slightly till 2050s, and then increase to some extent till 2100s;following the same pattern of outdoor average PM_{10} levels.

It is also approximated that mean indoor contaminant exposures are:

- Constant for CO (with substantial indoor sources, as indoor and outdoor emissions are not varied).
- Decreased for $PM_{2.5}$ and NO (those with periodic indoor sources that are naturally ventilated with decreased outdoor concentrations).
- Increased for NO_2 (slightly), PM_{10}, and O_3 (those with dominant outdoor sources which are naturally ventilated with increased outdoor concentrations).

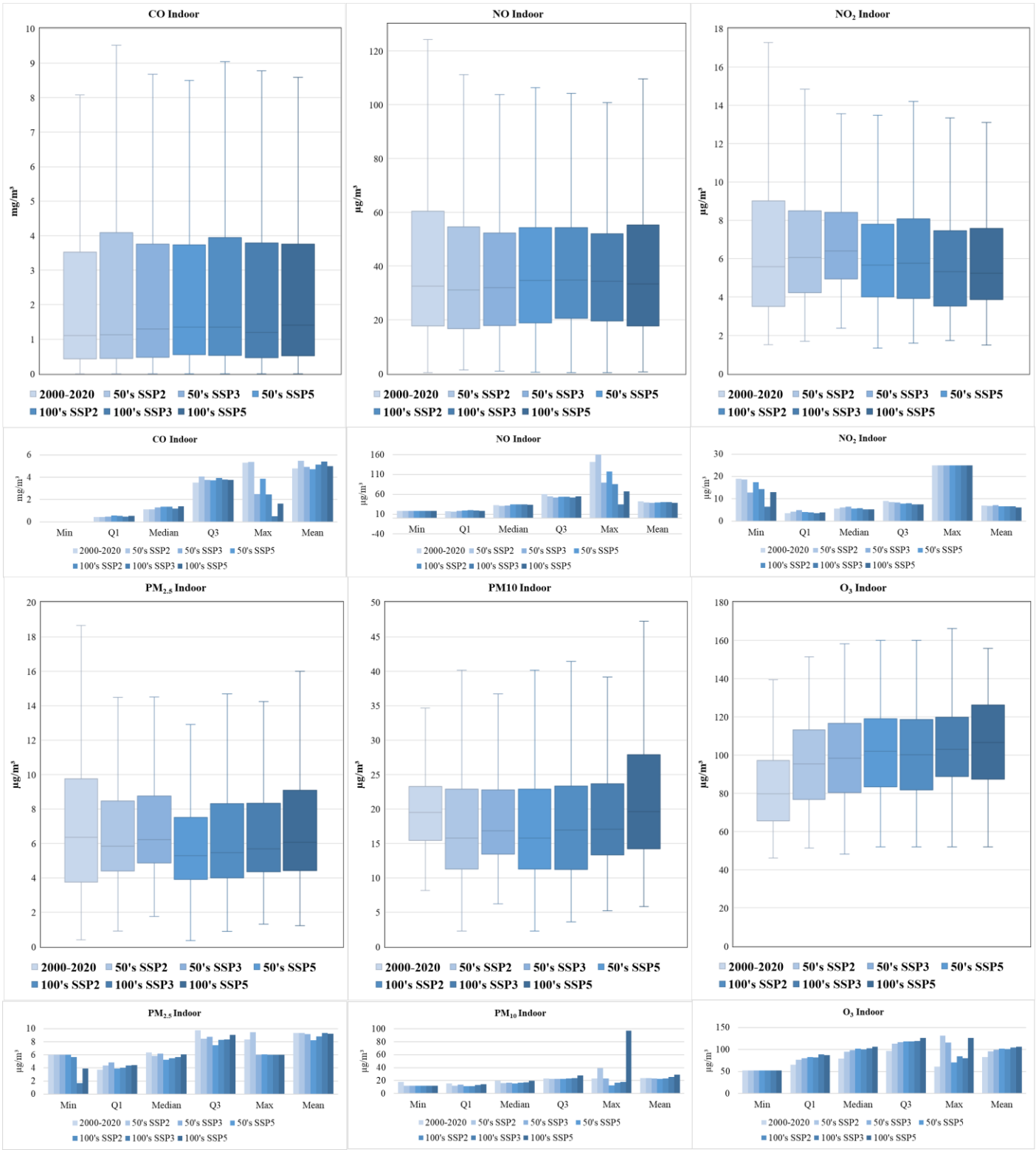

Fig 7.1. Indoor pollutant concentrations of Arlon test-house (CONTAM), for TMYs: "2000-2020" and "2040-2060, 2080-2100: SSPs 2-4.5, 3-7.0, and 5-8.5", and corresponding statistics.

7.2. Climate Change-IAQ Index(IAQ-CC Index: *CAPI*)

To provide a decision support tool, and objectivize and quantify the importance of climate change effects on IAQ, a novel IAQ-CC index is presented as follows: $\boldsymbol{CAPI} = \frac{\text{DCPI}}{\text{DCE}}$

$$\textbf{“}\textbf{\textit{C}}\textbf{limate Change }\textbf{\textit{A}}\textbf{ffected }\textbf{\textit{P}}\textbf{oor }\textbf{\textit{I}}\textbf{AQ” Ratio} = \left(\frac{\text{Days of } \textit{CC Correlated} \text{ Poor IAQ}}{\text{Days of CC Events}}\right) \qquad [0,1]$$

Based on the classification of IAQ indices, *CAPI* is considered a “Class-M1” type index (Pourkiaei & Romain 2023). This index describes the portion of days with climate change effects (e.g., heat waves and Ozon peak episodes), in which, poor IAQ occurs due to those specific events. In other words, the targets are indoor air ELV exceedances that are triggered by outdoor air ELV exceedances due to climatological events. This assumptions relies on the facts that climatological extreme events by impacting outdoor air quality can potentially affect IAQ. For this aim only those poor IAQ states which are solely correlated to the outdoor air quality conditions (outdoor air quality conditions are potentially impacted by extreme events, more likely for PM_{10} and O_3). Therefore, applying this index is sensible after a specific time period, such as a month or a season. Considering the structure of this index, it is applicable for each indoor zone, or to the entire building indoor environment as a whole. As the *CAPI* index is closer to the lower limit (0), the smaller portion of heat-wave and Ozone peak events are followed by correlated poor IAQ. On the other hand, the *CAPI* closer to the upper limit (1), indicates the higher portion of heat-wave and Ozone peak events are followed by correlated poor IAQ.

The definition of a poor IAQ is a challenge by itself since there is no comprehensive integrated reference available for all indoor pollutants (Pourkiaei & Romain 2023). In this regard, Table 7.1. presents the guidelines which are employed in this study for IAQ assessment, based on “ISO 16000-6:2011 Indoor Air”, and the newly updated “WHO global air quality guidelines 2021” (ISO16000-6 2011, WHO 2021). Accordingly, the identification of the poor IAQ state, with

respect to each pollutant, should follow the corresponding defined time scale as presented in the Table 7.1.

Table 7.1. Recommended 2021 AQG levels of pollutants and 2005 air quality guidelines (daily).

Pollutants	Averaging time	2005 air quality guideline	2021 AQG level
$PM_{2.5}$, µg/m³	24-hour	25	**15**
PM_{10}, µg/m³	24-hour	50	**45**
O_3, µg/m³	8-hour	100	**100**
NO_2, µg/m³	24-hour	-	**25**
CO, mg/m³	24-hour	-	**4**
TVOC, mg/m³			**ISO 16000-6:2011 ; 10-25**

7.2.1. Heat-Waves & Ozon-Peaks

The IRM characterizes a heat wave as a duration of at least 5 consecutive days that the maximum temperature is at least 25°C (summer days), in which at least 3 days exceeds the maximum temperature of 30°C (tropical days) (Doutreloup et al. 2022, Dodona 2022). On the other hand, the Ozon peak events (alarm phase) are defined based on the daily Ozone measurements and ozone forecasts, as follows: "On the previous day, in at least one weather station, an hourly mean O_3 concentration reaches higher than 240 µg/m³ (EU limit value) AND for the present day, for at least one weather station, an hourly mean O_3 value predicted higher than 180 µg/m³ (EU information threshold)". The IRCEL - CELINE has reported that the alarm phase criteria of O_3 have never taken place, afterward the very beginning of their recordings, in 2005 (Irceline 2022).

7.2.2. *CAPI* Results

To calculate the *CAPI* index, firstly, the number of days with climate change events should be determined. As mentioned earlier, the alarm phase criteria of O_3 have never taken place in Belgium, since the beginning of the recordings (2005) to date. Hence, ozone criteria are not practical since its peak episodes are rare conditions, even for the highest predicted future outdoor O_3 level (174 µg/m³ for 2100s, SSP-3). Therefore, future summer heat waves of each weather scenario were extracted based on the definition of IRM in the range of 20 June - 31 August (73 days), and are presented in Table 7.2. and Figure 7.2. In the next step, the number of days with poor IAQ in the heat wave periods, are extracted based on ELVs of Table 7.2., and are presented

in Table 7.3. The exceedance of limits due to other sources than the outdoor environment (e.g., given occupants' behaviors) is not considered (eliminated based on the target of CAPI).

Table 7.2. Different summer HW events date and duration extracted from corresponding weather scenario.

Weather Scenario	HW Events Dates	Days Number
Arlon TMY 2000-2020 – MAR	-	**0**
Arlon 2021 Real Data	[11-15 Aug]	5
Arlon 2022 Real Data	[16-25 Jul, 7-19 Aug]	**23** = (10+13)
Arlon TMY 2041-2060_SSP-2	-	**0**
Arlon TMY 2041-2060_SSP-3	[21-30 Jul]	**10**
Arlon TMY 2041-2060_SSP-5	[17-23 Jul, 2-7 Aug]	**13** (=7+6)
Arlon TMY2081-2100_SSP-2	[17-23 Jul, 13-17 Aug]	**12** (=5+7)
Arlon TMY2081-2100_SSP-3	[29 Jul - 8 Aug]	**11**
Arlon TMY2081-2100_SSP-5	[20-25 Jun, 13-23 Jul, 14-21 Aug]	**25** (=6+11+8)

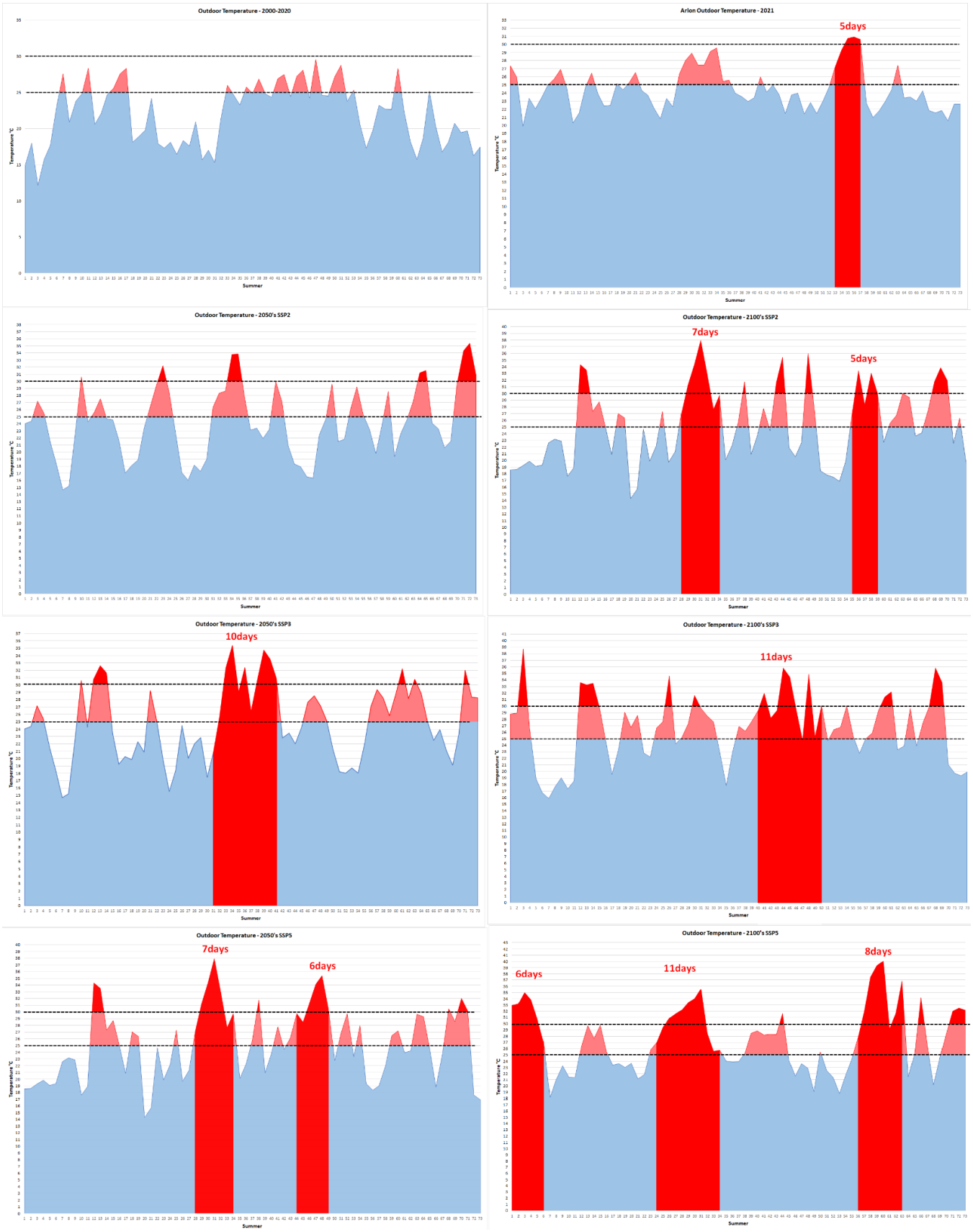

Fig 7.2. Heat-wave events over different weather scenarios in the context of changing climate.

Table 7.3. Different climate change correlated poor-IAQ days of summers, extracted from future IAQ.

Weather Scenario	CC-correlated poor-IAQ Dates	Days Number
Arlon TMY 2000-2020 – MAR	No heat events	**-**
Arlon 2021 Real Data	0	**0**
Arlon 2022 Real Data	3	**3**
Arlon TMY 2041-2060_SSP-2	No Heat events	**-**
Arlon TMY 2041-2060_SSP-3	[22-30 Jul]	**9**
Arlon TMY 2041-2060_SSP-5	[17-22 Jul, 2-7 Aug]	**12** (=6+6)
Arlon TMY2081-2100_SSP-2	[17-20 Jul, 14-17 Aug]	**8** (=4+4)
Arlon TMY2081-2100_SSP-3	[29 Jul - 6 Aug]	**9**
Arlon TMY2081-2100_SSP-5	[20-25 Jun, 13-22 Jul, 14-21 Aug]	**24** (=6+10+8)

Finally, the *CAPI* index is calculated as the ratio of climate change-correlated poor-IAQ days, over the CC-events days (in here heat waves duration), and is presented in Table 7.4. and Figure 7.3.

Table 7.4. *CAPI* final step calculation.

Weather Scenario	*CAPI* Ratio	*CAPI*
Arlon TMY 2000-2020 – MAR	No CC Events	-
Arlon 2021 Real Data	$^{0}/_{5}$	**0**
Arlon 2022 Real Data	$^{3}/_{22}$	**0.13**
Arlon TMY 2041-2060_SSP-2	No CC Events	-
Arlon TMY 2041-2060_SSP-3	$^{9}/_{10}$	**0.9**
Arlon TMY 2041-2060_SSP-5	$^{12}/_{13}$	**0.92**
Arlon TMY2081-2100_SSP-2	$^{8}/_{12}$	**0.67**
Arlon TMY2081-2100_SSP-3	$^{9}/_{11}$	**0.81**
Arlon TMY2081-2100_SSP-5	$^{24}/_{25}$	**0.96**

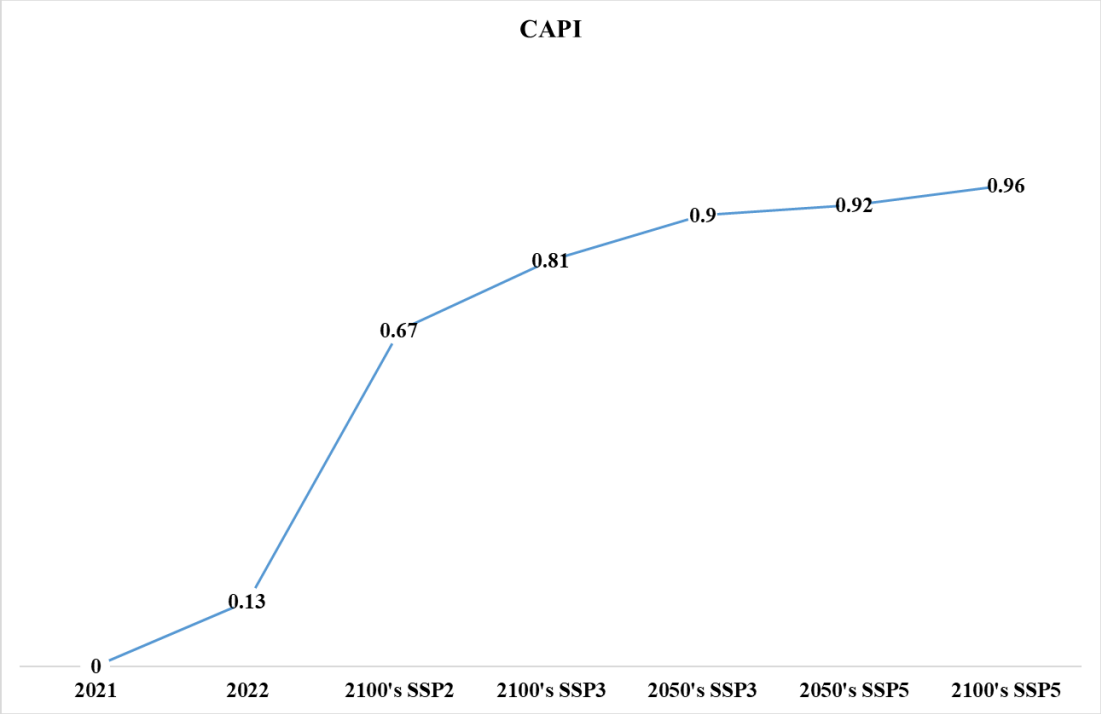

Fig 7.3. The evolution of *CAPI* index over different future weather scenarios in the context of climate change.

Regarding the *CAPI* index results, primarily, we try to take a deeper look into its components. The number of heat wave events, duration, and intensity were increased by the temporal evolution of climate predictions of the MAR model (2021 actual measurements < 2050's < 2100's). This trend is also followed in the SSP scenarios of each future weather forecast period (SSP2 < SSP3 < SSP5). Also, 100% of investigated heat waves are concurrent with outdoor Ozon pick episodes. Concerning the future "*CC correlated"* poor IAQ days, the estimated IAQ results by CONTAM were compared to the guideline values presented in Table 1. Accordingly, linked exceedances to the ambient pollutant concentrations were extracted (Table 3). Figure 7.4. depicts the *CAPI* projections via SSP2, 3, and 5 between 2021, 2050s, and 2100s.

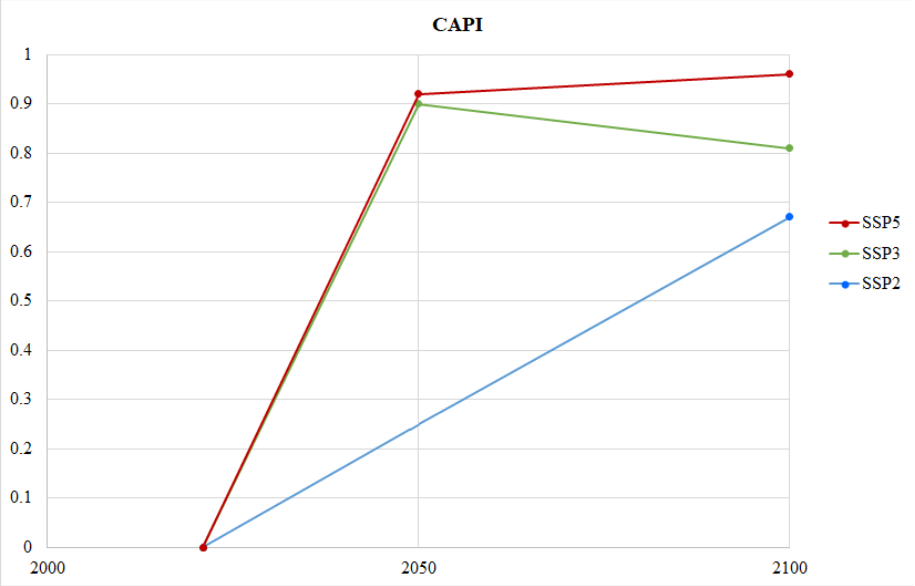

Fig 7.4. *CAPI* projections via SSP2, 3, and 5 between 2021, 2050s, and 2100s.

7.3. Implications For IAQ "Climate Adaptation And Mitigation Actions"

This section (5.3) is mainly inspired and drafted from the Handbook of Indoor Air Quality-Springer (Zhang et al. 2023, chapter 72). "IAQ is likely to be impacted both by climate change itself (direct) and the corresponding adaptation and mitigation strategies (indirect). Both adaptation and mitigation efforts are likely to lead to tighter buildings with less natural ventilation. Therefore, alongside energy efficiency and thermal comfort measures, it is crucial to identify and reduce indoor pollution sources, incorporating air cleaning or local ventilation where necessary.

Rising temperatures will significantly affect indoor thermal comfort, altering the patterns of window use and air conditioning to maintain internal comfort. These changes are likely to impact indoor concentrations of pollutants from both indoor and outdoor sources.

Air conditioning effectively reduces indoor heat exposure and protects health during heatwaves. However, prolonged AC use can prevent physiological adaptation to moderate heat increases, increasing risk if individuals must leave the AC environment or during power outages. Extensive AC use also strains the power grid, potentially causing blackouts and contributing to the UHI.

Mitigation efforts, including commitments to a net-zero carbon economy, suggest a shift towards an all-electric energy system based on renewable sources. This shift implies lower ambient air pollution (particularly NO_2 and PM), no indoor gas cooking emissions, and tighter building envelopes for energy efficiency. However, reduced ventilation can increase the impact of indoor pollution sources. Tighter buildings may require engineered retrofits to ensure effective ventilation. As global temperatures rise, space heating energy needs will diminish, potentially increasing the use of renewable wood-based fuels, which could impact IAQ if not properly ventilated. There may also be population migrations to cooler regions, establishing new communities closer to the poles.

Natural ventilation, modifiable via window opening by occupants, is another option. Encouraging natural ventilation at night could help since pollution concentrations tend to be lower, though less so in a warming climate.

Adaptive, intelligent control ventilation systems that monitor various indoor and outdoor conditions and adjust fresh air infiltration could maximize comfort and IAQ while being energy efficient. These systems could minimize infiltration during extreme air pollution episodes, preserving IAQ. Demand-controlled mechanical exhaust ventilation can reduce indoor CO_2 concentrations and save energy during the heating season.

Effective source control or elimination will be critical in tighter, energy-efficient homes to maintain IAQ. Air cleaners can be effective but require frequent maintenance and appropriate scaling to the space volume and AER." (Zhang et al. 2023, chapter 72)

7.4. Conclusions

Considering long-term IAQ measurement campaigns with LCS, establishing IAQ databases are crucial for better insight and future studies. The proposed hybrid deep-learner algorithm is capable of drawing out and learning the high-dimensional spatial and temporal features of air quality data time series in different regions. Our model performance is satisfactory since it can

adopt regional pattern features by 1D-CNN, and long-term temporal reliance features by Bi-LSTM.

It is also approximated that mean indoor contaminant exposures are:

- Constant for CO

  (with substantial indoor sources, as indoor and outdoor emissions are not varied).

- Decreased for $PM_{2.5}$ and NO

  (those with periodic indoor sources that are naturally ventilated with decreased outdoor concentrations).

- Increased for NO_2 (slightly), PM_{10}, and O_3

  (those with dominant outdoor sources which are naturally ventilated with increased outdoor concentrations).

The mean indoor level of contaminants, those with dominant indoor origins not only for CO, but also for VOCs (which was not considered in this study due to the lack of outdoor data) show the significance of ranking extensive endeavors to decrease and control indoor emission sources, advancement of ventilation systems, and applying high-performance air cleaners (purifiers) to increase the IAQ levels in residential buildings. It should be mentioned that CONTAM (and no other IAQ model to the best knowledge of authors) doesn't reflect the temperature variations in terms of emission rates, as its implemented contaminant source/sink elements are independent by temperature (constant coefficient model, pressure driven model, cutoff concentration model, and dispersion rate sink model) (Dols & Polidoro 2020). No physical chemistry-based emission model considering the temperature parameter has been developed to date, even for VOCs, but semi-empirical models based on correlation/regression case studies (De Jonge et al. 2018, De Jonge & Laverge 2019)

A set of final rather than random results is obtained, based on the mean hypothesis for model input elements which do not explain the essential uncertainties in the estimations. It was assumed

that some parameters to be fixed in the future, even though they seem to be different and changed to a certain level. In other words, the effects of forecasted variations of meteorological and outdoor air quality levels are kept aside, by making the correlated parameters in the model scenarios fixed. For instance, whole-house-average emission rates would be different in the future, but they rather change by some means unpredictable and consequently arduous to integrate in the future building IAQ models. The assumption of the well-mixed zone for pollutant concentration prediction was taken, though the experiments for developing/tuning the model were punctual (rather than well-mixed sampling). The taken assumptions allowed a quantitative evaluation of climate change effects on IAQ, for the mid-term and long-term future by a limited set of accessible infrastructures and resources.

References

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- De Jonge, K., Janssens, A., & Laverge, J. (2018). VOC exposure in Belgian dwellings: evaluation with a temperature and humidity based emission model. In ISIAQ Indoor Air 2018 conference.
- Dodona, 2022, Heatwave, UGhent, https://dodona.be/en/activities/1765918609/
- Doutreloup, S., Fettweis, X., Rahif, R., Elnagar, E. A., Pourkiaei, M. S., Amaripadath, D., & Attia, S. (2022). Historical and Future Weather Data for Dynamic Building Simulations in Belgium using the MAR model, 1-19, https://doi.org/10.5194/essd-14-3039-2022
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- ISO, K. (2011). 16000-6: Indoor air--Part 6: Determination of volatile organic compounds in indoor and test chamber air by active sampling on Tenax TA sorbent, thermal desorption and gas chromatography using MS. FID (ISO/DIS 16000-6).
- Pourkiaei, M., & Romain, A. C. (2023). Scoping review of indoor air quality indexes: Characterization and applications. *Journal of Building Engineering*, 106703, https://doi.org/10.1016/j.jobe.2023.106703
- Pourkiaei, M., Rahif, R., Falzone, C., Elnagar, E., Doutreloup, S., Martin, J., ... & Romain, A. C. (2024). Systematic Framework for Quantitative Assessment of Indoor Air Quality Under Future Climate Scenarios; 2100s Projection of a Belgian Case Study. *Journal of Building Engineering*, 109611, https://doi.org/10.1016/j.jobe.2024.109611
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- Rogelj, J., Popp, A., Calvin, K. V., Luderer, G., Emmerling, J., Gernaat, D., ... & Tavoni, M. (2018). Scenarios towards limiting global mean temperature increase below 1.5 C. *Nature Climate Change*, *8*(4), 325-332, https://doi.org/10.1038/s41558-018-0091-3
- WHO, World Health Organization, & European Centre for Environment. (2021). WHO global air quality guidelines: particulate matter (PM2.5 and PM10), ozone, nitrogen dioxide, sulfur dioxide and carbon monoxide. World Health Organization.
- Zhang, Y., Hopke, P. K., & Mandin, C. (Eds.). (2022). Handbook of indoor air quality. Springer Nature, https://doi.org/10.1007/978-981-16-7680-2

8. GENERAL CONCLUSIONS , PERSPECTIVES AND LINK WITH RESEARCH QUESTIONS

8. General Conclusions , Perspectives & Link With Research Questions

8.1. General Conclusions

This research as part of a PhD study within the OCCuPANt project at ULiège, investigated the impacts of climate change on IAQ during the summer months in a naturally ventilated house located in the south of Belgium. The findings highlight the significant influence of outdoor climatic conditions on indoor pollutant levels with direct contributions to outdoor-indoor natural AERs, and outdoor air pollution levels (in the context of changing climate), while less focusing on the critical role of mechanical ventilation systems, future occupant's behavior scenarios, and building characteristics. Our data analysis revealed that elevated outdoor temperatures and increased frequency of heatwaves, both consequences of climate change, contribute to higher indoor concentrations of certain pollutants, such as O_3 and PM_{10}. The naturally ventilated nature of the house allows for greater impacts of outdoor pollutants, particularly during periods of high outdoor concentrations. This is exacerbated during heatwaves when windows and doors are often kept open to cool the indoor environment based on wrong habits. Moreover, the study demonstrated a clear diurnal pattern in pollutant levels, with peaks corresponding to outdoor activity and traffic patterns. Indoor activities, such as cooking, heating, and cleaning, also contributed to short-term spikes in pollutant concentrations, highlighting the interplay between indoor and outdoor sources. The correlation analysis between indoor and outdoor pollutant levels underscored the significant influence of outdoor air quality on indoor conditions, particularly for pollutants like NO_2 and O_3. Despite the natural ventilation, indoor pollutant levels were mostly lower than outdoor levels, indicating the building's unappropriated active natural ventilation performances. These findings emphasize the need for adaptive strategies to mitigate the impacts of climate change on IAQ. Recommendations include enhancing building designs to improve ventilation performance without compromising IAQ, implementing real-time IAQ monitoring systems, and promoting behavioral changes to minimize indoor pollutant sources.

Conclusively, climate change could poses a significant challenge to maintaining healthy IAQ, particularly in naturally ventilated buildings. Proactive measures and continuous monitoring are essential to protect occupant health and improve resilience against the evolving heat events and climatic conditions. Future research should focus on developing and testing these adaptive strategies in various building types and climatic regions to ensure broader applicability and effectiveness.

Although the black box deep-learner model for future outdoor air pollution doesn't take the "different future GHG emission scenarios" to consideration directly, it is employing the *future input data* (which are) highly-correlated with those scenarios. So, different GHG scenarios (based on SSP criteria: technology, population, policies, etc.) are taken into account in our future regional ambient air pollution prediction as depicted in the Figure 7.6.:

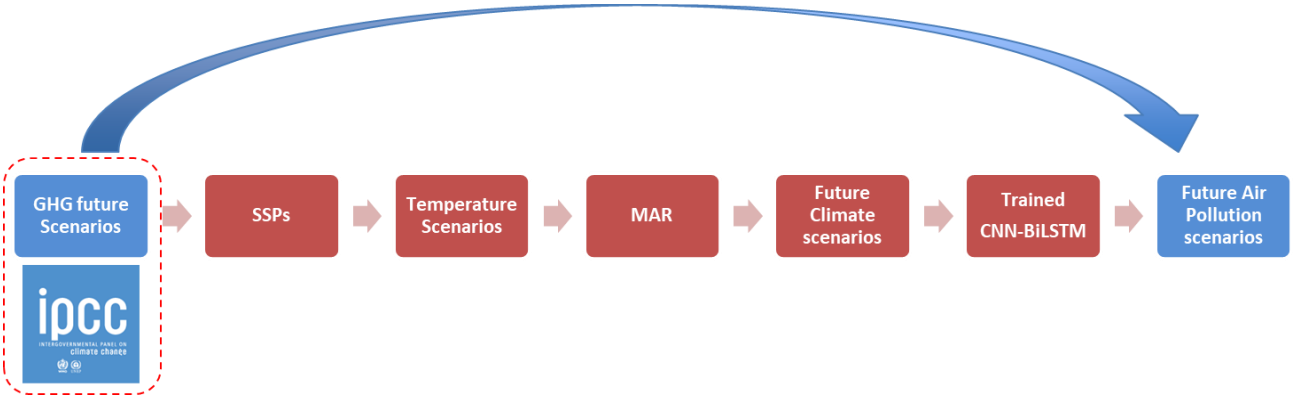

Fig 7.6. Th process of indirect consideration of GHG emission scenarios in future outdoor air pollution prediction. SSP5 scenario (Taking the Highway) = 100% direct consideration of GHG emission scenarios.

Finally, to provide a decision supporting tool and objectivize the assessment of climate change impacts on IAQ, a hybrid climate change-IAQ index (CAPI) was designed. CAPI integrates the state of IAQ, outdoor air pollution, and heat waves simultaneously. Both experiments and future temporal estimates of CAPI till 2100 showed an increased trend of declining IAQ levels in the context of increasing extreme heat events. CAPI's results for the chosen case study were derived by the exceedances of O_3 levels, though the other pollutants were also considered and applied.

8.2. Perspectives And Link With Research Questions

In this section, firstly thesis Research Questions (RQs) are represented and then the brief link to the thesis manuscript and summarized answers are provided.

8.2.1. RQ1

. ***RQ1.*** *How do current methods assess time-integrated IAQ information in residential buildings in temperate climates in the context of climate change?*

The second chapter was dedicated to answer to this question. Current methods for assessing time-integrated IAQ information in residential buildings in temperate climates, in the context of climate change, typically involve a combination of continuous monitoring and modeling techniques. These methods employ sensors to measure concentrations of key pollutants such as $PM_{2.5}$ and PM_{10}, VOCs, CO_2, and NO_2 over extended periods. Data from these sensors is then integrated with building simulation models, like CONTAM or EnergyPlus, which account for variables such as ventilation rates, building envelope characteristics, and occupant behavior. Additionally, these models incorporate climate projections and future air pollution to simulate future IAQ scenarios under varying weather and ambient air quality conditions driven by climate change. By combining real-time monitoring with predictive modeling, these methods provide a comprehensive assessment of IAQ over time, helping to identify trends, potential health risks, and the effectiveness of mitigation strategies in maintaining healthy indoor environments amidst changing climatic conditions.

8.2.1.1. Key References:

Seppänen, O. A., & Fisk, W. J. (2006). Some quantitative relations between indoor environmental quality and work performance or health. *HVAC&R Research*, 12(4), 957-973.

Discusses the impact of indoor environmental quality on health and productivity, which provides a foundation for understanding the importance of monitoring IAQ.

Wargocki, P., & Wyon, D. P. (2013). Providing better thermal and air quality conditions in school classrooms would be cost-effective. *Building and Environment*, 59, 581-589.

Highlights the significance of maintaining good IAQ for health and performance, underpinning the need for comprehensive IAQ assessment methods.

Batterman, S. (2017). Review and extension of CO2-based methods to determine ventilation rates with application to school classrooms. *International Journal of Environmental Research and Public Health*, 14(2), 145.

Reviews methods for assessing ventilation rates using CO2 measurements, relevant to evaluating IAQ in residential settings.

Kumar, P., Druckman, A., Gallagher, J., Gatersleben, B., Allison, S., & Eisenman, T. S. (2019). The nexus between air pollution, green infrastructure, and human health. *Environment International*, 133, 105181.

Discusses the interaction between air pollution, green infrastructure, and health, highlighting the broader context of IAQ assessment.

Fisk, W. J. (2015). Review of some effects of climate change on indoor environmental quality and health and associated no-regrets mitigation measures. *Building and Environment*, 86, 70-80.

Reviews the potential impacts of climate change on IAQ and proposes mitigation measures, providing context for current assessment methods.

Gupta, A., & Mittal, A. (2021). Indoor air quality monitoring systems and COVID-19 risk mitigation: A systematic review. *Environmental Research*, 198, 111205.

Systematic review of IAQ monitoring systems, relevant to understanding current methods used in residential buildings.

U.S. Environmental Protection Agency (EPA). (2018). Report on the Environment: Indoor Air Quality.

Provides comprehensive information on IAQ, including monitoring and assessment methods, particularly relevant in the context of climate change.

8.2.2. RQ2

. ***RQ2.*** *How to efficiently employ low-cost sensors for IAQ model development?*

The third and fourth chapters were dedicated to answer to this question. To efficiently employ LCS for IAQ model development, it is essential to strategically deploy these sensors to capture high-resolution spatial and temporal data on key pollutants. First, proper calibration of the sensors against reference-grade instruments to improve accuracy must be ensured. A network of these sensors should utilized and placed in various indoor locations to gather comprehensive data reflecting different sources and activities. Afterwards, gathered data must be integrated with advanced computational models, like CONTAM or EnergyPlus, to simulate IAQ dynamics under varying conditions. Advanced machine learning algorithms can further enhance model accuracy by identifying patterns and correlations in the collected data. Regular maintenance and validation of sensor performance are crucial to ensure data reliability. This approach not only reduces costs but also provides robust data to inform effective IAQ management strategies.

8.2.2.1. Key References:

Wang, S., & Song, G. (2020). Calibration of low-cost particulate matter sensors: Model development for a multi-pollutant monitoring instrument. *Sensors*, 20(18), 5177.

Gupta, A., & Mittal, A. (2021). Indoor air quality monitoring systems and COVID-19 risk mitigation: A systematic review. *Environmental Research*, 198, 111205.

Castell, N., Dauge, F. R., Schneider, P., Vogt, M., Lerner, U., Fishbain, B., ... & Bartonova, A. (2017). Can commercial low-cost sensor platforms contribute to air quality monitoring and exposure estimates? *Environment International*, 99, 293-302.

8.2.3. RQ3

. ***RQ3.*** *How to determine future regional values of IAQ influential parameters following pre-defined scenarios of climate change?*

The sixth chapter was dedicated to answer to this question. To determine future regional values of IAQ-influential parameters, such as future weather, air pollution, building characteristics, and occupant behavior under predefined climate change scenarios, a comprehensive approach is necessary. Firstly, climate models (e.g., CMIP6) must employed to project future weather patterns and temperature changes specific to the region. For future air pollution levels, outputs from chemical transport models (e.g., CMAQ) that consider both emission scenarios and atmospheric chemistry changes must be integrated. Future building characteristics can be projected using scenarios developed by building energy models (e.g., EnergyPlus) that incorporate advancements in energy efficiency, construction materials, and ventilation systems. Future occupant behavior can be estimated through sociological studies and surveys, combined with agent-based modeling to simulate changes in lifestyle, energy usage, and indoor activities. These projections can be integrated into IAQ models (e.g., CONTAM) to simulate IAQ under various climate scenarios, providing a detailed understanding of potential future conditions.

8.2.3.1. Key References:

IPCC. (2021). Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change.

Jacob, D. J., & Winner, D. A. (2009). Effect of climate change on air quality. *Atmospheric Environment*, 43(1), 51-63.

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8.2.4. RQ4

. *RQ4.* *How to quantify and evaluate the IAQ performance of buildings under the overheating impact of climate change, using a decision-supporting tool?*

The seventh chapter was dedicated to answer to this question. To quantify and evaluate the IAQ performance of buildings under the overheating impact of climate change, a hybrid climate change-IAQ index can be developed and utilized as a decision-support tool. This index integrates climate projections (e.g., temperature, humidity) from climate models with IAQ parameters (e.g., concentrations of target pollutants) measured through sensors or simulated via building energy and IAQ models such as EnergyPlus and CONTAM. The developed hybrid IAQ and climate change index (CAPI) employ these data points to assess the combined effect of external climatic conditions and internal pollutant sources on IAQ. By applying this type of index, stakeholders can compare different building designs, ventilation strategies, and retrofitting measures to determine their effectiveness in maintaining acceptable IAQ levels under future climate scenarios. This tool supports evidence-based decision-making to enhance building resilience against overheating and protect occupant health.

To find the most influential factor on IAQ in the context of climate change, a sensitivity analysis is essential. However, (pollutant-dependently), due to the stronger local emissions of indoor sources, these are likely more influential unless climate change alters the typical patterns of outdoor air concentrations during time (e.g., O_3 & PM).

On the other hand, the crucial aspect of occupants' behavior in the context of climate change will remain the ventilation performance rather than common indoor activities themselves. Because

indoor human activities are less likely to face impactful changes in terms of processes and temporal patterns (e.g., cooking, cleaning, etc.). This presents a significant challenge particularly without a systematic social analysis of natural/mechanical ventilation use in response to rising outdoor temperatures. The IPCC predicts future increases in outdoor temperatures ranging from 1.0 to 1.8°C under the SSP1-2.6 scenario, and from 3.3 to 5.7°C under the SSP5-8.5 scenario.

8.2.4.1. Key References:

Hamilton, I., Milner, J., Chalabi, Z., Das, P., Jones, B., Shrubsole, C., ... & Wilkinson, P. (2015). Health effects of home energy efficiency interventions in England: a modelling study. *BMJ Open*, 5(4), e007298.

Zusman, M., Schumacher, C. S., Gassett, A. J., Spalt, E. W., Austin, E., Larson, T. V., ... & Sheppard, L. (2020). Calibration of low-cost particulate matter sensors: Model development for a multi-pollutant monitoring instrument. *Environment international, 134, 105329.*

Castell, N., Dauge, F. R., Schneider, P., Vogt, M., Lerner, U., Fishbain, B., ... & Bartonova, A. (2017). Can commercial low-cost sensor platforms contribute to air quality monitoring and exposure estimates? *Environment International*, 99, 293-302.

APPENDIX

Publications Contributed To The Thesis

1. First Author – Conference Paper
   Pourkiaei, et al. 2022. Exploring the Indoor Air Quality in the Context of Changing Climate in Residential Buildings—Part A: Developed Measurement Devices of Low-Cost Sensors. https://www.aivc.org/sites/default/files/2_C48.pdf

2. First Author – Conference Paper
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3. Co-Author – Journal Paper
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