MOEEBIUS

Modelling Optimization of Energy Efficiency in Buildings for Urban Sustainability

D3.5 MOEEBIUS Indoor Air Quality Assessment Models

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Authors:

António Santos, Ricardo Rato, Cláudia Mafra – ISQ

Georgios Kontes - THN

Jana Trojanova – HON

Víctor Sanchez, Pablo de Agustín – TECNALIA

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Glossary

Acronym	Full name
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
BEPS	Building Energy Performance Simulation
BIM	Building Information Modelling
DCV	Demand Controlled Ventilation
DER	Distributed Energy Resources
EMS	Energy management system
EPA	U.S. Environmental Protection Agency
HVAC	Heating, Ventilation, and Air Conditioning
IAP	Indoor Air Pollution
IAQ	Indoor Air Quality
IEQ	Indoor Environment Quality
KPI	Key Performance Indicator
MF	Mixing Factor (γ_F)
MPC	Model Predictive Control
MOEEBIUS	Modelling Optimization of Energy Efficiency in Buildings for Urban Sustainability
PCB	Polychlorinated biphenyls
PPM	Parts Per Million
RH	Relative Humidity
TVOC	Total Volatile Organic Compound
VOC	Volatile Organic Compound

Definitions

The following definitions were obtained from ANSI/ASHRAE Standard 62.1-2010 Ventilation for Acceptable Indoor Air Quality:

Acceptable indoor air quality: air in which there are no known contaminants at harmful concentrations as determined by cognizant authorities and with which a substantial majority (80% or more) of the people exposed do not express dissatisfaction.

Air-cleaning system: a device or combination of devices applied to reduce the concentration of airborne contaminants, such as microorganisms, dusts, fumes, respirable particles, other particulate matter, gases, and/or vapours in the air.

Air conditioning: the process of treating air to meet the requirements of a conditioned space by controlling its temperature, humidity, cleanliness, and distribution.

Air, ambient: the air surrounding a building; the source of outdoor air brought into a building.

Air, exhaust: air removed from a space and discharged to outside the building by means of mechanical or natural ventilation systems.

Air, indoor: the air in an enclosed occupiable space.

Air, makeup: any combination of outdoor and transfer air intended to replace exhaust air and exfiltration.

Air, outdoor: ambient air that enters a building through a ventilation system, through intentional openings for natural ventilation, or by infiltration.

Air, recirculated: air removed from a space and reused as supply air. air, return: air removed from a space to be then recirculated or exhausted.

Air, supply: air delivered by mechanical or natural ventilation to a space, composed of any combination of outdoor air, recirculated air, or transfer air.

Air, transfer: air moved from one indoor space to another.

Air, ventilation: that portion of supply air that is outdoor air plus any recirculated air that has been treated for the purpose of maintaining acceptable indoor air quality

Concentration: the quantity of one constituent dispersed in a defined amount of another. conditioned space: that part of a building that is heated or cooled, or both, for the comfort of occupants.

Contaminant: an unwanted airborne constituent that may reduce acceptability of the air.

Demand-controlled ventilation (DCV): any means by which the breathing zone outdoor airflow (Vbz) can be varied to the occupied space or spaces based on the actual or estimated number of occupants and/or ventilation requirements of the occupied zone.

Exfiltration/air leakage: uncontrolled outward air leakage from conditioned spaces through unintentional openings in ceilings, floors, and walls to unconditioned spaces or the outdoors caused by pressure differences across these openings due to wind, inside-outside temperature differences (stack effect), and imbalances between supply and exhaust airflow rates.

Infiltration: uncontrolled inward air leakage to conditioned spaces through unintentional openings in ceilings, floors, and walls from unconditioned spaces or the outdoors caused by the same pressure differences that induce exfiltration.

Mechanical ventilation: ventilation provided by mechanically powered equipment, such as motor-driven fans and blowers, but not by devices such as wind-driven turbine ventilators and mechanically operated windows.

Natural ventilation: ventilation provided by thermal, wind, or diffusion effects through doors, windows, or other intentional openings in the building.

Occupiable space: an enclosed space intended for human activities, excluding those spaces that are intended primarily for other purposes, such as storage rooms and equipment rooms, and that are only occupied occasionally and for short periods of time.

Odour: a quality of gases, liquids, or particles that stimulates the olfactory organ.

Ventilation: the process of supplying air to or removing air from a space for the purpose of controlling air contaminant levels, humidity, or temperature within the space.

Volume, space: the total volume of an occupiable space enclosed by the building envelope, plus that of any spaces permanently open to the occupiable space, such as a ceiling attic used as a ceiling return plenum.

Ventilation zone: any indoor area that requires ventilation and consists of one or more occupiable spaces with similar occupancy category

1 Executive summary

This task focuses on the provision of enhanced Indoor Air Quality (IAQ) Models that are able to evaluate indoor hygienic and health/well-being conditions through identifying contamination of the air with various compounds, such as carbon dioxide (CO_2), carbon monoxide (CO), and volatile organic compounds (VOCs). This was accomplished through the development of an improved IAQ model to be integrated in the Energy Management System (EMS) program. Consequently, adequate Key Performance Indicators (KPIs) can be generated to assess the IAQ which is one of the main aspects for the user's comfort conditions.

This document details the IAQ model development and all the relevant parameters and inputs that the model should take into account to run properly. This model is adapted for direct integration in EnergyPlus (E+) through specific EMS programs developed using the E+ run time language functionality. At the building level the IAQ Model will play a key role for the *Local energy performance model*.

This document starts with a brief introduction and definition of the IAQ, a literature review and importance of the IAQ for human health, followed by the characterization of the main pollutant sources which are key factors to improve in the IAQ model developed. Then, the modelling methodology adopted is introduced and the IAQ model inputs are detailed and finally the numerical solution, which is adapted for direct integration in E+ language, is presented.

The main outcome of this document is a proposal of an improved mathematical model for the indoor air pollutant concentration prediction adapted for the calculation engine of the Building Energy Performance Simulation (BEPS) - E+.

2 Objectives of the report

The objective of this deliverable is to describe the development of an improved Indoor Air Quality Model that is able to evaluate indoor hygienic and health/well-being conditions through identifying contamination of the air with various compounds, such as carbon dioxide (CO2), carbon monoxide (CO) and volatile organic compounds (VOCs).

The mathematical model developed aims to predict accurately the indoor air pollutants concentration.

2.1 Scope of the document

This deliverable aims to, by extending explain the strategies adopted to develop the IAQ model and emphasise the improvements obtained. With the results obtained from the mathematical model developed it is possible to generate indoor air quality KPI's and simulate different ventilation rate to evaluate the HVAC system energy performance and IAQ levels.

Moreover, this task defines in detail the relevant parameters to predict all indoor air pollutants concentrations and provides an extensive explanation in order to adapt the model to the EMS program (in E+ language).

2.2 Relevance to other deliverables

The Indoor Air Quality Model (described in the present document), along with the Occupants Comfort Model (D3.4), the Distributed Energy Resources (DER) model (D3.3) and Enhanced Building Information Model (BIM) (D3.2) will be integrating the Local energy performance model (D3.6 - Local and Global Energy Performance Modelling).

The model generates an estimation/prediction of the IAQ KPIs evolution, selected in D2.3 - MOEEBIUS Energy Performance Assessment Methodology, which is compared in the MOEEBIUS framework with the actual evolution of these KPIs.

2.3 Deliverable Structure

The document is structured as follows:

- A brief introduction is presented in **Chapter 3**;
- What Air Quality is, the importance of IAQ for human health and the contaminants sources are described in **Chapter 4**;
- **Chapters 5** is related to the numerical modelling and the description of the mathematical indoor air quality model developed;
- Finally, main conclusions of the current work are presented in **Chapter 6;**

3 Introduction

In recent years, Model Predictive Control (MPC) strategy for building HVAC system is getting increasing attention. Development and integration of HVAC system MPC requires thorough understanding of the HVAC system working principles, interactions of the building envelope to the surrounding environment both internally and externally as well as thermal comfort and IEQ requirements.

In the IEQ field, the study of indoor air pollution (IAP) as a unique discipline requires knowledge in several areas, such as the fundamental principles of fluid mechanics, species transport, heat transfer, and systems engineering. Currently, the buildings systems complexity provide high levels of electronic control features embedded within the structures. Of particular concern are issues involving contaminants that routinely enter or lie dormant within building interiors, and their effects upon human health. Articles can be commonly found in newspapers throughout the world describing groups of people becoming sick while staying in a hotel, cruising on a ship, or traveling in planes or buses. Today, efforts to define and describe pollutant transport within buildings and interiors have become complex. Modelling pollutant transport within indoor environments now requires knowledge of computational tools and techniques that were utilized only in research laboratories a few years ago. Knowledge of fundamental principles of ventilation and building systems, including HVAC, must now be coupled with computational fluid dynamics techniques in order to accurately assess human health and predict contaminant exposure. We begin with a brief background in understanding exactly what is meant by IAP.

The study of IAP involves dealing with the emission, accumulation, and assessment of pollutants generally attributed to poor ventilation and air exchange. Of particular concern are issues involving air quality and human comfort within buildings. Toxic fumes and airborne diseases are known to produce undesirable odours, eye and nose irritations, sickness, and occasionally death. Other products such as tobacco smoke and carbon monoxide can also have serious health effects on people exposed to a poorly ventilated environment; studies indicate that indirect or passive smoking can also lead to lung cancer. Recommendations for outdoor airflow rates to dilute indoor polluted air vary considerably.

4 Importance of Indoor Air Quality

4.1 Air Quality

A precise definition of air quality is subjective and based on ASHRAE it can be defined as "air in which there are no known contaminants at harmful concentrations as determined by cognizant authorities and with which a substantial majority (80% or more) of the people exposed do not express dissatisfaction" (ANSI/ASHRAE Standard 62.1-2010). In a real environment, several pollutants co-exist. Various studies have shown associations between indoor air quality (IAQ) and human performance in addition to the potential health risk due to poor air quality (Wyon DP, 2004)

4.2 Overview and literature review

Most people are aware that outdoor air pollution can impact their health, b can have more significant and harmful health effects than expected. The U.S. Environmental Protection Agency (EPA) studies of human exposure to air pollutants indicate that indoor levels of pollutants may be two to five times — and occasionally more than 100 times — higher than outdoor levels. These levels of indoor air pollutants are of particular concern because most people spend about 90 percent of their time indoors. For the purposes of this guidance, the definition of good IAQ management includes:

- Control of airborne pollutants.
- Introduction and distribution of adequate outdoor air.
- Maintenance of acceptable temperature and relative humidity.

Research work (Fisk, 2002) estimated he potential gain of productivity from improved IAQ to be between 20 to 160 Billion Dollars in US considering only office workers. To achieve acceptable IAQ, combinations of the following actions are essential: contaminant source control, proper ventilation, humidity management and adequate filtration. Source control of contaminants can be achieved by either reducing the possible source of the contaminant in the building or by filtering the incoming air to the building. Regarding proper ventilation, various strategies have been implemented in the past several years. ASHRAE 62.1-2010 sets the minimum ventilation rate needed for buildings during occupied hours. In the ASHRAE 62.1 2004 version, determination of minimum outdoor ventilation rate is changed to be based on both occupancy level and floor area from its previous version that sets minimum outdoor ventilation rate based on either occupancy or floor area.

Most traditional ventilation systems provide fixed minimum outdoor ventilation rate based on design occupancy level and this could result in loss of energy or discomfort when the building operates in off-design conditions. A more advanced control strategy called Demand Controlled Ventilation (DCV) varies ventilation rate

based on occupancy. Most DCV systems use indoor CO_2 concentration level as a mean to control ventilation rate due to its direct association with presence of occupants. Even though CO_2 as a pollutant is not that hazardous except at very elevated concentration (≥5000 ppm), studies suggested that indoor concentration of 700 ppm above outdoor CO_2 concentration is believed to create unacceptable level of human body odor and is used as the permissible CO_2 limit according to ASHRAE 62.1.2010 Some of the commonly present indoor air contaminants with their acceptable indoor concentration are given in Table 1.

Temperature and humidity cannot be overlooked because thermal comfort concerns underlie many complaints about "poor air quality." Furthermore, temperature and humidity are among the many factors that affect indoor contaminant levels.

Outdoor sources should also be considered since outdoor air enters buildings through windows, doors and ventilation systems. Thus, transportation and grounds maintenance activities become factors that affect indoor pollutant levels as well as outdoor air quality on grounds.

Table 1 – Common air pollutants.

	Indoor Generation Rate	Permissible Indoor Concentration	Deposit Rate
CO_2	$\frac{0.0028 \times A_D \times M \times RQ}{0.23 \times RQ + 0.77}$	700 ppm	0
CO		10 mg/m^3	
Formaldehyde	61 µg/hr.m^2	0.027	0
Toluene	36 µg/hr.m^2	0.07 ppm	0
PM 2.5		35 µg/m^3	0.2

Where A_D is Dubies Body (DuBois D, DuBois EF, 2016) surface area (m^2), *M* is metric of metabolic rate, *RQ* is respiration quotient (0.83 for an adult engaged in a light activity).

A number of studies have attempted to understand the quantitative relationship between occupant overall satisfaction and the building's performance on individual indoor environment quality (IEQ) factors such as thermal comfort, acoustic quality, air quality and visual comfort, primarily to find out which has the most significant effect on occupant satisfaction. Based on a comprehensive literature review (Frontczak and Wargocki, 2011) report that thermal comfort is slightly more important than other IEQ factors. However, Figure 1 indicates that this finding was not universally consistent across all research papers on this question (Frontczak and Wargocki, 2011) and that IAQ assumes an important role for the occupant's satisfaction.

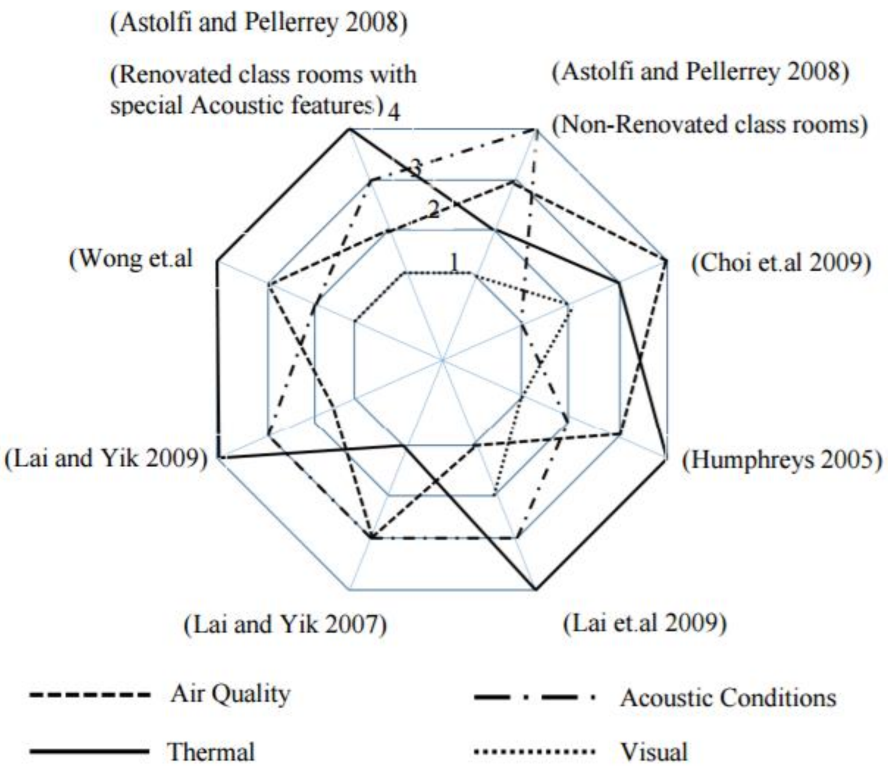

Figure 1 - Previous researchers' attempts at ranking (higher number indicates higher ranking) of importance of IEQ factors for overall satisfaction (Frontczak and Wargocki, 2011).

4.3 Risks to public health

In recent years, comparative risk studies performed by EPA and its Science Advisory Board have consistently ranked IAP among the top five environmental risks to public health. Good IAQ is an important component for a healthy indoor environment.

Failure to prevent or respond promptly to IAQ problems can increase long- and short-term health problems for building occupants such as:

- Cough;
- Eye irritation;
- Headache;
- Allergic reactions;
- In rarer cases, life-threatening conditions such as Legionnaire's disease, or carbon monoxide poisoning.

Indoor air problems can be subtle and do not always produce easily recognized impacts on health, well-being, or the physical plant. The following symptoms might be caused by a poor IAQ:

- Headache
- Fatigue
- Shortness of breath
- Sinus congestion
- Coughing
- Sneezing
- Dizziness
- Nausea
- Irritation of the eye, nose, throat and skin

These symptoms are not necessarily due to air quality deficiencies, but may also be caused by other factors—poor lighting, stress, noise and other factors. Due to varying sensitivities among building occupants, IAQ problems may affect a group of people or just one individual. In addition, IAQ problems may affect people in different ways.

4.4 Contaminants

Contaminants consist of gases, solids, or liquids (or combinations) and come in many types and forms. Some of the more common contaminants typically attributed to indoor air quality include smoke and odors attributed to perfumes, tobacco, and the cooking of food. The variety of contaminants are as plentiful as their source locations and origins. We begin with a brief description of the types of contaminants, followed by a discussion of the concentration equation and its various terms and units.

4.4.1 Types of contaminants

Contaminants in buildings generally consist of either particles or gases. Particles can either be in the form of solids or liquids. Gases are generally gaseous or exist as a vapor, both of which obey the perfect gas law. Indoor contamination is generally due to humans and animals, including contaminant released from furnishings and processes within interior spaces, and by intrusion of contaminants from outside air. Another form of contaminants is mold (fungal material). Humans and animals (mammals) exhale CO_2; this can become very troublesome in confined spaces (such as submarines) or heavily occupied interiors since it serves as an indicator of poor ventilation. The other major culprit to human health damage/risk is carbon monoxide (CO), which is highly toxic. CO results from incomplete combustion of hydrocarbon fuels and tobacco smoking (Darrell W Pepper, David Carrington. (2009)).

Table 2 – Types of contaminants [Darrell W Pepper, David Carrington. (2009)].

Dusts	Solid particles typically created from crushing, handling, detonation, and impact of organic or inorganic materials; particles do not diffuse in air but settle under the influence of gravity.
Gas	Material state of matter with very low density and viscosity that respond to changes in temperature and pressure; diffuses and uniformly distributes itself throughout any enclosure.
Vapors	Gaseous form of substances normally in solid or liquid state at room temperature and pressure; vapors diffuse and mix with the environment – vaporization is the changing of a liquid into a vapor state.
Aerosols	Liquid droplets or solid particles that are dispersed in air with average diameter mostly smaller than 1 μm, - remain suspended in air for some time.
Fume	Particulate created from the evaporation of solid materials and dispersed into the air; fumes are usually less than 1 μm in diameter.
Mists	Suspended liquid droplets generated from condensation as a gas transforms to a liquid state or by a liquid dispersing into the air due to foaming, splashing, or atomizing; mist forms when a finely divided liquid becomes suspended in air.
Smoke	Particles (suspension of aerosols in air) created from combustion or sublimation and consists of droplets as well as dry particles, e.g., tobacco produces a wet smoke composed of tarry droplets; carbon or soot particles are generally less than 0.1 μm in size and result from incomplete combustion of carbon-based materials.

The sources of building contamination and the multitude of contaminants are numerous. Many of the indoor pollution problems stem from construction activities of operations within a facility. Such contaminants include VOCs, pesticides, biological contaminants promoted by moisture, asbestos, radon, lead, and Polychlorinated biphenyls (PCBs). A variety of units are used for concentration, which is discussed in the next section.

Three commonly available indoor air contaminants were selected for the study: VOC's (Toluene, Formaldehyde, etc.), CO and CO_2 (used as a surrogate for occupant-generated pollutants). Toluene is selected as a representation of the total volatile organic compound (TVOC) level as it is commonly used as a reference compound for TVOC quantification. Formaldehyde is considered because of the high health risk associated with it even at very low concentration level.

Generation rate and allowable indoor concentrations of the three contaminants considered were summarized previously in Table 1.

4.4.2 Units

It is important to understand the common forms of units used to describe concentration. Concentration is essentially a quantity of material per unit of volume, per unit of mass, or per unit of moles. However, one must be careful when referring to a concentration within the air, within water, or soil (which is a multiphase media).

Concentration in air is usually given in units of partial pressure at one atmosphere of total pressure. Since the pressure of a gas is proportional to the number of molecules in a given volume:

$$\frac{partial\ pressure}{total\ pressure} = \frac{molecules\ of\ compound}{total\ molecules} = \frac{moles\ of\ compound}{total\ moles} \quad (1)$$

The most common "unit" found in the literature is parts per million (PPM) in air: PPM by weight (mg/L or g/m^3) and PPM by volume (mL/m^3 or 10^{-6} atm/atm).

4.4.3 Source Materials

The major portion of indoor air contaminants come from building materials and equipment. VOCs resulting from the manufacturing and installation processes typically migrate into the air. VOCs can be mainly classified into the following categories (Darrell W Pepper, David Carrington, 2009):

Table 3 – Classification of VOCs sources [Darrell W Pepper, David Carrington, 2009].

Adhesives, sealants, and architectural coatings	These types of coatings are installed wet and dry or cure on the premises; the solvents used in the formulation of these materials directly relate to the VOCs emitted. The resins used in the base of adhesives are either natural or synthetic and range from low to high emission rates; sealants consist of putties, caulking compounds, rubber, acrylic latexes, and silicones while architectural coatings include paints, stains, sealers, and varnishes.
Particleboard and plywood	Particleboard is a composite produce made from wood chips or residues that are bonded together with adhesives and typically come from milling or woodworking waste. Plywood consists of several thin layers or plies of wood that are bonded by adhesive and are generally classified as either softwood or hardwood; the IAQ effects of softwood and hardwood vary with the adhesive (resins).

Carpet, resilient flooring, and wall covering	These types of materials bring VOC-emitting composition into the building interior along with the use of adhesives to attach the material to various surfaces. Carpets typically consist of fibers of either wool or synthetics. Resilient flooring is generally either tile or sheet (vinyl or rubber). Wall coverings are made from paper, fabric, and vinyl.
Insulation, acoustical ceiling tile, and furnishings	These types of materials include a variety of paints, adhesives, backing, fabrics, and fibrous materials all of which combine to contribute VOCs. Insulation is commonly thermal oriented, but acoustical and fireproofing also are used; these usually exist in the form of batt and rigid foam consisting of fiberglass or mineral wool. Furnishings include such items as prefabricated movable partitions, workstations, desks, chairs, couches, photocopiers, computers, etc.

4.4.4 Pollutants transportation

The most common carriers of pollutants are ventilation systems and the human body (general work activity and socialization). The ventilation system serves as an ideal transport mechanism for dispersing particulates and gaseous compounds throughout a building. Similarly, the human body acts as a repository form transporting all forms of pollutants within a room as well as to other humans.

Operations commonly found in many industrial and office environments include such processes as maintenance and housekeeping, which permit dust or particulate buildup that leads to indoor air contamination. Likewise, office equipment, including such devices as wet and dry copying machines, computers, laser printers, and color inkjet printers, emit VOCs during operation. Pest control, construction activities in occupied buildings, moisture leaks, and many industrial activities including chemical spills, grinding, pouring, and sprays lead to indoor contamination. Operations involving food preparation and consumption are particularly sensitive to emissions and unsanitary conditions that lead to indoor air quality problems. Even the natural process of evaporation and diffusion of volatile liquids stored in rooms are common contributors to overall air quality.

4.5 Ventilation System

Ventilation systems are designed to either prevent contaminants from entering a room or remove contaminants from interior sources within the room. Since ventilation systems are integral to the study of indoor air pollution, it is prudent to at least identify them. A ventilation system consists of several key components: contaminant source, an exhaust hood, an air mover, ducts and fittings, makeup air, exhaust air, a pollutant removal device, a discharge stack, and air recirculation. Variations of these components are typically found in most ventilation systems designed to deal with indoor air quality and pollutant removal. Figure 2 shows a schematic overview of a general ventilation system.

The different components that can be found in ventilation systems are following described. An exhaust hood is used to contain contaminants emitted from a source and after cleaned, e.g., hoods are used to cover grills in kitchens. An air mover or fan is used to draw air into hood ducts. Makeup air is air that is brought into the room from the outside – this air is usually temperature and humidity controlled. Exhaust air is the air discharged from the room, and a pollutant removal device is a specific piece of equipment used to remove excess contaminant from the room (when environmental standards are exceeded), a discharge stack is a stack that exhausts air into the atmosphere, and air recirculation is air that is returned into the room (clean air).

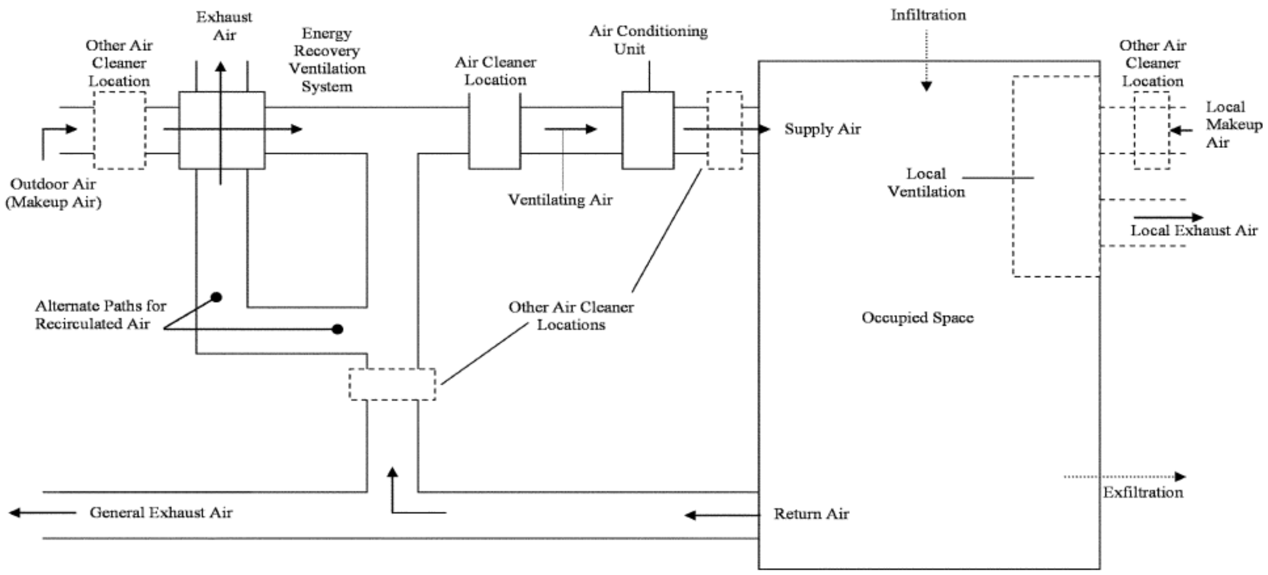

Figure 2 - ANSI/ASHRAE Standard 62.1-2010 : ventilation system.

To achieve an acceptable IAQ level, the ventilation system plays a key role where combinations of the following actions are essential:

- Contaminant source control;
- Proper ventilation;
- Humidity management;
- Adequate filtration.

Besides maintaining acceptable IAQ, it is also necessary to keep the associated energy consumption and costs as low as possible. In this research, effort has been made to develop an IAQ model to help assess the energy-efficient ventilation strategy that is capable of controlling the concentration levels of multiple contaminants typically found in indoor air handling at the same time the best efficacy point of the HVAC system.

5 Indoor Air Quality Modelling

5.1 Indoor Air Quality Assessment

Recently IAQ is getting more attention due to its impact on health and performance of the occupants. Various regulation and standards are in place to limit the concentration of indoor air contaminants in acceptable range. The building HVAC system should be able to clean the air as well as dilute the indoor air contaminant concentration to the level required by the set standards. Assuming mass flow rate of supply and return air to be the same in each zone, indoor air contaminant concentration over time can be estimated by eq.2.

$$V\frac{dC_i}{dt} = rate\ of\ change\ in\ mass\ due\ to\ [(inflitration\ of\ outdoor\ air) + (indoor\ pollutant\ generation) - (indoor\ air\ exfiltration) - (indoor\ removal\ of\ pollutant)] \qquad (2)$$

Where V is the total zone volume and C_i is the indoor concentration.

There are several factors that influence the indoor air quality. For instance, as a physical factor, the temperature influences the indoor thermal comfort which could have a profound impact upon the perception of the Indoor Air Quality (IAQ). Associated to the thermal comfort are the occupational activity, clothing, relative humidity (RH) and indoor wind speed (from mechanical or natural ventilation), what is addressed in the Occupants Comfort Model (D3.4). However, temperature above the acceptable thermal comfort range 20 – 26 °C (Olesen, Bjarne W., 2000) may increase the initial outgassing of Volatile organic compounds (VOC) from materials (Brooks, Bradford O. Davis, William F., 2000). Concerning RH, values over 70% are often associated with microbial growth and contamination, for that reason ASHRAE recommends that the RH must be kept below 60% (Olesen, Bjarne W., 2000). Other physical parameters such as Artificial Lighting, Vibration and Noise, could trigger off some symptoms commonly associated with poor IAQ (e.g. eye irritation, headache).

Furthermore, the buildings operation (occupancy, activities), building envelope and materials, equipment (HVAC systems) and the surrounding environment are the most important elements in the indoor air contaminant concentration prediction. It is crucial to refer that the presence of a contaminant or pollutant in indoor air does not mean necessarily a poor indoor air quality. A lot of airborne contaminants are normal air constituents, what influences the health effect of them is their concentration which could be determined by the variability in indoor infiltration rates, indoor generation rates, ventilation rates, and reaction rates. Usually these rates are used in a mass balance approach to summarize the variables that influence IAQ. This methodology was followed in this task, where was developed a robust model by modification and refinement of other

mathematical models based on simple mass balance equations. From the general point of view, this methodology consists in the substitution of applied mathematical expressions for terms on the right side of the mass balance equation (eq.2).

The HVAC filtration, dilution ventilation and exhaust ventilation are the most relevant HVAC design factors to IAQ control. The operation strategy and maintenance activities are intended to ensure acceptable low concentrations of contaminants from outdoor and from contaminants generated inside the spaces. In the other hand air filtration and contaminant emissions reduction from materials, equipment's and supplies begin to have greater attention by the legislators and manufactures. These two mains aspects are summarized in the mathematical model developed.

5.2 Methodology adopted

Simple models typically consist of either first order approximations which may crudely define the problem domain or elegant, sophisticated analytical solutions for ideal conditions. Rarely do such models exist which can provide intricate details at minute levels within an interior. However, the use of simple modeling tools can quickly provide great insight and an overall grasp of the problem. Such models are useful in establishing at least an order of magnitude assessment, and in some instances may be sufficient for determining IAQ values.

There are generally two concepts used when developing simple models for indoor air quality calculations: well-mixed and partially mixed ventilation models. In a well-mixed model, the concentration is spatially uniform within the enclosure; in a partially mixed model, the concentration is non-uniform generally due to poor mixing. Well-mixed conditions are produced by fans; the natural mixing occurs as a result of natural air currents. Unfortunately, most real world situations involve dealing with partially mixed hypothesis. Analytical procedures are available for these situations as well, but they are somewhat limited; a mixing factor (γ_F) is generally employed to modify the equations for a well-mixed model to account for the non-uniform distribution of concentration.

Assuming an enclosed space exists in which the concentration Ci is considered to be spatially uniform, as shown in Figure 3.

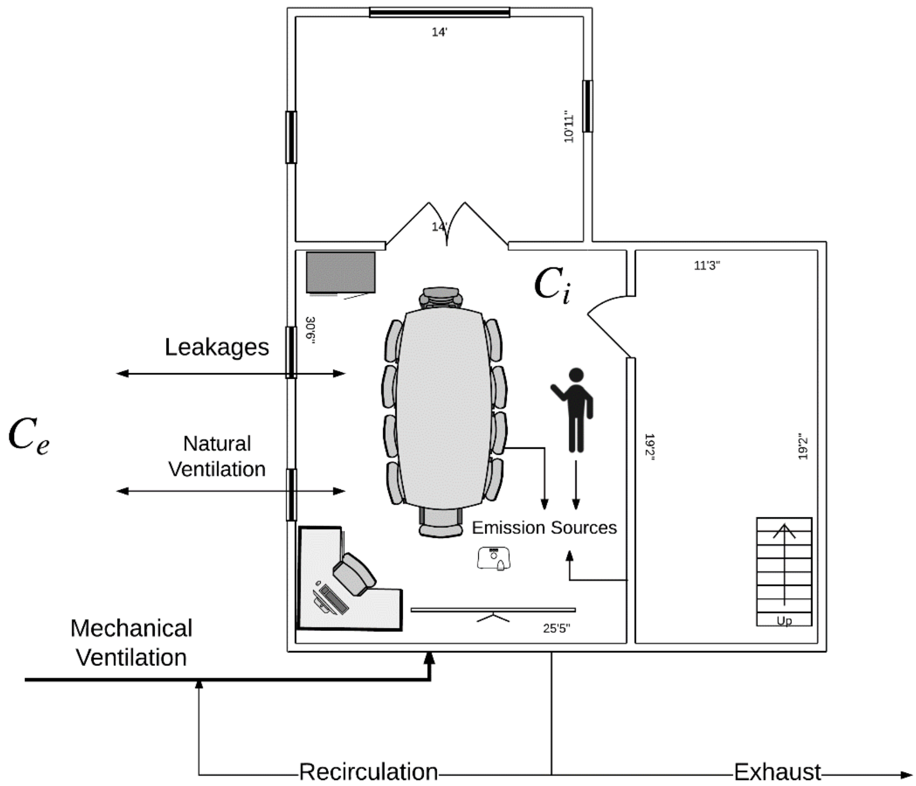

Figure 3 - Mass conservation and space flow dynamic for IAQ

5.3 MOEEBIUS IAQ MODEL

At instant t=0 the indoor contaminant mass concentration is C_o. A source begins to generate contaminants at a constant rate (S). Outside air with contaminant concentration C_e is added to the enclosure at a constant volumetric flow rate Q – contaminated air is removed from the space at the same rate. Applying the equation for conservation of mass, the governing equations for the contaminant concentration entering and leaving the enclosure can be written as

$$\frac{d}{dt}\int_{cv} CdV + \int_{Cs} (Ce - C)vdA + S = 0, \qquad (2)$$

Where C is the concentration, V is volume, v is the flow speed and A is the flow inlet/outlet area, cv denotes the control volume, and Cs is the control surface. Letting $Q \equiv Av$ (flow rate), can be simplified to the relation of Eq.3.

$$V\frac{dC_i}{dt} = \sum QC_e + S - \sum QC_i \qquad (3)$$

To account for wall losses, i.e., removal of contaminant by solid surfaces the model includes the adsorption rate (K_{ads}) of contaminant on materials and the contaminant decay rate.

The generic model is represented in the following differential equation:

$$V\frac{dC_i}{dt} = A + B - C + S - R - D \tag{4}$$

Where:

$$A = Q_m C_e \gamma_{Fm} \left(1 - \eta_{f0}\right) + Q_n C_e \gamma_{Fn} + Q_L C_e \gamma_{Fl} \tag{5}$$

***A* – Fresh air** from the mechanical ventilation, natural ventilation and leakages, where

- Q_m is the mechanical flow from the HVAC system (Q_n and Q_L are the flows from natural ventilation and Leakages/infiltration/exfiltration respectively)
- C_e is the outdoor pollutant concentration
- γ_{Fm} is the mixing factor for the mechanical flow, for this particular type of situation, setting γ_{Fm} = 1 indicates a well-mixed model while γ_{Fm} < 1 implies non uniform mixing and spatial variations in concentration, i.e., γ_{Fm} = 0.5 is used for a perforated ceiling, γ_{Fm} = 0.166 is for natural draft and ceiling exhaust fans, γ_{Fm} = 0.10 is used for infiltration and natural drafts.
- η_{f0} is the pollutant removal efficiency by the air handler, and the typical values are shown in Table 4 or must be used the filter efficiency values.

Table 4 - Ventilation Efficiency [Ioan Sârbu, Calin Sebarchievici, 2010].

System type	$t_e - t_i$ [°C]	ε_v
0	1	2
up–up	<0	0.9…1.0
	0…2	0.9
	2…5	0.8
	>5	0.4…0.7
up–down	<–5	0.9
	–5…0	0.9…1.0
	>0	1.0
down–up	<0	1.2…1.4
	0…2	0.7…0.9
	>2	0.2…0.7

Regarding the outdoor concentration C_e, unless the outdoor concentrations values are known by real time measurements, the standards values must be used. The standard values must be corrected for specific zones. In Annex I it is possible to find values for Urban and Suburban to VOC's, CO and CO_2 typical outdoor concentrations.

$$B = Q_r C_i \gamma_{Fm} \left(1 - \eta_{f1}\right) \tag{6}$$

***B* – Recirculated air**, where Q_r is the recirculated flow, C_i is the indoor pollutant concentration. For η_{f1} is the pollutant removal efficiency in the recirculation circuit, must be used the filter efficiency values.

$$D = (Q_m + Q_n + Q_L)\, C_i \gamma_{Fm} \tag{7}$$

***D* - Exhausted air**

$$S = \text{Metabolic Rate (M)} + \text{Activities(Ac)} + \text{Materials emission(Mat)} \tag{8}$$

***S* – Emission rate** (human activities and materials) Variable equations from transient models from Abadie M.O., Blondeau P. 2011 provided in excel format.

Metabolic Rate (*M*) is strictly linked to the CO_2 generation rates. Both the relationship between indoor CO_2 concentrations and IAQ and the relationship between indoor CO_2 concentrations and ventilation are based on the rate at which people generate CO_2. People generate CO_2 and consume oxygen at a rate that depends primarily on their physical activity and their size. The relationship between activity level, size and the rates of CO_2 generation and oxygen consumption is summarized below.

The rate of oxygen consumption, V_{O2}, in L/s, of a person is given by the following equation:

$$V_{O2} = \frac{0{,}00276 A_d M}{(0{,}23 RQ + 0{,}77)} \tag{9}$$

Where A_D is the DuBois surface area in m^2 (estimated below) (DuBois D, DuBois EF.) *RQ* is the respiratory quotient, i.e., the relative volumetric rates of CO_2 produced to oxygen consumed; *M* is the level of physical activity, or the metabolic rate per unit of surface area, in met (1 met = 58,2 W/m^2).

The DuBois surface area can be estimated by the following equation:

$$A_D = 0{,}203 H^{0{,}725} W^{0{,}425} \tag{10}$$

Where *H* is the body height in m and *W* is the body mass in kg.

Table 5 presents typical metabolic rates (in met) for different activity levels.

Table 5 – Typical Met Levels.

Activity	Met
Seated, quiet	1.0
Reading and writing, seated	1.0
Typing	1.1
Filling, seated	1.2
Filling, standing	1.4
Walking at 0,9 m/s	2.0
House Cleaning	2.0-3.4
Exercise	3.0-3.4

The CO_2 generation rate of an individual is therefore equal to V_{O2} multiplied by *RQ*. *RQ* value depends on the diet, the level of physical activity, and the physical condition of the person and is equal to 0,83 for an adult of average size adult (Steven J. Emmerich Andrew K. Persily, 2001).

$$CO_2 = V_{O2}RQ \qquad \text{(L/s)} \qquad (11)$$

The rates for the pollutants due to the indoor activities(Ac) and materials (Mat) will be supplied by the database available from Abadie M.O., Blondeau P. 2011., and multiplied by the number of activities and material area in contact with air. A short help guide to read Pandora database is presented in Annex III.

$$R = E\, VC_i \qquad (12)$$

***R* – Decay rate**, where *E* is the specific decay rate.

For the emission rate the surface area of the room ($A_{surf\text{-}walls}$) must now be considered to account for the contaminant sticking to the walls (for gases or vapours, this is called adsorption; for particles, this is referred to as deposition). It is very evident when one cleans a room after someone has been smoking in the room – various surfaces absorb tobacco smoke and then desorption occurs when the smoking ceases.

$$C = A_{surf}K_{ads} \qquad (13)$$

***C* – Adsorption factor**, where A_{surf} is the surface area (walls, furniture) and k_{ads} is the specific adsorption rate. Concerning k_{ads} was tested an one-phase models which consider the materials as homogeneous solid media and, consequently, hold that adsorption/desorption processes occur at the material surface exposed to the room air. In Annex IV is available is present a table with a non-exhaustive compilation of relevant sorption data based on the previous remarks (P. Blondeau, A. L. Tiffonnet, F. Allard and F. Haghighat, 2008).

Since the flow of air into and out of the enclosure is in equilibrium, it is easy to obtain an expression for *C*. If we now integrate over time eq.4.

$$\int_{C_0}^{c(t)} \frac{dC}{A + B - C + S - R - D} = \frac{1}{V} \int_{0}^{t} dt \tag{14}$$

Equation 14 must be solved numerically. Numerical solution of model equations generally mimics the processes described in the model. For difference equations, numerical solution is exact since we can use the rules laid down in the equations to follow the evolution of the system. Differential equations provide a rather more difficult problem to implement in the E+ language. The basic method is to divide continuous time into discrete intervals, and to estimate the state of the system at the start of each interval. Thus the approximate solution changes through a series of steps. The crudest method for calculating the steps is to multiply the step length by the derivative at the start of the interval. This is called Euler's method. More sophisticated techniques are used in performing the Runge-Kutte types of integration. Fourth order Runge-Kutte is both commonly used and sufficiently accurate for most applications (Lawson, Daniel. Marion, Glenn, 2008). In EnergyPlus the solution for the CO_2 Prediction Model and the Generic Contaminant Prediction is obtained with a Third order backward difference [EnergyPlus Documentation].

5.3.1 Numerical solution

For a time-varying source or ventilation flow rate, Eq.14 can be rewritten as

$$\frac{dC_i}{dt} = \frac{Q_m C_e \gamma_{Fm} \left(1 - \eta_{f0}\right) + Q_n C_e \gamma_{Fn} + Q_L C_e \gamma_{Fl}}{V} + \frac{Q_r C_i \gamma_{Fm} \left(1 - \eta_{f1}\right)}{V} - \frac{A_{sup} K_{ads}}{V} + \frac{(M \times Occ + Ac \times n_a + Mat \times n_s)}{V} - \frac{E\ C_i}{V} - \frac{(Q_m + Q_n + Q_L)\ C_i \gamma_{Fm}}{V} \tag{15}$$

Where O_{cc} is the number of occupants, n_a is the number of the same activities sources, n_s is the number of the same material sources.

Equation 15 must be solved numerically. Using a simple difference scheme and averaging *C* between unknown and known values – $(C^{n+1} + C^n)/2$ – on the right hand side, Eq. 15 can be solved in order to C^{n+1} as:

$$C^{n+1} = \frac{\frac{Q_m C_e \gamma_{Fm} \left(1 - \eta_{f0}\right) + Q_n C_e \gamma_{Fn} + Q_L C_e \gamma_{Fl}}{V} - \frac{A_{sup} K_{ads}}{V} + \frac{(M \times Occ + Ac \times n_a + Mat \times n_s)}{V} + \frac{C^n \times V}{\Delta t} + \frac{C^n Q_r \gamma_{Fm} \left(1 - \eta_{f1}\right) - EV - (Q_m + Q_n + Q_L)\gamma_{Fm}}{2}}{\frac{V}{\Delta t} - \frac{(Q_r \gamma_{Fm} \left(1 - \eta_{f1}\right) + EV + (Q_m + Q_n + Q_L)\ \gamma_{Fm}}{2}} \tag{16}$$

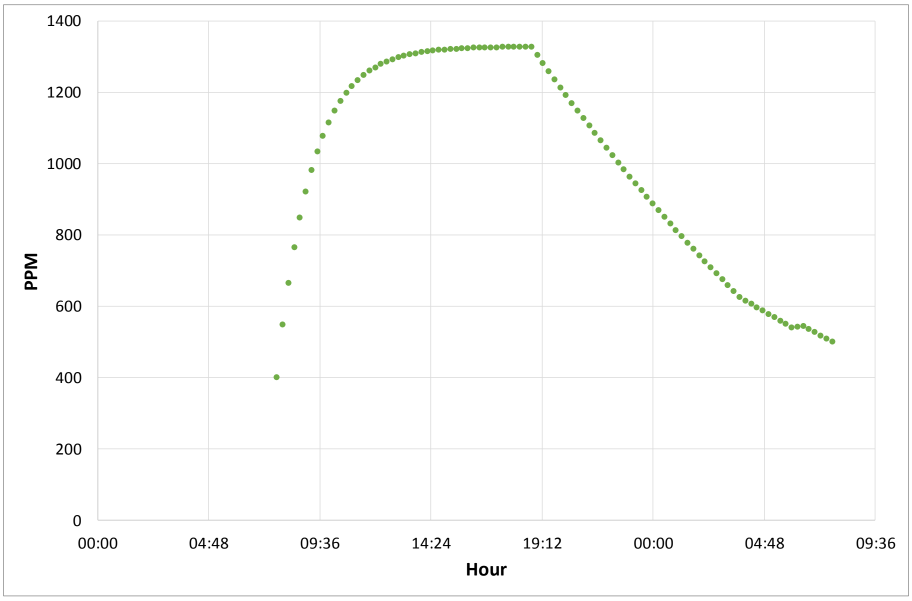

Figure 4 – MOEEBIUS IAQ model output example.

6 Conclusions

This report presents the MOEEBIUS indoor air quality modelling framework with the associated specifications. A state of the art analysis was performed as the starting point for the definition of the proposed framework, where the importance of IAQ and all the relevant parameters were highlighted. Then, the main aspect of the modelling framework was presented: the mathematical modeling based in mass balance with improved inputs. Detailed specifications were given for this mathematical development.

Within MOEEBIUS, the detailed IAQ model will assess the indoor air pollutants concentration for each occupied building zone and could be periodically updated in order to reflect changes that may occur on building's occupancy patterns, environmental standard values for exterior compounds concentrations and in the mechanical ventilation or in natural ventilation due to changes in occupancy behavior (e.g. open a window). The modeling approach allowed the development of the IAQ model in compliance with the MOEEBIUS sensor for indoor air compounds.

The model is defined at a zone level granularity by taking into account HVAC systems, occupancy profiles, occupancy activities, along with the characteristics of the building envelope and internal materials.

The major modifications and improvements in the MOEEBIUS IAQ model are related with its adaptability and with the inputs considered. The IAQ model is based on a mass balance, giving the model the possibility to be adapted for any pollutant compound. In the other hand, the model is supported for an extensive emission rate models database and the state of art review allowed the collection of an extensive list of materials adsorption rates in compliance with the IAQ model. The next step will consist in the validation of the IAQ model with experimental tests.

The IAQ model equations have been translated and tested in Java Programming Language (overview and classes diagram in Annex II). The IAQ model will be further integrated in the BEPS engine (to be specified as a whole in D3.6 Local and Global Energy performance models and developed in D5.1 MOEEBIUS Building Energy Performance Simulation System).

7 References

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8 ANNEX I

Table 6 - VOC's outdoor concentrations in µg/m3 (adapted from: Gianluigi de Gennaro, Genoveffa Farella, Annalisa Marzocca , Antonio Mazzone, Maria Tutino. (2013). Indoor and Outdoor Monitoring of Volatile Organic Compounds in School Buildings: Indicators Based on Health Risk Assessment to Single out Critical Issues, ISSN 1660-4601).

	VOC's Outdoor Concentrations										
	Urban	Suburban	Suburban	Suburban	Urban	Urban	Suburban	Suburban	**Avgd**	**AvgU**	**AvgSub**
Benzene	0,6	0,6	0,4	1,0	0,8	0,6	0,4	0,1	**0,57**	**0,7**	**0,5**
Toluene	**2,1**	**1,3**	**0,7**	**5,6**	**2,5**	**1,6**	**0,7**	**0,8**	**1,92**	**2,1**	**1,8**
Limonene	32,2	10,3	1,0	10,5	0,4	0,1	1,2	1,0	**7,08**	**10,9**	**4,8**
Tetrachloroethylene	0,4	0,2	0,1	0,7	0,1	0,3	0,1	0,2	**0,27**	**0,3**	**0,3**
Ethyl-benzene	0,4	0,3	0,2	1,7	0,5	0,4	0,2	0,2	**0,48**	**0,4**	**0,5**
Trimethylbenzene	0,3	0,3	0,1	0,8	0,3	0,2	0,2	0,1	**0,29**	**0,3**	**0,3**
Decane	2,8	1,6	0,5	4,7	0,4	0,4	0,4	0,5	**1,42**	**1,2**	**1,6**
Styrene	0,5	0,2	0,1	1,3	0,2	0,3	0,2	0,1	**0,35**	**0,3**	**0,4**

Table 7 - CO outdoor concentration in µg/m^3 (adapted from http://qualar.apambiente.pt/index.php?page=2).

CO (octo-hourly average) (µg/m^3)	
Urban	Suburban
298,8	218

Table 8 – Standard Value for CO2 outdoor concentration (Lee, J.Y., et al.,2016)

CO2 mean value for outdoor concentration in ppm
400

9 ANNEX II: Code

9.1 Overview

There are two main types of data utilized in the code: the Configuration Parameters and the Virtual Sensor data.

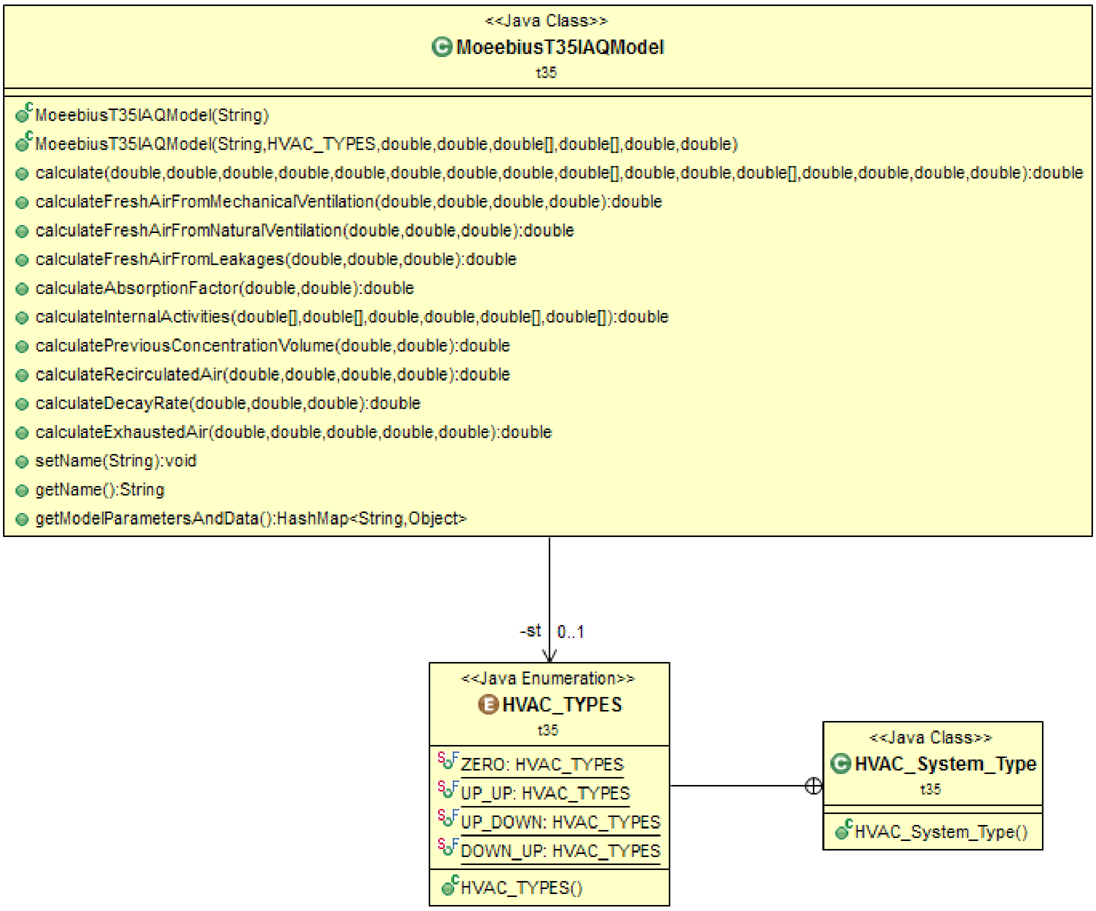
The Configuration Parameters express in general static information that is associated with each building zone. These are the following

1. The HVAC System Type;
2. The Zone Surface Area;
3. The Specific Absorption Rate;
4. A vector with the different material sources in a Zone for calculating the Internal Activities;
5. A vector with the different material types in a Zone for calculating the Internal Activities;
6. The Volume of the Zone;
7. The Specific Decay Rate.

The Virtual Sensor data are sensor data (or properties) that are required from the EnergyPlus simulation engine in each time-step of the simulation, such as the number of occupants. We refer to them as virtual sensor data, since the simulation engine is capable of providing information that would have been nearly impossible to measure in each application zone of the building. These are the following:

1. The mechanical flow from the HVAC system;
2. The outdoor pollutant concentration;
3. The mixing factor for the mechanical flow;
4. The pollutant removal efficiency of the air handler;
5. The natural ventilation flow;
6. The mixing factor for natural ventilation;
7. The leakages/infiltration/exfiltration flow;
8. The mixing factor for leakages/infiltration/exfiltration;
9. A vector with the different activity sources in a Zone for calculating the Internal Activities;
10. The number of occupants;
11. The metabolic rate;
12. A vector with the different Activity Indicators in a Zone;
13. The Concentration Level of Contaminants calculated in the previous simulation time-step;
14. The recirculated flow;
15. The pollutant removal efficiency of the recirculated air;
16. The simulation time-step in minutes.

9.2 Class Diagram



10 ANNEX III

Additional information about the structure of Data_Exported_from_PANDORA

- CATEGORY NAME: Occupants and Occupant Activities, Cleaning Products and Air Fresheners, Construction and Decoration Materials…

- GLOBAL TYPES NAME: Carpeting, Acoustical Materials, Finishes, Flooring, Air Fresheners, Using Incenses, Using Candles…

- TYPES NAME: Carpet 004, Carpet 005, Particle Board 006, Particle Board 005, Desktop 003, Printer 001, Shoes (sneakers) 001, Incense (aromatic) 002…

- DESCRIPTION: Carpet, commercial, Olefin, 1&2 backing: woven synthetic, latex laminate….

- LOCATION: Day-care, Hospital, Office, Residence, School…

- COUNTRY: location of the measurement and/or origin of the source

- REFERENCE: see LIST OF REFERENCES

- CONTAMINANT NAME: Pollutant name

- CONTAMINANT GROUPS NAME: VOC, PM...

- CASN: CAS number

- EMISSION MODEL: name of the emission model... Example: "Gas - Transient - Peak Model (mg/m^2.h)"

- C1 to C15: parameter values of the emission model

- EQ: equation of the emission model (parameters as letter, see below for the correspondence with C1 to C15)… example: S = a1*exp(-0.5*(ln(t/tp)/a2)^2)

- EU: unit of the emission given by the model

- N1 to N15: letter used in the emission model equation (related to the values in C1 to C15)

- U1 to U15: unit of the parameters (related to the values in N1 to N15)

11 ANNEX IV

Compilation of sorption and diffusion coefficients: Data fit with one-phase models (P. Blondeau, A. L. Tiffonnet, F. Allard and F. Haghighat, 2008).

REFERENCE	MATERIAL/CONTAMINANT	K	D (M²/S)	COMMENTS
Little et al (1994)	Carpet 1a/styrene	4200	4.1×10^{-12}	*K* in units of $m^3{}_{air}/m^3{}_{mat}$
	Carpet 1b/styrene	6500	3.6×10^{-12}	
	Carpet 1a/4-ethenylcyclohexene	1400	5.2×10^{-12}	
	Carpet 1a/ethylbenzene and xylenes	1500	10.2×10^{-12}	The numbers following 'carpet' identify different samples
	Carpet 1b/ethylbenzene and xylenes	2400	4.3×10^{-12}	
	Carpet 1a/4-phenylcyclohexene	81,000	0.59×10^{-12}	*K* and *D* determined as the best fit of published emission data
	Carpet 1b/4-phenylcyclohexene	67,000	0.50×10^{-12}	
	Carpet 3/formaldehyde	11,000	3.2×10^{-12}	
	Carpet 3/acetaldehyde	1	6.4×10^{-12}	
	Carpet 3/2,2,4-trimethylpentane	59,000	0.060×10^{-12}	
	Carpet 3/1,2-propanediol	180,000	0.065×10^{-12}	
	Carpet 3/2-ethyl-1-hexanol	450,000	0.088×10^{-12}	
	Carpet 4/styrene	5700	3.1×10^{-12}	
	Carpet 4/4-ethenylcyclohexene	1700	2.1×10^{-12}	
	Carpet 4/ethylbenzene and xylenes	5300	1.5×10^{-12}	
	Carpet 4/4-phenylcyclohexene	170,000	1.2×10^{-12}	
Bodalal et al (2000)	Carpet backing material/toluene	6171	43.10×10^{-12}	*K* in units of $m^3{}_{air}/m^3{}_{mat}$
	Carpet backing material/nonane	6216	28.30×10^{-12}	T = 23°C ± 1°C
	Carpet backing material/decane	14,617	5.42×10^{-12}	RH = 50% ± 5%
	Carpet backing material/undecane	24,255	2.79×10^{-12}	
	Plywood/cyclohexane	348	155×10^{-12}	
	Plywood/ethylbenzene	1636	40.4×10^{-12}	
	Plywood/decane	6948	12.8×10^{-12}	
	Floor tile/ethylbenzene	1920	16×10^{-12}	
	Floor tile/nonane	2142	14.8×10^{-12}	
	Floor tile/decane	13,045	2.09×10^{-12}	
	Floor tile/undecane	26,647	0.85×10^{-12}	
Cox et al (2001b)	Vinyl flooring/n-butanol	810 ± 77		T=25.6±0.3°C
	Vinyl flooring/toluene	980 ± 34		Dry conditions
	Vinyl flooring/phenol	120,000 ± 3000		
	Vinyl flooring/n-decane	3000 ± 420		
	Vinyl flooring/n-dodecane	17,000 ± 260		
	Vinyl flooring/n-teradecane	120,000 ± 1300		
	Vinyl flooring/n-pentadecane	420,000 ± 38,000		

REFERENCE	MATERIAL/CONTAMINANT	K	D (M^2/S)	COMMENTS
Yang et al (2001)	Gypsum board/ethylbenzene	1550		*K* in m^3_{air}/m^3_{mat}
	Gypsum board/ethylbenzene	10.05		T = 23°C ± 1°C
	Gypsum board/ethylbenzene	34.90		RH = 50% ± 2%
Tiffonnet et al (2002)	Acrylic paint/acetone	2.80 at 20°C		*K* in g_{air}/g_{mat}
		2.56 at 25°C		(original data in
		2.53 at 30°C		units of g_{air}/g_{mat})
He et al (2005)	ACT2/tetradecane	400	500×10^{-12}	ACT: acoustic ceiling tile
	ACT3/hexanal	5524	109×10^{-12}	CRP: carpet
	CRP1/4-phenylcyclohexene	66,833	235×10^{-12}	GB: gypsum board
	CRP1/heptane	300	609×10^{-12}	OSB: oriented strand board
	CRP2/dodecane	986	192×10^{-12}	PB : particle board
	CRP2/limonene	1441	163×10^{-12}	PLY : plywood
	CRP2/styrene	268	364×10^{-12}	*K* in units of m^3_{air}/m^3_{mat}
	CRP3/4-phenylcyclohexene	10,512	117×10^{-12}	Partition coefficients
	CRP3/dodecane	3840	174×10^{-12}	Determined
	CRP3/limonene	1400	325×10^{-12}	Simultaneously
	CRP3/styrene	275	455×10^{-12}	with diffusivities
	CRP3/tetradecane	22,476	12×10^{-12}	and initial
	CRP3/tridecane	7336	81×10^{-12}	concentrations
	CRP4/dodecane	42,549	75×10^{-12}	by fitting one-phase
	CRP4/iso-octane	50,000	9×10^{-12}	model to various
	CRP4/tridecane	69,942	72×10^{-12}	emission data
	CRP5/iso-octane	84,151	1×10^{-12}	measured in
	CRP6/tridecane	71,560	136×10^{-12}	small chamber tests
	GB1/α-pinene	80,329	10×10^{-12}	Proposed values
	GB2/α-pinene	80,200	5×10^{-12}	are optimal values
	GB3/α-pinene	52,744	16×10^{-12}	from the best fit
	OSB1/α-pinene	194,080	0.2×10^{-12}	of emission
	OSB2/α-pinene	21503	38×10^{-12}	Profiles
	OSB2/furan	60,256	6×10^{-12}	
	PB0/α-pinene	849	99×10^{-12}	The numbers
	PB0/camphene	1090	106×10^{-12}	following the
	PB0/hexanal	550	74×10^{-12}	material name
	PB0/limonene	334	126×10^{-12}	identify different
	PB4/α-pinene	86	800×10^{-12}	Samples
	PB4/camphene	1470	1052×10^{-12}	

REFERENCE	MATERIAL/CONTAMINANT	K	D (M²/S)	COMMENTS
	PB5/α-pinene	492	655×10^{-12}	
	PB5/camphene	1570	1011×10^{-12}	
	PB5/hexanal	70,927	16×10^{-12}	
	PB5/limonene	1898	900×10^{-12}	
	PB6/camphene	564	63×10^{-12}	
	PB6/hexanal	19,650	66×10^{-12}	
	PLY1/3-carene	37,562	388×10^{-12}	
	PLY2/3-carene	125,632	0.4×10^{-12}	
	PLY2/α-pinene	80,560	0.4×10^{-12}	
	PLY2/*p*-cymene	29,736	0.4×10^{-12}	
	PLY3/3-carene	19,676	22×10^{-12}	
	PLY3/α-pinene	6749	0.1×10^{-12}	
	PLY3/limonene	11,454	36×10^{-12}	
	PLY3/*p*-cymene	15,974	44×10^{-12}	
Elkilani et al (2003)	Carpet fibres/toluene	0.86 at 25°C		Dry conditions
		0.73 at 30°C		
		0.50 at 35°C		Original data in
		0.34 at 45°C		units of m –
	Carpet fibres/1,2-dichlorobenzene	1.60 at 25°C		converted to
		0.83 at 30°C		g_{air}/g_{mat} using
		0.74 at 35°C		the specific
		0.36 at 45°C		surface area
	Carpet fibres/1,1,1-trichloroethane	0.18 at 25°C		of the carpet
		0.16 at 30°C		fibres provided
		0.13 at 35°C		by the authors