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Modelling VOC levels in a new office building using passive sampling, humidity, temperature, and ventilation measurements

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ABSTRACT

New buildings often have high initial concentrations of VOCs that, although not necessarily harmful, may be disturbing and cause discomfort among occupants. In new buildings, running the ventilation system continuously and at full rate during the first year is common practice to reduce VOC levels. However, the drawback of such an arbitrary strategy is the risk of over-ventilating with unnecessary heat losses as a consequence. In this article, a new approach, a VOC-passport, is developed where early measurements of VOCs together with a calculation model are used to find an optimized ventilation strategy. The proposed calculation model is tested on two newly built office rooms where VOCs were measured using passive samplers, together with temperature, humidity and ventilation rates, and it shows good agreement with measurements. An example of how a daily ventilation schedule may look like if optimized with the prosed model is presented. The example illustrates that in buildings where VOC levels are allowed to increase periodically, VOC levels can be kept at acceptable levels during occupancy hours if the effective storage capacity is known. The proposed method has a potential to improve the indoor air quality in new buildings without compromising energy efficiency.

1. Introduction

Poor indoor air quality in offices is of major importance since it may cause adverse health effects, and influence work performance and perceived indoor air quality [1]. Malodours are often caused by volatile organic (VOCs), for example formaldehyde and other, larger aldehydes with low odour thresholds [2]. VOCs are considered one of the main pollutants found in the indoor environment [3]. Some common sources for VOCs are building materials, paints, solvents, wood preservatives, aerosol sprays, cleansers, petroleum related products, furnishing materials and disinfectants [4,5]. Typical impacts from odour or sensory irritation are: annoyance, breathing pattern, reaction time on tasks, mood and distraction [6]. Low levels of volatile organic compounds (VOCs), malodours or other air pollutants contribute generally to a better mental performance among office workers [7–9].

Levels of non-occupant related VOCs that comes from new materials and products are often higher in new buildings and it may take several months after the building is put into use before VOC levels declines to acceptable levels [10–14]. These early VOCs are often easily sensed and sometimes referred to as a characteristic "new-smell". There is, to the authors knowledge, no published studies on the strategies commonly used to handle excess levels of VOCs in new buildings. Our insights

are based on private communications with experts from *Akademiska hus AB* and *Gothenburg City Premises Administration*. These organizations administrate large stocks of academic- and school buildings in Gothenburg, respectively. Both organizations practice running the ventilation systems continuously and at full rate during the first 6–12 months after their buildings are put in use, with the purpose of reducing VOC levels. [15,16]. Such a general strategy is based on experience because VOC sensors that are installed in the ventilation system cannot distinguish between non-occupant and occupant related VOCs. However, with this strategy it is not sure that VOCs are kept at acceptable levels at all times while, at the same time, there is a risk of over-ventilating leading to unnecessary energy losses. Instead, an alternative approach is needed that can reduce energy losses from ventilation and ensure good indoor air quality.

The concentration decay of VOCs in new buildings is non-linear and depends on internal diffusion within the emitting material [17]. Sorption of VOCs in porous materials may dampen concentration variations and reduce the peak concentration in a room [18,19]. The emission rate from a material depends on the temperature and humidity in the room, where increased temperature or humidity increases the emission rates [20,21]. To control VOC levels in a building, it may, therefore, be

important to consider not only ventilation rates, but also temperature and humidity. For example, in an experiment by Liang et al. [22] VOC emissions from a medium-density fibreboard were measured in an experimental room. Results showed lower VOC levels in the room soon after the fibreboard was introduced compared to a following period when the temperature inside the room was higher [22].

After a new building is put in use, the owner is responsible for the indoor environment and for maintaining the building operation. The Swedish national regulations on healthy indoor environments specify the functional performance of a building, but there is no information about how this can be achieved. To meet the requirements in the regulations, low-emitting building materials are commonly used to reduce VOC-levels indoors [23]. However, using only low-emitting building materials may not be enough to keep VOCs at acceptable levels if ventilation rates are low [24]. In addition, new offices are often furnished with new products that also emit VOCs into the environment. This is not mentioned in the regulations and there is no information about the combined effects of emissions from both building materials and furniture.

In this article, we propose a method, 'VOC-passport', for prediction of VOC concentration in indoor air based on on-site measurement of early-stage VOCs. The benefit of the proposed method is that it does not need a material emission database. Instead, the measurements provide insights into the total VOC-performance or VOC-footprint that is specific for a particular room or building. The proposed method stems from an unforeseen result in an earlier project [25].

In the *method* section an overall description of the method is given. Also, the methods used in field and the numerical model are described in detail. The *results and discussion* section presents results from both measurements and simulations, and provides a verification of the method. The results and methods are analysed and discussed. The section *ventilation strategy — example* provides an example of how the proposed method could be used to optimize the ventilation schedule. Finally, the *conclusion* section summarizes the main findings in the paper.

2. Established methods

Setting an optimum ventilation rate with regards to energy consumption and indoor air quality can be challenging and requires information about the emission loads in the room. There are several methods proposed that utilizes emission data from the database provided by NRC (National Research Council Canada) to estimate the required ventilation rate [26–28]. For example, Ye et al. proposes two methods for determining required ventilation rates in residential buildings and offices. Ventilation rates are, in both methods, calculated based on material emission data from a database provided by NRC and concentration limits based on several indoor air quality Refs. [28]. In one of the two methods, the ventilation requirement is split in two steps where the first step handles initial high emission rates and the latter handles lower long-term emissions. The motivation for splitting the ventilation requirement in two steps is to reduce over-ventilation at the later stage when emission rates are lower. The authors point to the material emission database as an important source for the method uncertainty. Since the database does not cover all materials currently available on the market, the usability of the method is limited in real world applications. Also, the data uncertainty that arises from variability between tested specimens is not accounted for in the proposed methods. The authors suggest obtaining a more representative emission data that covers a wider range of materials in order to improve the accuracy. Despite the uncertainties, the study points at the importance of accounting for material emissions when adjusting ventilation rates and illustrates the risk of over-ventilating if ventilation rates are not decreased as the emission rates decline.

2.1. VOC-sensing technology

In office buildings, VAV (variable ventilation volume) is commonly used to decrease energy losses, and CO_2 is often used as a control signal for the ventilation system to reduce occupancy related pollutants. However, the same control signal cannot be used to indicate non-occupant related pollutants [29]. Besides, excess ventilation rates may not have a significant effect on the emission rates and, thus, ventilating during non-occupancy hours will not reduce the off-gassing time [30, 31]. Instead, intermittent ventilation may be a better choice where the VAV-system is used to increase the ventilation rates during occupancy hours and minimize it during non-occupancy hours. The challenge with such a strategy is to determine appropriate ventilation rates and the length of the pre-ventilation time, which may vary from several minutes to several hours [32].

Development in gas sensing technologies in recent years have resulted in cheap and readily available real-time VOC-sensors [33,34]. One of the sensor technologies that have gained attention in the ventilation community is the metal oxide semiconductor (MOS), mainly because of its low price and potential advantage over CO_2-sensors, since they are claimed to detect not only presence of people but also other odorous events, generated by VOC, such as cleaning and cooking. The intended use for these sensors is usually to provide an alternative to CO_2-sensors with additional capabilities. However, they are not intended to provide indications of harmful contaminants since they cannot distinguish one VOC from another [35–37]. In addition, MOS-sensors are typically more sensitive to one or several gases compared to others and may react more strongly to for example detergents, paints or human present and less strongly to emissions that originate from building materials [36]. This means that there are uncertainness of the usability of these sensors when it comes to monitoring the concentration decay of VOCs from materials and equipment in new buildings and more research is needed. However, it should be noted that work on improving the selectivity of MOS-sensors have been performed with promising results which may lead to MOS-sensors being more useful for monitoring VOC emissions in new building in the feature [38,39].

2.2. Numerical modelling

Several models have been developed to predict VOC concentrations in buildings and there are generally two types of models, non-physical models and physical models. Non-physical models typically describe statistical regularities derived from measurements, for example Markov process models, autoregressive moving average, or autoregressive integrated moving average models [40]. The major drawback of non-physical models is the lack of transferability between different testing conditions, which is also the reason why physical models often are preferred over non-physical ones. Most physical models treat the volume of air in a room as a balanced system where the total sum of VOCs entering and leaving the room is zero. Such models often assumes that VOCs are well mixed with the air in the room. Emissions are added using source terms (or removed using sink terms), which may be formulated as a constant or with some dependency on for example pressure or temperature. However, sinks and sources can also be modelled using Fick's second law to more accurately describe the diffusion within materials. These models vary in complexity depending on the number physical processes that are considered. More simple diffusion models account mainly for diffusion processes and assume constant material properties, while complex models account for non-constant material properties and may also include for example surface adsorption [41, 42]. Although diffusion models often can describe the emission source more accurately than for example empirical models [41], the main drawback is the need of material VOC emission properties which may not always be available [43].

Fig. 1. Room 1 (left), room 2 (middle) and both rooms seen from the outside (right).

3. Methods

In this article, a method, 'VOC-passport' is developed. The method combines on-site measurements of early-stage VOCs with numerical simulations to make concentration predictions dependent on ventilation rates. Measurements are performed shortly after a new or renovated building is completed and used to calibrate a mathematical model that is used for the predictions. The model accounts for material emissions, emission storage in the room and ventilation rates.

The hypothesis is that an effective storage capacity of the room together with a lumped source strength can be found and used to model the time dependent non-occupant related VOC concentration in the room. The model can be used to optimize an intermittent ventilation strategy (implemented in a VAV-system) so that non-occupant related VOC concentrations are kept at acceptable levels without over-ventilating with unnecessary energy losses as a consequence.

The method consists of two major steps. The first step is field measurements where temperature, humidity and ventilation rate is measured by the ventilation system in a room while VOCs are measured using passive samplers. In the second step, the results from the field measurements (first step) are used to calibrate a physical model that can be used to simulate non-occupant related VOC levels in the room based on ventilation rates, temperature and humidity.

It is important to note that non-occupant related VOC emissions from materials act on a longer timescale than occupant related emissions. While emissions from materials can be understood by measuring on longer timescales such as weeks, occupant-related emissions cannot. This is similar to how built-in moisture in concrete constructions can be understood by measuring on a weekly basis, while occupant related moisture production must be captured on a much shorter timescale such as minutes or hours.

Following the first step in the methodology, measurements and simulations of volatile organic compounds (VOCs) and C1–C10 straight chain aldehydes are performed in two rooms (room 1 and room 2) in a newly built office building at Chalmers campus Johanneberg in Gothenburg, Sweden. The building was put in use in October 2019 and is a low energy building, certified with the highest rank in the Swedish building certification system, Miljöbyggnad [44]. The load bearing walls are made of cross laminated timber and steel frames, and the floors are made of concrete. The ventilation system is demand-controlled and equipped with temperature and humidity logging capabilities.

The test rooms (room 1 and room 2), Fig. 1, are two identical meeting rooms placed on floor 3 and 4. The size of the rooms are about 3.0×4.0×3.5 m. Furnishing is identical in both rooms. Walls are covered with painted gypsum boards and there is a suspended ceiling of wooden acoustic panels. There is a carpet on the floor, a whiteboard, a table, 8 chairs, a low shelf, a coat hanger, a projector, a ceiling lamp, speakers and spotlights.

In addition, temperature, absolute humidity and ventilation rates are measured continuously by the ventilation system in each room.

Table 1
Sampling schedule for the VOC measurements.

Date	Week	Measurement
2019-10-14 → 2019-10-20	1	1
2019-10-28 → 2019-11-03	3	2
2019-11-04 → 2019-11-10	4	3
2019-11-11 → 2019-11-17	5	4
2019-11-25 → 2019-12-01	7	5
2019-12-16 → 2019-12-22	10	6
2020-01-13 → 2020-01-19	14	7
2020-02-24 → 2020-03-01	20	8
2020-04-20 → 2020-04-26	28	9

Results from measurements are used to calibrate a *source model* which accounts for dependency on temperature and absolute humidity. The source model is then implemented in a *physical model* that calculates the concentration inside the room. Input parameters for the mass balance model are found by comparison with measured VOC concentrations using a fitting algorithm in MATLAB. The flowchart in Fig. 2 shows an overview of the method.

The method is illustrated in four steps:

1. Temperature, absolute humidity and ventilation airflow are measured by the ventilation system and VOCs are measured using passive samplers.
2. Average temperature, average absolute humidity and median ventilation airflow are calculated for each sampling period where a sampling period is the period for which passive samplers have been used.
3. The source model, Eq. (4) and Eq. (5) in Section 3.2 is calibrated by fitting against measured VOC using the values from the previous step.
4. Model parameters (initial concentration and effective storage capacity) in Eq. (6) are determined by fitting simulation output to measured VOC concentrations.

3.1. Sampling and chemical analysis

The sampling of volatile organic compounds (VOCs) and aldehydes in the two test rooms were performed during more than six months. Time schedule for the whole experimental part is presented in Table 1. The sampling period for each measurement was one working week. The samplers were installed in the sampling locations on Monday early morning and they were collected on Friday late afternoon.

VOCs are passively sampled on Tenax TA (PerkinElmer) adsorbent tubes and analysed in compliance with ISO 16017-2 [45]. The Tenax tubes are thermally desorbed (Markes International, Unity 1 and Ultra, 5 min, 250 °C) and analysed by gas chromatography/mass spectrometry (GC/MS). The gas chromatograph (GC) is an Agilent 6890 equipped
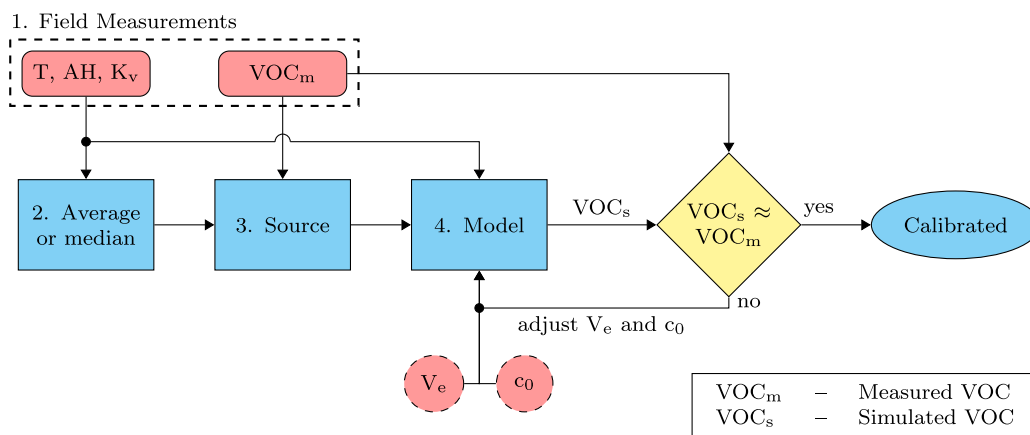
Fig. 2. Flowchart showing an overview of the method, VOC-passport.

with a mass selective (MS) detector (Agilent 5973N) in electron impact mode for compound identification and quantification. The GC is equipped with a CP Wax 52C (Agilent) capillary column (Polyethylene glycol phase, 60 m, 0.32 mm i.d., 1.2 mm film thickness) and used helium as carrier gas. The GC oven temperature program is started at 50 °C and increased to 100 °C at 4 °C/min. then increased to 220 °C at 8 °C/min. and maintained for 10 min. The results are expressed as TVOC (Total Volatile Organic Compounds) and quantified as toluene equivalents, i.e using uptake rate and the response factor of toluene. Terpenes, α-pinene and 3-carene are quantified using their compound specific uptake rates and response factors. Calibration is achieved by application of microlitre amounts of solution of the compounds in methanol on Tenax tubes. The VOC calibration standards were analysed with each batch of samples from the particular sampling occasion. The limit of quantification (LOQ) for the individual VOC 0.5 μgm^{-3} based on 3 times the signal-to-noise ratio. Aldehydes (straight chain C1–C10) are measured using passive samplers — DSD-DNPH Aldehyde Diffusive sampling Device (Supelco, Bellefonte, PA). The sampling procedure and the analytical technique (solvent extraction and high performance liquid chromatography) followed the ISO 16000–4 standard [46]. Standard calibration curves for the C1–C10 aldehydes were used for the quantification of the substances in each batch of samples from the sampling occasion. The LOQs for the aldehydes ranged from 0.08 μgm^{-3} (formaldehyde) to 1.8 μgm^{-3} (decanal). The analysed results are then an average concentration of the compounds over the entire sampling period. Results of other studies state that the active and passive sampling techniques in the field compare reasonably well [47, 48].

3.2. Model description

The concentrations in the room are modelled with the following mass balance equation:

$$V_e \frac{\partial c}{\partial t} = K_v \left(c_{bg} - c \right) + S \tag{1}$$

where c_{bg} [kg m^{-3}] is the background VOC concentration, t [s] is the time, S [kg s^{-1}] is the source strength, K_v [m^3 s^{-1}] is the ventilation airflow rate and V_e [m^3] is the effective air volume or effective storage capacity that describes short-term storage of VOC as the concentration in the room fluctuates. Typically, these are VOCs stored on surfaces and inside materials in the room and are quickly released back to the room when VOC concentrations decreases.

The effective volume, V_e, describes the total VOC storage capacity of the room, including both the indoor air and emitting materials, in a unified and comprehensible way. It is derived in an analogy with moisture buffering volume of a ventilated space [49,50]. When V_e is compared to for example the physical volume of the room, it clarifies

the magnitude of the room's VOC capacity. Since the buffering of VOC may work differently for different VOCs, V_e may have different values for different VOCs in the same room.

With $c_{bg} = 0$ the solution for Eq. (1), for one time period with constant ventilation rate, becomes:

$$c(t) = c_0 \cdot e^{-nt} + \frac{S}{K_v} \left(1 - e^{-nt} \right) \tag{2}$$

where c_0 [kg m^{-3}] is the initial VOC concentration and n is given by:

$$n = \frac{K_v}{V_e} \tag{3}$$

In practice, the background concentration of VOCs in buildings will never be zero, it may range from values below the laboratory reporting limits up to several hundreds of μgm^{-3} [51]. However, since the model is calibrated against measured values, any actual background concentration will be handled indirectly by the source term.

To quantify the source strength from measured data the following two equations are used. First, the flow of VOCs out of the room is calculated from measured data with:

$$S_A = \check{K}_v \cdot c \tag{4}$$

where S_A [kg s^{-1}] is the flow of VOCs, $\check{K}_v$ [m^3 s^{-1}] is the median ventilation rate and c [kg m^{-3}] is the VOC concentration. During longer measurement periods, with only small variations in concentration and ventilation air flow, Eq. (4) can be interpreted as the average source strength of emissions in the room. When several VOCs are lumped together, S_A is simply the lumped source strength for those VOCs.

The rooms are situated entirely within the building, see Fig. 1, and, therefore, the only driving force for air leakage is the pressure difference caused by mechanical ventilation. Air leakage in energy efficient and acoustically well-designed buildings like the one used in this study usually makes up a small, but not insignificant part of the total ventilation rate [52], and generally varies with the pressure. Unfortunately, there are no measurements of how airtight the rooms are and, therefore, to account for air leakage, estimations are made based on the authors experience. It is assumed that each room has a specific air leakage, q$_{50}$, of 0.1–0.2 l/s per m^2 room area at 50 Pa pressure difference. Translated to normal conditions, where the pressure difference is 1–2 Pa, this assumption gives a total air leakage of 0.5 l/s to 1.5 l/s in each room, (compared to 10–20 l/s which is the mechanical ventilation rate during occupancy). Therefore, an air leakage of 1.0 l/s is added to K_v in all calculations. The authors are aware that using a constant rate for air leakage may cause some inaccuracy, for example, overestimation of air leakage when mechanical ventilation rates are low. However, given the lack of measurement data, the proposed method is the most feasible without introducing large errors.
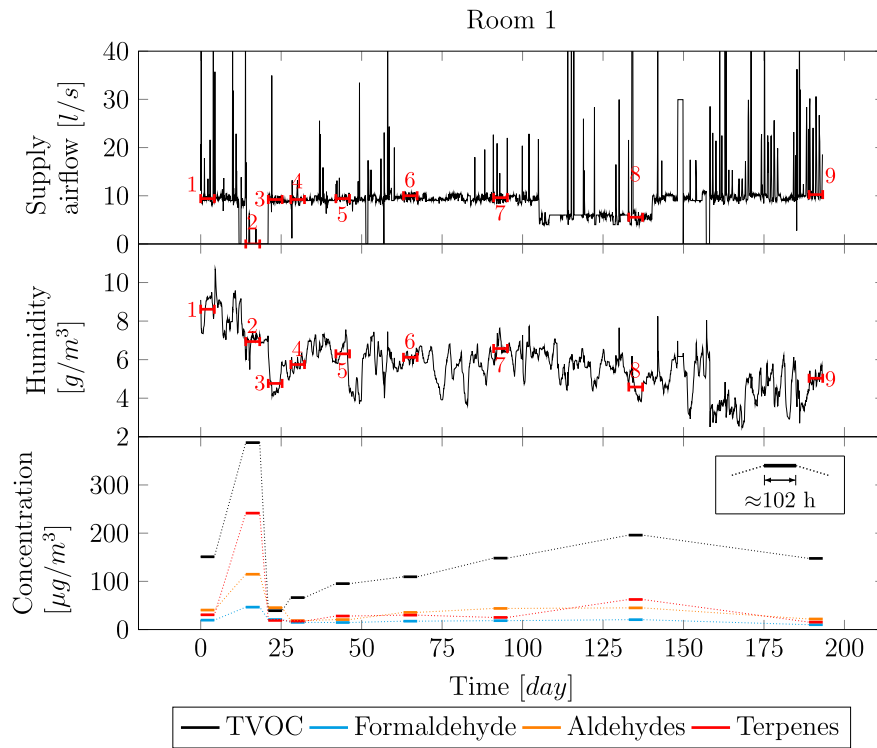
Fig. 3. Measured supply ventilation, humidity and measured VOC concentrations in room 1. Sampling periods are numbered from 1 to 9. The horizontal bars show the measured average concentration during each measurement period and the dashed lines, between each measurement, are added to visualize trends. The length of each measurement period is 4 days and 6–8 h ($\approx$102 h).

In accordance with the work of Xiong et al. [20] and Liang et al. [22] we have also tested a correlation between emission strength and humidity in the indoor air. In contrast to Liu et al. we found no major difference in the correlation between using *relative humidity* or *absolute humidity*. However, we find it more practical to continue with absolute humidity since it, in contrast to relative humidity, is decoupled from temperature. Therefore, in the next step, the following model is used for relating the average source strength, S_A, to temperature and absolute humidity:

$$S = S_1 \cdot T^{0.75} \cdot e^{S_2 \cdot AH - \frac{S_3}{T}} \tag{5}$$

where S_1, S_2 and S_3 are coefficients that can be determined by curve fitting, AH [kg m^{-3}] is the absolute humidity and T [K] is the temperature. Both notations, S_A and S, refer to the VOCs source strength. S_A denotes the source strength derived from measurements, Eq. (4), and S is a general source term in the mass balance, Eq. (5).

In short, first the average source strength is calculated using Eq. (4). Then, the coefficients in Eq. (5) are adjusted to fit the calculated source strength for the measured average temperature and humidity. The fitting algorithm used is the fit() function in MATLAB [53].

Finally, by substituting Eq. (5) into Eq. (2) we get:

$$c_t = c_{t-1} \cdot e^{-n_t \Delta t} + \frac{S_1 \cdot T_t^{0.75} \cdot e^{S_2 \cdot AH_t - \frac{S_3}{T_t}}}{n_t V_e} \left(1 - e^{-n_t \Delta t}\right) \tag{6}$$

$$t = 1, 2, \ldots N \tag{7}$$

where, Δt is the length of the time step and t is the index for the time step. Each time step has its corresponding temperature, absolute humidity and ventilation rate.

The effective volume, V_e, and initial concentration, c_0, can be found by fitting the calculated concentration to the measured concentrations. This is done by using the *Global Optimization Toolbox* in MATLAB to minimize the difference between model output and measured results.

4. Results and discussion

Several VOC's are measured using the passive sampling technique described above. However, only a selection of the measurements are presented; TVOC, formaldehyde, sum of terpenes (α-pinene, β-pinene, 3-carene, limonene, camphene, myrcene) and sum of aldehydes (butanal, pentanal, hexanal, heptanal, octanal, nonanal, decanal).

The results from measurements together with supply ventilation and humidity are shown in Fig. 3 (room 1) and Fig. 4 (room 2). Temperature and supply ventilation airflow is measured by the ventilation system and presented as hourly values as well as average values over the sampling periods.

As indicated earlier, during the second sampling period the ventilation rate is set close to zero (both in room 1 and room 2 which results in increased concentrations. The idea is that a clear peak in concentration followed by a decrease when the ventilation is turned back on would facilitate finding an effective storage capacity for the room to use in the calculation model. Also, by setting the ventilation rate to zero it is possible to get an idea of the highest achievable average concentration.

For the remaining sampling periods (after the second period) the ventilation rate is kept at predefined levels except during periods when the room is occupied. These periods can be recognized by much larger ventilation flows, which are automatically controlled by the presence and temperature sensors in the room. Also, for some shorter periods, the ventilation system is undergoing maintenance and is therefore turned off. For this reason, the median K_v is used rather than its average value when calculating the source strength with Eq. (4).

In room 1 (Fig. 3) concentrations increases during the second measurement period, when the ventilation is running at a lower rate. When the ventilation rate is increased in the following sampling period, concentrations decrease towards the levels found before the ventilation rate is reduced. However, in the remaining sampling periods, except from the last one, there is a small gradual increase in concentration for all TVOCs.
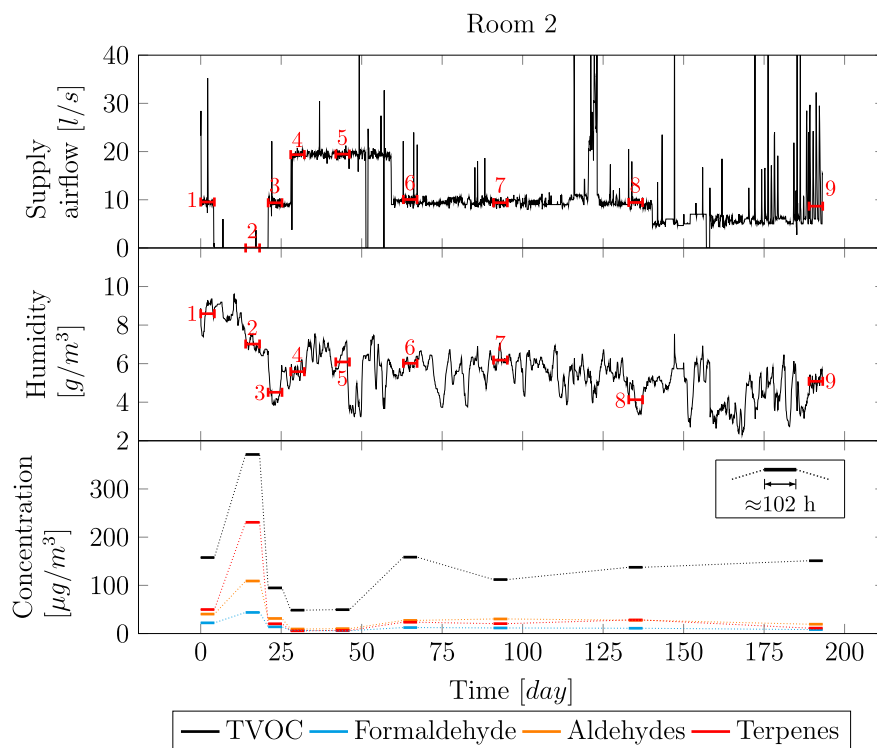
Fig. 4. Measured supply ventilation, humidity and measured VOC concentrations in room 2. Sampling periods are numbered from 1 to 9. The horizontal bars show the measured average concentration during each measurement period and the dashed lines, between each measurement, are added to visualize trends. The length of each measurement period is 4 days and 6–8 h (≈102 h).

As in room 1, the ventilation rate in room 2 is set close to zero during the second sampling period. Concentrations decrease from their peak values to lower values during period 4 and 5 when ventilation rates are higher. When the ventilation rate decrease again after period 5 concentrations increase and reach relatively steady levels throughout the remainder of the measurements. Similar to room 1, there is no clear tendency towards a further decrease in concentration. However, there is no clear trend towards increased concentrations either, as observed in room 1. Instead, concentrations reach relatively steady levels after about 60 days.

4.1. Source strength and humidity dependency

Figs. 5 and 6 show average source strength calculated with Eq. (4) and plotted against average absolute humidity. The sampling periods are numbered from 1 to 9 where 1 is the first sampling period and 9 is the last sampling period. The blue curve shows Eq. (5) fitted against average source strengths and measured average temperature and average absolute humidity. The R-square value in the title of each plot indicates the fitting degree of the source model. Red data points are values that lowers the fitting degree significantly and are therefore considered outliers, these values are excluded from the fitting process.

To simplify the visualization of results, the predicted values (blue curve) are calculated, using Eq. (5), for an average temperature rather than the actual measured temperatures. Since the influence from temperature on the source strength is much smaller than the influence from humidity, this simplification does not result in any major loss of information.

In both rooms, Figs. 5 and 6 (room 1 and room 2), measurement point 2 is excluded when fitting the source model. During this sampling period the ventilation rate is close to zero and the source strength can for this reason not be described by Eq. (4). In room 1 (Fig. 5), also measurement point 3 is an outlier and is, therefore, removed when fitting the source model.

Since the calculation of the source strength is based on steady state conditions, there can be errors if the concentration during a significant part of the measurement period has not reached steady state. For example, such situations may occur when there are larger and more permanent changes in ventilation rates between two measurement periods. This can explain why the measurement periods 2 and 3 seem to be underestimated and overestimated, respectively. Prior to measurement period 2, there is a lower concentration which increases rapidly when the ventilation rate is turned down. The average concentration during the period is then lower than what it would be at steady state and the source strength becomes underestimated in the calculation. Similarly, for the measurement period 3, the concentration is changing from a higher level to a lower level as the ventilation rate is increased, and the source strength becomes overestimated.

The concentration of terpenes is unexpectedly high during sampling period 8, while concentrations for the remaining VOCs were not. In addition, α-pinene was found in a higher concentration within the group of terpenes during period 8. This compound may be related to, for example, fragrances or cleaning agents used for office cleaning. Similarly, the concentration of terpenes during sampling period 8 is somewhat higher also in room 1. Therefore, cleaning of the room is considered the most likely explanation.

In both rooms there is a positive correlation between the increased absolute humidity and source strength. The fitting degrees are decreasing with the complexity of the compounds considered. The two groups of chemically similar compounds, aldehydes and terpenes, show a high correlation and formaldehyde show the highest correlation. However, TVOC show a weaker correlation compared to formaldehyde, aldehydes and terpenes. This is not surprising since TVOC represent the total sum of measured VOCs where each of the VOC may respond differently to both humidity and temperature. Interestingly, the TVOC source strength shows better correlation with temperature if expressed in degree Celsius rather than degree Kelvin. This is not shown in the figures but was tested earlier in the project.
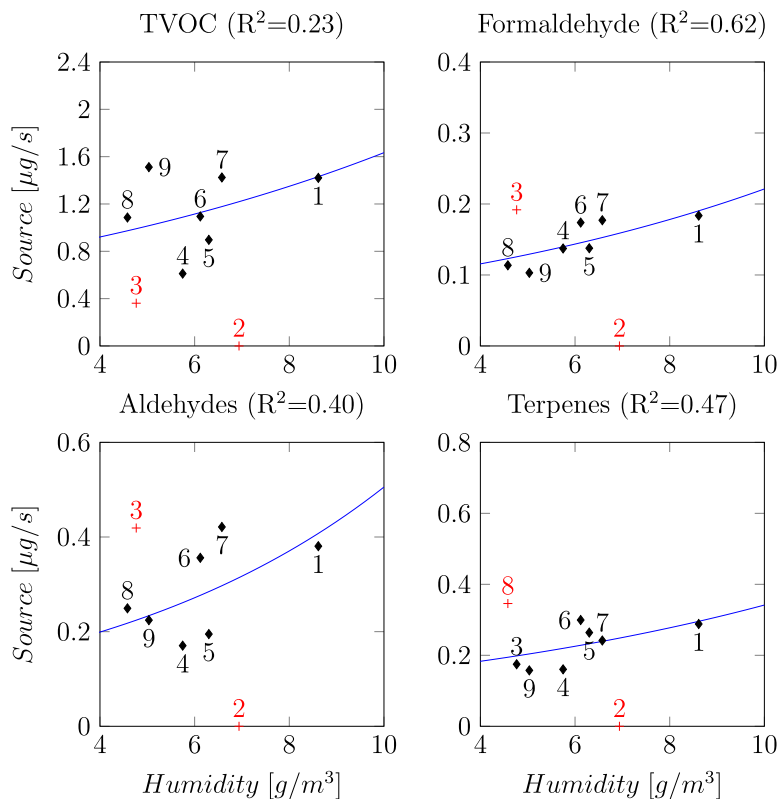
Room 1

Fig. 5. Calculated source strengths plotted against absolute humidity together with model predictions. The latter is plotted for an average temperature of 22.4 °C. The points were calculated from measurement data using Eq. (4) and the blue line is calculated with Eq. (5).

4.2. Simulations of room concentrations

Figs. 7 and 8 show the results from calculations of formaldehyde and sum of aldehydes using Eq. (6) together with average concentrations and corresponding results from measurements. Simulations are performed for both rooms and all four categories of VOCs. However, only simulations of formaldehyde and sum of aldehydes in room 2 are presented here since room 2, in comparison with room 1, have one more value that is not considered an outlier in the calculation of the source strength.

When determining the effective volume and initial concentration, the second sampling period is excluded in both simulations. During this period the ventilation rate was very low, see Fig. 4. At low ventilation rates, the air leakage becomes a large share of the total air change rate of the room and, therefore, the estimated effective volume and initial concentration become sensitive to the choice of air leakage. By excluding the second sampling period, results become less sensitive to how leaky the room is assumed to be.

Both simulations show high fitting degree with the measured data although somewhat higher for aldehydes, $R^2=0.93$ compared to $R^2=0.89$ for formaldehyde. The estimated effective volumes in both simulations are quite similar, 37 m^3 for formaldehyde and 45 m^3 for aldehydes. The initial concentration in both simulations had no effect on the fitting degree since the concentration decayed in time for the first measurement period as long as the initial concentration was not set extremely high. For simplicity, the initial concentration was therefore set to zero in both simulations.

For a closer view of the results, the section marked with an orange rectangle in Fig. 8 is enlarged and shown in Fig. 9. Three additional simulations are also added with either ventilation rate, absolute humidity or temperature set to its average measured value during the entire simulation period. This way, the effect of each of these parameters can

be compared. It should be noted that Fig. 9 only shows a section of the entire measurement period. However, several sections have been studied and they all show similar behaviour.

As can be seen in Fig. 9, temperature, during the chosen period, has negligible effects on the concentration since the curve calculated with averaged temperature closely follow the original, simulated concentration ($R^2 \approx 1.0$). However, this does also depend on how much the temperature varies during the period and one can expect that larger variations in temperature may have larger impact. The difference between *simulation* and *averaged ventilation rate* can be interpreted as the influence that absolute humidity has on the concentration. Likewise, the difference between *simulation* and *averaged absolute humidity* can be interpreted as the influence that ventilation rate has on the concentration. The fitting degree between *simulation* and *averaged ventilation rate* is $R^2=0.28$ and the fitting degree between *simulation* and *averaged absolute humidity* is $R^2=0.91$. Thus, ventilation is more influential on concentration than absolute humidity. However, it is important to note that this is just a section of the entire simulation period (shown in Fig. 8), and that the effects from humidity and ventilation rate depend also on their variations during the chosen simulation period.

5. Ventilation strategy — example

With a known room specific VOC storage capacity (effective volume), V_e, and a known source strength the concentration response to a change in ventilation rate can be simulated using Eq. (6). Given that the declination in source strength is negligible over shorter time spans, such as days or weeks, then it is possible to optimize the ventilation schedule to minimize energy losses while keeping VOC levels below a specified value during occupancy hours. Fig. 10 shows an example of what such an optimized ventilation strategy could look like. Here, model input
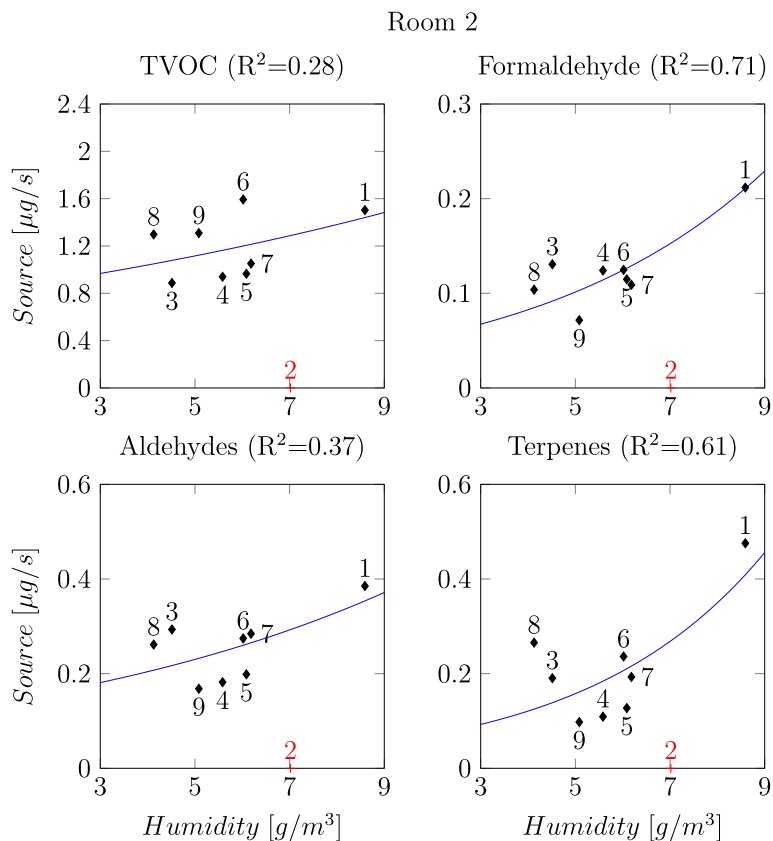
Fig. 6. Calculated source strengths plotted against absolute humidity together with model predictions. The latter is plotted for an average temperature of 21.3 °C. The dots are calculated from measurement data using Eq. (4) and the blue line is calculated with Equation.
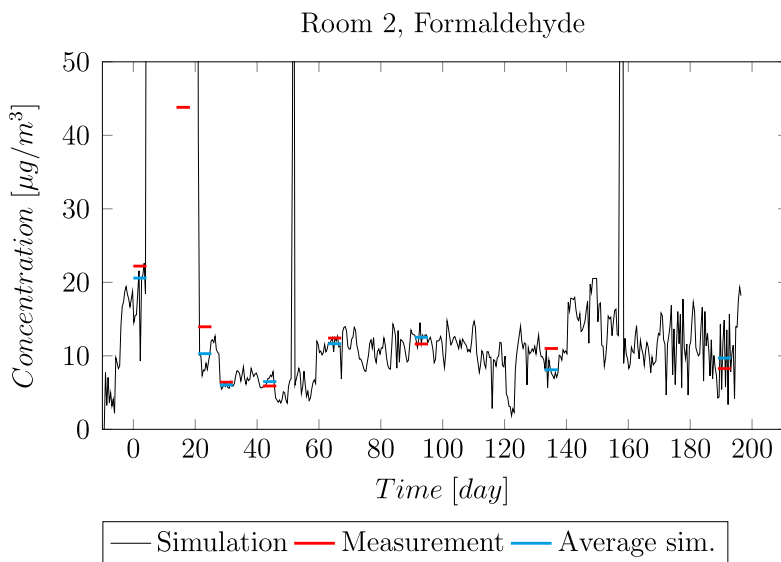

Fig. 7. Model prediction and measured formaldehyde concentrations. Input parameters: $c_0=0$, $V_e=37$ m³ and fitting degree: $R^2=0.89$.

parameters V_e, S_1, S_2 and S_3 are those determined in previous stages and used in Fig. 8.

In indoor air quality guidelines published by *Public Health England* it is recommended that the long-term exposure (1 year) of formaldehyde levels do not exceed 10 μgm⁻³ [54]. This recommendation is therefore used in the simulation in Fig. 10 as a maximum value for indoor formaldehyde levels during occupancy hours.

As can be seen, the ventilation rate is heavily reduced during non-office hours, to minimize energy losses, and set to normal rates during office hours (shaded areas). However, before the start of each working day, a ventilation "pulse" is forced to quickly reduce the concentration below the target threshold (10 μgm⁻³). The blue dashed line shows the average ventilation rate, 11.2 l/s, calculated from the scheduled ventilation rate. This can be compared with 15–20 l/s which is the
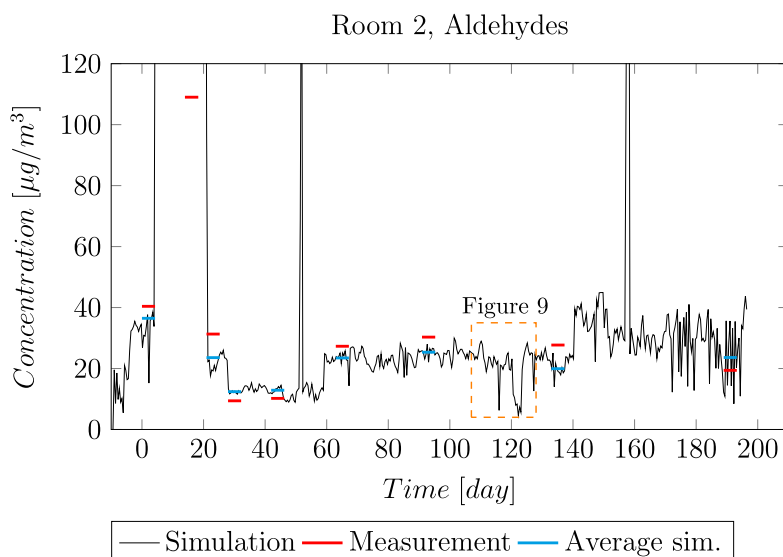
Fig. 8. Model prediction and measured aldehyde concentrations. Input parameters: c_0=0, V=45 m³ and fitting degree: R^2=0.93. The orange dashed rectangle marks the section that is enlarged in Fig. 9.
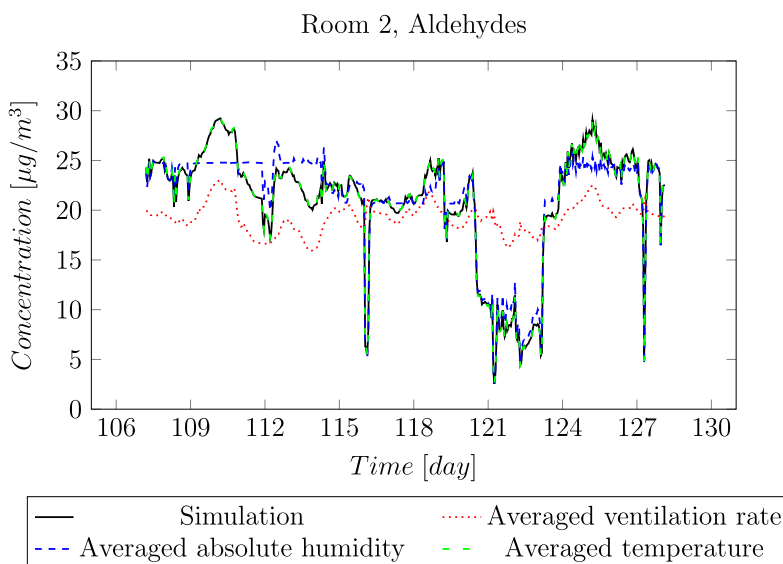

Fig. 9. Model prediction (orange dashed rectangle in Fig. 8) with sensitivity analysis for input parameters, ventilation rate, absolute humidity and temperature.

ventilation rate that would have been used if the ventilation schedule is not optimized.

Fig. 10 illustrates also two key concepts; (1) increased overall ventilation to reduce the total time with increased VOC concentrations may be unnecessary if concentrations can be allowed to increase above a given threshold for short periods of time, (2) if the source strength and storage capacity is known, a ventilation strategy can be used that reduces the overall ventilation rate without increasing VOC-levels during occupancy hours.

While the model also works for other timescales than those presented here, its major limitation is that spatial distribution of VOCs is not included and, thereby, transport mechanisms like diffusion within materials are not accounted for. The advantage of calibrating the model with time-averaged measured values for longer time periods such as hours or days is that occupancy related emissions, which are temporary and fluctuating, are averaged out while non-occupancy related emissions from materials are still accounted for. These are deliberate limitations to make the model feasible for the intended use, which is early stages of new buildings before normal activities have started.

6. Conclusions

This paper proposes a new alternative approach, VOC-passport, to control indoor concentrations of VOCs in the early stages of new- or newly renovated buildings. A model for calculating indoor VOC concentrations that accounts for ventilation rates, temperature and humidity is proposed where input parameters are determined from measurements in the field by using passive samplers. The model shows good agreement with measurements when TVOC is separated into individual compounds or groups of compounds, formaldehyde, aldehydes and terpenes. However, correlations between source strength and humidity show higher fitness degree when fewer VOCs are grouped together. A deeper analysis of the results suggests that indoor humidity and ventilation rate have major impacts on the early-stage concentration levels while temperature is less important. Air leakage may influence the results, especially if the ventilation rate is low, and it is therefore advisable to avoid near zero ventilation rates during measurements.

The proposed method is used to give an example of how a daily ventilation schedule may look like if the short-term VOC storage of the
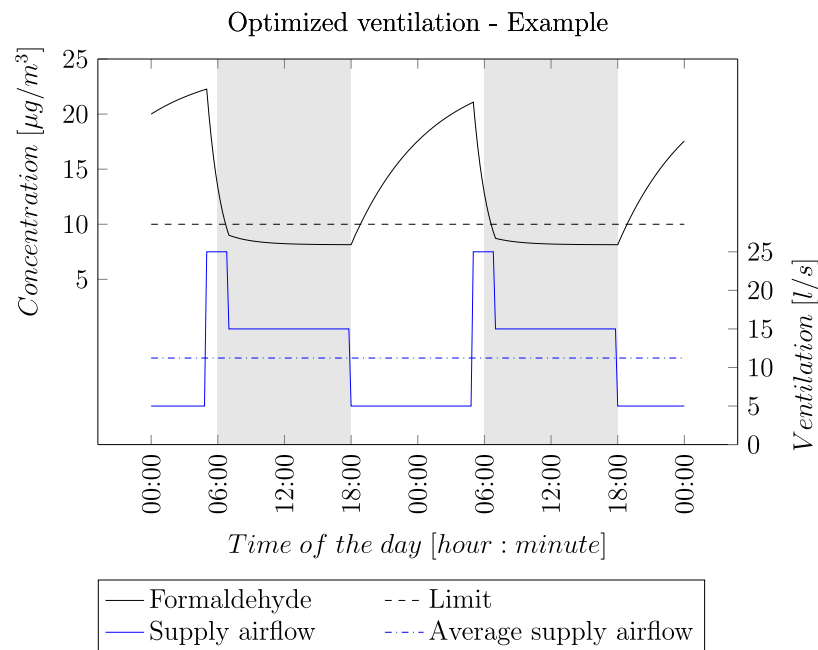
Fig. 10. Example of optimized ventilation strategy to keep formaldehyde levels below 10 μgm⁻³ during occupancy hours.

room is taken into account. The example illustrates that in buildings where VOC levels are allowed to increase periodically, VOC levels can be kept at acceptable levels during occupancy hours if the effective storage capacity is known. With the proposed method, there is no need to determine long-term source degradation, focus is instead on short term VOC storage and the reduction of VOC levels during occupancy hours while minimizing energy losses from ventilation.

This paper demonstrates successfully how numerical modelling together with early on-site measurements can be used to reduce energy losses by ventilation while ensuring a good indoor environment. The strength of the proposed method is that it does not rely on a database with material properties, instead it uses standardized on-site measurement methods. Future work will include both field- and laboratory measurements. Focus will be on further validation of the method for estimating effective storage capacity and method applicability for optimizing ventilation schedules.

CRediT authorship contribution statement

Fredrik Domhagen: Writing – review & editing, Writing – original draft, Data collection, Concept- and method development. **Sarka Langer:** Supervision, Review & editing, Data collection, Concept- and method development, Fund raising. **Angela Sasic Kalagasidis:** Supervision, Review & editing, Data collection, Concept- and method development, Fund raising.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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