

Modeling Dynamic Behavior of Volatile Organic Compounds in a Zero Energy Building

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ABSTRACT

With increasing building airtightness, the design of an adequate ventilation system gains importance. The first generation of ventilation systems, based on continuous supply of the nominal airflow rate, are now being replaced by Demand Controlled Ventilation (DCV). These systems, often H₂O and/or CO₂ controlled, do not take into account the emissions of Volatile Organic Compounds (VOCs) to the indoor environment.

A small, airtight, zero energy building that has been designed as the Belgian contribution to the international Solar Decathlon competition (2011) was rebuilt afterwards in Ostend, Belgium. This building will be used as test facility for the development and validation of a holistic VOC source model. In this study, results are obtained from thermal, airflow and contaminant simulation models of the test facility. The different models and modeling assumptions are discussed. A dynamic VOC source model, derived from literature, is used as proxy of possible VOC concentrations.

The results show an important influence of environmental parameters on the indoor VOC levels with VOC concentrations exceeding health guidelines. It is therefore important to design DCV systems and controls taking into account possible elevated VOC levels and while doing so, incorporate the dynamic behavior (influence of temperature and humidity) of the VOC emissions.

1 KEYWORDS

Modeling, VOCs, Case-study, Test facility

2 INTRODUCTION

Today's newly built and extensively renovated dwellings are built very airtight to reduce unwanted infiltration of cold air and as a consequence reduce heat losses. To safeguard the health of the occupants by keeping the Indoor Air Quality (IAQ) acceptable, ventilation systems must be installed in these homes. The first generation of ventilation systems are systems that supply outdoor air to 'dry' spaces (e.g. living room, bedroom) and extract contaminated air from the 'wet' spaces (e.g. kitchen, bathroom, toilet) both at a continuous volume flow rate. In Belgium, the nominal flow rate, depends on the type and size of the space and assumes worst case situations (BIN 1991). This constant flow of air dilutes the contaminants that are emitted indoors and by doing so, keeps the IAQ acceptable.

An issue with these systems is the fact that they provide the nominal airflow rate regardless of the actual need for dilution. By doing so, during the heating season, there will be more cold air that needs to be heated for thermal comfort, driving up the *ventilation heat losses*.

An efficient way to lower these ventilation heat losses is to install a second generation ventilation system, namely Demand Controlled Ventilation (DCV). These systems measure CO₂ and/or H₂O continuously and allow the volume flow rate to be lowered when the demand for dilution/ventilation is low. How the controls for these systems are set up is crucial to make sure the IAQ stays acceptable. That is why the Belgian legislation includes a '*method of equal performance*' which assesses the proposed controls based on Monte-Carlo, dynamic simulations of the system in a standardized reference house with average occupation. This method is developed by Heijmans et al. (Heijmans, Van Den Bossche, and Janssens 2007) and Laverge et al. (Laverge 2013).

Most of the current DCV systems as well as the assessment *method of equal performance* only consider CO₂ and H₂O as both are good indicators for comfort. The health aspect of IAQ is therefore overlooked in the development and assessment of these systems. A first step towards including this aspect in the assessment method is the consideration of Volatile Organic Compounds (VOCs) that are emitted by building materials, furniture and by performing certain activities. To do so, it is necessary to be able to simulate the emissions of VOCs to the indoor environment, including the dynamic behavior with relation to temperature and humidity. A holistic approach is necessary to be able to correctly model the exposure to VOCs of a simulated occupant and account for the interaction between outside conditions, the building, materials and HVAC systems.

To validate such a model it is necessary to have a reliable test setup outside of laboratory conditions which allows to account for all possible external influences on the VOC emissions and VOC concentration in the room. In this study, a thermal and airflow simulation model of a test facility, including a simplified temperature and humidity VOC model, are used to prove the importance of the external parameters and to evaluate the potential of this facility in performing VOC tests.

3 E-CUBE

In 2011, Ghent university participated in the Solar Decathlon competition. A zero energy house has been designed, named the 'E-cube' (Figure 1).



Figure 1 - E-cube test facility © UGent, photo Nic Vermeulen

After the competition, it was rebuilt in the Greenbridge science park in Ostend (Belgium). The E-cube will be used as a testing facility. All characteristics and HVAC systems of this building are well known and because the building is subject to real environmental conditions it is ideal for a series of measurements providing data for the validation of the VOC source model. Because of the open-plan design, the building can be assumed to be single-zone. Using the E-cube, several scenarios of increasing complexity can be measured under real, in-situ dynamic conditions.

The construction of the E-cube is made using pre-fab elements, which are a series of almost identical panels with a surface area of 2.5 m² each. A wall panel is either a closed panel, a fixed window panel or a operable window/door panel. The closed panels are built using a wooden frame and two plywood boards (1.2 cm) are enclosing 18 cm of PIR insulation. Roof and floor panels are similar but consist of 1.8 cm plywood boards. The windows are triple-glazed with low emissivity coatings and Argon filling. The frames are Aluminium CS104 which are specially developed for passive-house standard buildings (De Loof, Rottiers, and van de Walle 2011). Table 1 shows the overall dimensions of the floor, roof and facades.

Table 1. Surface area of boundary surfaces

	Total [m²]	Opaque [%]	Fixed window [%]	Operable window [%]
North Wall	44.6	78	6	17
East Wall	45.1	83	11	6
South Wall	44.6	61	28	11
West Wall	45.1	94	0	6
Roof	61.7	100	0	0
Floor	61.7	100	0	0

4 EMISSION MODEL

Research concerning VOC modeling started in 1979, in 1987 a procedure was developed to test material emissions (Sanchez, Mason, and Norris 1987). Based on these results Dunn published the first attempt to model VOC emissions (Dunn 1987). Based on the theory of Dunn his ‘deep source model’ Little et al. proposed a model based on physical parameters instead of statistical correlations (Little, Hodgson, and Gadgil 1994). This model still serves as a basis for more detailed and numerical models (Huang and Haghghat 2002; Xu and Zhang 2003; Yang et al. 2001). In 2004, the findings of different variations on the model of Little et al. were brought together by Deng et al. forming a new ‘standard’ for VOC emission models (Deng and Kim 2004). Today, new variations still occur taking into account more details (e. g. multi-layer situations (Deng et al. 2010)) or trying to simplify the existing models (Qian et al. 2007). All recent models can predict VOC emissions with good correlation in steady state conditions (constant temperature and humidity). However, almost all studies and measuring campaigns found that the VOC emission rate is strongly dependent on temperature and humidity, but in emission models these parameters are never really taken into account (Deng, Yang, and Zhang 2009; Lee and Kim 2012; Liang, Yang, and Yang 2015; Nazaroff et al. 2018; Salthammer and Uhde 2009; Sanchez, Mason, and Norris 1987; Zhang et al. 2007).

Emission rates from building materials are dependent on three material characteristics, diffusivity D_m , starting concentration C_0 and partitioning coefficient K_m . These parameters are dependent on temperature and humidity. Although this dependency was known from the start

of research concerning this subject, only recently, good correlations were found to take into account the dynamic character of D_m , C_0 and K_m (Deng, Yang, and Zhang 2009; Liang, Lv, and Yang 2016; Zhang et al. 2007).

The emission model used in this study, formula 1, is derived from literature and includes the temperature dependency for D_m and the temperature and humidity dependency for C_0 (De Jonge 2018). An important note is the fact that the emission model and the temperature and absolute humidity dependency have only been validated with measured data as separate models.

$$E(t) = 2.1 \frac{\left[d_1 T^{1.25} e^{\frac{d_2}{T}} \right] \left[(1 + C_1 AH) C_2 T^{-0.5} e^{\frac{-C_3}{T}} \right]}{\delta} e^{-2.36 \frac{\left[d_1 T^{1.25} e^{\frac{d_2}{T}} \right] t}{\delta^2}} \quad (1)$$

$E(t)$	[mg/m ² /h]	Emission rate
T	[K]	Material temperature
AH	[g/kg]	Absolute humidity
δ	[m]	Material thickness
t	[h]	Time since start of emissions
d_1, d_2	[varies]	Diffusivity material constants for VOC-material system
C_1, C_2, C_3	[varies]	Initial concentration material constants for VOC-material system

The chosen VOC to model was formaldehyde as, because of the high occurrence and related risk, it has been found to be the priority pollutant to assess (Kotzias et al. 2005; Brouwere et al. 2009). The material characteristics (d_1 , d_2 , C_1 , C_2 , C_3) are specific to the pollutant-material system and are not broadly available yet.

The proposed model will be used to model formaldehyde from Medium-Density Fiberboard (MDF). The amount of emissions from plywood might be different, but the overall reaction of emissions to external factors will be similar and makes it suitable for the intended purposes.

5 SIMULATION MODELS

In this study two simulation models are made: (1) a thermal model and (2) an airflow and contaminant model. The software used is Dymola and CONTAM respectively.

5.1 Thermal model

The thermal model in Dymola is modeled using the IDEAS v2.1 library which has been developed as part of IEA EBC Annex 60 (Jorissen et al. 2018). The open plan characteristic of the building makes it suitable for a 1-zone modeling approach. Only the external boundaries (external walls, windows and doors, floor and roof) of this zone are considered. Internal partition walls are not modelled.

The goal of this simulation model is achieving realistic surface temperatures of the walls, floor and ceiling. This surface temperature will later be used as input of the respective VOC-

source model of that component in CONTAM. The simulations will also provide a transient temperature profile to the zone which otherwise would be constant. Table 2 shows the characteristics of the materials used in construction.

Table 2. Material characteristics used for thermal simulations

		Multiplex	PIR-insulation
Thermal Conductivity	[W/(m.K)]	0.17	0.023
Specific Heat Capacity	[J/(kg.K)]	1 880	1 470
Density	[kg/m ³]	400	30
Longwave emissivity		0.86	0.8
Shortwave emissivity		0.44	0.8

The optical properties of the real installed glazing system of the E-cube were not documented. Based on the available description a similar glazing system is chosen from the catalogue of the LBL Window software (*Triple low-e (argon) - deflected*). The U-value of the simulated glazing system is 0.692 UNIT and has a g-value of 0.32 UNIT.

The U-value of the window CS 104 frame depends on the fact if they are operable windows or have a fixed frame. The operable window frame has a U-value of 1.16 whereas the fixed frame window has a U-value of 0.88.

On figure 2, the overall room temperature profile, the outside temperature profile and the different surface temperature profiles can be seen. The graph shows that the inside air temperatures are prone to variations of outside temperatures. This can be explained by the lack of available thermal mass of this construction type. This illustrates one of the common characteristics of lightweight constructions. Because of this, the risk of overheating will be higher. The detailed results show that the surface temperatures and thus temperatures influencing the emissions will be different for every surface but will follow the inside air temperature quite well.

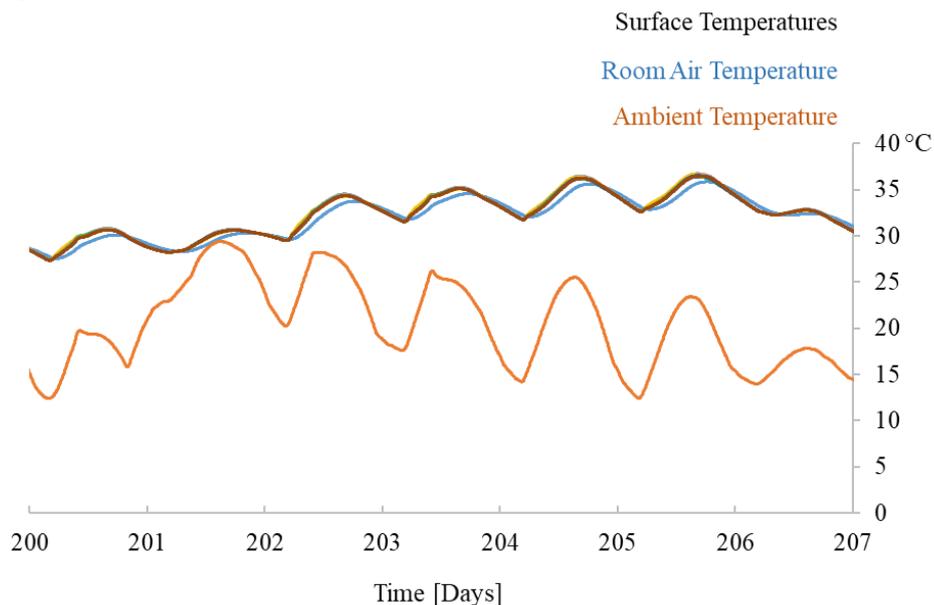


Figure 2 - Detail of ambient temperatures and temperature profiles obtained from thermal simulations (room air and surface temperatures)

5.2 Airflow model

The airflow and contaminant model has been made using CONTAM, a software especially developed for this purpose. This is a freely available simulation software developed by NIST (Dols and Polidoro 2015). The modelling approach is based on the model developed by (Heijmans, Van Den Bossche, and Janssens 2007) which has been used repeatedly to study CO₂ and H₂O controlled DCV ventilation (Laverge 2013; De Jonge, Janssens, and Laverge 2018; Caillou et al. 2014).

In this model, the E-cube is also modeled as being 1-zone. The leakiness of the boundary walls is modelled by the use of 4-airflow paths, each representing the air-leakage of 1/4th of what that wall would have. The wall is divided in four horizontal bands and each node is placed in the middle of that band.

The airflow element represents the cracks in 1 m² of wall for a building with a q50 value of 3 m³/h·m² multiplied by the surface area it represents. The wind pressure profile of this component is obtained from table A2.2 - Face 1-p. 258 (Liddament 1996).

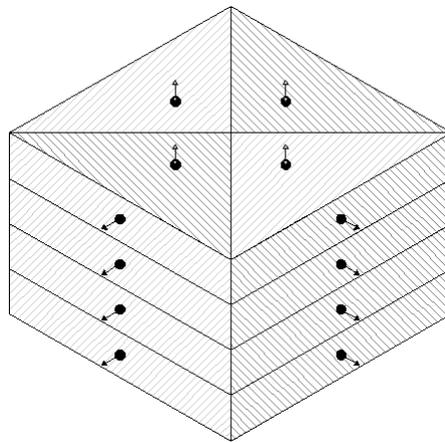


Figure 3 - Schematic drawing of the E-cube with positioning of airflow elements and the surface that each airflow element represents

Four airflow elements represent the leakiness of the flat roof as illustrated in figure 3. The wind pressure profile used for these elements is based on the same table (Table A2.2 – Roof <10°- p.258 (Liddament 1996). Although the roof is flat, a certain azimuth angle must be provided for every node. It was decided to give every element a different orientation (N, E, S and W). For the leakiness of the floor, a similar approach is adopted.

5.3 Contaminant model

The model represented by formula 1 is implemented in CONTAM as a super node with two transient input parameters: absolute humidity and temperature. As already stated, the five fixed parameters, which are the material characteristics, are not known for a broad range of materials yet. The emission model for MDF is therefore used as proxy for the VOC emissions coming from plywood.

For the humidity, no internal sources are considered as there will be no activity or human presence in the room during the experiment. A humidity buffering model is implemented using the ‘boundary layer diffusion model’. The buffering capabilities of wood are described by Heijmans et al. (Heijmans, Van Den Bossche, and Janssens 2007) and shown in table 3.

The absolute humidity used as input for the VOC emission model is assumed to be the same as the absolute humidity in the room.

Table 3. Input parameters of humidity buffer model for 1 m² wooden surface area

Film transfer Coefficient	[m/s]	0.0003
Film Density of Air	[kg/m ³]	14.34
Surface Mass	[kg]	0.00171
Partition Coefficient	[-]	0.684

The input temperatures of the emission model are the surface temperatures of the different surfaces and are obtained using the previously described thermal simulations. Transient temperatures are linked to CONTAM using a CVF file.

6 RESULTS

Figure 4, 5 and 6 show the running average of the results over 24 hours of the final simulation. The choice to plot the running average is made to get a better view on the yearly trends and overall better readability than the otherwise fast changing hourly data.

The black line is the same for each graph and is the formaldehyde concentration in the room air in mg/m³, the recommended maximum value by WHO for formaldehyde is 0.1 mg (Liteplo and World Health Organisation 2002). The Belgian indoor air quality decree also defines an intervention value of 0.1 mg/m³ ('Binnenmilieubesluit - Besluit van de Vlaamse Regering van 11 juni 2004 houdende maatregelen tot bestrijding van de gezondheidsrisico's door verontreiniging van het binnemilieu' n.d.). In a free-floating situation without any means of forced ventilation, this recommended value is exceeded for large periods of the year.

The first graph, figure 4, shows the indoor temperature profile. As shown in figure 2, this temperature can be seen as a good proxy for the different surface temperatures in the room because of the low thermal mass of the simulated protected volume. It is clear that the temperatures and the indoor VOC concentrations correlate.

The second graph, figure 5, shows the absolute humidity. As no events (e.g. showers, cooking) or humans are present (moisture in human breath), this humidity profile, even with buffering, follows the typical yearly outdoor profile. Less humid air during winter and highest peak humidity during summer. Because of the lack of events, the influence of humidity on the emission rate is less noticeable. Nevertheless, on closer investigation, it is clear that the effect of humidity may not be ignored. The trend of higher VOC concentrations during summer is also linked to the elevated humidity level.

The third graph, figure 6, shows the air change rate (ACH) per hour calculated with the outgoing air volume. On a yearly basis, the ACH will be lower during summer. This is directly related to the lower air speeds during this season. In general, an inverse correlation of the ACH and the VOC concentration can be seen. This makes sense: if the ACH rises the emitted VOCs will be diluted more efficiently thus lowering the VOC concentration.

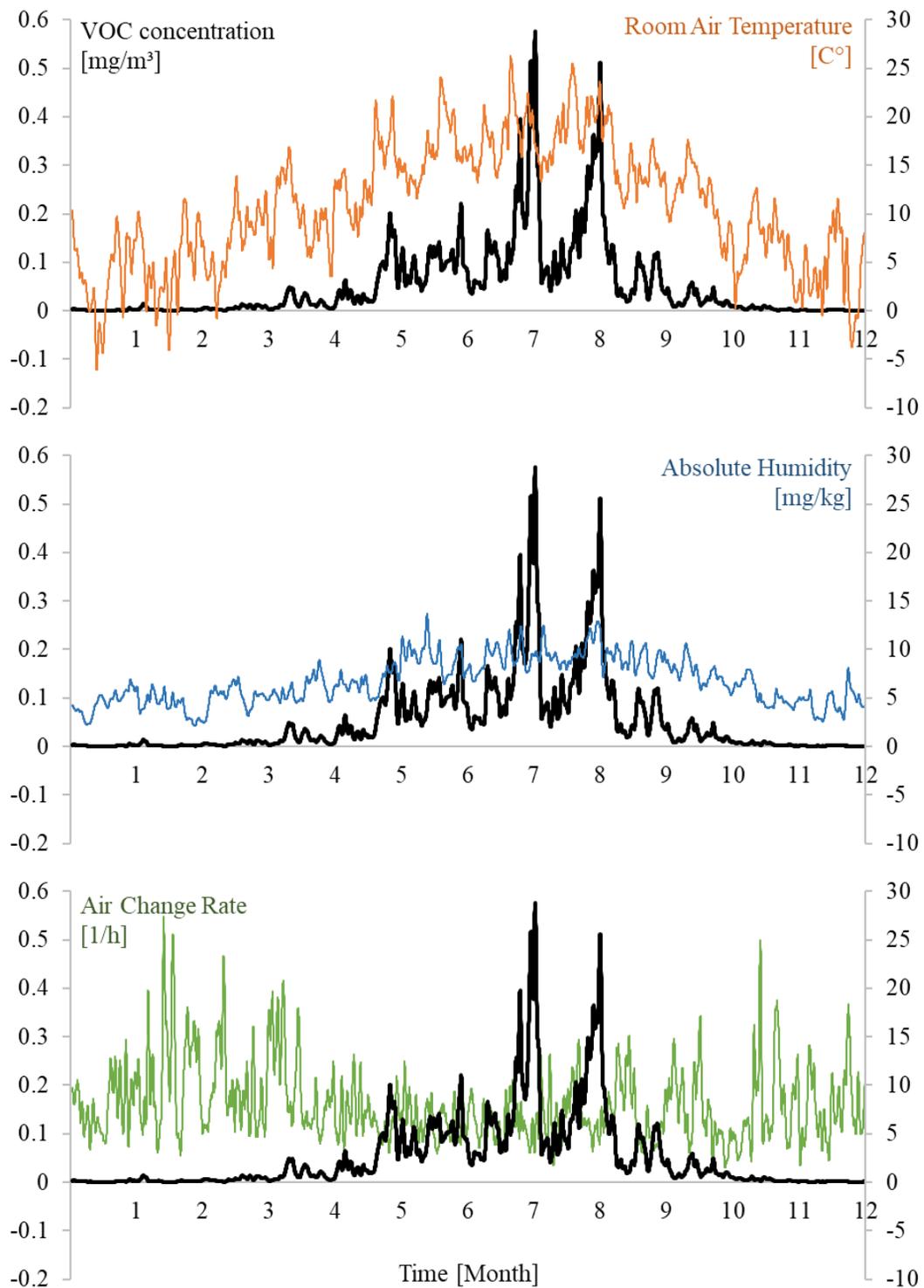


Figure 4-6 - Air Temperature (orange), Absolute Humidity (blue) and the Air Change Rate (green) together with the corresponding indoor VOC concentration

Figure 7 shows a detail of the simulated results for a hot summer week in June (not moving average). Depending on which moment of the year is looked at, other parameters appear to have the biggest influence. Overall, the detailed graph shows the same behavior as can be seen on yearly basis. When ACH goes up, VOC concentrations go down. When temperature and humidity rise, VOC concentrations go up.

A good example can be seen from day 205 to 206. On this day ACH stays relatively low all day. Combined with high emission rates, related to the high temperatures and humidity, the VOCs are accumulating and reaching a peak value, five times above the recommended value.

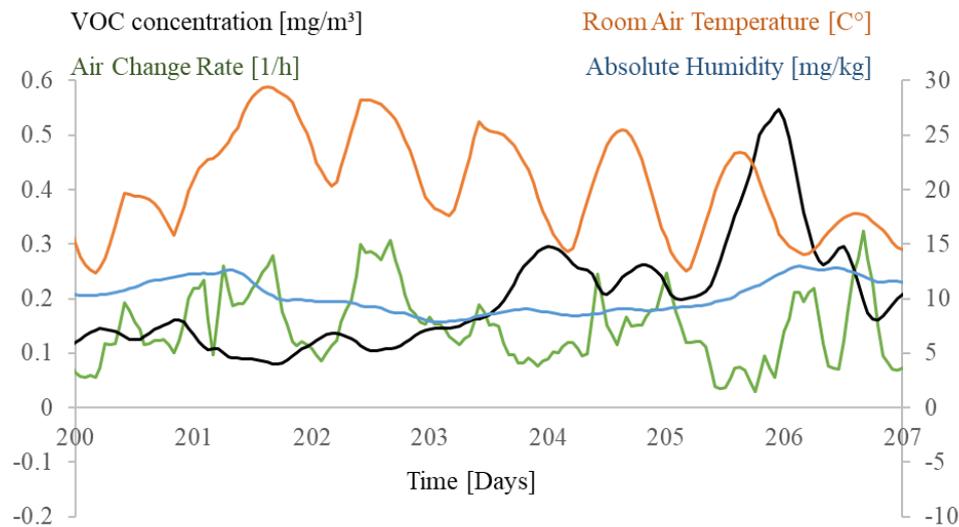


Figure 7 - Detail (one week) of VOC concentrations, Room Air Temperatures, Absolute Humidity and Air Change Rate

7 CONCLUSIONS

Like expected, temperatures and humidity are influencing the VOC concentrations to a large extend. The influence of these factors may not be underestimated and will have to be monitored alongside with the VOC content in the E-cube test facility to be able to fully understand the indoor VOC behavior.

This combined simulation is not taking into account the internal walls, local heat islands due to direct solar irradiation and temperature stratification. The internal walls might have a big impact on the actual indoor VOC levels: not only will it provide additional VOC source surfaces, it will also provide more thermal mass which will store more heat and will buffer more moisture.

IDEAS does take into account the solar gains by dividing the solar gains through the window over the entire surface. In reality however, the temperature rise will be more local with locally elevated VOC emissions as a consequence.

The last possible important factor that is not considered is temperature stratification. By decoupling the thermal and pressure/airflow simulations and the 1-zone assumption, thermal stratification along the height of the zone is not considered. This could have an important effect on both temperature driven airflows and surface temperatures of the test-facility and their influence on the ACH and VOC emissions respectively. For pressure differences due to stack effect, only the relative height of the different airflow elements is considered.

The high formaldehyde content can be explained by different factors. First of all, the amount of exposed wood in this construction is very high. Floor, ceiling and walls are all finished with plywood. Considering the fact that for the simulations the characteristics for (highly polluting) MDF is used instead of the characteristics of plywood, high VOC levels could be

expected. Secondly, no forced ventilation is simulated which will lead to situations of very low ACH for long times and the opportunity for VOCs to accumulate.

Nevertheless do the simulations show the important influence of external factors on VOC emissions and indoor VOC levels. It shows the need for test-facilities outside laboratory conditions, like the E-cube, as they are able to give insight in all possible factors. By monitoring real, in-situ but well controlled buildings, with lab-grade equipment, this set-up will provide data needed to validate the holistic VOC source model. With such a model, it will be possible to give reliable estimations of real, dynamic indoor VOC levels which are hard to measure using compact sensors. Such a model can be used during design of buildings, ventilation systems and ventilation system controls or can be used for legislative purposes.

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