Implementing Volatile Organic Compounds in CONTAM for assessment purposes: a review

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Abstract

Today's common demand controlled ventilation systems lower the ventilation airflow rate based on real-time CO₂ and H₂O measurements. Both ventilation system design and the Belgian assessment method for such systems, based on Monte-Carlo simulations, only consider these two comfort parameters. The health aspect of indoor air quality is thereby overlooked. A first step towards adding this aspect is the addition of Volatile Organic Compounds (VOC). As part of this research, eight different methods to model VOC emission and behavior in the airflow simulation software CONTAM are discussed: two methods to model event-based emissions, five methods to model continuous VOC emissions and one additional method to model sorption behavior. The overview illustrates the lack of an adequate, ready-to-use method that can be used to update the simulation based assessment method. Two methods (.CVF and TCP/IP) hold the potential to be used for this purpose but need to be further investigated.

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 (living room, bed room) and extract contaminated air from the 'wet' spaces (e.g. kitchen, bathroom, toilets) 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 (2007) and J. Laverge et al. (2011,2013) and is often performed using the airflow simulation software CONTAM developed by NIST (Dols and Polidoro 2015).

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 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, sorption effects and instantaneous emissions from events. A holistic approach is necessary to be able to correctly model the exposure to VOCs of a simulated occupant and allow the assessment of controls based on VOC monitoring.

This research and the development of this method is intended to make the research from material sciences directly available for engineering/design applications in DCV systems and legislation. Because the existing method has been developed using CONTAM, the extension for VOCs should ideally be done in CONTAM as well.

The implementation of such a VOC source model is not a standard option in the available CONTAM source/sink models. This paper gives an overview of the standard and less standard possibilities to model VOC emissions to the indoor environment.

Evaluation criteria

The evaluation of the different implementation methods is done based on the practicality for both research and industrial applications, the possibility to assess VOC controlled DCV systems and the possible accuracy for holistic assessment of long-term VOC exposure. The assessment criteria can be summarized in five categories:

- Location: is the source location fixed or virtually moving?
- Emission rate: is the emission rate scheduled, simulated (steady state/dynamic) and can it account for long-term emissions?
- Integration: is it implemented in the CONTAM software framework or is external software necessary?
- Possible emission models: does the implementation method allow for empirical, semi-empirical and/or numerical emission models?
- Other feature: is it possible to simulate a ventilation system controlled based on room VOC concentrations?

Table 1 summarizes the findings of each implementation method based on these criteria.

Review of implementation methods

Common VOC emissions in dwellings can be categorized in two ways: instantaneous, burst emissions and continuous, diffusion controlled emissions. The first group are emissions linked to events like cooking on a gas stove or cleaning (Logue et al. 2014; Nazaroff and Weschler 2004; Bonnet et al. 2018), the second are the VOCs that are emitted continuously from building materials and furniture as they diffuse out of the material (Salthammer, Mentese, and Marutzky 2010; Salthammer and Uhde 2009; Gene Tucker 1991; Bluyssen et al. 1997). Both cases are considered.

Burst emissions

Because the burst emissions are event-specific, the effect of temperature and humidity does not need to be considered here. CONTAM allows two ways to easily model this kind of behavior.

The first approach is the standard *CONTAM Burst Source Model*. This model allows the attachment of a schedule that controls, for every time step, if the model releases a pre-defined mass of VOC contaminant to the zone air or not. By altering the schedule value, it is possible to emit the pre-defined value multiplied with the factor defined in the schedule. This schedule, like any other, is always completely defined at the start of the simulation but can be used by several components operating with such a node. The Burst Source model is added to a certain room and is therefore always room specific. For modelling events with a fixed location, like cooking on a gas stove, this model is ideal. For events with a less-defined location, the second approach is more suitable.

This following, second, approach is *coupling VOC emissions to an occupant*. CONTAM allows virtual occupants to go from room to room. It also allows these occupants to be a source of contaminants. Usually, this function is used to simulate moisture and CO₂ production from breathing and transpiration. However, the software allows the addition of other contaminants and to couple these emissions to a schedule comparable to the one used in the Burst Source Model. By doing so, it is possible to simulate a moving source of VOCs coupled to the occupant performing the activity. For example, when someone is mopping the floor, the addition of VOC

contaminant mass will follow the person who is cleaning as that person moves from room to room.

Continuous emissions

Several measurement campaigns have named building materials as the biggest contributor of VOCs to the indoor air. Although the dependency of emissions on temperature and humidity has been known from the start of research concerning this subject (van Netten, Shirtliffe, and Svec 1989; Sanchez, Mason, and Norris 1987; Pickrell et al. 1984), to simplify testing procedures and modelling, steady state conditions were assumed for quite some time. Recently, several efforts were made to obtain temperature and humidity dependent material characteristics that influence the VOC emissions (Wal, Hoogeveen, and Wouda 1997; Liang, Lv, and Yang 2016; Q. Deng, Yang, and Zhang 2009; Y. Zhang et al. 2007). Other research then tried to model the emissions temperature and humidity dependent based on chamber emission testing (Xiong et al. 2016) or by updating an existing model including the newly specified material characteristics (De Jonge, Janssens, and Laverge 2018).

These semi-empirical models are specific for each VOC-material system and lack physical correlations. These models are therefore not satisfactory accurate for assessment purposes and thus it makes sense to look into all the different ways to implement VOC emission models in CONTAM, and not limit the overview to the implementation of these models.

Source-Sink model

From the several emission models integrated in CONTAM, there are two models closely resembling models currently found in literature about VOC emission modelling. The *Decaying source model* and the *Boundary layer diffusion model*.

The Decaying source model, models the emission of VOCs as a source with known initial emission rate and an exponential decay based on a given first-order decay constant (1).

$$S_a(t) = \text{mult. ctrl. } G_0 \cdot e^{\frac{-\Delta t}{t_c}} \quad (1)$$

With

$S_a(t)$ = Source strength of contaminant a at time t [kg_a/s]

G_0 = Initial generation rate [kg_a/s]

Δt = Elapsed time since the start of emission [s]

t_c = time constant [s]

mult = Source/sink multiplier [-]

ctrl = Schedule or control value [-]

(Dols and Polidoro 2015)

This model closely resembles the steady state, decaying behavior of early, semi-empirical analytical VOC emission models based on chamber emission testing (Dunn 1987; Reitzig et al. 1998; J. S. Zhang and Shaw 1997). Two major downsides are that it does not include the effect of temperature and humidity and that it assumes the decay as a function of time instead of as a function of

the VOCs left in the material. By adding a control node (see super-node approach later) which scales this function in relation to the temperature and humidity levels in the room, the effect of these parameters can be taken into account to some extent. The long term emissions will however not be modelled correctly.

The Boundary layer diffusion model (2), implemented in CONTAM is derived from the model presented by Axley (1991).

$$S_a(t) = ctrl.h.d.A_s \cdot \left[\frac{C_a(t) - C_s(t)}{k} \right] \quad (2)$$

With

h = film mass transfer coefficient over the sink [m/s]

d = film density of air [$\text{kg}_{\text{air}}/\text{m}^3$]

A_s = surface area of the adsorbent [m^2]

C_a = concentration in air [$\text{kg}_a/\text{kg}_{\text{air}}$]

C_s = concentration in the adsorbent surface [$\text{kg}_a / \text{kg}_s$]

k = Henry adsorption constant or the partition coefficient [$\text{kg}_{\text{air}}/\text{kg}_s$]

$ctrl$ = Schedule or control value

(Dols and Polidoro 2015)

This Boundary layer diffusion model only models the transport from the contaminant at the material surface to the bulk air and vice versa. Modelling the transition resistance at the surface and modelling the boundary layer above the material are two phases of the emissions often considered. The third aspect is the transport of the contaminants from inside the material to the surface by means of diffusion (Huang and Haghighat 2002). The diffusion characteristics of the specific contaminant-material system are not considered in this model. Because of this, together with the steady state assumptions for all parameters, the model is not adequate for the intended purposes (cfr. Introduction).

The assessment method should be able to assess the IAQ over periods of several year. The long term emissions are thus significantly more important than the (well-studied) initial emissions. Both models discussed here, are developed based on the initial emission behavior and are not able to capture the long-term emission behavior (even if scaled according to temperature and humidity). A more complex method will be necessary. Although not always intended for this purpose, CONTAM does allow some other methods to implement material VOC emissions.

Super-node control

One of the possibilities is the use of 'Control nodes'. A control node is intended to, as the name states, control certain elements in the software. It can also be used to control certain source/sink elements. If a control node is attached, the output of the connected source/sink element only emits its value times the value of the control.

Apart from well-known controls (e.g. Limit and band switches, Limit and band controllers, Proportional controllers, P/I controllers), one simple mathematical or

logical operation or a predefined function can be assigned to a node (e.g. addition, multiplication, AND, OR, EXP(x), SQRT(x)). With these nodes, a network can be constructed that can eventually equal a certain mathematical equation. This network can be bundled in a super-node to visually hide the network of control nodes and connected to control a constant emission source/sink node.

$$RH = \frac{P_w}{P_{ws}} \cdot 100\%$$

$$AH = \frac{B \cdot P_w}{P_{tot} \cdot P_w} \quad (3)$$

$$\ln\left(\frac{P_{ws}}{P_c}\right) = \frac{T_c}{T} \left(C_1 \cdot v + C_2 \cdot v^{1.5} + C_3 \cdot v^3 + C_4 \cdot v^{3.5} + C_5 \cdot v^4 + C_6 \cdot v^{7.5} \right)$$

where $B = 621,9907 \text{ g/kg}$ and $AH [\text{g/kg}]$

$$v = 1 - \frac{T}{T_c}$$

$$C_1 = -7.85951783$$

$$C_2 = 1.84408259$$

$$C_3 = -11.7866497$$

$$C_4 = 22.6807411$$

$$C_5 = -15.9618719$$

$$C_6 = 1.80122502$$

$$T_c = 647.096K$$

$$P_c = 220640hPa$$

(Wagner and Pr 2002)

Figure 1: CONTAM super-node equivalent to equation 3 (3) as it is implemented and visualized in CONTAM.

Although this approach seems promising, there are some serious limitations. Every node is programmed in a straight forward manner: input-operation-output, the signals are unidirectional. The equation to implement should therefore only have one unknown, should be written analytically and can only contain the mathematical operations that are included in CONTAM.

Because of the arguments mentioned above, implementing complex formulas is practically impossible. One node, not implemented correctly can make for false results that are hard to correct. The value of a control node or operation performed by a certain control node can only be viewed when opened for editing. Figure 1 and equation 3 show a formula and how it takes shape as a network of control nodes. The example is the conversion from AH to RH derived from the formulas by Wagner and Pruß (2002).

The advantage of this approach on the other hand is the ability to use the zone temperature and humidity as input signals. It is possible to implement a dynamic, but simplified, VOC emission model using this method.

Figure 2 shows the behavior of two models which are able to simulate VOC emissions: a decaying source model (generation rate: 10 µg/h, decay constant: 1/dy) and a T and AH dependent emission model implemented using the super-node control method (De Jonge, Janssens, and Laverge 2018). The results shown in Figure 2 are calculated relative to the values of a constant VOC emission model (generation rate: 10 µg/h), by doing so, the influence of varying air change rates due to the influence of ambient air/wind conditions are filtered out.

Figure 2: Left axis: Comparison of the relative behaviour of a decaying source model and a T and AH dependent VOC emission model (De Jonge, Janssens, and Laverge 2018) implemented using the super-node control method.

Right axis: temperature profile in the room in [°C].

The currently implemented input values for the different models are of less importance as it is the behavior of the models which should be looked at. As only the super-node approach allows for the influence of T and AH to be taken into account, only these results show the important correlation between rising temperatures and rising VOC

concentrations (Liang, Yang, and Yang 2015). Because of this influence and the necessity to take this effect into account, the super-node model will be, of the options which do not require external software, more accurate to model long term emission rates.

CVF control node

Another way to control a source/sink node is to connect it to a CVF node. Such a CVF node references to an external CVF file. This is a text file with a '.CVF' extension, and is not part of the project file. The way this file should be written is explained in the CONTAM manual and can, be made by using a spreadsheet program. In this file, a number of schedules can be defined and a control value linked to the different time steps of the simulation. Figure 2 shows the structure of such an CVF file.

For the purpose of implementing a complex VOC emission model, this file could contain a schedule containing the emission rates for every moment in time and be linked to the different source/sink nodes of the respective rooms. At the start of each simulation, CONTAM will use the values of the CVF file. By changing the values in the CVF file, new emission rates are introduced in the simulation.

ContinuousValuesFile ContamW 2.1					
CVF file used to implement VOC emissions in CONTAM					
1/1	12/31				
4					
VOC_E_LivingRoom					
VOC_E_Bedroom1					
VOC_E_Bedroom2					
VOC_E_Kitchen					
1/1	00:00:00	0.0174	0.0157	0.0174	0.0157
1/1	00:05:00	0.0510	0.0453	0.0510	0.0453
1/1	00:10:00	0.2779	0.2268	0.2779	0.2286
1/1	00:15:00	0.0825	0.0715	0.0825	0.0717
1/1	00:20:00	0.1116	0.0948	0.1116	0.0951
1/1	00:25:00	0.1382	0.1155	0.1382	0.1159
1/1	00:30:00	0.1623	0.1339	0.1623	0.1345
1/1	00:35:00	0.1839	0.1504	0.1839	0.1512
1/1	00:40:00	0.2031	0.1651	0.2031	0.1661
1/1	00:45:00	0.2201	0.1783	0.2201	0.1794
1/1	00:50:00	0.2350	0.1901	0.2350	0.1914
1/1	00:55:00	0.2480	0.2007	0.2480	0.2022
1/1	01:00:00	0.2594	0.2103	0.2594	0.2119
1/1	01:05:00	0.2693	0.2190	0.2693	0.2207
1/1	01:10:00	0.2779	0.2268	0.2779	0.2286

Figure 3: Start of a .CVF file which includes four VOC emission schedules (example). Each of the four columns on the right can be referred to by the names given at the start. For example, the first name, 'VOC_E_LivingRoom' column refers to the values of the 4th columns counting from the right.

To use this approach, two CONTAM simulations of the same project should be run. First, the simulation is run without any inputs to the VOC emission nodes. Results (including temperature and humidity) in all rooms can be exported. Based on these boundary conditions, the VOC emission rates can be calculated in an external software or programming language. If the CVF file is updated with these results and the CONTAM simulation is run again, the source/sink node will refer to these emission rates. Human exposure and internal contaminant transport can

be simulated together with for instance burst mode emissions from standard emission nodes.

The downside of this method is twofold. First, it will not be possible to use the room air contaminant concentration as boundary condition as it will not be possible to export these results from the initializing, first simulation. Secondly, the controls for other components (e.g. ventilation flow rates) cannot be controlled based on the room concentration. If done so, the airflow rates will become different and temperature and humidity levels will change to the point where the scheduled VOC emission rates based on the boundary conditions of the initial simulation are not valid anymore. If the dependencies are linear, this can be solved by doing multiple iterations. For this approach however, simulation time is much longer because the whole simulation has to be run several times.

TCP/IP method

CONTAM allows communication with other software by using TCP/IP socket communication. To do so, a project should be run directly in CONTAMx, which is the project solver, and activate the bridge mode. The other software will act as a server and predefined messages are sent back and forth between them.

If a named *constant* type control node is defined in the project file that controls a source/sink model, the value of this control node can be initialized using the *INPUT_CTRL_INFO_MSGTYPE* message type and modified during the simulation using the *ADJ_CTRL_NODE_MSGTYPE* message type. In other words, if for every time step the needed input values or boundary conditions are communicated to the external software, than that software can calculate the emission rate and send it back to CONTAM. With such a set-up it is possible to link controls to the indoor VOC levels as these will be calculated dynamically. The possible formulas that can be used for VOC emission modelling are only limited by the capabilities of the external software.

The downside of this method is that it will, most likely, require more computational power or take more time to simulate because it has to communicate with the external software. A second argument against this method is the fact that CONTAM, based on the available information in the manual (Dols and Polidoro 2015), only seems to allow one bridge mode. To correctly model the temperatures present in the building connections with TRNSYS and EnergyPlus are available based on the bridge mode TCP/IP communication. If the bridge is used for the VOC emission model, this connection will not be available anymore. Modelling the VOC emissions in one of those softwares will potentially resolve this issue but limits the possibilities for the VOC model to those of the chosen software.

Sorption modelling

Sorption effects (short for adsorption/desorption) have been repeatedly investigated and found to have an important buffering effect on the indoor air contaminant concentrations like VOCs (Axley 1991; B. Deng, Tian,

and Kim 2006; Matthews, Hawthorne, and Thompson 1987). It should therefore not be neglected.

Although ideally, the sorption effect is part of the simulated VOC transport and emissions, this effect could be modelled separately as a whole or to compensate for non-emitting surfaces that will act as extra area with sorption behavior.

The standard CONTAM source/sink model implemented for this buffering behavior is the deposition/resuspension model. Equation 4 shows how this model is described in CONTAM.

$$R_a(t) = v_d \cdot (mult \cdot A_s) \cdot \rho_{air}(t) \cdot C_a(t) \quad (4)$$

$$S_a(t) = (ctrl \cdot r \cdot A_r) \cdot L_a(t)$$

where

- $R_a(t)$ = Removal rate (by deposition) of contaminant a from zone air to surface at time t [kg_a/s]
 - v_d = Deposition velocity [m/s]
 - A_s = Deposition surface area [m²]
 - $\rho_{air}(t)$ = Density of air in the source zone at time t [kg_{air}/m³]
 - $C_a(t)$ = Concentration of contaminant a in zone air volume at time t [kg_a/kg_{air}]
 - $S_a(t)$ = Source (resuspension) rate of contaminant a from surface to zone air at time t [kg_a/s]
 - r = Resuspension rate [1/s]
 - A_r = Resuspension surface area [m²]
 - $L_a(t)$ = Concentration of contaminant a on the deposition surface at time t [kg_a/m²]
 - $mult$ = Source/sink multiplier [no units]
 - $ctrl$ = Schedule or control value [no units]
- (Dols and Polidoro 2015)

When this model is used separately from the continuous emission models to simulate two phenomena occurring on/with the same material, the interaction between both will not be accounted for. The resuspension rate in this case is independent of the deposition rate, which does not reflect the governing physics. An intermediate solution to model the sorption effect separately, is the boundary layer diffusion model (see continuous emission model). Modelling the sorption behavior as part of the continuous emission model should be preferred.

Discussion

Two of the possibilities discussed in this paper have the potential to serve the assessment method if some 'workarounds' are used, the .CVF method and the TCP/IP method. Although these approaches both seem promising. They both have distinct downsides and, at the time, are not readily available.

Generally, if several VOC emission model options should be tested for research purposes, a convenient way to implement numerical models of VOC source models is lacking.

For the purpose of this research (and possibly other engineering or design applications), the building and system model will probably have to be run hundreds of times. Especially, as is the case, when Monte-Carlo simulations come into play. Additionally, the assessment method this model will serve, should be easy to use by the industry.

CONTAM is not an open-sourced software. Because of this, the quality and speed of simulations can be guaranteed which is, of course, appreciated. For this research however, this can become a problem as the complexity of the desired model rises. An integrated solution for the VOC source model will therefore, in the end, be the best solution. If this could be possible in the

future, all calculation concerning airflow, contaminant transport and human exposures will stay integrated in CONTAM. Co-simulation with other software will only be necessary for the thermal calculations which, today, is already possible with TRNSYS and EnergyPlus.

Conclusion

This paper discussed the different possible ways to implement a VOC emission model in CONTAM. With the use of this model in an assessment method for DCV systems, based on Monte-Carlo dynamic simulations, the overview showed that none of the currently available options are adequate. This is because the integrated source/sink models always assume steady state, do not model the internal diffusion or are empirical models. Using several control nodes in a network only allows for simplified, analytical solutions but allows dynamic controls to VOC concentrations in the air.

Table 1: Scheme of discussed models and their features.

		Event emissions		Continuous emissions					Sorption behavior*	
		Burst Mode	Occupant Schedule	Existing Source/Sink		Super-node control	.CVF	TCP /IP	Existing Source/Sink	
				Decaying source	Boundary layer diffusion				Deposit /Resus.	Boundary layer diffusion
Location	Fixed	+		+	+				+	+
	Moving		+							
Emission rate	Scheduled	+	+				+			
	Simulated: Steady state			+	+	+	+	+	+	+
	Simulated: Dynamic (incl. T&H)			++	++	+	+	+		
	Long term E.	N/A	N/A				+	+	N/A	N/A
Integration	Integrated in contam	+	+	+	+	+			+	+
	External software						+	+		
Possible emission models	Empirical	N/A	N/A	+	+	+	+	+	N/A	N/A
	Semi-empirical					+	+	+		
	Numerical						+	+		
Other feature	Vent. Syst. Control linked to VOC	+	+	+	+	+	***	+	+	+

* If modelled separately

** Scaled according to T and H with super-node control

*** When multiple, whole simulation, iterations are done between CONTAM and the external software.

N/A – Not applicable

Two options with links to external software do hold the potential to provide the degrees of freedom necessary for the further development of the assessment method because the complexity of the VOC emission models is not limited by CONTAM anymore. For the .CVF file method, the approach with multiple iterations will be necessary to capture possible dynamic behavior due to controls related to the simulated VOC and will, as mentioned previously, require more time/computing power. The TCP/IP method, in combination with thermal calculations, will only be possible when the 'other' software being used is TRNSYS or EnergyPlus.

Table 1 gives an overview of the capabilities of all discussed methods to implement VOC emission behavior. Everything considered, as mentioned in the discussion section, does integrating a new Source/Sink model directly in CONTAM hold the greatest potential. This is not possible for non-developers as this software is not open-sourced. From all options discussed in this paper, does the use of TCP/IP socket communication and the .CVF method hold the most potential but both are yet to be developed in practice.

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