Dynamic Simulation Of Long-term Indoor VOC Concentrations In A Newly Renovated Residential Unit: A Pilot Study

Jun Guan[1], Weihui Liang[1], Xudong Yang[1, *]

[1]Tsinghua University, Beijing, China
[*]*xyang@tsinghua.edu.cn*

ABSTRACT
Dynamic simulation of indoor volatile organic compound (VOC) concentration variation in the long term would be an economical and effective approach for estimating the long-term exposure and related risk. And yet, most existing numerical studies either neglect the time factor, or only focus on short-term behaviors. In this study, we attempted to build a single zone air quality model of long-term indoor VOC concentration variation. For further analysis, a newly renovated apartment unit was selected for a preliminary case study of simulating the long-term trend of VOCs decay over one and a half years, with on-site measurements done once every one or three months. The results indicated that both previous experiment research and the modeling results show similar long-term decaying trend of VOCs indoors. However, the decay rate of simulated concentration curve was found to be faster than that of the measured trend. Possible interpretations of the above results were given in light of existing knowledge base. The work performed in this paper would be useful to understand the long-term VOC behavior in actual buildings, and offer a preliminary case study how to apply a simplified physical model to simulate the real world complex phenomenon.

KEYWORDS
Material emission, Volatile organic compound, Long-term decay, Indoor air quality, Simulation

1 INTRODUCTION

There have been scientific research findings about exposures and the risk of volatile organic compound (VOCs) derived from building materials, furnishings or other sources in indoor environment (Saijio and Kishi, 2004, Haghighat et al., 1994). In addition to experimental measurement methods, indoor air quality (IAQ) simulation seems to be a more convenient and fast way to understand the VOC behavior in actual buildings. Until now, there have been various IAQ simulation programs available, such as CONTAM3.0 by NIST (Walton and Dols, 2010), IAQX1.0 (U.S. EPA, 2000),ACCESS-IAQ (Yang and Chen, 2001) and CHAMPS-BES (Andreas and Zhang, 2007). And yet, most existing studies either neglect the time factor, or only focus on short-term behaviors. In fact, a few field measurement researches indicate that understanding how indoor VOC concentrations actually vary with long time would be helpful to estimate the long-term exposure and related risk (Guan et al. 2012, Parkand Ikeda 2006).

In this study, we attempted to build a single zone air quality model and to predict the long-term trend of VOC decay by numerical method. The simulated results would be compared with the previous research of a long-term observation on a newly renovated apartment unit for over one and a half years (Guan et al., 2012). Further discussion and conclusion were given for the IAQ model improvement.

2 METHODS

2.1 Mathematical model

To simplify the problem, well-mixed room model assumption is adopted in this study for our study of VOC concentrations in a residential unit within a multi-family residential building. Mass balance equation of the contaminant in a well-mixed space can be written as

$$V\frac{dC_a}{dt} = QC_{in} + \sum_i \dot{E}_{soi}A_{soi} - \sum_j \dot{S}_{sij}A_{sij} - QC_{out} \quad (1)$$

Where V is the volume of the zone, m^3;C_a is the VOC concentration in the zone, ug/m^3; t is time, s; Q is the ventilation rate of the zone, m^3/s; C_{in} is the VOC concentration at the supply inlet, ug/m^3; $\dot{E}_{soi}$ is the emission rate per square meter of the source material i, $ug/m^2/s$; $A_{soi}$is the area of the source material i, m^2; $\dot{S}_{sij}$ is the sorption rate per square meter of the sink material j, $ug/m^2/s$; $A_{sij}$is the area of the sink material j, m^2; C_{out} is the VOC outlet concentration, ug/m^3. For a well-mixed zone, $C_{out}=C_a$.

The ventilation rate (Q) should be obtained by simulation or on-site measurements. The values of $\dot{E}_{soi}$ and $\dot{S}_{sij}$ in equation (1) are determined using the emission source and sink models, respectively. For building materials as emission sources, models are divided into different categories. Detailed description of the emission source models used in this study can be found in Yang (1999) and Yang and Chen (2001).

2.2 Simulation procedure

To simulate indoor VOC concentrations in a single-zone residential unit, some information and key parameters in equation (1) need to be obtained. The basic simulation procedure can be generally divided into four steps: (1) collection of basic information, (2) selection of major emission sources, (3) environmental chamber tests to obtain the key emission parameters of each major emission source, and (4) dynamic simulation of indoor VOC levels (Liang et al., 2012). Detailed discussion of each step is given in the following case study section.

3. CASE STUDY

3.1 Basic information collection

In this study, a newly renovated apartment unit was selected for observation and simulation for over one and a half years, with on-site measurements done once every one or three months. The layout of the residential unit, located in Beijing, China, is shown in Fig. 1. The basic information needed includes the room volume "V" and ventilation rate "Q". Another important piece of basic information is to obtain a list of materials as potential VOC emissions sources. The area and volume of each room are given in Table 1. The total volume of the entire unit is 174.65 m^3.

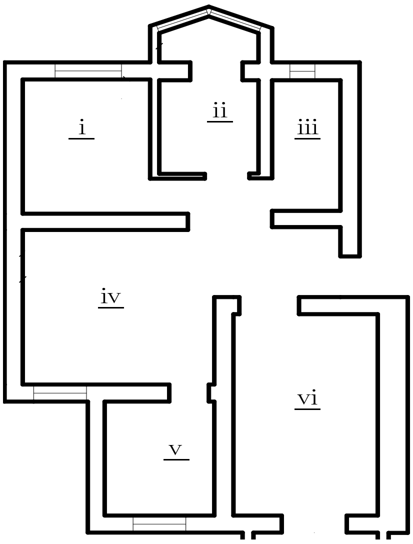


Figure1.*Layout of the selected residential unit*

As natural ventilation rate fluctuated with a certain random in real case, we measured the averaged air exchange rate (ACH) several times during the 1.5 years and the result was around 0.16 h^{-1} with all windows closed by means of tracer gas decay method (Sherman, 1990). In this case, CO_2 was used as the tracer gas. Thus, the simulation scenarios of the case study were simplified for two cases in Table 2. The equivalent air change rates at non-measurement period of Case 1 and Case 2 are set as 0.5h^{-1} and 2h^{-1}, which were represented for smaller and larger window/door opening range, respectively.

Table 1. *The area and volume of each room in the residential unit*

Room No.	*Name*	*Area (m^2)*	*Volume (m^3)*
i	Bedroom (North)	9.24	23.56
ii	Kitchen	7.4338	18.96
iii	Toilet	4.815	12.28
iv	Living & dining room	21.7772	55.53
v	Bedroom (South)	6.748	17.21
vi	Master bedroom	18.4761	47.11
Total	-	68.49	174.65

Table 2. *Simulated scenarios of the case study*

Item	Equivalent	Air change rate	Starting	Cut-off time	Total time of

	air change rate (h^{-1})	(all windows closed, h^{-1})	time of observation	of observation	observation (day)
Case 1	0.5	0.16	2010-5-19	2011-12-06	566
Case 2	2	0.16	2010-5-19	2011-12-06	566

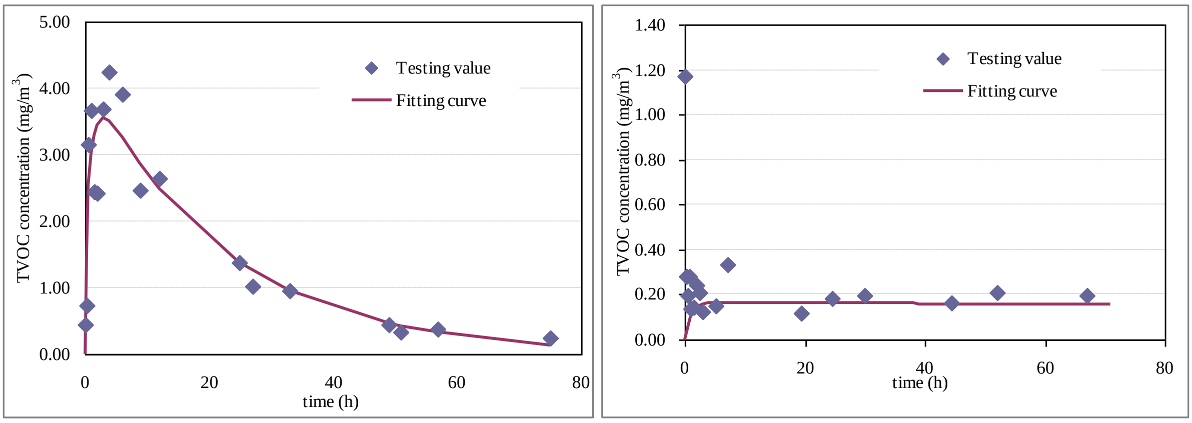
3.2 Main emission sources selection and tests

A single-zone model was attempted to simulate the long-term trend of VOC decay. Key emissions parameters of major VOC sources, including the diffusion coefficient, partition coefficient and initial concentration of VOC were obtained by previously verified small-scale environmental chamber method (ASTM, 1990). Details about these parameters, the source models, the test conditions and procedures can be found from the literature (e.g., He and Yang, 1999). The convective mass transfer coefficient was adopted to be 0.0003 m/s (Li and Niu, 2005).

The mainlyselected emission sources and their corresponding decoration record are shown in Table 3. Material test results and regression parameters of the materials are shown in Fig.2 and Table 4. For comparative analysis, all the input information for this single zone room model was attempted to be consistent with the real case (See table 1, 2, 3 and 4).

***Table 3**. Main decoration materials list*

Material	*Area of material(m^2)*	*Decoration date*
Wall paint	303.24	May 20, 2010
Wood door	9.41	May 25, 2010
Wood floor	56.24	June 1, 2010



(a) Wall paint+putty assembly; (b) Wood floor

***Figure2.** Small-scale environment chamber test results of different decoration materials and their corresponding regression results*

***Table 4.** VOC regression results of selected decoration materials*

Emission materials	*Parameter*	*Value*
Wood floor	D (m^2/s)	$6.31*10^{-14}$
($\dot{m}=E_1e^{-k_1t}+E_2e^{-k_2t}$)	K (-)	4873.2
	C_0 (mg/ m^3)	571973

Putty+wall paint assembly	hm(m/s)	0.0025
	k_{11}(h^{-1})	2.087908
	k_{12}(h^{-1})	0.045286
	E_1 (ug/m^2.h)	15.34638
	E_2(ug/m^2.h)	10.19546

3.3 Modeling results

Fig. 3 gives the modeling results for long-term observation in this case. For a comparison, on-site measurement values were also presented in the figure (Jun Guan et al., 2012). It is evident that the decay trend of VOC both by modeling method (Case 1 and 2) and on-site measurement method is verified by modeling methods. Note that only total VOC is presented as an example to illustrate the simulation method.

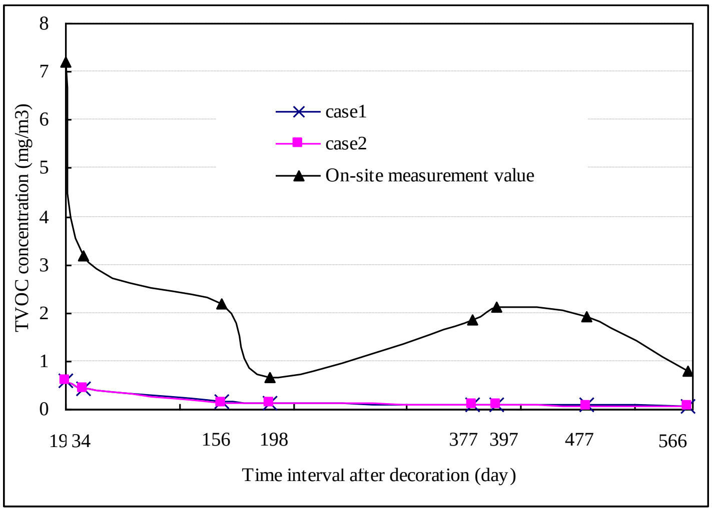


Figure3. *Modeling results for long-term observation*

In this figure, the values in case 1 are close to those in case 2. It indicate that air change rates contribute a little to VOC concentration of selected residential unit no matter what air change rate is lower (e.g, 0.5h^{-1}) or higher (e.g., 2h^{-1}) in the two cases. Furthermore, VOC concentration values of modeling results are far below those of on-site measurements.

The above-mentioned results in Fig.3 also show the inconsistency between on-site measurement and modeling. Combining with Fig.2, it just confirms that the impact of long-term decay for main decoration materials is much less than that of short-term decay as it resulted in fast decay of VOC concentration to the low level in few days after decoration.

4 DISCUSSION

Although the results from modeling results shows the similar decay trend comparing with those of on-site measurement, the evident inconsistency of decay rate between above two methods indicates that the single zone air quality model and its procedures need to be advanced for better accuracy with actual condition. And then, possible interpretations of the above results were accordingly given in light of existing knowledge base.

4.1 Mathematical model simplification

To simplify and clarify the problem, besides that a single zone air quality model was applied for simulation, the sink effect was neglected, though sink materials can also play a significant role in indoor VOC concentrations (Won et al 2001; Deng et al 2012). Notice that although the model can incorporate the sink effect into the IAQ model, sink model help to reduce the concentration level and enlarge the gap of the results between the two methods.

4.2 Ventilation information collection

ACH as an important ventilation parameter should be classified and obtained for the modeling process. However, the ACH can vary over a wide range depending on building type and materials used, openings configuration (Gao and Lee 2011), outdoor environment (Ghiaus et al. 2006) and occupant behavior (Roetzel et al. 2010). In this study, two modeling cases under ACHs of 0.5 and 2 h^{-1} show the similar decay trend and rate. And thus it is indicated that lower sensibility happens to long-term decay of VOC concentration than short-term decay. However, notice that renovated materials are main VOC emission sources in this study. It can be concluded that material emission sources might be negligible for long-term decay simulation except that some individual VOCs in materials have the properties of long-term emission. Further sensibility analysis for other different or specific VOC emission sources under different ACHs should be conducted for modeling improvement.

4.3 Source information collection and depiction

The higher concentration level by on-site measurements also indicates some unknown VOC sources were not concerned in this study except the renovated materials. Thus, it should get a more effective attempt to find other potential factors, such as human activity, family chemicals, ventilation or other purification strategies, etc. On the one hand, the source information should be noted down in time, and VOC emission model for the main sources should be figured out and incorporated into the IAQ model. One the other hand, above impact factors should be eliminated or quantified in process of on-site measurements if model validation will be done.

Notice that there has some uncertainty for natural ventilation, uniformity of room VOC concentration in this case, etc. Thus, experimental and modeling methods should be revised for better application to real buildings in light of above complex phenomenon in the future.

5 CONCLUSION AND IMPLICATION

In this paper, we tracked the long-term indoor VOC concentration decay of a newly renovated apartment unit, and attempted to simulate the long-term trend of VOC decay by applying a single zone air quality model. While both experiments and modeling results show a long-term decaying trend of VOCs indoors, the decay rate of simulated concentration curve was found to be faster than that of the measured trend. Possible interpretations of the above results were given in light of existing knowledge base. The work performed in this paper would be useful to understand the long-term VOC behavior in actual buildings, and offer a preliminary case study how to apply a physical model to simulate the real world complex phenomenon.

6 ACKNOWLEDGEMENT

This project is supported by the National Natural Science Foundation of China (No. 5087811) and China Postdoctoral Science Foundation (No. 2012M510458).

7 REFERENCES

Andreas Nicolai, Zhang J.S. and John Grunewald. 2007. Coupling strategies for combined simulation using multizone and building envelope models. In: Proceedings of the 10th International IBPSA Conference - Building Simulation 2007, Beijing, 1506-1513.

ASTM. 1990. *ASTM, D5116*, Standard Guide for Small-scale Environmental Chamber Determinations of Organic Emissions from Indoor Materials/products. Philadelphia: American Society of Testing and Materials.

Deng Q, Yang X, Zhang JS. 2012. Key factor analysis of VOC sorption and its impact on indoor concentrations: The role of ventilation. Building and Environment, 47: 182-187

Gao C, Lee WL. 2011. Evaluating the influence of openings configuration on natural ventilation performance of residential units in Hong Kong. Building and Environment, 46: 961-969.

Ghiaus C, Allard F, Santamouris M, Georgakis C, Nicol F (2006). Urban environment influence on natural ventilation potential. Building and Environment, 41: 395-406.

Guan J, Liang W, Yang X, Li Z. 2012.Long-term observation on indoor VOC concentrations in a newly renovated residential unit.In: Proceedings of 10th international conference of Healthy Buildings, Brisbane.

Haghighat F, Jiang Z, Zhang Y. 1994. The impact of ventilation rate and partition layout on the VOC emission rate: time-dependent contaminant removal. *Indoor Air*, 4: 276-283.

He G, Yang X. 2005.On regression method to obtain emission parameters of building materials.*Building and Environment*, 40: 1282-1287.

Li F, Niu J. 2005. Simultaneous estimation of VOCs diffusion and partition coefficients in building materials via inverse analysis.*Building and Environment*, 40:1366–1374.

Liang W, Gao P, Guan J, Yang X. 2012. Modeling volatile organic compound (VOC) concentrations due to material emissions in a real residential unit. Part I: Methodology and a preliminary case study. Building Simulation: An International Journal, DOI: 10.1007/s12273-012-0083-6.

ParkJ. S., IkedaK. 2006. Variations of formaldehyde and VOC levels during 3 yearsin new and older homes.Indoor Air, 16: 129-135.

Roetzel A, Tsangrassoulis A, Dietrich U, Busching S (2010). A review of occupant control on natural ventilation.Renewable and Sustainable Energy Reviews. 14: 1001-1013.

Saijo Y, Kishi R, Sata F, Katakura Y, Urashima Y, Hatakeyama A, Kobayashi S, Jin K, Kurahashi N, Kondo T, Gong YY, Umemura T. 2004. Symptoms in relation to chemicals and dampness in newly built dwellings. International Archives of Occupational and Environmental Health, 77:461-470.

Sherman MH. 1990. Tracer-Gas techniques for measuring ventilation in a single zone. Building and Environment, 25(4): 365-374.

United States Environmental Protection Agency. 2000. Simulation tool kit for indoor air quality and inhalation exposure (IAQX) Version 1.0 user's guide (EPA-600/R-00-094)

Walton GN, Dols WS. 2010. CONTAMW 3.0 user manual. Gaithersburg, MD, USA: National Institute of Standards and Technology.

Won D, Sander DM, Shaw CY, Corsi RL (2001). Validation of the surface sink model for sorptive interactions between VOCs and indoor materials. Atmospheric Environment, 35: 4479–4488.

Yang X. 1999.Study of building material emissions and indoor air quality, PhD Dissertation, Department of Architecture, Massachusetts Institute of Technology, USA.

Yang X, Chen Q. 2001. A coupled airflow and source/sink model for simulating indoor VOC exposures. Indoor air, 11:257-269.