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Evaluation of indoor air quality based on qualitative, quantitative and olfactory analysis

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In studying indoor atmospheric pollution, the concentration of air pollutants is considered to be the primary factor in judging indoor pollution level, while sensory effects accessed by olfactory analysis has not been paid enough attention. In this paper, twenty living rooms in Beijing including newly decorated, 3 months and 6 months after decoration were sampled once a day for 10 d, and qualitative analysis, quantitative analysis and olfactory analysis of volatile organic compounds were carried out. The results showed the concentrations of the 6 main compounds surpassed the limitation values released by World Health Organization; the pollutants with highest chemical concentrations were not the most odor active odorants. Olfactory analysis which measured the odor characters such as odor detection threshold (ODT), odor active value (OAV) and odor quality was a helpful tool to identify possible chemicals which cause indoor smelling issues, and it was necessary to access indoor air quality in combination with their chemical concentrations to give a comprehensive judgment on indoor air quality.

indoor air pollution, chemical concentration, odor detection threshold (ODT), odor active value (OAV), odor quality

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In recent years, pollution caused by indoor decoration has become more and more serious. As most people spend about 90% of their time indoors [1], the influence of indoor air contamination is long-termed and consecutive. Prolonged exposure to indoor toxicants can potentially lead to a variety of health issues such as dysthesia, transient morbidity, disability, disease, and even death in extreme cases [2]. Lots of studies have been performed and great public concerns have been drawn to the indoor air contamination, and the results showed that volatile organic compounds (VOCs) are the main and ubiquitous pollutants [3].

In studying indoor VOCs, with respect of connection between pollutants and human health, the toxicities of pollutants were the principal issue [4], the chemical concentration was considered to be the primary factor in judging the intensity of indoor odor pollution [5]. Therefore, series of guidelines and regulations released in many countries were concentrated on the concentration limitation of indoor air pollutants based on toxicities [6,7].

However, some VOCs that commonly detected indoor are associated with odor [8], among which some pollutants with concentrations even lower than the limitation can strongly impact the overall sensory impression. Odor can also cause a variety of undesirable reactions among people, ranging from annoyances to documented health issues [9]. Therefore it is necessary to investigate the odor characters of pollutants combining with the concentration.

Odor characters are tested by sensory measurement by human olfactory system. Two factors including odor active value (OAV) and odor quality are usually used in odor evaluation. OAV, which is defined as the concentration of chemical pollutant divided by its odor detection threshold (ODT) [10], is calculated to identify possible pollutants causing malodors or to express the odor activity of one odorous compound [11]. Among odor chemicals, only those with concentrations exceeding odor thresholds (OAVs are

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higher than 1) can be perceived. Odor quality is the characteristic of the smelled odor and is reported using odor description, which provides a referencing vocabulary for odor character and reflects the hedonic tone [12]. As odorants with the same OAV but with different odor qualities may smell significantly different, it is necessary to give the odor quality in odor description. Still, characterization of odors (qualitative and quantitative) can help to identify pollution sources and play an important role in evaluating indoor air quality due to great human sensitivity to odor [13].

In this study, twenty living rooms in Beijing including newly decorated, 3 months and 6 months after decoration were sampled once a day for 10 d. Qualitative, quantitative, and olfactory analysis of VOC pollutants were carried out. The results showed that a variety of organic odor pollutants including alkane, halogenated alkanes, alcohols, aldehydes, ketones, esters, ethers, and benzene series compounds were detected in the samples. The compounds with the highest concentrations in the samples were not the most odor active pollutants. Odor quality of a sample was complicated, which was different from any of the components or the sum of all. Olfactory analysis was helpful to give a comprehensive judgment on indoor air quality in combination with quantitative analysis.

1 Materials and methods

1.1 Material and instrument

β-Phenylethyl alcohol, isovaleric acid, methyl cyclopentanone, γ-undecanoate, β-methylindole, alkanes, aldehydes and ketones were all analytical grade reagents and purchased from J&K SCIENTIFIC LTD; alcohols, esters and benzene series compounds were analytical grade reagents and obtained from Beijing Chemical Reagents Company.

APSG-MW tubes (a glass tube filled with multi-walled carbon nanotubes bonding on the external surface of porous silica gel particulates), prepared by our laboratory [14]; Constant flow air sampler, (Beijing Municipal Institute of Labour Protection, China); Solid Phase Micro Extraction (SPME) (Supelco, USA); 1, 5, 10, 20 μL and 100-mL syringe (Agilent); thermal desorption (TD) and GC-MS (Thermo TRACE GC 2000, TRACE DSQ), (Thermo Electron Corporation, USA); dynamic olfactometer, (Stillwater, Minnesota, USA).

The desorption temperature of TD was 250°C, and helium (purity 99.999%) was used as carrier with a flow rate of 0.1 L/min. GC/MS was equipped with a DB-5MS capillary column (30 m in length, 0.25 mm in diameter, with a 0.25-μm thick film). Helium (purity 99.999%) was used as carrier, with a constant flow rate of 0.9 mL/min. The injection port was maintained at 220°C with a 15:1 split ratio. The initial oven temperature was 50°C and kept for 10 min, and then increased to 200°C at a rate of 10°C/min. The temperature of the ion source in the MS was 250°C.

1.2 Sampling and samples analysis

Twenty resident domiciles in Beijing including newly decorated, 3 months and 6 months after decoration were sampled and analyzed for consecutive 10 days in August. Doors and windows were kept closed for 24 h before sampling. Sampling was performed by APSG-MW tubes connected with air sampling pump at room temperature, with a flow-rate of 0.5 L/min and sampling time of 10 min.

Samples were subsequently analyzed by GC-MS. The desorbed samples were carried out from APSG-MW tubes by carrier gas of TD after pre-heating for 2 min [14]. At the same time, the desorbed gas was collected with a 100-mL syringe and the VOCs were extracted by a SPME device for 15 min. Then samples extracted in SPME were desorbed in the injection port of the GC, and the sample analysis was done by GC-MS. Compound identification was based on target ions and qualifier ions of mass spectrum, retention times and comparison with library spectra. Quantification was based on regression lines, which were calculated over a range of 6 levels of concentrations versus the corresponding abundances.

1.3 Olfactory analysis

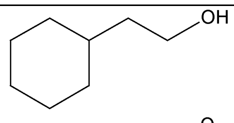
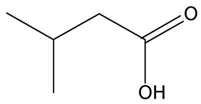
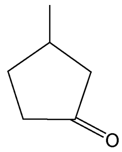
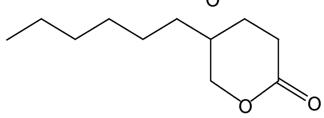
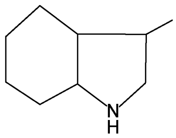
The medical ethics committee of University of Science and Technology Beijing (USTB) approved the protocol prior to the start of this study. All the research was performed in accordance with the Declaration of Helsinki.

Subjects between 22 and 32 years old who do not smoke were invited to attend a screening test [15]. At the start of this session, all subjects signed informed consent. They thereupon screened with 5 standard odorous dilution liquids with certain concentrations as shown in Table 1. Their odor qualities were also described.

At first, 5 odorless tapes (size: 14 cm×7 mm) were prepared, and the top 1 cm of each tapes were marked as test part, the test parts of 2 tapes were soaked in a standard stimuli liquid. The remaining 3 tapes were soaked in the odor-free liquid using the same method. When the 5 soaked tapes were presented to the subjects, they were instructed to distinguish the 2 tapes containing the odorant. Each subject tested the 5 standard odorants using the same method. The subjects who could distinguish all the 5 standard odorants correctly from other 3 odorless tapes in each trial could pass the panel screening test and perform the further study.

(1) Experimental condition. Sixteen participants composed of 8 males and 8 females were finally selected. The test was carried out in an odor-free room with a temperature of 20°C and a relative humidity of 35%. The duration of smelling was less than 2 s, which was considered long enough to collect information of odors [16]. To avoid the participants from fatigue smelling, there was a 2 min break between tests of each stimulus, which was considered to be long enough to allow the olfactory epithelium recovery

Table 1 Standard odorant and standard density used for the screening test

	Standard odorant	Structural formula	Concentration (w/w)	Odor type
A	*β*-Phenylethyl Alcohol		$10^{-4.0}$	Flowery, floral
B	Isovaleric acid		$10^{-5.0}$	Bromidrosis
C	Methyl cyclopentanone		$10^{-4.5}$	Sweet rice crust
D	*γ*-Undecaractone		$10^{-4.5}$	Fruit aroma
E	*β*-Methylindole		$10^{-5.0}$	Manure smelly

from sensory adaptation [17]. During the break, the participants reported their results.

(2) Procedure. Triangle odor bag method [15] was used with some modification for the assessment of odor detection threshold (ODT) of single VOC: when deciding the testing order of samples with different odor strengths presented to the panel, we took into account the fact that a weak odor (higher dilution) becomes more difficult to detect after introducing a strong odor (lower dilution). A descending order of odor strength is prone to intrigue olfactory adaptation of panelists. Therefore, an ascending order presentation was used in the present study.

Three odorless bags were filled with the same volume of odor-free air until the bags were almost full and closed with silicone rubber stoppers. And then certain amount of objective substance was injected into one of the 3 bags through its label with a syringe. The injection volume should meet the required concentration, at which detection occurred by chance, i.e., sub-threshold level. The other 2 bags were filled only with odor-free air (the same volumes as the first one). The 3 bags were delivered together to a subject, and he or she was instructed to smell all the 3 bags and reported from which he or she sensed an odor. The selection was mandatory, so the participants had to pick one sample based on their own olfactory senses from three sample bags at each level.

When his or her answer was incorrect, the same procedure was carried out at the next stage in which the amount of the odor was added 3 times more than the first sample. This procedure continued until the panel gave a correct answer.

The threshold was calculated for each panelist using the following formula:

$$\mathrm{ODT}_A = \frac{\log a1 + \log a2}{2}, \quad (1)$$

ODT_A, odor detection threshold for panelist A; $a1$, correct maximum dilution ratio; $a2$, incorrect minimum dilution ratio.

The mean threshold values calculated for each panelist excluding minimum and maximum values was taken as the threshold value for a group of all the panelists.

For the assessment of odor quality of VOCs presented singly with certain concentration, 2 μL of analytical grade objective substance was injected into a Teflon bag filled with 10 L of purified air at room temperature and normal pressure. When completely volatilized, the gas mixture was diluted by dynamic olfactometer to the desired concentration (the concentration of target compound tested in the real sample). Odor participants were instructed to smell at the sniffing port and describe the odor quality and evaluated whether it was easy to perceive. There were 4 levels could be used to access the difficulty for perception: easy, relatively easy, relatively hard and hard.

2 Results and discussion

2.1 VOCs detected by qualitative and quantitative analysis

TD-GC-MS analysis was firstly carried out to determine the main VOCs in the samples. Two hundred and fourty-two VOCs were detected, which could be classified as alkanes, esters, aromatics, alcohols, ketones, olefins, aldehydes, halohydrocarbo, cycloalkanes, ethers and other four types as shown in Table 2. The number of chemicals in certain class and the percentage of the number of chemicals in certain class attribute ratios to the total 242 chemicals are also listed in descending order. It shows clearly that the detected indoor compounds are in very large quantity and various types. And the most abundant VOCs are alkanes, esters, aromatics, alcohols and ketones. Compared to pollutants detected in office rooms [8], there are much more alcohols, ketones and esters, which may released by finishing material and fumes from the kitchen [18].

Considering the abundance and complexity of the pollutants indoors, only 40 pollutants with the presence percentage greater than 9.5% were listed in Table 3. The presence percentages was calculated by dividing the times that a pollutant be detected in the samples by the number of total samples collected, which was 200, and the compounds were listed in the decreasing order of their presence percentages According to the results, the detected VOCs could be classified as alkane, halogenated alkanes, alcohols, aldehydes, ketones, esters and benzene series compounds, which were also the most abundant classes shown in Table 2. Among them, benzene, naphthalene, tetrachloroethylene, trichloroethylene has been set as indoor pollutant with health risk by World Health Organization (WHO); toluene and *m,o*-xylene are in the way to be regulated by WHO [19].

Obviously the most frequently detected compounds were toluene, *m*-xylene, benzene, ethyl benzene, butyl acetate,

Table 2 Chemical class of compounds detected and their attribute ratio

Chemical class		Number of chemicals in certain class	Attribute ratio (%)[a]
Alkanes		66	27.2
Esters		35	14.4
Aromatics		34	14.0
Alcohols		22	9.1
Ketones		19	7.9
Olefins		18	7.4
Aldehydes		16	6.6
Halohydrocarbons		14	5.8
Cycloalkanes		10	4.1
Ethers		7	2.9
Others	3,5-Dihydroxybenzamide 1,2-Diaminopropane 6-Aminoundecane *p*-Benzoquinone	4	1.7

a) Number of the chemicals in certain type/the number of total chemicals detected (242).

Table 3 Compound detected from the samples of 20 living rooms and its detectable rate

Compounds	Frequency	Detectable rate (%)	Compounds	Frequency	Detectable rate (%)
Toluene	184	92.0	*n*-Decane	41	20.5
m-Xylene	162	81.0	Cyclohexanone	41	20.5
Benzene	150	75.0	Cyclohexane	40	20.0
Ethyl benzene	132	66.0	Nonanal	37	18.5
Butyl acetate	109	54.5	Styrene	35	17.5
o-Xylene	108	54.0	Nonane	31	15.5
α-Pinene	94	47.0	Decanal	31	15.5
Tetradecane	89	44.5	Ethanol	31	15.5
Dodecane	84	42.0	D-limonene	30	15.0
Tridecane	74	37.0	Cyclopentane	30	15.0
n-Pentadecane	70	35.0	Butane	25	12.5
Naphthalene	65	32.5	2-Butoxyethanol	25	12.5
Ethyl acetate	64	32.0	Dichloroethane	24	12.0
Hexanal	64	32.0	Tetrachloroethylene	24	12.0
Butanol	61	30.5	2-Ethyl-1-hexanol	23	11.5
Hendecane	59	29.5	Trichloroethylene	22	11.0
Pentane	58	29.0	Octyl aldehyde	22	11.0
Hexane	51	25.5	Butyraldehyde	20	10.0
Hexadecane	49	24.5	Isopropanol	19	9.5
1,2,3-Trimethylbenzene	48	24.0	Pentanol	19	9.5
Dichlorobenzene	44	22.0	Hendecanal	19	9.5

and *o*-xylene as their detectable rates were much greater than 50%. Most of them are ubiquitous VOCs in indoor air measured in European and North American field except for butyl acetate [3]. The 6 compounds with the highest mean chemical concentrations were listed in Table 4. The results showed toluene was the most abundant VOC in the indoor air, with a mean value of 0.34 mg/m^3; the concentrations of *m, o*-xylene was 0.32 mg/m^3, and the rest ranged from 0.040 to 0.090 mg/m^3. The relative standard deviations (RSD) of the relative response factor (RRF) ranged from 1.5% to 11.6%. The relative error for nine measurements (accuracy) ranged from 3.7% to 19%, and the precision for seven parallel samples ranged from 1.8% to 13.6%. According to the guidelines released by WHO [19], the contents of all the 6 main compounds surpassed the limit value set in the long-term guideline, which was 0.01 mg/m^3 to prevent potential malignant effects in the airway.

2.2 Odor characteristics of the main VOCs tested by olfactory analysis

Odor characteristics such as odor threshold and odor quality were tested by the method described in the Section of 1.3. Odor active values were calculated by the following equation:

$$\mathrm{OAV} = \frac{C}{\mathrm{ODT}}, \tag{2}$$

where C is the chemical concentration of the target compound. The results were listed in Table 4.

ODTs of the 6 main VOCs ranged from 0.077 to 8.8 mg/m^3; while OAVs ranged from 0.0046 to 1.8. The most odor active stimulus, *m*-xylene, with the highest OAV value of 1.8, was not the most abundant composition, neither the one with the lowest ODT. Therefore it was inadequate to evaluate the odor effect of VOCs only by their chemical concentrations or odor threshold. Combination of chemical analysis with olfactory analysis could provide considerably more information. It was also helpful in the management of indoor odor pollution by finding out the most odorous pollutants.

Table 4 Odor characteristics of the 6 main single VOCs

Stimulus	Mean concentration (mg/m^3)	Odor detection threshold (mg/m^3)	Odor active value
Toluene	0.34	1.3	0.27
m-Xylene	0.32	0.18	1.8
Benzene	0.040	8.8	0.0046
Ethylbenzene	0.080	0.75	0.11
Butyl acetate	0.090	0.077	1.2
o-Xylene	0.32	1.7	0.19

2.3 Analysis of change in odor quality

We also investigated correlation of measured odor qualities of the whole samples associated with the 6 main VOCs. The odor qualities of the 200 samples and the 6 main compounds whose detection frequencies were higher than 50% were measured. The perceived results were listed in Table 5.

The perceived results of the 200 indoor samples showed they were all irritating, unpleasant and easy to perceive, although the odor levels were not exactly the same. Most of the 6 main compounds were described as slightly sweet, except for ethyl benzene which was irritating.

The samples were mixtures of some compounds including the 6 main components. However, the result showed the perceived odor of the samples changed dramatically compared to those only containing one of the 6 main components: all the 200 samples smelt irritating. The odor preference reduced compared to the single substance. It was because the olfactory system recognized complex mixtures of odorants as single entities due to odor blending, but the perception of an odorant mixture is not a simple integration of the percepts of the unmixed components [20]. A mixture of odorants could elicit a novel odor percept through configural processing (i.e., perceptual odor blending) [21].

Moreover, we noticed that odors of the compounds with high concentrations such as toluene (0.34 mg/m^3) and *m*-xylene (0.32 mg/m^3) were difficult to be perceived. With regard to certain compounds such as benzene (0.04 mg/m^3), butyl acetate (0.09 mg/m^3) and ethyl benzene (0.080 mg/m^3), even low concentrations could produce strong odors which

Table 5 The perceived odor character of the whole samples and the main pollutants

Stimulus	Odor quality and hedonic tone	Level of difficulty for perception
The whole samples	Irritating, unpleasant	Easy
Benzene	Fragrant, pleasant	Easy
Toluene	Slightly bitter, relatively unpleasant	Hard
Butyl acetate	Sweet, pleasant	Easy
Ethylbenzene	Slightly spicy, relatively unpleasant	Easy
m-Xylene	Slightly sweet, pleasant	Relatively hard
Styrene	Slightly sweet, pleasant	Relatively easy

were easy to perceive. In traditional means, the hazardous effects were estimated only by judging their chemical concentrations [22]. However, compounds with low concentration could also be harmful, such as releasing irritate odor. By combining chemical analysis and olfactory tests, it was able to provide a comprehensive recognition of pollutants, and was helpful in harm prevention and control. On the other hand, the result confirmed the fact that odor quality is an important influence factor in environmental assessment when there are odorants and it is helpful in understanding which VOCs might sensory irritation.

3 Conclusions

The present study showed the indoor pollutants with highest chemical concentrations were not the most odor active odorants. Olfactory analysis which measured the odor characters such as ODT, OAV and odor quality was a helpful tool to identify possible chemicals which cause indoor smelling issues, and it was necessary to access indoor air quality in combination with their chemical concentrations. In addition, odor qualities of samples were complex and different from any content or the sum of all. Further investigations on multiple odor interactions are currently underway in our laboratory to unravel more details of odor quality.

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