CO_2 and volatile organic compounds as indicators of IAQ

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ABSTRACT

The trend toward minimizing ventilation of houses in order to reduce energy consumption for heating and cooling leads to an increase in indoor air pollution. The deterioration of indoor air quality (IAQ) negatively affects human health, safety, productivity and comfort. In order to evaluate the scale of this influence IAQ assessment has to be performed. However, the IAQ itself is not well defined and a number of parameters are considered as its indicators. In this work we compared carbon dioxide and volatile organic compounds as indicators of indoor air quality. In order to examine the problem, time series of CO_2 concentrations were considered as the source of information about IAQ. The data were obtained from continuous measurements of CO_2 and total volatile organic compounds (TVOCs). The following analytical instruments were applied: the non-dispersive infrared (NDIR) sensor – for CO_2 measurements, the photoionization detector (PID) and semiconductor gas sensors – for TVOCs determination. The correlation and regression analysis were applied to examine the relationship between measured quantities in two time scales, namely one day and 30 minutes. They reflect different time scales of CO_2 and volatile organic compounds (VOCs) concentration variation. Based on the analysis, we concluded that CO_2 and TVOCs measurements conveyed different information about IAQ, as a function of time. The analytical method had strong influence on the information obtained. In particular, the discrepancy was observed when comparing NDIR and PID methods. Also techniques applied for VOCs measurements provided different information about these substances. The results of our work entitle to conclude that the total concentration of VOCs should be taken into account as the indicator of IAQ in addition to CO_2.

KEYWORDS

Indoor air quality, correlation, sensor, time series, carbon dioxide, VOCs

1 INTRODUCTION

The fundamental requirement imposed on a heat, ventilation and air conditioning system is to assure appropriate indoor air quality (IAQ), thermal comfort and acoustic environment. This goal should be achieved cost-effectively (ASHRAE 62.1:2007; ISO 16814:2008). The attention is particularly focused on energy savings (Burman et al., 2014). The recent trend toward minimizing ventilation within houses in order to reduce energy consumption for heating and cooling leads to an increase in indoor air pollution level (Daisey et al. 2003; Crump, 2011; Yu et.al., 2009; Chung et al., 2001). The deterioration of indoor air quality negatively affects human health, safety, productivity, and wellness (Turune et al., 2014; Haverinen-Shaughnessy et al., 2015). One of main roles in IAQ assessment is played by indicators. In practice, it is difficult to determine the reference parameters describing chemical properties of air inside a building, because the "quality" of indoor air is not well defined. In case of thermal comfort, the situation is relatively simple. The main indicator for thermal comfort is room temperature or sometimes, a combination of temperature and humidity (specific enthalpy). Chemical indoor air quality may be characterized by a set of values and parameters extracted from qualitative and quantitative analysis of air. However, in many cases the link between the perception of air quality and the chemical composition as well as concentration levels of various substances is still unclear. The problem is also related to the possibilities to measure the indicators. The qualitative sensory analysis of indoor air is complex and subjective. The quantitative and qualitative analysis of indoor air composition is difficult to perform since this gas is a mixture of many substances. Usually, their concentrations are low. In addition, indoor air constituents are strongly affected by many factors. Due to it they display considerable temporal changes. For that reason, the applicability of traditional analytical methods is limited. Even if there are available measuring techniques for determination of the required parameter, the measuring device must fulfil certain requirements in order to be applicable for the ventilation control. For example, it should provide fast, stable and reliable output signals. They have to correspond to the value of the specified reference quantity which is determined. Incorrect measurements can lead to uncomfortable indoor microclimate or excessive use of energy as an effect of under- or over-ventilation of rooms.

The aim of work is to compare carbon dioxide (CO_2) and volatile organic compounds (VOCs) as indicators of IAQ.

2 CO_2 AND VOCs

Carbon dioxide is one of the most important constituents of indoor air. In many buildings, a major source of this gas is human occupancy. Occupants emit CO_2 through exhalation. The emission rate depends on the number of people and their level of activity. Carbon dioxide at very high concentrations (greater than 5000 ppm) can pose a health risk. At concentrations commonly found in buildings, direct influence of this gas on human health is minimal, although symptoms such as drowsiness and decrease of perception are observed. Current technology enables easy and relatively inexpensive measurement of CO_2 (Mahyuddin etal., 2012). As the indicator, the carbon dioxide concentration level inside a building is considered from two points of view. Firstly, this quantity is closely related to the ventilation rate and therefore it can be useful to estimate building air exchange rates and the percentage of outdoor air intake at an air handler. CO_2 measurements are often used in demand controled ventilation (Fisk et al., 2010). Generally speaking, this system adapts the airflow rate continuously to the actual pollutant emissions from activities and processes in the room. In practice, it allows to adjust ventilation rates according to the actual CO_2 concentration, rather than using pre-determined rates e.g. based on maximum occupancy. Currently, CO_2 concentrations remain a rough and easily measurable surrogate for ventilation rate. Secondly, under some circumstances CO_2 is proposed as an indicator of general indoor air quality. This approach is justifiable only in buildings where metabolic or combustion sources of CO_2 are predominating. It means that this gas may be an indicator only for air quality related to human occupancy. Therefore the proposition to use CO_2 concentration as an indicator of occupant odors (odorous bioeffluents) and the acceptability of a space in terms of human body odor is controversial. Indoor CO_2 concentrations are particularly poor indicators of health risks in rooms with strong pollutant emissions from the building or building furnishings, particularly when occupant densities are low. For that reason, indicators which allows to adjust ventilation rates based on the measurement of other parameters are needed. This requirement can be fulfilled by volatile organic compounds.
VOCs include a variety of chemicals, some of which may have short- and long-term adverse health effects (Tucker, 2000; Wolkoff et al., 2006). They are emitted by a wide array of products numbering in thousands, e.g. paints and lacquers, paint strippers, cleaning agents, pesticides, building materials and furnishings, office equipment such as copiers and printers, correction fluids and carbonless copy paper, graphics and craft materials including glues and adhesives, permanent markers, and photographic solutions. Lack of standards for non-industrial buildings describing acceptable concentrations of many common volatile organic compounds is the limitation for the application of these substances as indicators of IAQ. On the other hand, the

choice of an indicator based on VOCs is to a great extent dependent of the possibilities to measure this parameter. It is relatively simple to measure just one substance e.g. CO_2. However, regarding VOCs, indoor air is a combination of many different organic compounds at different concentrations. The commercially available gas sensors measure non-selectively a wide range of volatile substances and they do not provide selective information. Therefore indicator such a total concentration of VOCs is proposed. The serious disadvantage of this approach is the interpretation of measuring results.

3 EXPERIMENTAL

The analysis presented in this work was based on the experimental data collected during an indoor air quality study, performed in a university classroom. Nine days in the winter season 2014/15 were taken under consideration.

The classroom is located on the third floor of the building which was erected in 70-ties. Recently, it has been renovated, including thermo-isolation. Airtight windows were mounted. The room size is 9.6 x 7.2 x 3.2 m. It may host up to 40 students. Air exchange is realized by a natural ventilation.

The study focused on teaching hours. Measurements were performed from early morning till the evening in a continuous manner. They consisted in monitoring air parameters using following sensors: temperature sensor, relative humidity sensor, CO_2 sensor, photoionization detector (PID) sensor and semiconductor gas sensors (SGS). The last two techniques are considered as applicable for determining VOCs in indoor air. The measurement characteristics of the applied instruments are presented in Table 1. The temporal resolution of data collection was 1 min.

Table 1: Measuring characteristics of sensor devices applied in IAQ study

Sensor	Measuring principle	Measuring range	Accuracy	Resolution
Temperature sensor	thermistor NTC 10 Ω	-20 – 60 °C	±0.2 °C ± 0.15 % display reading	0.1 °C
Relative humidity sensor	capacitive sensor	5 – 100 %RH	±2 % (10 – 90 %RH); ±2.5 % outside	0.1 %
CO2 sensor	non dispersive infrared (NDIR)	0 – 5000 ppm	±50 ppm + 3 % display reading	1 ppm
Semiconductor gas sensor, TGS822	semiconductor gas sensor	5-10000 ppm organic solvents	N/A	N/A
Photoionization detector	Photoionization detection, 10.6 eV Krypton PID lamp	0.1 - 5000 ppm	± 5% display reading ± one digit	0.1 ppm

All measuring devices were located in one place, at the back of the classroom 1m over the floor, out of the direct influence of classroom occupants. In parallel with measurements, the number of people in the classroom was counted. In addition, there were noted down the times of windows/ doors opening or setting windows ajar.

4 METHODS

4.1 Pearson correlation

Sample correlation coefficient for two data vectors **p**=(x_1, x_2, …, x_n) and **q**=(x_1, x_2, …, x_n) in *n*-dimensional vector space is given by (Navidi, 2011):

$$R = \frac{\sum_{i=1}^{n}(y_i - \bar{y})\sum_{i=1}^{n}(x - \bar{x})}{\left(\sum_{i=1}^{n}(y_i - \bar{y})^2 \sum_{i=1}^{n}(x - \bar{x})^2\right)^{1/2}} \tag{1}$$

where, $\bar{x}$ and $\bar{y}$ denote the sample mean of vector **p** and **q** respectively. In statistics and other sciences, R it is widely used as a measure of the degree of linear dependence between two variables. Correlation coefficient belongs to an interval <-1,1>. It is commonly accepted that values close to 1 indicate strong positive correlation, values close to -1 indicate strong negative correlation and values close to zero announce lack of correlation. A precise determination of the statistical significance/insignificance of the correlation coefficient is based on *t*-test (for $n \geq 3$).
If the null hypothesis H_0: R=0 is true, the test statistic (Navidi, 2011):

$$t = \frac{R}{(1-R^2)^{1/2}}(n-1)^{1/2} \tag{2}$$

has t distribution with $\nu = n-2$ degrees of freedom. In case of testing the null hypothesis against the alternative H_a: $R \neq 0$, at the significance level α, the critical interval is $I = \left(-\infty, -t_{\alpha/2,\nu}\right\rangle \cup \left\langle t_{\alpha/2,\nu}, \infty\right)$. If sample test statistic belongs to critical interval, correlation coefficient may be considered statistically significant at the significance level α.

4.2 Simple linear regression

The formula (Navidi, 2011):

$$y = ax + b + \varepsilon \tag{3}$$

describes a simple linear regression of variable *y* with respect to variable *x*. This model is widely applied in science to quantitatively determine a linear relationship between two variables. The parameters *a* and *b* are the slope, and offset, respectively. Only the deterministic part of the dependent variable variability may be explained by linear transformation of *x* (i.e. the term *ax*+*b*). Random component, ε represents the part which is not explained. The parameters of simple regression are typically calculated using least squares method.
We examined the quality of fit for regression models developed in this work using coefficient of variation of the RMSE. It is given by (IDRE, 2015)

$$CV = \frac{RMSE}{\bar{y}} \tag{4}$$

where RMSE is the root mean square error and $\bar{y}$ is the mean of the dependent variable. *CV* compares the size of RMSE in relation to the average value of the variable described by a model. RMSE is computed from

$$RMSE = \left(\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}\right)^{1/2} \tag{5}$$

where y and $\hat{y}$ are the dependent variable and the output of regression model, respectively.
All calculations utilized in this work were done in MATLAB environment.

5 RESULTS AND DISCUSSION

The postulate that CO_2 and VOCs could be considered as alternative indicators of indoor air quality is based on the assumption that both have common source - building occupants. Hence, it could be expected that the temporal variation of the two indicators follows a similar pattern. In consequence, they may be highly correlated. In this paper, we have analyzed this issue in detail.

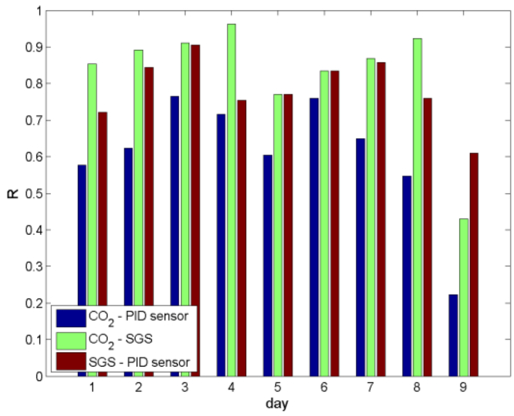

Figure 1: Pearson correlation between CO_2 concentration (NDIR sensor), PID sensor and semiconductor gas sensor responses. Correlation coefficients refer to the time scale of one day.

In Fig. 1 we compare Person correlation between the time series of CO_2 concentration, PID sensor and semiconductor gas sensor responses, which were recorded during nine days. The presented correlation coefficients correspond to the time scale of one day (strictly - working hours). Based on the bar plot we see that, in this time scale, correlations between the considered variables were usually relatively high; in particular for pairs: CO_2 – SGS and SGS – PID sensor. In spite of day to day differences, such results could be interpreted as indicating an overlap in information provided by CO_2 measurement and VOCs indication based on semiconductor gas sensor (green bars), as well as the interchangeability of VOCs assessment based on two techniques – semiconductor gas sensing and photoionization detection (brown bars). Contrarily, the information shared by CO_2 data and PID sensor responses was quite small (blue bars).

However, the assumption that observations based on correlation analysis which refers to the time scale of one day are true in any time scale may not be valid; In particular for shorter time scales. In fact, such scales are more important from the point of view of providing a useful information about air quality to the ventilation system control. Lack of validity may be caused by the fact that indoor air parameters usually display a substantial temporal variation during the day, especially during working (teaching) hours. In our study, we also noted this phenomenon, as illustrated in Fig. 2 for an exemplary day 9.

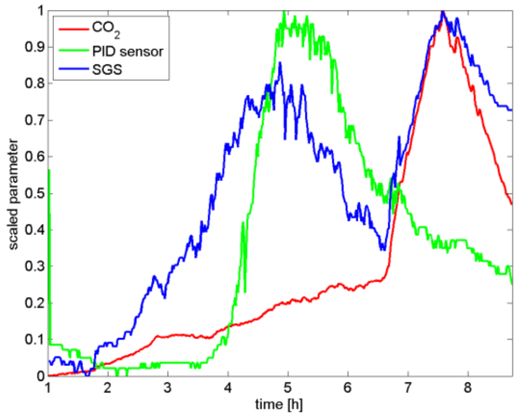

Figure 2: Temporal variation of CO_2 concertation, PID sensor and SGS responses in the time scale of one day (working hours at the university, day 9). Due to fact that the orders of magnitude of parameters are different measurement data was scaled to the range <0,1> for displaying it in one plot.

While displaying temporal variability, CO_2 concentration, PID sensor and SGS responses generally did not behave in the same way, as shown in Fig. 2. Namely, their increase, decrease or lack of change were not synchronized. Hence, it couldn't be expected that the correlation between the parameters is maintained at the same level over entire period of several hours.

In further analysis, there were considered correlations referring to shorter time scale. We chose 30 minutes. This scale was a compromise between the minimum duration of two major events which take place in the studied object, the break (15 minutes) and classes (45 minutes). The time window of this size was moved along the time series of data collected over the period of one day in order to cut out 30 min long time subseries. Correlation coefficients were calculated for the set of subseries associated with each position of the window. The results of the analysis for an exemplary day 9 are shown in Fig. 3. We distinguished statistically insignificant correlation coefficients (α=0.01) using red markers.

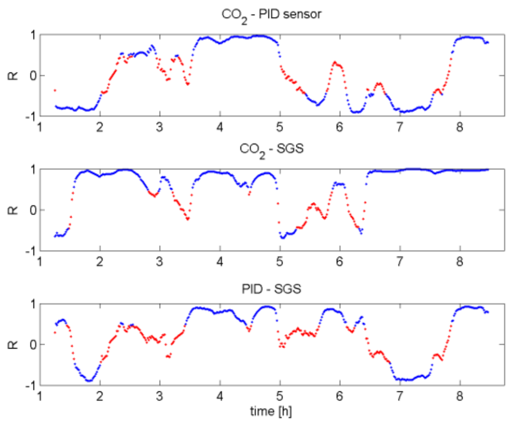

Figure 3: One day evolution of Pearson correlation between CO_2 concentration, PID sensor and SGS responses, computed in the time scale of 30 min (day 9). The results were obtained using moving time window technique.

The results shown in Fig. 3, confirmed that correlation between the examined indoor air parameters was neither constant nor high during the day. Correlation coefficients calculated using time scale of 30 min exhibited high temporal variation and they took values from a full available range of <-1,1>. One shall draw special attention to the fact that, in some periods of time, the coefficients were not statistically significant (red markers in Fig. 3). Insignificant correlation means that the co-variation of the two variables is negligible. This in turn implies that unknown changes of one variable may not be deduced based on the known behavior of the other variable. In other words, the parameters carry mutually irrelevant information. In Fig. 4 we summarized the fractions of daytime, when the 30 min time scale correlations were statistically insignificant. The results obtained for 9 days were considered jointly.

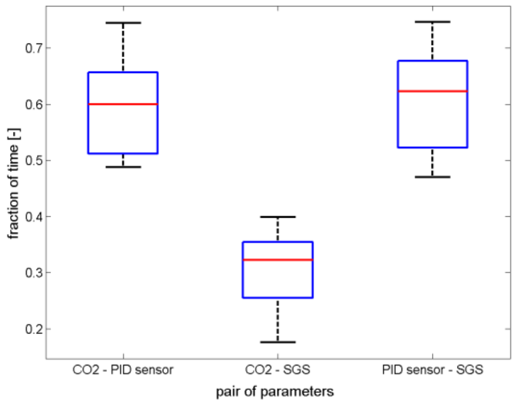

Figure 4: Fraction of daytime when Person correlation between CO_2 concentration, PID sensor and SGS responses was statistically insignificant. The plot summarizes nine days of IAQ study.

As shown in Fig. 4, on average, short time scale correlations CO_2 – PID sensor as well as PID sensor – SGS were statistically insignificant during as much as 60 % of daytime. For the CO_2 – semiconductor gas sensor pair the respective time fraction was more than 30 %. Based on these results, we may infer that in short term perspective, time series of CO_2 concentration conveyed different information than the corresponding time series of PID sensor responses. In addition, the PID sensor responses were not a credible source of information provided by gas sensors.

Further, we estimated the error of inference about one IAQ indicator based on other parameter, using a univariate linear regression model. Two approaches were compared. In the first approach, one regression model was parameterized based on the data collected during one day. This model was later applied to infer about all values of the dependent variable on that day. The corresponding errors are shown in Fig. 5a. In the second approach a set of regression models was applied. An individual model was parameterized, based on the data associated with one 30 min time interval, and it was applied to infer about the value of the dependent variable in the middle of this interval. A set of models was obtained using moving time window technique. The corresponding errors are shown in Fig. 5b.

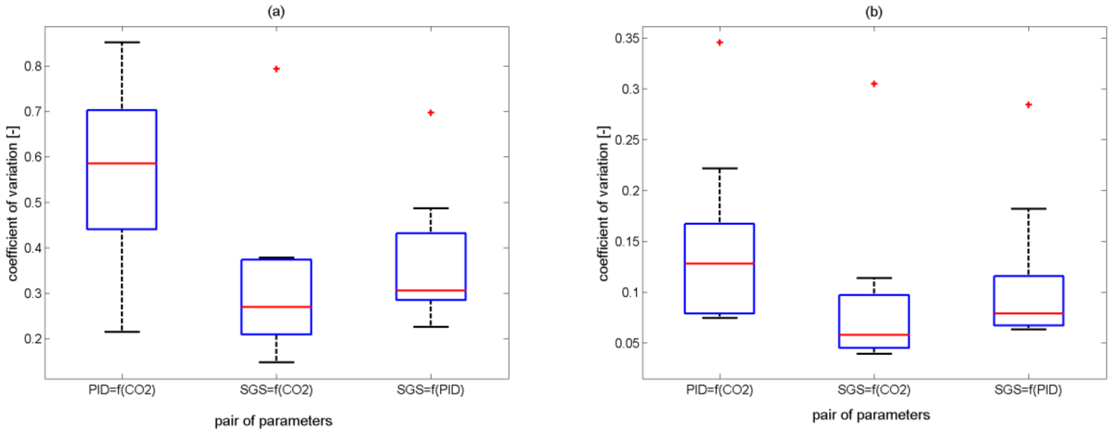

Figure 5: Error of inference about the measured values of CO_2 concentration, PID sensor and SGS responses using: a) simple linear regression model – parameterized for the time scale of one day, b) set of simple linear regression models – parameterized for the time scale of 30 min, using moving time window technique. The plot summarizes nine days of IAQ study.

In Fig. 5 we see that the application of model developed for the period of one day resulted in high errors. The average coefficient of variation when inferring about PID responses based on CO_2 concertation was 60 %. In case of modeling semiconductor gas sensor responses using CO_2 concentration the error was about 25 %. Reconstruction of SGS responses based on PID sensor responses was loaded with CV=30 %. These unacceptably hing errors were a consequence of the fact that the models developed for the period of 1 day were not able to cope with explaining the short term variability of the dependent quantities. They flattened their variation, as shown in Fig. 6.

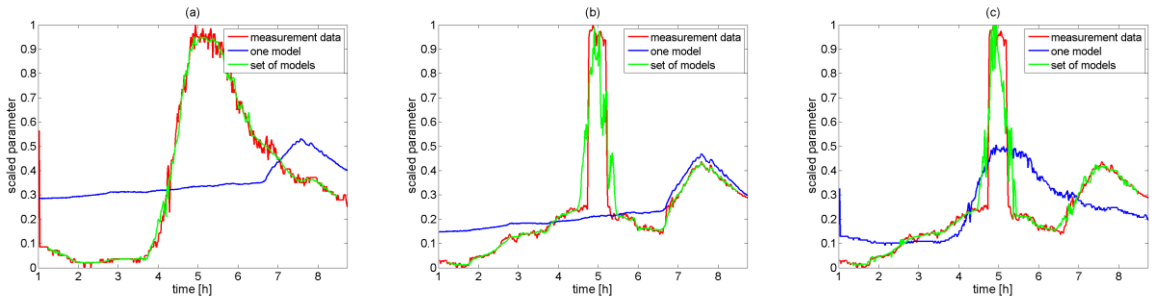

Figure 6: Results of modeling: a) PID=f(CO_2), b) SGS=f(CO_2) and c) SGS=f(PID) using simple linear regression model –parameterized for the time scale of one day and set of models – parameterized for the time scale of 30 min, using moving time window technique.

When applying short time scale models, the results of mutual inference about IAQ indicators were very good. In all considered cases coefficients of variation were smaller than 15 %. However, we observed that models coefficients were highly dependent on the position of moving time window. Therefore, if one wanted to deduce accurately changes of one variable, based on the other indicator, the model would have to be reparametrized every 30 min. Hence, the instruments providing data on both IAQ indicators would have to be available permanently. It is against the logics of the alternative use of indicators.

6 CONCLUSIONS

Several conclusions were drawn based on the results obtained in this work. (1) The co-variation of measured quantities showed high temporal variability. It means that the results of CO_2 and TVOCs measurements conveyed different information about IAQ, as a function of time. (2) The analytical method had strong influence on the information obtained. In particular, the discrepancy was observed when the NDIR and PID method were compared. (3) Techniques applied for VOCs measurements provided different information about these substances. This fact was reflected in the behaviour of correlation between PID and semiconductor gas sensor measurements. VOCs contained in indoor air have different properties and variously affect IAQ. Therefore, a wide spectrum of information about air composition is required to control the quality of this gas. (4) Room occupancy was not clearly related to the direction or magnitude of correlation between the considered quantities.
The results of our work entitle to conclude that the total concentration of VOCs should be taken into account as indicator of IAQ in addition to CO_2. It is already possible from the technological point of view. Current sensor technology allows to provide information about these substances in air, easily and relatively inexpensively.

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