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Estimation of Space Air Change Rates and CO₂ Generation Rates for Mechanically-Ventilated Buildings

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1. Introduction

It is well known that people spend 80-90% of their life time indoors. At the same time, pollution levels of indoors can be much higher than outdoor levels. Not surprisingly, the term 'sick building syndrome' (SBS) has been used to describe situations where occupants experience acute health and comfort effects that are related to poor air in buildings (Clements-Croome, 2000). It is an increasingly common health problem which has been acknowledged as a recognizable disease by the World Health Organization (Redlich et al., 1997, Akimenko et al., 1986).

Since its recognition in 1986, many efforts have been put to try to identify the causes to eliminate SBS. The causes may involve various factors. Mainly, it is thought to be a direct outcome of poor indoor air quality (IAQ) (Clements-Croome, 2004). In most cases ventilation system is found to be at the heart of the problem as well as high carbon dioxide (CO₂) levels (Redlich et al., 1997). Since 70's energy crisis, buildings have been tried to build with tight envelopes and highly rely on mechanical ventilation so as to reduce energy cost. Due to tight envelopes, a big portion of energy contributes to ventilation. In most cases SBS occurs in mechanically-ventilated and commercial buildings, although it may occur in other buildings such as apartment buildings. It has been estimated that up to 30% of refurbished buildings and a significant number of new buildings suffer from SBS (Sykes, 1988). However, the solutions to SBS are difficult to implement by the complexity of ventilation system and the competing needs of energy saving.

Hence the issue about ventilation efficiency is getting more and more people's attention. It is useful to evaluate ventilation in order to assess IAQ and energy cost. A number of techniques are available to perform such evaluations. Among them, the measurement and analysis of CO₂ concentrations to evaluate specific aspects of IAQ and ventilation is most emphasized. CO₂ is a common air constituent but it may cause some health problems when its concentration level is very high. Normally CO₂ is not considered as a causal factor in human health responses. However, in recent literatures, it has been reported that there is a statistically significant association of mucous membrane (dry eyes, sore throat, nose congestion, sneezing) and lower respiratory related symptoms (tight chest, short breath, cough and wheeze) with increasing CO₂ levels above outdoor levels (Erdmann & Apte,

2004). Elevated levels may cause headaches and changes in respiratory patterns (Environment Australia, 2001). Although no hard evidences have shown direct causal link between indoor CO₂ level and the above symptoms, indoor CO₂ level should be concerned regarding human health risk. Because occupants are the main source of indoor CO₂, indoor CO₂ levels become an indicator to the adequacy of ventilation relative to indoor occupant density and metabolic activity. In order to keep a good IAQ, indoor CO₂ concentration must be reduced to a certain level. Therefore, CO₂ is often used as a surrogate to test IAQ and ventilation efficiency.

Many works contributed to use indoor CO₂ concentration to evaluate IAQ and ventilation. Nabinger et al. (Nabinger et al., 1994) monitored ventilation rates with the tracer gas decay technique and indoor CO₂ levels for two years in an office building. Their aims were to assess the operation and performance of the ventilation system and to investigate the relationship between indoor CO₂ levels and air change rates. However, the assessment was done for a whole building without detaining individual rooms. Lawrence and Braun (Lawrence & Braun, 2007) used parameter estimation methods to estimate CO₂ source generations and system flow parameters, such as supply flow rate and overall room ventilation effectiveness. They examined different parameter estimation methods from simulated data and the best-performed method was applied to field results. Their goal was to evaluate cost savings for demand-controlled ventilation (DCV) system for commercial buildings. Wong and Mui (Wong & Mui, 2008) developed a transient ventilation model based on occupant load. Similar as Lawrence's work (Lawrence & Braun, 2007), they used optimization method to determine model parameters from a year-round occupant load survey. Their interest was also energy saving. Miller et al. (Miller et al., 1997) used nonlinear least-squares minimization and tracer gas decay technique to determine interzonal airflow rates in a two-zone building. But they didn't apply their method to field measurement. Other similar works have been done by Honma (Honma, 1975), O'Neill and Crawford (O'Neil & Crawford, 1990) and Okuyama (Okuyama, 1990).

Despite extensive studies, there is sparse information available regarding the use of field measured CO₂ concentrations to estimate ventilation rates (i.e. space air change rates) and CO₂ generation rates for a particular space, such as office room, in commercial buildings. Particularly there lacks a simple and handy method for estimating space air change rates and CO₂ generation rates for a particular space with indoor CO₂ concentrations. A strong limitation of the existing models in the literature is either they focus on the effect of ventilation over a whole building without considering particular spaces or they are too complicated for practical use. A big number of field measured data are required in these models to determine several model parameters, such as ventilation effectiveness, ventilation rate, exfiltration rate, occupant-load ratio and so on. Therefore, their interests lie mainly with overall and long-term efforts - energy saving. This is understandable, but it is generally not practical as it does not provide any information relevant to indoor air for a particular space, and hence cannot serve as some kind of guidance from which a good IAQ can be derived. In addition, in the above models, ventilation rates are mostly determined using the tracer gas technique. Although the tracer gas technique is powerful, in practice the technique is not easy to implement and in some way is not economical (Nabinger et al., 1994).

In this paper, we develop a new method to estimate space air change rates and transient CO₂ generation rates for an individual space in commercial buildings using field measured CO₂ concentrations. The new approach adopts powerful parameter estimation method and

Maximum Likelihood Estimation (MLE) (Blocker, 2002), providing maximum convenience and high speed in predicting space air change rates with good accuracy. With MLE, the model enables us to use obtained space air change rates for further estimating CO₂ generation rates in a great confidence.

Additionally, a novel coupled-method is presented for predicting transient CO₂ generation rates. Traditionally, transient CO₂ generation rates are directly computed by solving mass balance equation of CO₂. In our coupled-method, we combine the traditional method and equilibrium analysis to estimate CO₂ generation rates. The coupled-method provides a simple and reliable method as an alternative to traditional methods. Importantly, the method proposed in this study also works well for general commercial buildings and other mechanically-ventilated buildings as the school building represents a common case for commercial buildings. The objectives of this study are:

- to develop a concise method to estimate space air change rate during a working day by directly applying field measured CO₂ concentrations from a particular and mechanically-ventilated space. Furthermore, the method should be able to be easily adapted for some complex ventilation systems, where ventilation rate (i.e. space air change rate) is not constant, e.g. variable air volume (VAV) and demand-controlled ventilation (DCV) systems;
- to propose a novel method for further predicting transient CO₂ generation rates during the day;
- to examine MLE's suitability in terms of ventilation rate prediction. MLE is widely used in a great range of fields, but rarely seen in predicting ventilation rates.

Overall, the method should be simple, economical and universal, and can be used as supplement tool to evaluate IAQ and ventilation efficiency for a particular space.

2. Methodology

Nowadays, except some spaces where occupants vary with time and are the main heat load and main pollutant source (e.g. conference rooms, assembly halls, classrooms, etc.), constant air volume (CAV) system is still primary way to ventilate spaces in commercial and residential buildings because of its simplicity and convenience. Moreover, a summary of data from mechanically ventilated commercial buildings suggests that for a given room in the building, the air is well mixed, although there are differences in the age of air in different rooms (Frisk et al., 1991). Therefore, the method discussed in this paper focuses on spaces with nearly constant air change rates and well-mixed indoor air. But the method can be easily adapted for time-varying ventilation systems, such as variable air volume (VAV) and demand-controlled ventilation (DCV) systems. In Section 4.1.1, we will offer an introduction about the application of the method in time-varying ventilation systems. For a well-mixed and mechanically-ventilated space, the mass balance of CO₂ concentration can be expressed as:

$$V \frac{dC}{dt} = Q(C_o(t) - C(t)) + G(t) \quad (1)$$

where

V = space volume,

$C(t)$ = indoor CO₂ concentration at time t ,

Q = volumetric airflow rate into (and out of) the space,

$C_o(t)$ = supply CO₂ concentration,

$G(t)$ = CO₂ generation rate in the space at time t .

The space with the mechanical ventilation system normally experiences infiltration when the ventilation is on, namely, the return airflow rate is slightly over the supply airflow rate to avoid any moisture damage to the building structures (for example most buildings in Finland) (D2 Finnish Code of Building Regulations, 2003). Therefore, the return airflow rate can be assumed to be the sum of the supply airflow rate and infiltration. If a well-mixed condition for the space is assumed and the space is served by 100% outdoor air, which is common phenomenon in Finnish buildings, the mass balance of CO₂, Eq. (1) does not change by including infiltration. In such setting, Q becomes the return airflow rate in Eq. (1). However, if the space is not served by 100% outdoor air and the infiltration cannot be ignored, Eq. (1) has to be extended by including infiltration and outdoor CO₂ concentration. Calculation procedures may be more tedious, but the model is not principally different from Eq. (1). In this study, Eq. (1) is sufficient for our investigated building, in which rooms are served by 100% outdoor air. Furthermore, the above arguments are also applicable to those commercial buildings whose spaces experience exfiltration rather than infiltration.

In practice, whether the space experiences exfiltration or infiltration, its rate is quite small compared with the supply or the return airflow rate in commercial buildings when the ventilation is on. Therefore, sometimes we can ignore it for simplicity in some commercial buildings when the ventilation is on. Note: Eq. (1) is used for the estimation of space air change rate, which may include not only outside but also recirculated air in supply air. In Finland, most rooms/spaces in commercial buildings are served by 100% fresh air and the recirculation of indoor air is in general not taken as a way to save energy due to concerns on IAQ. If the space is supplied by mixed air, the percent outdoor air intake has to be known before applying Eq. (1) to estimate the air change rate of fresh air.

If we assume Q , $C_o(t)$ and $G(t)$ are constant, Eq. (1) can be solved as follows:

$$C(t) = C_o + \frac{G}{Q} + (C(0) - C_o - \frac{G}{Q})e^{-It} \quad (2)$$

where

$C(0)$ = indoor CO₂ concentration at time 0,

$I = Q/V$, space air change rate.

When CO₂ generation rate G is zero, Eq. (2) can be expressed as:

$$C(t) = C_o + (C(0) - C_o)e^{-It} \quad (3)$$

The obtained Eq. (3) is the fundamental model to estimate space air change rate in this study. If CO₂ generation rate is constant for a sufficient time, the last term on the right side of Eq. (2) converges to zero, and the airflow rate can be expressed as:

$$Q = \frac{G}{(C_{eq} - C_o)} \quad (4)$$

where C_{eq} is equal to $C_o + \frac{G}{Q}$ and called the *equilibrium CO₂ concentration*. Eq. (4) is often used to estimate airflow rate (i.e. space air change rate) if an equilibrium of CO₂ concentration is reached. This method is called *equilibrium analysis*. The time required to

reach equilibrium state mainly depends on air change rate. It takes about three hours to reach 95% of the equilibrium CO₂ concentration at 0.75 ach if the CO₂ generation rate is 0.0052 L/s (approximately one person's CO₂ generation rate in office work) and the outside and initial CO₂ concentrations are 400 ppm for an 80 m³ space. In the same condition at 2.5 ach, it takes 35 minutes to reach 95% of its equilibrium value.

Furthermore, we split the working (i.e. occupied) period of a working day into *occupied working period* when staff is present and *unoccupied working period* when staff has left for home with the 'on' ventilation system. In our case, the ventilation system will remain 'on' and continue working for the duration after staff has left the office, much like a delay off timer. The space air change rate in the *occupied working period* can be evaluated through that of the rate in the *unoccupied working period* based on the assumption of an approximate constant air change rate for the occupied period of a working day as discussed previously. The space air change rate for an *unoccupied working period* is relatively easier to estimate as the CO₂ generation rate is zero. Therefore, we can take Eq. (3) as the governing equation of CO₂ concentration for an *unoccupied working period*. Note: Eq. (3) is derived based on the assumption that supply CO₂ concentration is stable, such as the case of spaces served by 100% outdoor air. If supply CO₂ concentration is unstable (e.g. mixed supply air), the measurement of supply CO₂ concentration has to be required.

2.1 Estimating space air change rate by Maximum Likelihood Estimation

For the determination of the model parameters from such measurements, such as the space air change rate from measured indoor CO₂ concentrations, we adopted Maximum Likelihood Estimation (MLE). Very often, such determination of the model parameters is executed through least squares fit (IEEE, 2000). The method fails when some assumptions (independent, symmetrically distributed error) are violated. More methods include χ^2 fits, binned likelihood fits, average calculation, and linear regression. In general, MLE is the most powerful one (Blocker, 2002). The idea behind it is to determine the parameters that maximize the probability (likelihood) of the sample or experimental data.

Supposing α is a vector of parameters to be estimated and $\{d_n\}$ is a set of sample or experimental data points, Bayes theorem gives

$$p(\alpha | \{d_n\}) = \frac{p(\{d_n\} | \alpha)p(\alpha)}{p(\{d_n\})} \quad (5)$$

What MLE tries to do is to maximize $p(\alpha | \{d_n\})$ to get the best estimation of parameters (i.e. α) from $\{d_n\}$. Because $p(\{d_n\})$ is not a function of the parameters and normally a range of possible values for the parameters (i.e. α) is known, $p(\{d_n\})$ and $p(\alpha)$ are left out of the equation. So only $p(\{d_n\} | \alpha)$ needs to be dealt with. Note that $\{d_n\}$ can be expressed in terms of

$$d(n) = f(n, \alpha) + \varepsilon_n \quad (6)$$

with ε_n being the measurement error and $f(n, \alpha)$ the true model. The error ε_n often trends to normal distribution:

$$p(\varepsilon_n) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{\varepsilon_n^2}{2\sigma^2}\right] \quad (7)$$

where σ^2 is the variance of the measurement errors and assumed to be independent of the time. The secret to finding the probability of a data set (i.e. $\{d_n\}$) is to have a model for the measured fluctuations in the data; i.e. the noise. Therefore,

$$p(\{d_n\} | \alpha) = p(\varepsilon_n) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(d(n) - f(n, \alpha))^2}{2\sigma^2}\right) \quad (8)$$

Commonly, the data set at each measurement point are statistically independent, so are the measured errors. Therefore, $p(\{d_n\} | \alpha)$ can be rewritten as

$$p(\{d_n\} | \alpha) = p(d_1 | \alpha)p(d_2 | \alpha)p(d_3 | \alpha)\dots p(d_n | \alpha) = \prod_n p(d_n | \alpha) \quad (9)$$

Since the logarithm of a function is the maximum when the function is the maximum, the logarithm of the probability is preferred for the sake of convenience. The logarithm of $p(\{d_i\} | \alpha)$ is given by

$$\log p(\{d_n\} | \alpha) = \sum_n \log p(d_n | \alpha) \quad (10)$$

In order to maximize $p(\alpha | \{d_i\})$, MLE only needs to maximize Eq. (10), namely to solve the set of equations

$$\frac{\partial \log p(\{d_n\} | \alpha)}{\partial \alpha_i} = 0, \quad i = 1, 2, 3, \dots, \quad (11)$$

subject to the usual constraints that the second derivatives be negative. The set of equations in Eq. (11) are called *Maximum Likelihood Equations*.

Substituting Eq. (8) into Eq. (10), we obtain

$$\log p(\{d_n\} | \alpha) = -\sum_n \frac{(d_n - f(n, \alpha))^2}{2\sigma^2} - 0.5 \sum_n \log 2\pi\sigma^2 \quad (12)$$

If the variance σ^2 is not a function of α , we just need to maximize the first sum in Eq. (12) in order to maximize Eq. (10). If the variance σ^2 is a function of α and/or n , all terms in Eq. (12) need to be kept. In our study, we assume the variance σ^2 of measurement errors to be constant but not a function of parameters. Hence Eq. (3) can be re-expressed as

$$f(n, \alpha) = C(n) = (C(0) - \alpha_0) \exp(-\alpha_1 n \Delta t) + \alpha_0 \quad (13)$$

where α_0 and α_1 are two unknown parameters, supply CO₂ concentration and space air changer rate respectively, and Δt is the time interval for each measurement count. Substituting Eqs. (12) and (13) into Eq. (11), the MLE equations are obtained as:

$$\frac{\partial \log p(\{d_n\} | \alpha)}{\partial \alpha_0} = \frac{1}{\sigma^2} \sum_n (1 - \exp(-\alpha_1 n \Delta t)) \left[d_n - (C(0) - \alpha_0) \exp(-\alpha_1 n \Delta t) - \alpha_0 \right] = 0 \quad (14)$$

$$\frac{\partial \log p(\{d_n\} | \alpha)}{\partial \alpha_1} = -\frac{(C(0) - \alpha_0) \Delta t}{\sigma^2} \sum_n n \exp(-\alpha_1 n \Delta t) \left[d_n - (C(0) - \alpha_0) \exp(-\alpha_1 n \Delta t) - \alpha_0 \right] = 0 \quad (15)$$

Solving these two equations, Eqs. (14) and (15), simultaneously allows for the estimation of the space air change rate (i.e. α_1) and supply CO₂ concentration (i.e. α_0) for a working day. MATLAB can be employed to obtain the solutions. Residuals are often used to examine the general and specific fit between the data and the model which are the differences between the observed and the predicted values:

$$\varepsilon_n = d(n) - f(n, \alpha) \quad (16)$$

Both the sum and the mean of the residuals of a correct model should be equal/or near to zero. In addition, the residual plot of a correct model should show no any trend and pattern and all residual points should scatter randomly. In this study, the residuals of the model fit were examined.

As previously mentioned, in practice MLE is often implemented through least squares fit. But unlike conventional least square method, MLE is more flexible and powerful by taking measurement errors into account, which can avoid any highly-biased result. MLE gives the answer with some probabilistic sense; i.e. the answer obtained from MLE is probably the best we can get, knowing what we know. In addition, if the variance of measurement errors is known, it is possible to use MLE procedure to estimate parameter errors. Taking space air change rate as example, we possibly can use MLE procedure to report not only expected value (i.e. space air change rate) but also a prediction interval for space air change rate with a certain confidence, meaning that the expected air change will fall within the predicted interval with a certain confidence (e.g. 95% confidence). Prediction interval provides more knowledgeable information on space air change rate. About how to estimate predict interval is out of the scope of this study, we will reserve it for our future work.

2.2 Estimating CO₂ generation rates

Theoretically, the obtained space air change rate by MLE (i.e. solving Eqs. (14) and (15)) can be used to estimate transient CO₂ generation rates by solving Eq. (1) where the derivative of indoor CO₂ concentration needs to be calculated. However, in practice, the derivative of indoor CO₂ concentration cannot be solved analytically. Numerical differentiation is often employed which is very unstable and inevitably produces errors and amplifies noise errors from the measurements. Moreover, the supply CO₂ concentration is often unknown. When all of these factors come together, Eq. (1) cannot be used alone. We will provide a solution for such problem in Section 3.2.2.

In our study, the supply CO₂ concentrations were not measured but estimated using MLE (i.e. solving Eqs. (14) and (15)). For a short period, supply CO₂ concentrations don't change much which can be considered as constant. However, for a long period, the supply CO₂ concentrations may have significant changes. Sometimes, morning and evening supply CO₂ concentrations can have up to 40 ppm difference or even more. That means actual supply CO₂ concentrations at other times of a working day, particularly at morning times, may have significant differences from the estimated supply CO₂ concentration. In order to account for these changes, we tried to compute the upper and lower bounds of indoor CO₂ generation rates when solving Eq. (1). In general, the supply CO₂ concentration ranges from 370 ppm to 420 ppm in buildings in Finland, but this range may change. Derivatives of indoor CO₂ concentrations were calculated using Stirling numerical differentiation (Lu, 2003, Bennett, 1996, Kunz, 1975).

The proposed method (i.e. solving Eqs. (14) and (15)) was first implemented and tested thorough simulated data and then applied to field site data.

3. Simulated data

All data were generated from Eq. (2) with five-minute intervals. Two cases were simulated with constant space air change rates and supply CO₂ concentrations:

Case 1: The ventilation rate is 0.7 ach and supply CO₂ 400 ppm;

Case 2: The ventilation rate is 2.5 ach and supply CO₂ 400 ppm.

The duration of the simulated indoor CO₂ concentrations for each case was four days with the following noise variance settings for each day: (day 1) constant variance=1; (day 2) constant variance=4; (day 3) constant variance=9; and (day 4) variable variances. Noise component was generated by a random number generator via a normal distribution. Fig. 1 displays the typical simulated indoor CO₂ concentrations for one day.

Hence, a total of eight day's simulated data were tested. The space air change rate is evaluated in the *unoccupied working period* (see Fig. 1) and then applied to the *occupied working period* to compute CO₂ generation rates as presented previously. Sections 3.1 and 3.2 will present the comparison results and discussions.

3.1 Results for space air change rates

Table 1 shows the results of the estimated space air change rates during *unoccupied working periods*, and Table 2 the model performances.

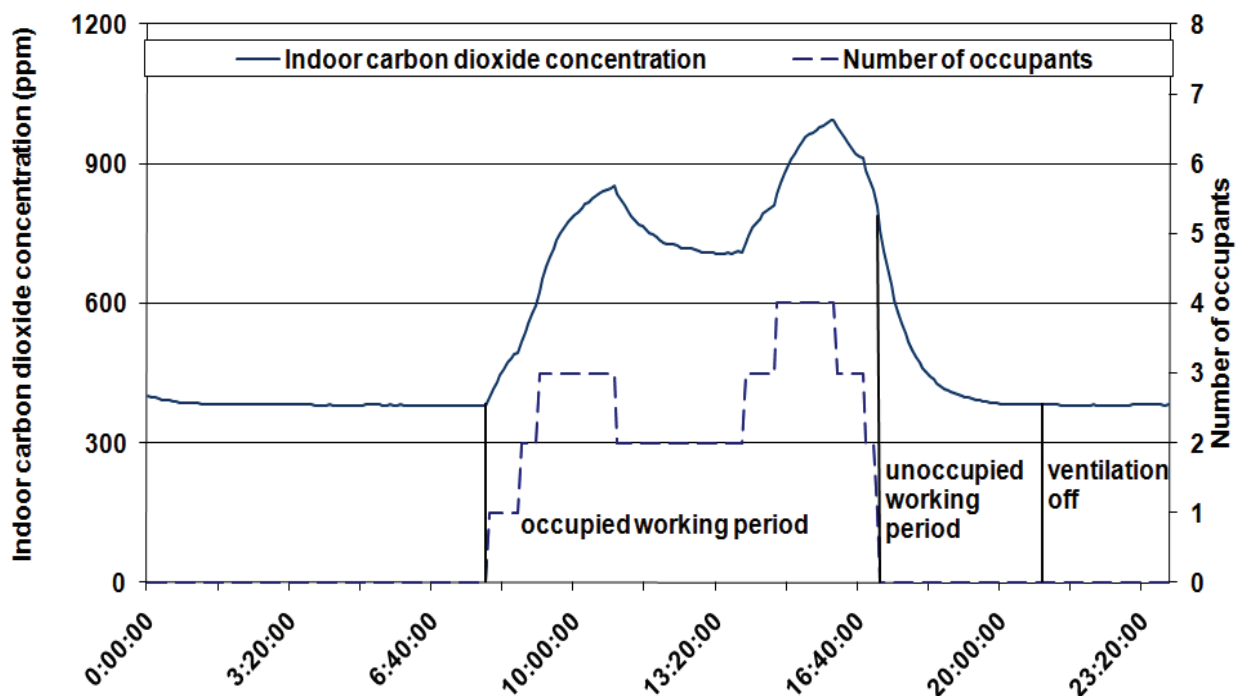


Fig. 1. Indoor CO₂ concentrations for a typical working day in an office.

In Table 1, the variances for variable noise were generated based on $\pm 1.5\%$ accuracy range with 95% confidence (e.g. standard deviation = $3.75 = 500 \times 1.5\% / 2$ for the simulated indoor CO₂ concentration of 500 ppm). Table 1 also demonstrates that even though Eqs. (14) and (15) are derived under the assumption of constant variances, both equations work well for variable noise variances as long as noise variances are not very big. An increase in noise variances does not seem to have an effect on the results, as all the estimated space air change

rates are close to the true values. However, an increase of the fitting error is observed in Table 2 with increased noise variances or variable noise variances, which implies that big noise variances can cause instabilities in estimated results of space air change rates. Due to space limitations, we only show here the comparison results for the cases with the largest variance of 9. Fig. 2 displays the fitting results of CO₂ concentrations based on the estimated space air change rates from MLE, and Fig. 3 the corresponding residuals.

Case	Parameter	Actual	Maximum Likelihood Estimation (MLE)			
			$\sigma^2=1^c$	$\sigma^2=4^c$	$\sigma^2=9^c$	σ^2 is variable ^d
Case 1	α_0 (ppm) ^a	400	399.96	404.8	402.2	406.1
	α_1 (ach) ^b	0.7	0.704	0.718	0.728	0.733
Case 2	α_0 (ppm) ^a	400	400.3	399.6	400.9	399.9
	α_1 (ach) ^b	2.5	2.5	2.45	2.55	2.61

^a Supply CO₂ concentration, see Eq. (13)

^b Space air change rate, see Eq. (13)

^c Constant noise variance.

^d Variable noise variance computed by $\frac{(CO_2 * 1.5\%)^2}{2}$. 1.5% is accuracy range for simulated CO₂ concentrations with 95% confidence.

Table 1. Estimated space air change rates for Case 1 and Case 2

Figs. 2 and 3 indicate a good fit of the model (i.e. Eq. (13)) to the simulated data. All residual plots in Fig. 3 show no pattern and trend. These results prove that in theoretical level the proposed model is suitable for the estimation of space air change rate which is near constant during the whole working period.

Case	Noise Variance	MSE (mean squared error)	R ² (coefficient of determination)
Case 1	$\sigma^2=1$	1.16	1
	$\sigma^2=4$	1.88	1
	$\sigma^2=9$	10.3	0.997
	σ^2 is variable	12.46	0.997
Case 2	$\sigma^2=1$	1.16	0.998
	$\sigma^2=4$	6.13	0.992
	$\sigma^2=9$	4.59	0.994
	σ^2 is variable	7.61	0.996

Table 2. Model performances for simulated data

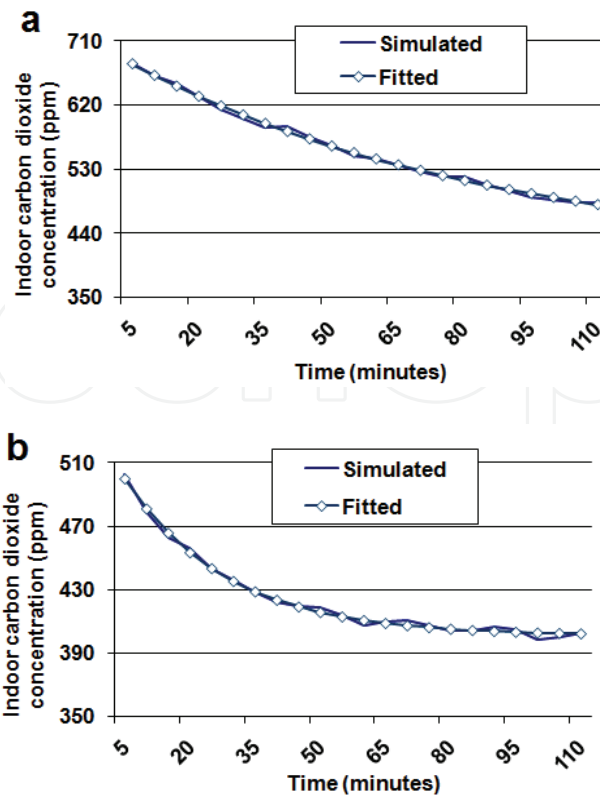


Fig. 2. Simulated and fitted indoor CO₂ concentrations during unoccupied working periods: (a) Case 1 ($\sigma^2=9$). (b) Case 2 ($\sigma^2=9$).

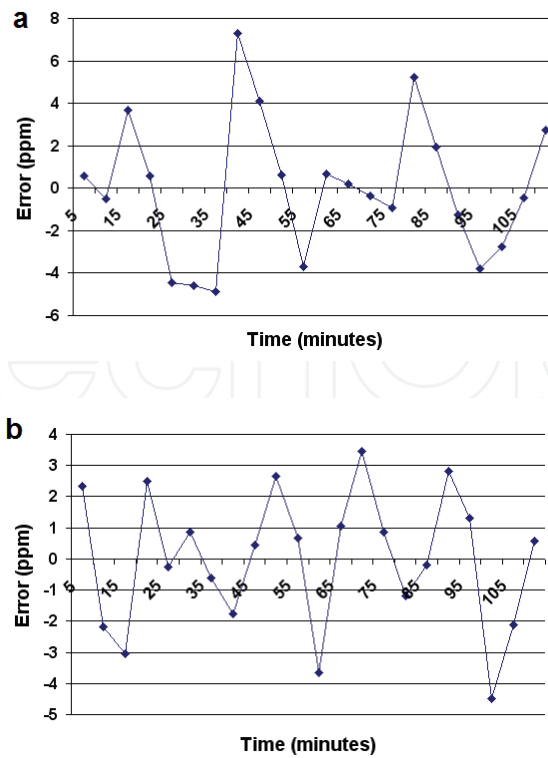


Fig. 3. Residuals for the CO₂ concentration fittings: (a) Case 1 ($\sigma^2=9$). (b) Case 2 ($\sigma^2=9$).

3.2 Results for CO₂ generation rates

3.2.1 Difficulties with estimation of CO₂ generation rates

For measured indoor CO₂ concentrations in which analytical derivatives are not available, numerical methods by finite difference approximation are probably the only choice. However, all the numerical differentiation is unstable due to the growth of round-off error especially for the noise contaminated data which further amplifies the measurement errors (Anderssen & Bloomfield, 1974, Burden & Faires, 1993) as demonstrated in Fig. 4 for Case 1 using Stirling numerical differentiation. Fig. 4 illustrates that the CO₂ generation rates oscillate with increasing noise. When the noise variance reaches 9, the CO₂ concentrations jump to the highest value 0.0083 L/s and drop to the lowest value 0.0032 L/s vs. the actual value 0.0052 L/s, resulting in instability. We need to develop a new strategy with regard to such problem.

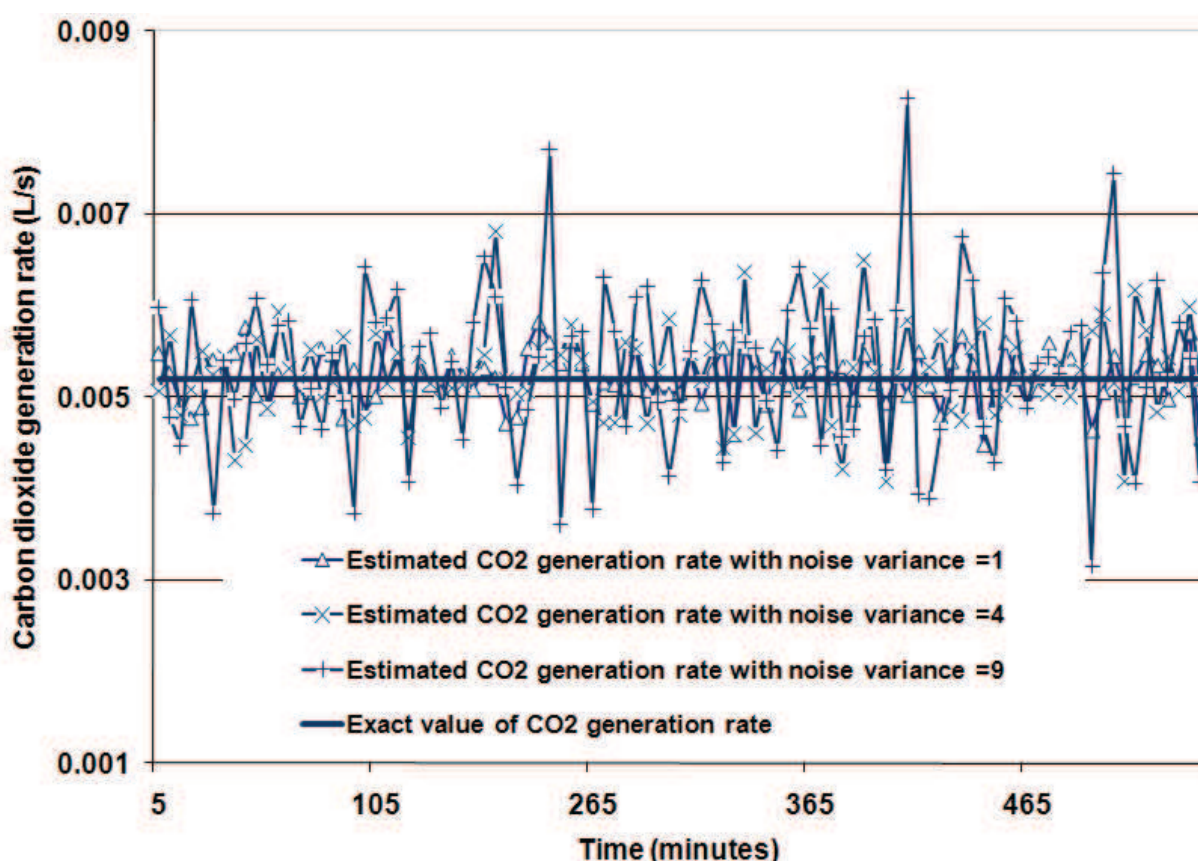


Fig. 4. Predicted CO₂ generation rates for Case 1 using Stirling numerical differentiation.

3.2.2 New strategy for estimation of CO₂ generation rates

Instead of directly estimating the CO₂ generation rates, we opted to evaluate the number of occupants. In fact, almost all ventilation regulations were stipulated based on the number of occupants. Another benefit of knowing the number of occupants is that it can somehow compensate for the losses from calculation errors. Taking Case 1 as an example (see Fig. 4), due to computation errors, the outcome can be as high as 0.0083 L/s vs. actual value, 0.0052 L/s. If we knew that the number of occupants was one, we could immediately obtain the corresponding CO₂ generation rate of 0.0052 L/s for an average-sized adult in office work. The new method is described with the following four steps:

- Step 1.** compute derivatives of all measured CO₂ concentrations for a range of supply CO₂ concentrations. In other words, we set the lower and upper bounds for the supply CO₂ concentrations and calculate the corresponding bounds for CO₂ generation rates. For instance, in this study, the supply CO₂ concentrations are normally between 370 ppm and 420 ppm which are then set as the lower and upper bounds respectively to compute the corresponding bounds for CO₂ generation rates. However, due to the errors of numerical round-off and measurement as well as the error from the estimated space air change rate, the actual CO₂ generation rates may fall outside the computed range. Nevertheless, the obtained range at least gives us some picture about the CO₂ generation rate at that point;
- Step 2.** identify significant jumps and drops from the measured CO₂ concentrations. In this study, we consider 10 plus ppm jump or drop as significant change. However, one significant jump or drop does not mean that the number of occupants has a change. Further analysis on derivatives of the measured CO₂ concentrations needs to be done. This is followed by Step 3;
- Step 3.** analyze derivatives of all measured CO₂ concentrations (i.e. CO₂ generation rates) at the jumped or dropped point as well as subsequent points;
- Step 4.** finally, further confirm the obtained possible numbers of occupants by computing the value of the equilibrium CO₂ concentration. This step mainly targets the complex in estimating the number of occupants described in Step 2.

To gain some insight into practical problems, we use one example from a field measurement to illustrate the above four steps.

Example 1: Suppose seven continuous measured points (indoor CO₂ concentrations, ppm) are

$$\begin{array}{ccccccc} P_1 & P_2 & P_3 & P_4 & P_5 & P_6 & P_7 \\ 503-> & 510-> & 526-> & 562-> & 579.6-> & 579.2-> & 578.8 \end{array}$$

- Step 1.** we set 380 ppm and 460 ppm as the lower and upper bounds for the supply CO₂ concentrations, and use these bounds to compute CO₂ generation rates for all points. We obtain:
 DP₁ (0.0047, 0.0099), DP₂ (0.0057, 0.01), DP₃ (0.017, 0.02), DP₄ (0.0148, 0.02),
 DP₅ (0.0123, 0.0175), DP₆ (0.0073, 0.0125), DP₇ (0.0077, 0.013).
 The first value in each parenthesis is the lower bound for CO₂ generation rate (L/s) at that point and the second one the upper bound;
- Step 2.** From these seven points, we identify three significant jumps: P₃, P₄ and P₅;
- Step 3.** We analyze P₃, P₄ and P₅ as well as their subsequent points: P₆ and P₇. From the results in Step 1, we can get the following guesses if we assume n as the number of occupants after the jumps:
 for P₃, $3 \leq n \leq 4$ for the lower bound, $3 \leq n \leq 4$ for the upper bound,
 for P₄, $2 \leq n \leq 3$ for the lower bound, $3 \leq n \leq 4$ for the upper bound,
 for P₅, $2 \leq n \leq 3$ for the lower bound, $3 \leq n \leq 4$ for the upper bound,
 for P₆, $1 \leq n \leq 2$ for the lower bound, $2 \leq n \leq 3$ for the upper bound,
 for P₇, $1 \leq n \leq 2$ for the lower bound, $2 \leq n \leq 3$ for the upper bound,
 where we assume that one person's CO₂ generation rate is 0.0052 L/s;
- Step 4.** Judging from P₃, P₄, and P₅, the number of occupants is more likely three while from P₆ and P₇ is close to two. But, due to no significant drop between P₅ and P₆, the

number of occupants at P₅ should be the same as at P₆. In addition, because the computed ranges of CO₂ generation rates at P₃, P₄ and P₅ are close, the number of occupants should be unchanged from P₃ to P₅. Now we can confirm that the number has changed at P₃. The possible number after P₃ is two or three based on the computed CO₂ generation rates at P₃, P₄, P₅, P₆ and P₇. If we assume that the space air change rate is 2.92 ach for an 80 m³ space, the lowest equilibrium CO₂ concentration for three occupants will be $610.411 \text{ ppm} = 370 + 3 \cdot 0.0052 \cdot 10^3 \cdot 3600 / (2.92 \cdot 80)$ which is significantly bigger than P₅, P₆ and P₇. If the number of occupants were three, CO₂ concentrations should have gone up continuously after jumps. However, actually CO₂ concentrations trend to be steady instead. So we can conclude that the number of occupants after jumps is two.

The above example shows how to estimate the numbers of occupants in this study. The proposed method is original. However, keep in mind that the proposed method is only applicable for the spaces where activity levels are relatively stable and occupants are present for long enough time, such as office room, lecture room, conference rooms and so on. In these spaces, minimum requirements of outdoor air per person are explicitly indicated by industry standards or building codes, therefore knowing the number of occupants is significant in order to fulfill minimum requirements of outdoor air for spaces. As for spaces where activity levels (occupants) change considerably with time, such as sporting halls, swimming pools and so on, it isn't recommended to use the proposed method to estimate the number of occupants, instead direct calculation of CO₂ generation rates from Eq. (1) is probably better way to evaluate occupants. Section 4.1.2 presents the results by applying this method to our field measurement. Section 4.1.1 provides results of estimations of space air changes rates using the method discussed in Section 2.1. The CO₂ generation rate for a typical office occupant in Finland is 0.0052 L/s.

4. Experimental data

The field measurement was set up in an office (27.45 × 2.93 m³, on the third floor) in a three-storey school building. The mechanical ventilation is supplied (100% outdoor air) in daytime on working day from 6:10 a.m. to 8:00 p.m. and shut down during nighttime, weekends, and public holidays. Three persons, two males and one female, work at the office regularly and the design airflow rate is around 200 plus m³/h (2.5 ach). In addition to indoor CO₂ concentrations, the pressure differences between the return air vent and room were also measured. Fig. 5 shows the office's layout as well as the measurement location. The measurement was categorized based on two stages. At the first stage (22.9.2008 – 28.9.2008), the existing ventilation system was examined. At the second stage (13.10.2008-19.10.2008), the ventilation system was reconfigured by blocking some holes at the supply and return air vents, aiming at reducing airflow rates. Finally, ten day's measurement data were obtained except for weekends. However, due to unexpected long working hours of the occupants which were beyond 8 p.m., there were no *unoccupied working periods* available for several days. Finally, five day's data were obtained which are displayed in Fig. 6. All data were measured within 5 min interval. The measurements show that the pressure differences, an important indicator to airflow rate, were almost constant for all working hours each day despite small fluctuations. This implies that space air change rates on each working day are near constant.

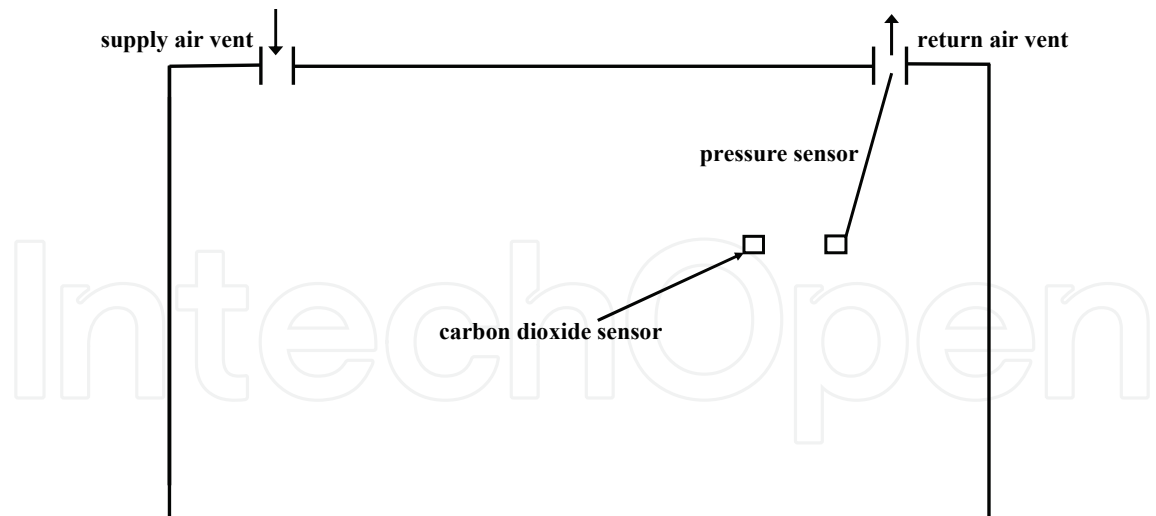


Fig. 5. The plan layout of the office.

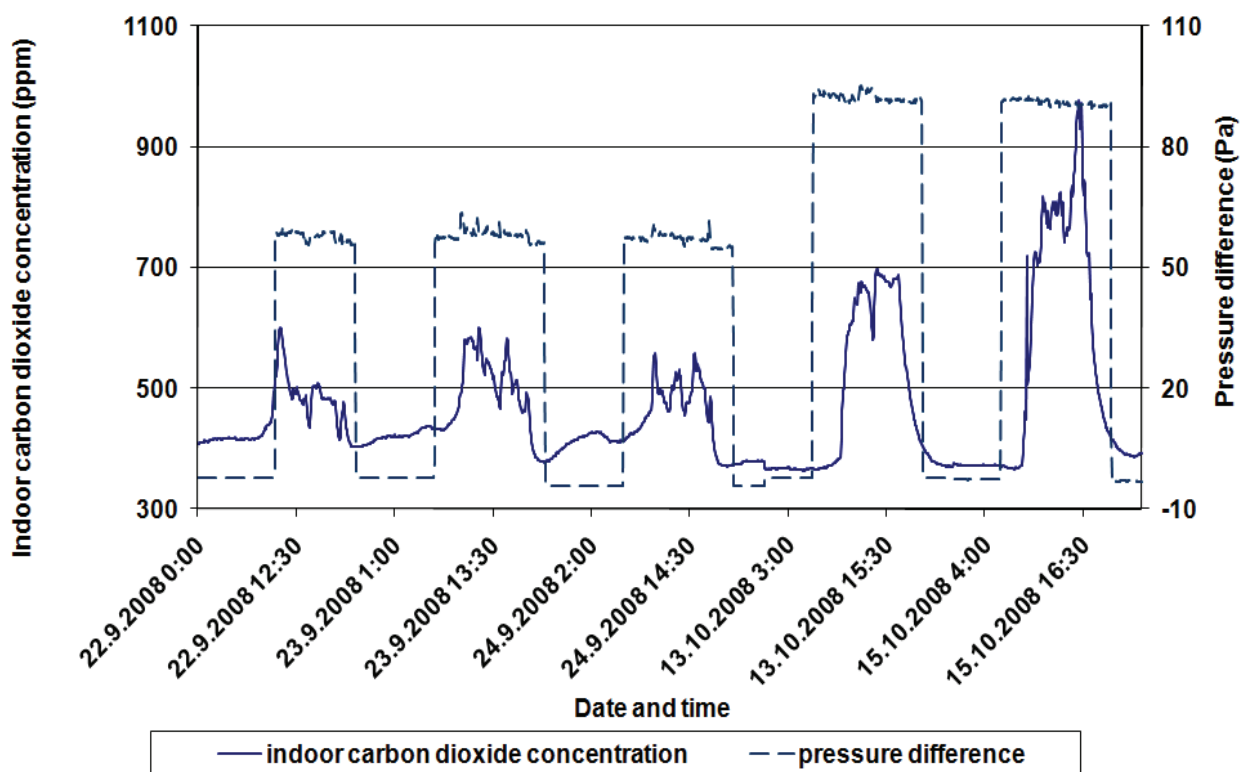


Fig. 6. Measured indoor CO₂ concentration and pressure difference between the return air vent and room.

4.1 Results and discussion

4.1.1 Results and discussion for space air change rates

Although we have measured pressure differences between the return air vent and space, there was no direct measurement available for airflow rate due to technical difficulties. Most literatures summarize the relationship between airflow rate and pressure difference across an opening as the following empirical formula (Feustel, 1999, Awbi, 2003):

$$Q = C(\Delta P)^n \quad (17)$$

where

Q = airflow rate, m³/s,

ΔP = pressure difference across the opening, Pa,

C = a constant value depending on the opening's geometry effects,

n = flow exponent.

Eq. (17) is called powerlaw relationship also. Theoretically, the value of the flow exponent should lie between 0.5 and 1.0. The values are close to 0.5 for large openings and near 0.65 for small crack-like openings. Supply and return air vents can be regarded as large openings. Note the 'unknown' value C is not essential for evaluating airflow rate if we use the following Eq. (18) based on Eq. (17)

$$\frac{Q_1}{Q_2} = \left(\frac{\Delta P_1}{\Delta P_2}\right)^n \quad (18)$$

However, we need an extra equilibrium analysis, Eq. (4), as a supplement tool to evaluate and analyze results. Fortunately, on 22.9.2008 and 13.10.2008, one person was present in the office for a long time which allowed reaching near-equilibrium. Table 3 illustrates the measurement situations during the period when the measures were taken.

On 22.9.2008, only one person worked in the office for nearly the whole afternoon with a number of visitors for less-than-five-minute visit during 14:05 - 15:35 when the indoor CO₂ concentrations (about 500 ppm) were higher than the average 481 ppm obtained at a near-equilibrium state during 15:40 - 17:20. The near-equilibrium was judged from the measured CO₂ concentration shown in Table 3 as no noticeable change was monitored within the period. It is worth mentioning that the person has been out shortly enough during the time 15:40 - 17:20 which allowed us to quantify the lower bound of CO₂ concentrations at near-equilibrium stage on a shorter time scale. The actual equilibrium CO₂ concentration value should lie between 478 ppm and 483 ppm. We took the average value, 481 ppm, as the equilibrium concentration value. The CO₂ generation rate for this person was estimated as 0.0052 L/s based on his size.

Similarly, the near-equilibrium was observed at an even longer period of 14:25-17:00 on 13.10.2008. The indoor CO₂ concentrations fluctuated around 680 ppm (almost unnoticeable) at the near-equilibrium state. The actual equilibrium value should be between 670 ppm and 690 ppm, we took the average value, 681 ppm, as the equilibrium concentration value. Again, Eq. (4) was used for the equilibrium analysis. Tables 4 and 5 show the estimated space air change rate results from the equilibrium analysis and MLE on 22.9.2008 and 13.10.2008 as well as comparisons with other days.

When proceeding MLE for one working day, we used only the measured CO₂ concentrations during *unoccupied working period*. The outliers in the measurement data were discarded since they can result in biased estimates and wrong conclusions (Boslaugh & Watters, 2008). The fitting results for five day's *unoccupied working periods* are shown in Fig. 7 and Fig. 8, and their residuals are presented in Fig. 9 and Fig. 10.

Essentially we evaluated space air change rates from MLE by: 1) the equilibrium analysis and 2) pressure differences based on the powerlaw relationship (i.e. Eq. (18)). In other words, if the pressure differences are close in all periods, nearly the same estimated space

air change rates result no matter what methods we employ, namely MLE or equilibrium analysis. Table 4 verifies this assertion. On 22.9.2008, 23.9.2008 and 24.9.2008, all periods have close pressure differences, the space air change rates estimated from MLE present nearness to those from the equilibrium analysis. Table 5 shows similar results for 13.10.2008 and 15.10.2008.

It is worth mentioning that Tables 4 and 5 also present somewhat violations against the powerlaw relationship. For instance, the space air change rate with 91-Pa pressure difference (13.10.2008) should be greater than that with 90-Pa pressure difference. However, Table 5 shows reverse results on 13.10.2008 and 15.10.2008. Such violations are quite natural in practice due to the calculation and measurement errors as well as underestimated equilibrium CO₂ concentrations. Those errors are ignorable. Additionally, numbers after one decimal place are meaningless in terms of mechanical ventilation.

Date	Time	CO ₂ concentration	The number of occupants
22.9.2008	9:55 - 13:40	From 526 ppm to 495 ppm	Ranging from 3 to 1
	13:45 - 14:00	Lunch break. From 488 ppm to 435 ppm	0
	14:05 - 15:35	From 435 ppm to 495 ppm	1 at most times, but there were some short-time visitors, less than five minutes
	15:40 - 17:20	From 488 ppm to 479 ppm. Near constant. The average is 481 ppm	1
	17:25-	Decaying	0
13.10.2008	9:40-13:15	From 386 ppm to 659 ppm	Ranging from 2 to 1
	13:15-13:40	Lunch break. From 659 ppm to 581 ppm	0
	13:50-14:20	From 581 ppm to 695 ppm	Ranging from 2 to 1
	14:25-17:00	From 688.4 ppm to 688.2 ppm. Stable and near constant despite of small fluctuation. The average is 680 ppm	1
	17:05-	Decaying	0

Table 3. Situations about indoor CO₂ concentration changes for 22.9.2008 and 13.10.2008

Date	Method	Space air change rate (α_1 , ach)	Supply CO ₂ concentration (α_0 , ppm)	Pressure difference (Pa) ^a
22.9.2008	Equilibrium analysis	2.93	401 ^b	58
	MLE	2.92	401 ^b	56
23.9.2008	MLE	2.94	378 ^b	56
24.9.2008	MLE	2.92	370 ^b	55

^a This is average pressure difference between the space and return air vent for the estimated period

^b Supply CO₂ concentration estimated by MLE

Table 4. Space air change rates estimated from equilibrium analysis and Maximum Likelihood Estimation (MLE) on 22.9.2008, 23.9.2008 and 24.9.2008

Date	Method	Space air change rate (α_1 , ach)	Supply CO ₂ concentration (α_0 , ppm)	Pressure difference (Pa)
13.10.2008	Equilibrium analysis	0.77	378	92
	MLE	0.74	378	91
15.10.2008	MLE	0.76	387	90

Table 5. Space air change rates estimated from equilibrium analysis and Maximum Likelihood Estimation (MLE) on 13.10.2008 and 15.10.2008

Table 6 illustrates excellent model performances from MLE for all five days. Figs. 7 and 8 demonstrate good fittings between the measured and estimated indoor CO₂ concentrations, and the residuals in Figs. 9 and 10 shows no trend and pattern. In practical applications, the following cases often make the parameter assessment methods more difficult to use:

1. A large number of parameters. This could lead to multiple solutions.
2. Inadequate governing equation. If the governing equation cannot model well the actual condition in a physical means, the parameter method could perform bad and the resulting parameters may have misleading interpretations.

In our study, there are only two parameters (i.e. space air change rate and the supply CO₂ concentration), and the range of supply CO₂ concentrations is often known. In practice, the range of supply CO₂ concentration can be narrowed by observation. Most importantly, the governing equation Eq. (1) in this study well reflects the physical reality as a well-mixed indoor air is a widely accepted assumption for an office with mechanical ventilation (Fisk et al., 1991). Therefore, satisfactory results were obtained which demonstrated the suitability of the governing equation. As such, the computational load was small and convergence took few seconds in our calculation. All these show that the proposed method is substantially simpler and faster than most traditional methods. In summary, the space air change rates estimated from MLE are accurate and the proposed method is simple and fast.

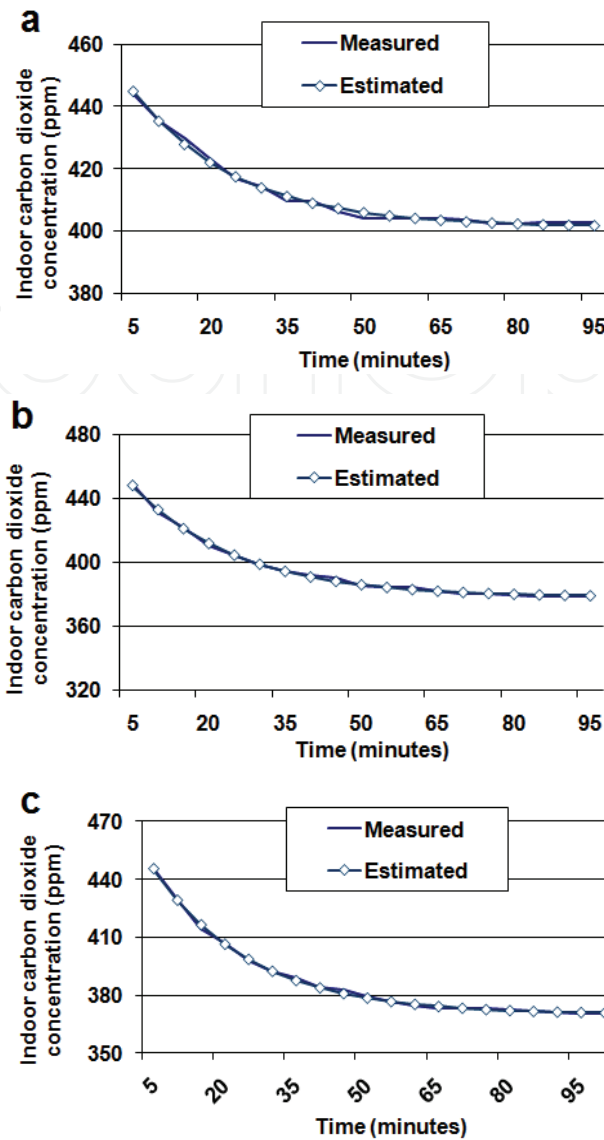


Fig. 7. Measured and estimated indoor CO₂ concentrations for unoccupied working periods on: (a) 22.9.2008, (b) 23.9.2008 and (c) 24.9.2008.

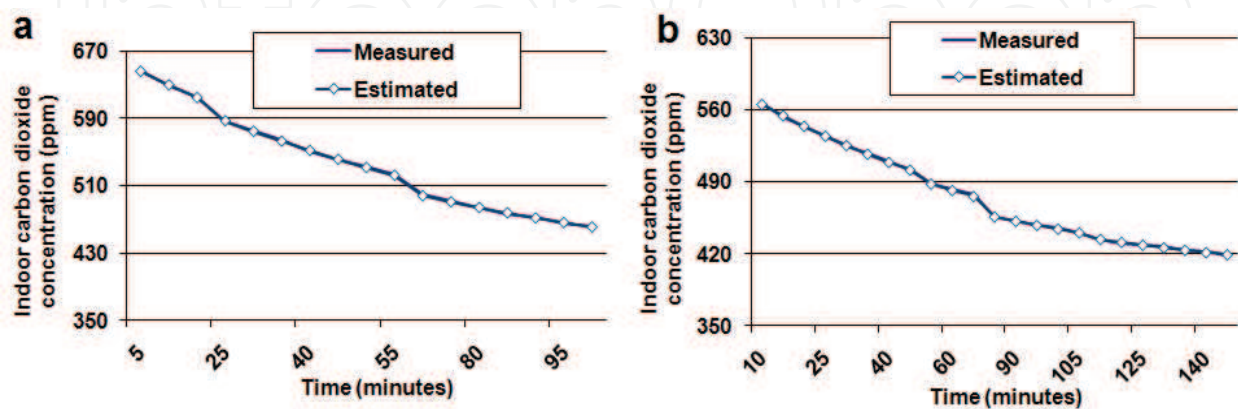


Fig. 8. Measured and estimated indoor CO₂ concentrations for unoccupied working periods on: (a) 13.10.2008 and (b) 15.10.2008.

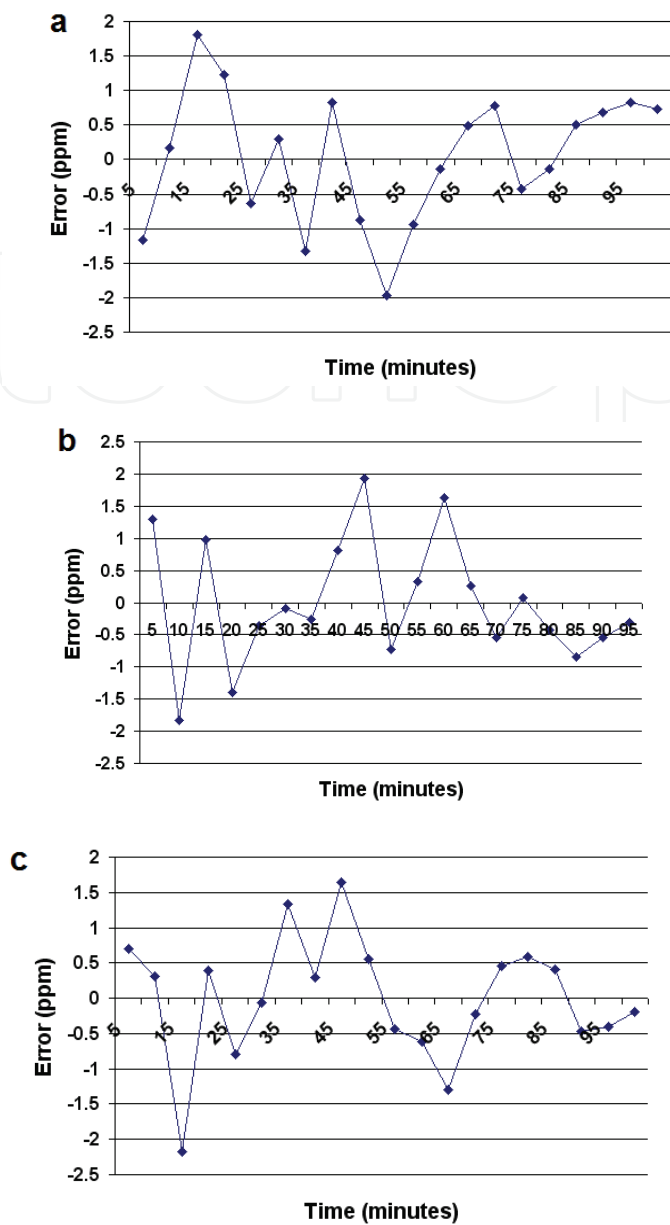


Fig. 9. Residuals from fittings on: (a) 22.9.2008, (b) 23.9.2008 and (c) 24.9.2008.

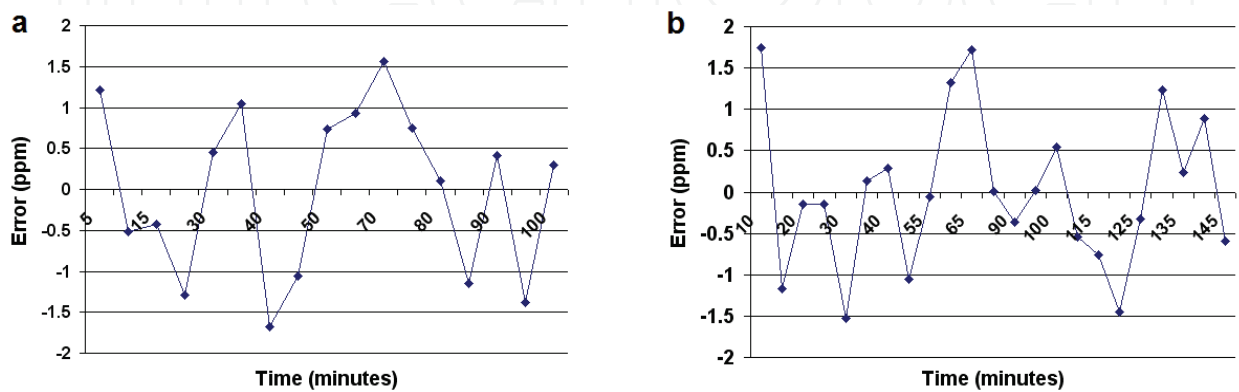


Fig. 10. Residuals from fittings on: (a) 13.10.2008 and (b) 15.10.2008.

Date	MSE (mean squared error)	R ² (coefficient of determination)
22.9.2008	0.95	1
23.9.2008	0.92	0.998
24.9.2008	0.63	0.998
13.10.2008	0.98	1
15.10.2008	0.82	1

Table 6. Model performances for experimental data

The proposed MLE method works more efficiently with spaces having big space air changes. These spaces, such as office rooms, lecture rooms, and alike, often have high demands on IAQ. But, as for the spaces with large volumes and small air changes rates (e.g. sporting halls), because air movements are slow sometimes sensors cannot catch changes of CO₂ concentrations within one or even more measurement intervals provided intervals are rather small. In this case, the measurement interval needs to be set a big value in order to avoid any form of stair-like curve from measured CO₂ concentrations, which obviously would bring big trouble for the estimation of space air change rate using MLE. The above assertion was verified by our later works. After this study, the proposed MLE method was further applied to estimate space air change rates for several sports halls. All these halls are served by full ventilation in daytime and half in nighttime, and space air change rates are small (<0.7). The first round of measurements started with small interval: 1 min. The graphs of measured CO₂ concentrations from the first round showed that there were many stairs existing in curves for *unoccupied working periods*, meaning that CO₂ concentrations remained the same within one interval (i.e. 1 min) or more during the decay due to small space air change rates and large volumes. Although the proposed MLE method still worked in this complex and difficult condition, fitting errors were so big that we cannot trust results. Actually estimated space air rates were near actual ones. Later on, the new round of measurements were conducted and the measurement interval was enlarged to 15 min. Measured CO₂ concentrations therefore presented continuously and smoothly decaying trends for *unoccupied working periods*, and fitting errors turned to be reduced significantly and become very small. Estimated space air changes rates were quite close to actual ones and trusted as a result. All these show that the propose MLE method can work well in some complex conditions as long as the measurement is well conducted.

In addition, although the method was primarily designed for constant air volume (CAV) system, it is easy to switch the method to time-varying ventilation system, such as demand-controlled ventilation (DCV) systems or variable air volume (VAV) system. But, as for a time-varying ventilation system, it is very difficult to estimate space air change rates only by measurements of indoor CO₂ concentrations. Some extra measurements must be needed. In most cases, we often take pressure differences between the return air vent and space as supplemental measurements due to technical simplicity in implementation. In order to proceed the estimation, some reference pressure difference between return air vent and space must be set first. This reference value can be selected randomly, such as 8 Pa. or 10 Pa. Moreover, Eq. (13) also has to be changed accordingly as followed:

$$f(n, a) = C(n) = (C(n-1) - \alpha_0) \exp\left(-\alpha_{ref} \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \Delta t\right) + \alpha_0 \quad (19)$$

where

- α_0 = supply CO₂ concentration for *unoccupied working period*,
 - ΔP_{ref} = reference pressure difference between the return air vent and space,
 - α_{ref} = space air change rate corresponding to ΔP_{ref} ,
 - ΔP_n = pressure difference between the return air vent and space at measurement count, n.
- Note that in the above equation we apply the powerlaw relationship (i.e. Eq. (18)) to account for changes of space air change rates. Therefore, Eqs. (14) and (15) are modified as follows:

$$\frac{\partial \log p(\{d_n\} | \alpha)}{\partial \alpha_0} = \frac{1}{\sigma^2} \sum_n (1 - \exp(-\alpha_{ref} \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \Delta t)) \left[d_n - (C(n-1) - \alpha_0) \exp(-\alpha_{ref} \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \Delta t) - \alpha_0 \right] = 0 \quad (20)$$

$$\frac{\partial \log p(\{d_n\} | \alpha)}{\partial \alpha_{ref}} = \dots \quad (21)$$

$$- \frac{\Delta t}{\sigma^2} \sum_n (C(n-1) - \alpha_0) \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \exp(-\alpha_{ref} \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \Delta t) \left[d_n - (C(n-1) - \alpha_0) \exp(-\alpha_{ref} \sqrt{\frac{\Delta P_n}{\Delta P_{ref}}} \Delta t) - \alpha_0 \right] = 0$$

Solve Eqs. (20) and (21) to estimate the space air change rate corresponding to the reference pressure difference and supply CO₂ concentration for *unoccupied working period*. And then take the reference pressure difference, ΔP_{ref} , and estimated corresponding space air change rate, α_{ref} , as reference values to estimate the space air change rate at any time step using the powerlaw relationship (i.e. Eq. (18)). For instance, assume that:

- reference pressure difference between return air vent and space = 8 Pa,
- space air change rate estimated from Eqs. (20) and (21) for the reference pressure difference = 1 ach,
- measured pressure difference at some time step = 50 Pa.

Hence we take 1 ach and 8 Pa as reference values to approximate the space air change rate at that time step as: 2.5 ach = 1 * (50/8)^{0.5} (see Eq. (18)). Clearly, our method is also applicable for time-varying ventilation system.

4.1.2 Results and discussion for CO₂ generation rates

We used the method described in Section 3.2.2 (four-step method) to estimate the number of occupants, and then compared the results with records from diaries. The diaries recorded the numbers of occupants. For short-time visitors with less than 5-minute stay, they were not recorded in diaries. Because diaries are incomplete for 13.10.2008 and 15.10.2008, here we just present the results for 22.9.2008, 23.9.2008 and 24.9.2008, totally three days in Fig. 11. Fig. 11 illustrates that even if the number of occupants didn't change, the indoor CO₂ concentrations could vary and sometimes show a decaying trend. In addition to the occupants and space air change rates, indoor CO₂ concentrations can be influenced by other factors, such as the supply CO₂ concentrations, short-time visitors and particularly changes on CO₂ generation rates. Activities have great influences on human CO₂ generation rates. When a person sits for long time, his CO₂ generation rate will turn to decrease steadily due to his fatigue, which results in a decaying trend of indoor CO₂ concentrations even if the number of occupants is unchanged.

Hence a significant change on indoor CO₂ concentrations does not necessarily mean a change on the number of occupants. For example, on 23.9.2008, one significant change from 461 ppm to 484.2 ppm was observed, which seemed to be associated the change of

occupants. However, with the developed model we evaluated that the number of the occupants was the same as before. Therefore, the changes might due to the occupant's activity. Indeed, an informal request from the person revealed that he actually did a little excise so as to alleviate the tiredness from the long-time work. Human activity does have a great impact on CO₂ generation rate, and sometimes misleads our judgments on the number of occupants. The developed model can correctly estimate the number of the occupants in such complicated case.

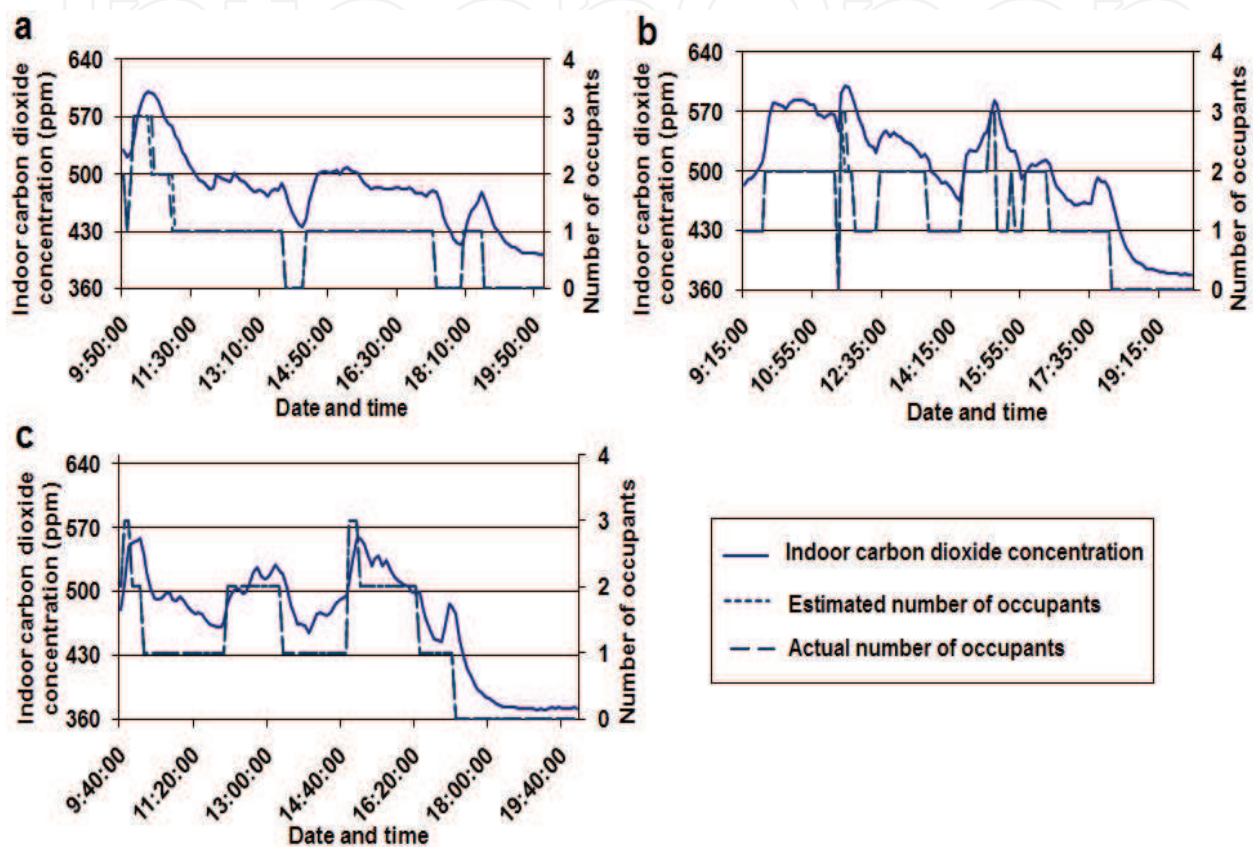


Fig. 11. The estimated and recorded numbers of occupants vs. measured indoor CO₂ concentrations on: (a) 22.9.2008, (b) 23.9.2008 and (c) 24.9.2008.

5. Conclusions

A simple and efficient model based on Maximum Likelihood Estimation (MLE) was developed to estimate space air change rates for an individual space in the commercial building. The results were verified by experimental measurements. The residuals from experimental results showed no trend and pattern, and all fittings between estimated and measured were satisfactory with at least 0.998 coefficient of determination (R^2). In addition, the estimated space air change rates were applied further to predict the numbers of occupants (see Fig. 11). The predicted numbers of occupants were the same as the actual numbers recorded in diaries. Moreover, the paper also shows the possibility that the model can be adapted for estimating time-varying space air change rates, which are common cases in demand-controlled ventilation (DCV) and variable air volume (VAV) systems. The methodology in the paper presents three new features which improve upon the current literature:

1. Bridging the gap between the Maximum Likelihood Estimation (MLE) and its application in estimating space air change rate. We estimated space air rates through MLE from a simplified mass balance equation of CO₂ concentration on the basis of ventilation schedule.
2. Estimating the number of occupants by coupling the traditional method and equilibrium analysis. In the traditional method, transient CO₂ generation rate is computed by solving the mass balance equation of CO₂ concentration. In this study, we combined the traditional method and equilibrium analysis to estimate the number of occupants.
3. Identifying a potential of the MLE method for evaluating time-varying space air change rates.

It is worth mentioning that the proposed model is based on the assumption of a well-mixed ventilated space, this restriction is chosen for convenience but can easily be relaxed. The model can be extended to more complicated configurations such as non-well-mixed space by changing the governing equations of CO₂ concentration (i.e. Eq. (3)) accordingly. A limitation of the model is that it relies on the *unoccupied working period* of a working day for estimating the space air change rate. If the *unoccupied working period* is too short or there is no *unoccupied working period* at all, the model will lose its ability in estimating the corresponding space air change rate. In our future work, we will tackle the above-mentioned limitation. One possibility is to use some global optimization method, such as genetic algorithm, to estimate the space air change rate and CO₂ generation rates during the whole occupied period. In addition, we will also extend our work to more complicated cases such as non-well-mixed and large spaces.

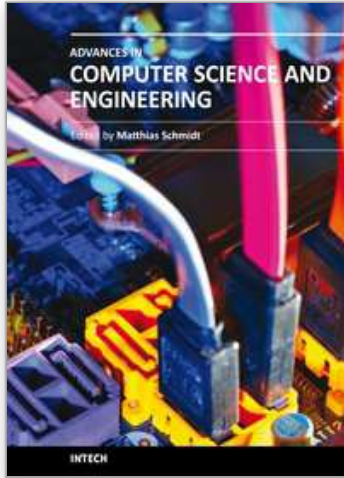
6. Acknowledgement

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