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SOURCE ESTIMATION OF INDOOR CONTAMINATION WITH VARIATIONAL CONTINUOUS ASSIMILATION METHOD

T. MATSUO[1], A. KONDO[1], H. SHIMADERA[2] and Y. INOUE[1]

[1] Graduate School of Engineering, Osaka University
2-1 Yamadaoka, Suita-shi, Osaka 565-0871, Japan
[2] Center for Environmental Innovation Design for Sustainability, Osaka University
2-1 Yamadaoka, Suita-shi, Osaka 565-0871, Japan

ABSTRACT

In order to manage and maintain hygienic indoor environment, it is necessary to know concentration of contaminants such as airborne particles and disease agents. If the Computational Fluid Dynamics (CFD) is used to estimate concentration of contamination, it requires information of the location and the intensity of contamination source. In the most cases, however, these details are unknown. Thus sometimes assimilation techniques are used to estimate these details together with observed data. In this study, the Variational Continuous Assimilation (VCA) method was used, and the validity was confirmed by numerical experiments. The VCA method assimilates observed data into CFD, and modifies the calculation. In the numerical experiments, quasi-observed data created by CFD were used, and the VCA method was applied to two-dimensional steady state flow fields which have different source locations. The main aim of the numerical experiments is to investigate the effect of positional relation between observation points and contamination source on source estimation. In the results, it was found that the positional relation between observed points and contamination source has significant effect to source estimation, and settling the observation points at suitable location can enlarge the area in which the VCA method can identify source location and intensity successfully.

INTRODUCTION

Indoor contaminants such as airborne particles and disease agents have an adverse effect on health of occupant. To assess, manage, and control the indoor hygienic environment effectively, it is necessary to know the concentration of contamination, and (if there is contamination) the location of the contamination source and its intensity.

Source estimations are typically carried out by measurements or CFD. However, both methods have some limitations. Measurements can obtain accurate values of observed location, but it is difficult to measure the whole field of objective room, and measurements of concentration cannot be used to simulate the spreading of the contaminants. On the other hand, CFD can calculate values of the entire field, and it also can predict or simulate the spreading of contamination. However, CFD requires accurate boundary conditions and source information such as the location and the intensity of the source which may be unknown in most cases. In order to overcome these limitations, various data assimilation methods have been developed.

The one of the most common assimilation method is called the nudging method, in which calculated values are modified directly by adding a “nudging” term into them to fit with the observed data. Nudging method is easy to apply, but it is difficult to select appropriate nudging coefficient because it has great impact to the estimations but little physical meaning. Thus the coefficient should be chosen carefully. For example, the work of Zou et al.(1) used a data assimilation method to determine the optimal nudging coefficient.

The methods which modify the calculated values directly have some problems. First, the modified values would fit observed data, but they may not satisfy the governing equations such as continuity equation. Second, the method can modify the calculated values only in the area which has observed value. In order to overcome the these problem, Kondo et al.(2) used the cost function consisting of not only the difference of calculated and observed values, but also residual of governing equation.

There are some assimilation methods which are different from aforementioned methods in a way that doesn’t modify the calculated values directly. For example, Le Dimet and Talagrand proposed the adjoint method(3), which modifies the initial boundary conditions instead of calculated fields. However, Toth and Peña(4) pointed out that if there are model errors, the result of calculation using correct initial conditions will “drift” from correct fields. Additionally, Kovalets et al.(5) found that if the “imperfect model” is used, much more observed data is needed to obtain good result with high probability than when the “perfect model” is used. The latter result is consistent with that of Wang et al.(6) which identifies the point source of gaseous contaminant by the coefficients of transport equations of steady fields, and their study also pointed out that the location of observation points has an impact on the area where the method can identify the source location successfully.

According to their conclusion, it is difficult to obtain accurate estimates with incorrect model, so that we should use a model as accurate as possible. When the model is accurate enough while the correct flow and temperature fields are available, inverse calculations can be used for source estimation. There are some methods which identify source location by solving convection diffusion equation reversely. Zhang and Chen(7,8) used the Quasi-Reversibility (QR) equation and Pseudo-Reversibility

(PR) equation to identify the source location and intensity. The QR method solves the convection diffusion equation with negative time step, in which second-order diffusion term is replaced by fourth-order stabilization term. On the other hand, the PR method doesn't reverse the time step but flow fields, and the method omits the diffusion term. Zhang and Chen(7) concluded that the QR method is slightly better than the PR method in term of accuracy, but the QR method requires more computational time. If the contaminant is air borne particles, the calculation required specified treatment. Chen et al.(8), for example, investigated the effect of near-wall heat source on particle deposition, and Tung et al.(9) investigated the behavior of different particles in radius in industrial clean rooms with various tool coverage. Zhang et al.(10) used the Lagrangian-Reversibility (LR) model in order to identify the release source of indoor airborne particles ,which performed a little better than PR method. These methods can identify the source location if the flow field is accurate enough. In most cases, however, errors occur in calculated flow field due to the errors of boundary conditions, initial conditions, discretization of governing equation, and so on.

The method employed in this study was the Variational Continuous Assimilation (VCA) method, which originally introduced by Derber(11), and modified in order to identify the source location and strength. In this study, VCA method was used only for identification of contamination source location and intensity, but the method can be used to correct flow and temperature fields at least in principle, and these versatility and expansibility for the future study are the reason why we used this method in this study.

The main aim of this study is to investigate the effect of positional relation between observation points and contamination source on source estimation of the VCA method, and to find the qualitative method to set observation points appropriately.

METHOD

The VCA method is an iterative method, which repeats the CFD calculation and the correction calculation. CFD calculate flow, thermal, and concentration fields, and then the decrease of the errors between calculated and observed values.

The governing equations of the VCA method

When observed values are available at P different times over the assimilation interval, the times are ordered such that $t_1 < t_2 < \cdots < t_p$. The model requires N time steps to cover the same interval.

The governing equation of the CFD calculation is given by

$$\Psi^n = A^n \Psi^{n-1} + \lambda^n \phi \tag{1}$$

where Ψ^n is the vector consisted of calculated values at time t_n, and A^n is conversion matrix acting upon Ψ^{n-1}. The correction term $\lambda^n \phi$ consists of a prespecified time-dependent variable λ^n and a spatially dependent vector ϕ. The variable λ^n is used to control the distribution of a correction vector over the assimilation interval. The VCA method corrects the calculation by optimizing the correction vector.

The size of the error is defined by the objective function, which is given by

$$I = \frac{1}{2}\sum_{p=1}^{P}\left(\Psi^p - \tilde{\Psi}^p\right)^{\mathrm{T}}\left(\Psi^p - \tilde{\Psi}^p\right) \tag{2}$$

where Ψ^p is the calculated vector at time t_p, and tilde denotes observed vector. Further, the $(\ )^{\mathrm{T}}$ notation denotes the transpose of a matrix.

In the correction calculation, the VCA method obtains an optimized correction vector by differentiating the error with respect to the correction vector.

Application of the VCA method for source estimation

The VCA method is used to obtain the optimal ϕ that corrects the calculation vector Ψ^n. In this study, the objective of applying the VCA method was to estimate the source location and intensity of contamination.

The convection diffusion equation of concentration is given by

$$\frac{\partial C}{\partial t} + \nabla \cdot (vC) = \nabla \cdot (\Gamma \nabla C) + S \tag{3}$$

where C is the concentration of contamination, v is the wind velocity, Γ is the coefficient of diffusion. The $\nabla \cdot$ notation denotes the divergence, and the ∇ notation denotes the gradient. S is the source intensity, which was assumed as a constant variable.

When the flow field is known but the contamination source is unknown, the differences between calculated and observed concentration are caused by the effect of the contamination source.

According to Eq. (1), an expression of Eq. (4) is given by

$$C^{n+1} = A^{n+1}C^n + A^{n+1}S^* \tag{4}$$

where S^* is expressed as $S^* = S \cdot \Delta t$ and Δt denotes the time step between time t_n and t_{n+1}.

Then, an expression of the correction term can be obtained by Eq. (5) as

$$\lambda^n \phi = A^{n+1} S^* \tag{5}$$

Therefore it can be assumed that $\lambda^n \phi$ is equivalent to the effect of source term at time t_n.

The numerical experiment of VCA method for indoor contamination estimation

The VCA method was applied to a simple two-dimensional field with steady flow. The objective room is shown in Fig. 1. The boundary conditions are displayed in

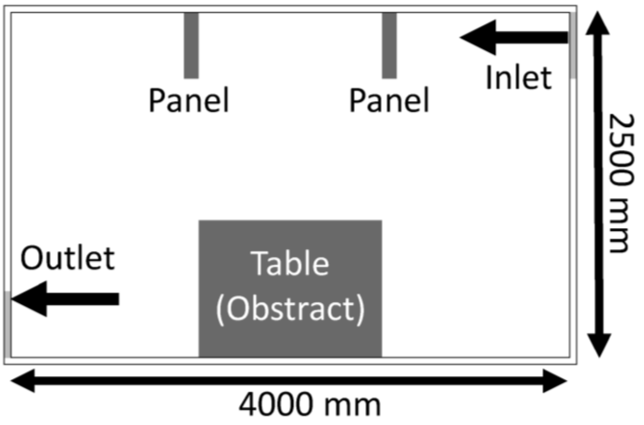

Figure 1. Objective Room

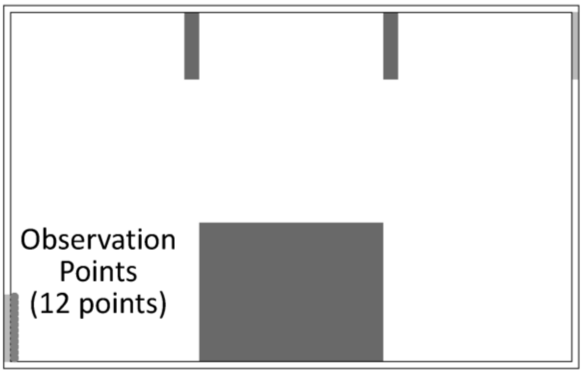

Figure 3. The location of the observation points.

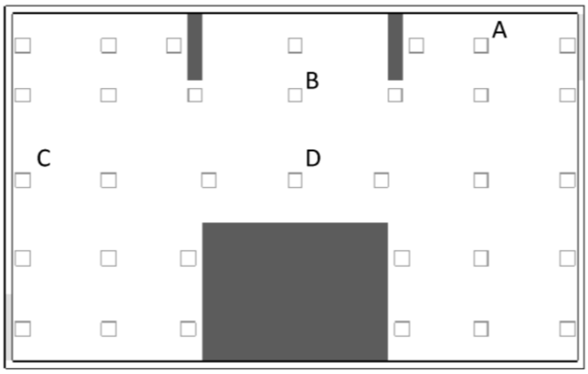

Figure 2. The location of contamination sources.

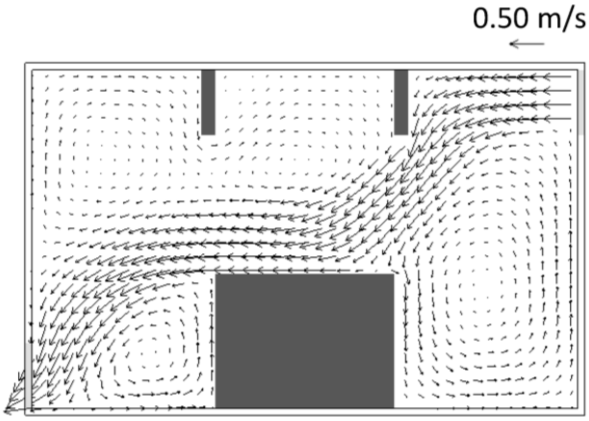

Figure 4. Flow Field

Table 1. Boundary conditions

Inlet	Constant flow: 0.50 m s^{-1}
Outlet	Free boundary
Contamination source	Intensity: 4.0 mg m^{-3} s^{-1}

Table 1.

The objective of the numerical experiments was to investigate the effect of the positional relation between observation points and contamination source. Therefore, in this experiment, 33 different simulation cases were carried out with different source locations.

The each case had only one contamination source, and the source locations are shown in Fig. 2. The contaminant was emitted for a second, and it was assumed that the time when the emission is started and ended was known. Therefore in the VCA method, time-dependent variable λ^n was 1 when the contamination was been emitting, and 0 when the contamination wasn’t been emitting.

Making the quasi-observed data

Because of the numerical experiment, the real observed data cannot be used. So we used quasi-observed data instead of real observed data. The quasi-observed data were created by extracting the data from the calculation result with correct source information.

Generally, the observation points should be set as downstream as possible because they can detect only the contaminant which emitted from the place more upstream than them. Thus the observation points were set at the outlet as shown in Fig. 3. The observation interval was set to 1 sec.

The flow field

When the source estimation is carried out in actual situation, the flow field is not well known in most cases. However, it is a commonplace technique to assume the calculated flow field is correct(2,6,7,8,12,13,14,15). In this study, we also assumed that the flow field is known, and the flow is steady. The flow field is shown in Fig. 4.

RESULT OF NUMERICAL EXPERIMENT 1

The time variation of concentration field in the case of the contamination source is located at center of the room (D in Fig. 2) is shown in Fig. 5. The contaminant was transported along the flow, and got diffuse with time. The quasi-observed data which used in the VCA method were extracted by these results.

The result of the VCA method applied to the case of the source location D is shown in Fig. 6, which shows the time variation of estimated concentration field. Figure 5 and 6 show that the time variation of concentration field was successfully estimated.

The distributions of correction vector are shown in Fig. 7 where the empty square is the correct location of the contamination source, and the area which colored dark gray enclosing 50% of the sum of the correction vector,

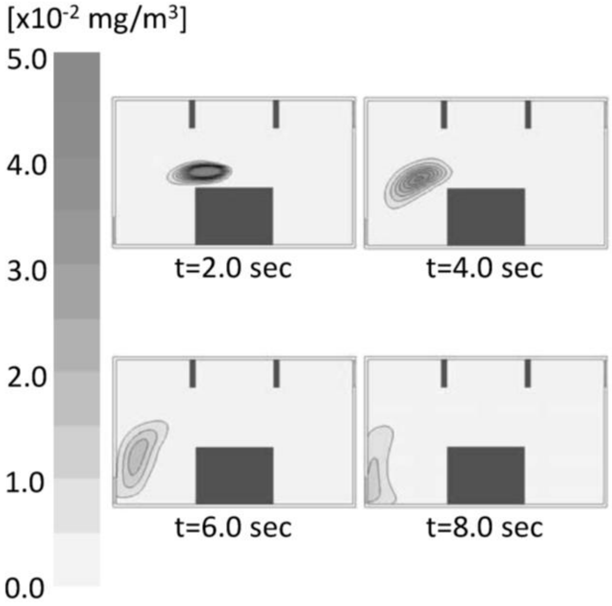

Figure 5. The correct time variation of the concentration of contamination source A. (a) t=2.0 sec (b) t=4.0 sec (c) t=6.0 sec (d) t=8.0 sec

and the area colored light gray enclosing 90%, which means most of the correction vector is highly concentrated near the correct contamination source. As previously explained, the distribution and the strength of the correction vector can be assumed as the location and intensity of the contamination source, respectively.

The assessment of the VCA results

In order to determine if the source estimation was successful or not, we used following criteria.

1. The correct source is located in the area of top 90% of the sum of correction vector (the light gray area).
2. There is only one peak of correction vector (dark gray area).

If the distribution of correction vector satisfies the criteria, the estimation was assumed “succeeded”. For example, the case of contamination source A and D shown in Fig. 7(a) and 7(d), respectively, was “succeeded”. However, the two cases shown in Fig. 7(b) and 7(c) were not succeeded. The case shown in Fig. 7(b) satisfy the second criterion but not the first one. In contrast, the case shown in Fig. 7(c) satisfy the first criterion but not second one.

The Effect of the positional relation between observation points and contamination source

In Fig. 8, the determination results of 33 the cases are shown, in which the contamination sources are represented as numbered squares, respectively. The filled squares represent the contamination source which can be estimated successfully, and empty squares represent the ones which cannot estimated successfully. This result indicated a hypothesis that only when a contamination source is located in main flow path, the estimation will be succeed.

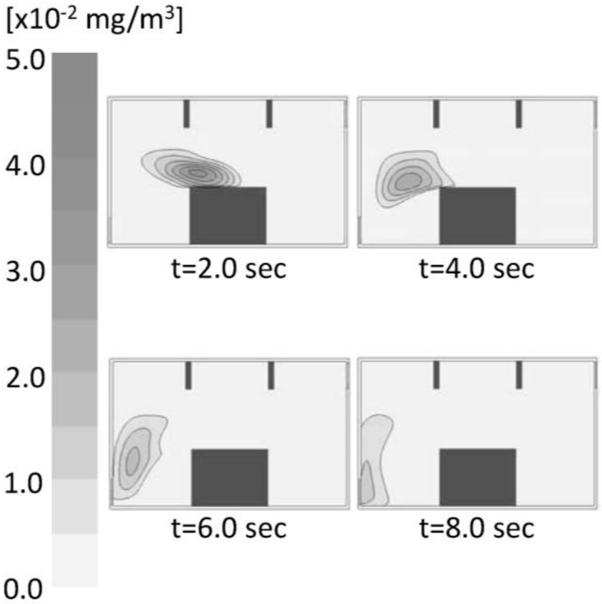

Figure 6. The estimated time variation of the concentration of contamination source A. (a) t=2.0 sec (b) t=4.0 sec (c) t=6.0 sec (d) t=8.0 sec

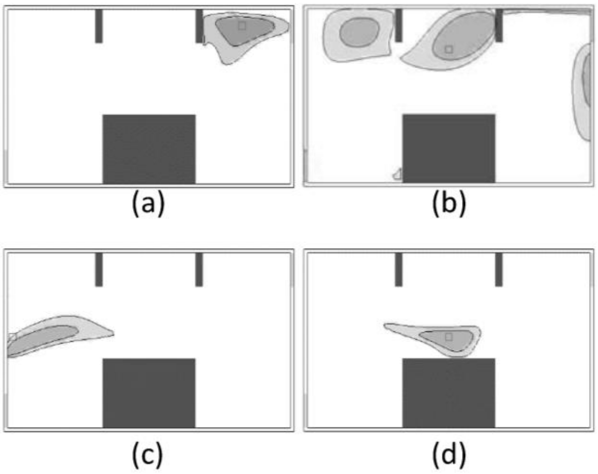

Figure 7. The distribution of correction vector. (a)The result of source location A. (b)The result of source location B. (c)The result of source location C. (d)The result of source location D.

The streamline shown in Fig. 9 corroborates this hypothesis. The source locations were estimated successfully only in the cases the contamination source and observation points were located on the same streamline.

The result of estimation of source intensity

The estimated source intensities are shown in Fig.10, and it indicates that when the source location was estimated successfully, the source intensity was also estimated successfully.

The reason why the intensity of the source no. 25 was underestimated is that the source is located at the edge of the streamline which pass through the outlet. Thus only a part of the emitted contamination could be observed.

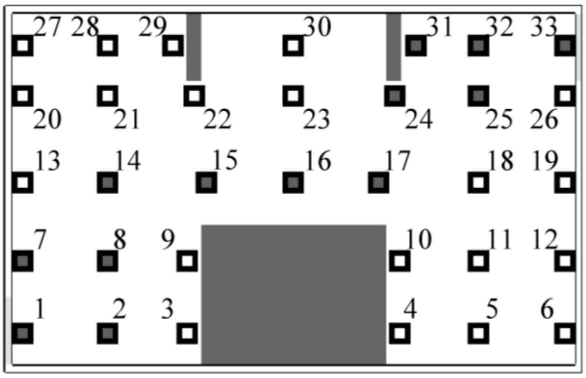

Figure 8. The result of 33 cases. (Filled squares are the location where can be estimated successfully, and empty squares are not.)

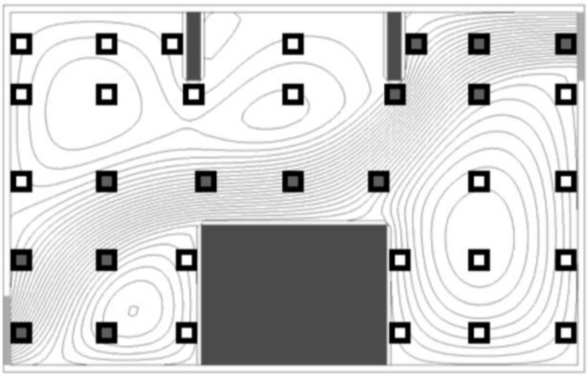

Figure 9. The result of judgments of 33 cases with the stream line.

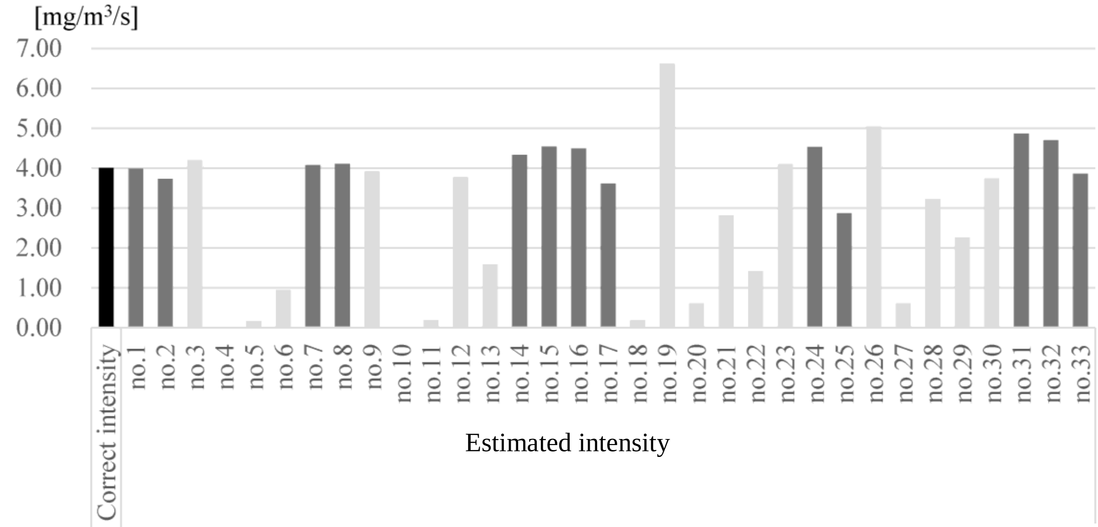

Figure 10. The estimated intensity of the contamination source.

RESULT OF NUMERICAL EXPERIMENT 2

The aforementioned hypothesis suggests that to set up observation points to cover more streamline will enlarge the area where the VCA method can estimate source location. Thus, in order to verify the hypothesis, second numerical experiment was carried out with additional observation points on which the locations were decided based on the aforementioned hypothesis.

The locations of observation points are shown in figure 11. The additional observation points were located on downstream of the eddies.

The results of the source location estimation

In the second numerical experiment, 33 simulation cases were carried out in the same way as the first experiment, and the results of the source location A, B, C and D in Fig.2 are shown in Fig. 12. It was found that the second experiment can evaluate source locations which couldn’t be evaluated in the first experiment (see Fig. 7 and 12).

The effect of the additional observation sources

The results of 33 simulation cases were also determined if the estimations were carried out successfully or not, respectively, and they are shown in Fig. 13 which shows that the representative numbers of contamination sources which could be evaluated was increased, which means that the additional observation points enlarged the area where the VCA method can identify the location of contamination source successfully.

The results of case E and F, in which the contamination source could not be estimated successfully, are shown in Fig. 14. Figure 14(a) and 14(b) show that they don’t satisfy the criterion 2 (there is only one peak), but the estimation were carried out almost successfully.

This result indicates that the additional observation points improved the estimation result dramatically. Therefore it is very important to consider the appropriate positional relation between the observation points and contamination sources, and if flow field is known, we can set the observation points appropriately.

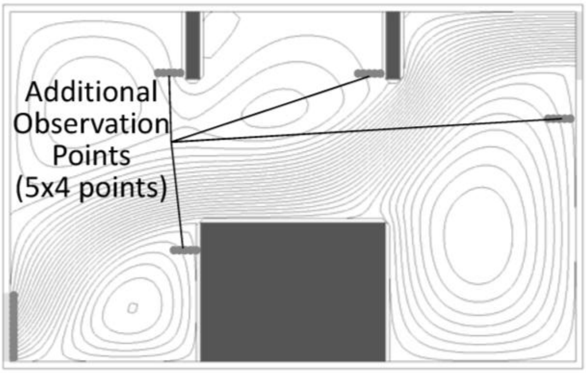

Figure 11. The locations of observation points.

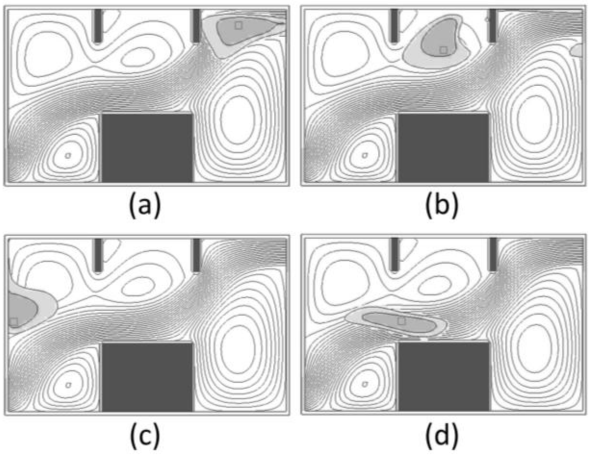
(a) (b)
(c) (d)

Figure 12. The distribution of correction vector with streamline. (a)The result of source location A. (b)The result of source location B. (c)The result of source location C. (d)The result of source location D.

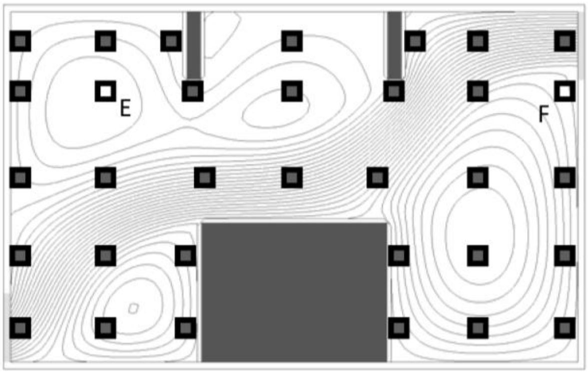

Figure 13. The result of judgments of 33 cases. (Filled squares are the location where can be estimated successfully, and empty squares are not.)

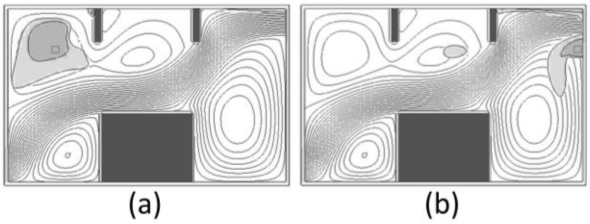
(a) (b)

Figure 14. The distribution of correction vector with streamline. (a)The result of source location E. (b)The result of source location F.

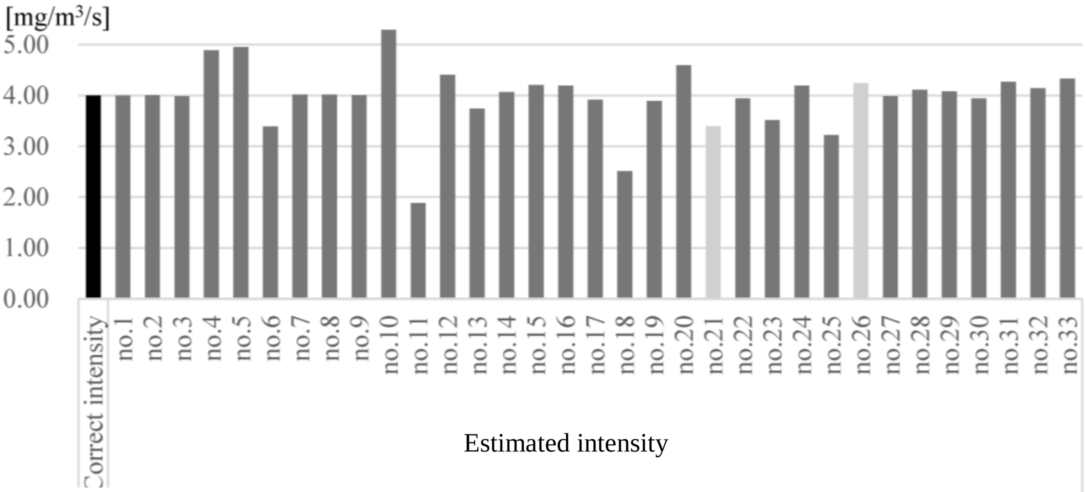

Figure 15. The estimated intensity of the contamination source.

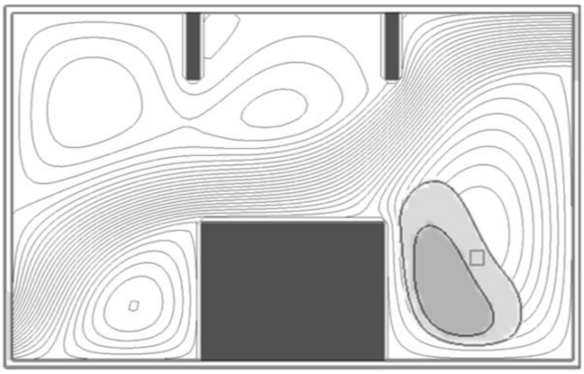

Figure 16. The distribution of correction vector of contamination source no.11.

The result of source intensity estimation

The estimated source intensities are shown in Fig. 15, which indicates that in the most cases when the source location is estimated successfully, the source intensity can be estimated successfully.

The intensity of the source no. 11 and 18 were underestimated, and the reason is that the sources are located inside of the streamline which pass through the observation points as shown in Fig. 16 and 17, respectively. Thus only a part of the emitted contamination could be observed, resulting underestimated intensity.

In contrast, the intensity of the source no. 10 was overestimated, because the estimated correction vector was distributed inside streamline which pass through the observation points (as shown in Fig. 18), and so that a part of the contamination emitted from the estimated source location wasn't transported to the observation points. Thus the overestimated source intensity couldn't be corrected.

In either case of under- or over- estimation, the error of estimated source intensity was caused by the error of estimated source location.

CONCLUSION

For estimation of indoor environment such as the distribution of contamination, a method of data assimilation is applied, and the method was modified in order to evaluate the location and the intensity of contamination source.

The main aim of this study was to investigate the effect of positional relation between observation points and contamination source on source estimation of the VCA method, and to find the qualitative method to set observation points appropriately. For this aim, two numerical experiments were carried out.

In the numerical experiments, the VCA method was applied to two-dimensional steady flow which has one contamination source whose location and intensity are unknown. Both experiments were carried out with 33 contamination sources, respectively.

In the first experiment, the observation points were set only at outlet of the objective room. The result of the numerical experiment indicated that the estimation of the source location will succeed only when the observation points and contamination source are on the same streamline.

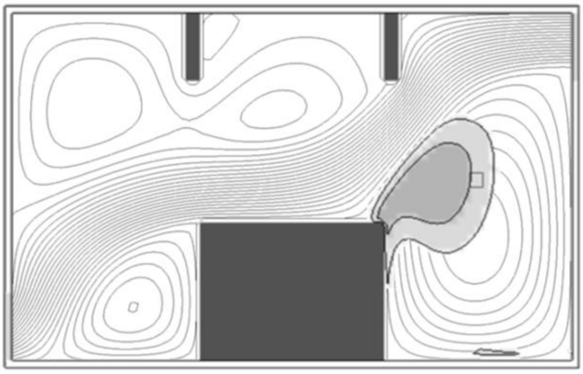

Figure 17. The distribution of correction vector of contamination source no. 18.

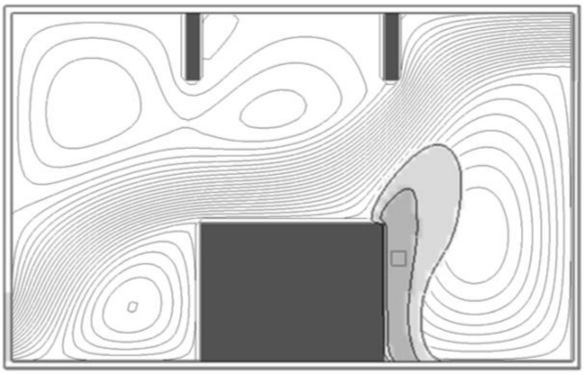

Figure 18. The distribution of correction vector of contamination source no. 10.

Therefore, in the second experiment, the additional observation points were set to cover the more streamline. In the result of the second experiment, the source locations were estimated successfully in 31 cases out of 33 cases, and the accuracy of the estimation of the source intensity was also improved.

From the results of the numerical experiments, followings were concluded.

1. The source location can be evaluated only when the contamination source and observation points are on the same streamline.
2. The source intensity also can be evaluated when the contamination source is evaluated successfully.
3. If the contamination source is located at the edge of streamline which pass through the observation points, the intensity of the contamination source will be underestimated.
4. When the correction vector distributes on the streamline which does not pass through the observation points, the source intensity tends to be overestimated.
5. When the location of the contamination source is unknown, the observation points are recommended to be positioned covering as much streamline as possible.

In this study, the VCA method was applied only to simple two-dimensional room. In addition, because of numerical study, the observation errors were omitted in this study. Further study is therefore necessary to validate the generality of our results.

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