18th International Conference on
Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes
9-12 October 2017, Bologna, Italy

IDENTIFICATION OF OUTDOOR CONTAMINATION SOURCES BY USING VARIATIONAL CONTINUOUS ASSIMILATION METHOD

Tomohito Matsuo[1], Takaya Matsumoto[1] Hikari Shimadera[1] and Akira Kondo[1]

[1]Osaka University, Osaka, Japan

Abstract: In this study, the variational continuous assimilation (VCA) method was applied to source estimation in outdoor condition. The VCA method is a kind of data assimilation methods, which minimizes the difference between calculated and observed concentration by adding the correction term onto the governing equation of the CFD model. The correction term can be assumed as the source term. The unknown source location and intensity were estimated by assuming the correction term as the source term. In order to validate the VCA method, a set of numerical experiments was conducted. The results shows that the VCA method could roughly reproduce the correct concentration fields.

Key words: *CFD, Data assimilation, Source estimation, Outdoor*

INTRODUCTION

In the case of accidental release of hazardous substances, it is important to investigate the distribution of the contaminants. In order to detect the released contaminants, some sensors are used. The sensors can observe the concentration of the contaminants at the points where the sensors are located. If the number of the sensors is enough, we can obtain the concentration field directly. The number of the sensors, however, is limited in most cases and we cannot estimate the concentration field with high resolution.

A data assimilation method that combines the observation data with computational fluid dynamics (CFD) may solve this problem. Recently, various data assimilation methods to estimate the contamination source location and intensity have been developed. Zhang and Chen (2007), for example, compared the quasi-reversibility (QR) method and the pseudo-reversibility (PR) method. The QR method solves the modified transport equation with negative time step. The PR method solves the transport equation with reversed airflow. The both method can estimate the contamination source location by observed concentration of the contamination. Zhang et al.(2012) used the QR model and the Lagrangian-reversibility (LR) model in order to estimate indoor particulate sources. Because these methods use a concept of the back trajectory, the methods will perform well in convection-dominated flow. Keats et al.(2007) and Liu and Zhai (2008) incorporated source receptor function (SRF) into Bayesian inference in order to estimate the source location and intensity. Kovalets et al. (2011) and Wang et al. (2013) used the variational method with SRF to search the stationary point source which minimizes the differences between observed and estimated concentration of contamination. These methods have an advantage that the methods can derive the relationship between potential contamination sources and the observed concentration before the observation, so that they can rapidly identify the source location and intensity after the release of the contaminant. The methods requires, however, much more calculation resources than the reversibility methods, especially when there are plural contamination sources. In this study, in order to estimate plural contamination sources, the variational continuous assimilation (VCA) method was employed. The VCA method was developed by Derber (1986), and modified by Matsuo et al. (2015). The method can estimate the distribution of contamination sources and their intensities.

METHODOLOGY

In this section, the concept of the VCA method and the numerical experiment in order to validate the method are explained.

The governing equations of VCA method

The VCA method is a kind of variation method, which minimizes the differences between observed and calculated values by modifying the governing equation. In this study, the governing equation is the mass conservation equation, which is given by,

$$\frac{\partial C_{cal.}}{\partial t}+\frac{\partial(\boldsymbol{U}C_{cal.})}{\partial \boldsymbol{x}}=\frac{\partial}{\partial \boldsymbol{x}}\left(D\frac{\partial C_{cal.}}{\partial \boldsymbol{x}}\right)+S, \tag{1}$$

where $C_{cal.}$ is the concentration of contaminant, $\boldsymbol{U}$ is wind velocity, D is the effective diffusion coefficient, and S is the constant source term.

The transport equation can be discretized as,

$$C_{cal.}^{n+1}=A^{n}C_{cal.}^{n}+S^{*}, \tag{2}$$

where A is a linear operator acting upon $C_{cal.}$, and S^* is expressed as $S^*=S\Delta t$.

The VCA method modifies the governing equation by adding the correction term $\lambda\phi$ as follows.

$$C_{cal.}^{n+1}=A^{n}C_{cal.}^{n}+S^{*}+\lambda^{n}\phi, \tag{3}$$

where λ is the correction matrix which means the time distribution of the correction, and ϕ is the correction vector which mean the spatial distribution. The correction matrix, which is assumed to be known, is unit matrix when the correction applied, and is zero matrix when the correction is not applied.

The difference between observed and calculated values is defined as follows.

$$I=\frac{1}{2}\sum_{p=1}^{P}\left(C_{cal.}^{p}-C_{obs.}^{p}\right)^{\mathrm{T}}\left(C_{cal.}^{p}-C_{obs.}^{p}\right), \tag{4}$$

where I is called the "objective function", P is the number of calculation steps, $C^{n}_{cal.}$ and $C^{n}_{obs.}$ are the calculated and observed concentration of contaminant at pth observation step, the $(\ )^{\mathrm{T}}$ notation denotes the transpose of a vector or a tensor.

The VCA method searches the correction term which minimizes the objective function I by optimizing the correction vector ϕ by the following equation.

$$\phi^{k+1}=\phi^{k}+\alpha\left.\frac{\partial I}{\partial \phi}\right|_{\phi=\phi^{k}}, \tag{6}$$

where ϕ^k is the kth iteration of ϕ, α is the parameter of step size.

Application of the VCA method to the source estimation

As mention above, the discretized mass conservation equation is given by equation (3). By substituting $S^*=S^*_{correct}$ and $S^*=S^*_{wrong}$ into equation (3), respectively, and equation (7) can be obtained.

$$C_{cal.}^{n+1}=A^{n}C_{cal.}^{n}+S_{correct}^{*}+\lambda^{n}\phi\big|_{S^{*}=S^{*}_{correct}}=A^{n}C_{cal.}^{n}+S_{wrong}^{*}+\lambda^{n}\phi\big|_{S^{*}=S^{*}_{wrong}} \tag{7}$$

When the difference between calculated and observed values is caused only by source term, the correction term which calculated with "correct" source term is zero. Thus the following equation is obtained by substituting $S^*_{wrong}=0$.

$$S_{correct}^{*}=\lambda^{n}\phi\big|_{S^{*}=0} \tag{8}$$

Therefore, assuming that the source term S^* is zero in calculation, the correction term $\lambda^n\phi$ will become equivalent to the correct source term. According to this, the distribution of correction term was assumed as the estimated source location and intensity in the numerical experiments.

Procedure of numerical experiment

In order to validate the VCA method applied to the source estimation, a set of numerical experiments was conducted. In the numerical experiments, unknown source location and intensity was estimated by using the known flow field, release time and concentration at limited points.

The experiments were performed with the following procedures: (i) "correct" concentration field was calculated by CFD with "correct" contaminant source; (ii) "observed concentration" was extracted from the "correct" concentration field; (iii) the VCA method was applied to the known flow field and "observed concentration" and release time in order to estimate "correct" concentration field; (iv) estimated concentration field and source location and intensity were compared with those of "correct" dataset.

Calculation domain

The calculation domain is shown in Figure 1. The height of the domain is 70 m. There are 6 buildings which are the same size (W × D × H = 15 m × 12 m × 6 m) in the domain. The horizontal mesh size is 1.5 m × 1.5 m in the analysis domain, and proportionally expanding outside the analysis domain. The vertical mesh size is 0.5 m from the ground to 12 m, and proportionally expanding above 12 m. The number of the meshes is 1,881,472.

In the experiments, the isothermal condition and the steady state flow was assumed. The wind blew from west to east, and the vertical distribution of the wind velocity at the west boundary followed the power law.

$$u(z) = u_r (z/z_r)^n \tag{9}$$

where z is the height, z_r is the reference height, u_r is the reference velocity and n is the constant which reflects the effect of the surface roughness. In the experiments, z_r = 10 m, u_r = 3 m and n = 0.25.

Calculation conditions

The governing equations of the CFD calculation are the conservation equations of momentum, mass and contamination. The equations were discretized by finite volume method. As the discretization scheme, the second-order upwind scheme was used for the convection term; the second-order central discretization scheme for the diffusion. The SIMPLE algorithm was employed to solve the velocity-pressure coupling. The standard k-ε model was used for the turbulence model.

Figure 2 shows the location of contamination sources and observation points. All the sources and observation points are located at 3.25 m high. The contamination sources are assumed to be a point source on the building. The intensity of a source is 1 g/m^3/s. The release of the contaminant occurs instantaneously (from t = 0 s to 1 s). The calculation period is t = 0 s to 100 s. The observation points are located at center of each two adjacent buildings and position away from a corner of each building by a distance D or W, as shown in figure 2. In each experiments, the one or two sources were selected and used as the "correct" source of contaminant, and all the observation points were used to the assimilation.

Figure 3 shows the flow field in the analysis domain. It shows the small wind velocity around building, and large eddies in the lee side of the buildings.

RESULTS

Figure 4 shows the "correct" and estimated concentration fields of contaminant when the "correct" contaminant source was located at source A in figure 2(a). The estimated concentration field could roughly reproduce the "correct" concentration field. The wrong high concentration, however, existed in the leeward of "correct" contamination source.

Figure 5 shows the "correct" and estimated concentration field when the "correct" sources are located at A and B in figure 2(a). The concentration field which comes from source A is similar to that shown in figure 5. The estimated concentration field which comes from source B occurs in windward of "correct" contamination source B. These slippages may be caused by the complicated flow near the buildings.

Figure 6 shows the estimated source location and intensity. The wrong high intensity appears in west side of lower-right building, which may be caused by the complicated flow between the lower two buildings. The estimated source location and intensity are not good for the source B, because observation points were not located in the lee of the source B, and could not detect the high concentration of the contaminant.

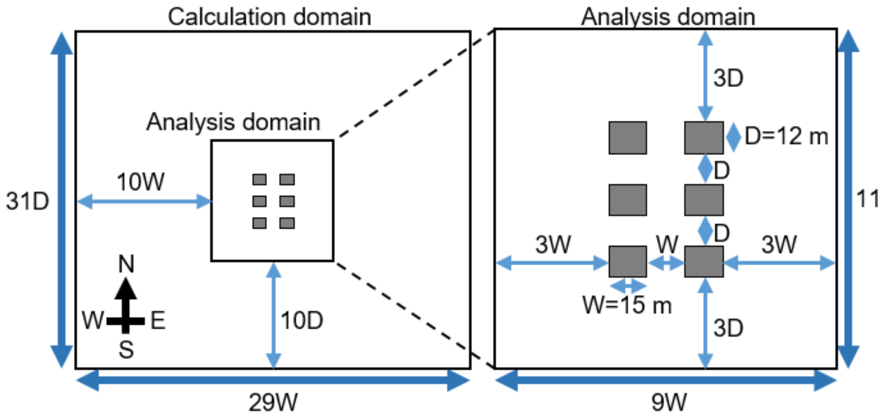

Figure 1. The objective field

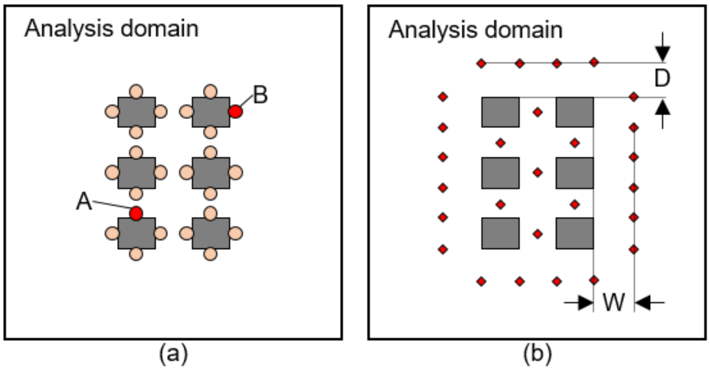

Figure 2. Locations of (a) contamination sources, (b) observation points.

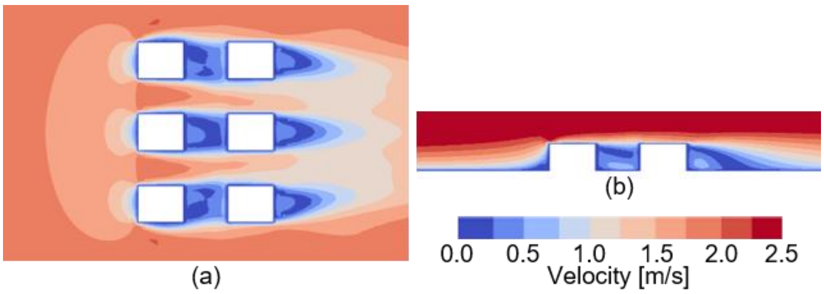

Figure 3. Velocity field at (a) 3.25 m high, (b) center of the north-south direction.

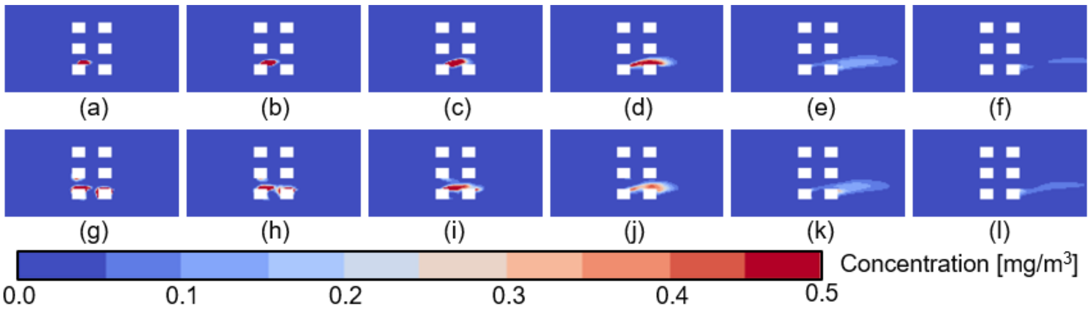

Figure 4. The concentration fields (a-f) calculated with “correct” source, and (g-l) estimated by VCA method, when the “correct” source is located A (figure 2(a), at t = 4, 8, 16, 32, 64, 96 s.

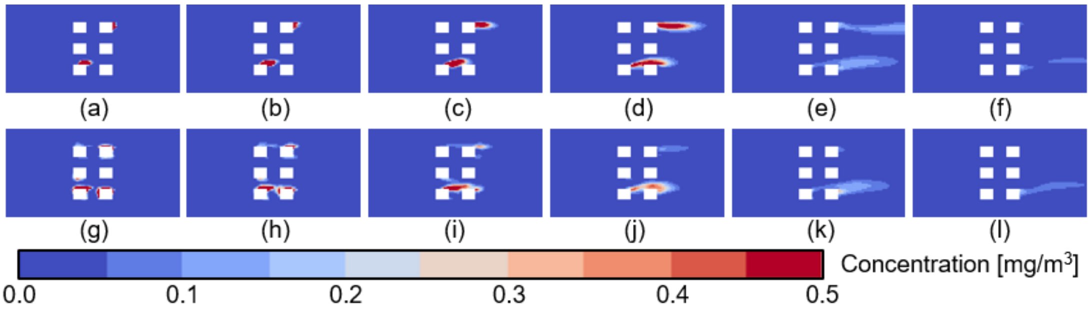

Figure 5. The concentration fields (a-f) calculated with "correct" sources, and (g-l) estimated by VCA method, when the "correct" sources are located A and B (figure 2(a)), at t = 4, 8, 16, 32, 64, 96 s.

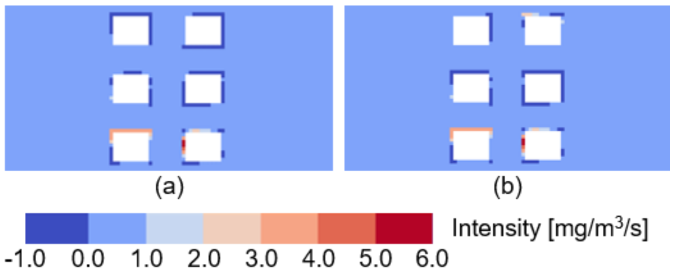

Figure 6. Estimated Source location and intensity when "correct" sources are (a) located at A in figure 2(a), (b) located at A and B in figure 2(a).

CONCLUSION

In this study, the VCA method was applied to source estimation in outdoor conditions. In order to validate the method, a set of numerical experiments was conducted. In the numerical experiments, the location and intensity of unknown contamination sources were estimated by known flow field, concentration at observation points, and release time. Though the results show that the method could roughly reproduce the concentration field, the estimated source location and intensity were not so good because of complicated flow field near the buildings and the location of the observation points.

REFERENCES

Derber, J. C, 1989: A variational continuous assimilation technique. *Monthly Weather Review*, **117**, 2437-2446.

Keats, A, E. Yee and F. Lien, 2007: Bayesian inference for source determination with applications to a complex urban environment. *Atmospheric Environment*, **41**, 465–479.

Kovalets, I. V, S. Andronpoulos, A. G. Venetsanos and J. G. Bartzis, 2011: Identification of strength and location of stationary point source of atmospheric pollutant in urban conditions using computational fluid dynamics model. *Mathematics and Computers in Simulation*, **82**, 244–257.

Liu, X, Z. Zhai, 2008: Location identification for indoor instantaneous point contaminant source by probability-based inverse computational fluid dynamics modeling. *Indoor Air*, **18**, 2-11.

Matsuo, T, A. Kondo, H. Shimadera, T. Kyuno and Y. Inoue, 2015: Estimation of indoor contamination source location by using variational continuous assimilation method. *Building Simulation*, **8**, 443-452.

Wang, X, W. Tao, Y. Lu and F. Wang, 2013: A method to identify the point source of indoor gaseous contaminant based on limited on-site steady concentration measurements. *Building Simulation*, **6**. 395-402

Zhang, T. and Q. Chen, 2007: Identification of contaminant sources in enclosed spaces by a single sensor. *Indoor Air*, **17**, 439-449.

Zhang, T, H. Li and S. Wang, 2012: Inversely tracking indoor airborne particles to locate their release sources. *Atmospheric Environment*, **55**, 328-338.