ESTIMATION OF SOURCE LOCATION OF OUTDOOR POLLUTION BY USING VARIATIONAL CONTINUOUS ASSIMILATION METHOD

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ABSTRACT

For the case where hazardous contaminants are emitted to the atmosphere, the understanding of the concentration fields and the source location is important to protect the surrounding environment from pollutant threat. In this study, based on Computational Fluid Dynamics (CFD), the data assimilation technique called the Variational Continuous Assimilation (VCA) method was utilized to estimate not only the concentration fields but also the source location and its intensity. In the VCA method, the correction term adds to the mass conservation equation. The correction term can be assumed to be the source term of the mass conservation equation.

In order to valid the accuracy of the VCA method, the numerical experiments were performed. In numerical experiments, observation datasets were created by the CFD simulation. The 'correct' concentration fields were calculated by the CFD simulation with the 'correct' boundary conditions. The observation datasets were extracted from the 'correct' concentration fields. The 'pseud' concentration fields were calculated by the CFD simulation with the 'pseud' boundary conditions, in which there was no contaminant source. By assimilating the observation datasets into the 'pseud' concentration fields, the 'pseud' concentration fields were revised. The revised concentration fields by the VCA method were compared to 'correct' concentration fields and the 'correct' source term. The use of the observation datasets on the windward side as well as on the downward side furthermore improved the accuracy of the concentration fields by the VCA method.

INTRODUCTION

If hazardous pollutant is emitted to the atmosphere, the understanding of the concentration dispersed from pollutant source is important in order to protect not only our human health but also the surrounding environment from the pollutant threat. When the source location of outdoor pollution is exactly known, the concentration fields can be easily calculated by the CFD simulation. In almost cases, however, the source location of outdoor pollution is unknown and the concentration at only several observed points is known.

In this study, the data assimilation method called variational continuous assimilation (VCA) method was used in order to estimate the source location from several observation data. The VCA method was originally developed by Derber⁽¹⁾, and was modified for the above purpose. In order to validate the accuracy of the VCA method, the numerical experiments were performed. From the theory of the VCA method, the location and the intensity of pollutant source, which continuously releases contaminants to the atmosphere, was estimated by assimilating the correct observation datasets into the pseud concentration fields.

METHOD

Governing equations and VCA method

In the numerical experiments, the governing equations of the CFD simulation was discretized by finite volume method. For the discretization scheme, the power low method was used for convection and diffusion term. The pressure was solved by SIMPLE method²). The k-ε model was used as the turbulence model.

The VCA method is the method that the correction term is added to the mass conservation equation in order to minimize the error between the CFD simulations and the observation data. The corrected mass conservation equation is given by

$$\Psi^{n} = A^{n}(\Psi^{n-1}) + \lambda^{n} \varphi \tag{1}$$

where *n* is the *n*th calculation step, and A^n is conversion matrix acting upon *n*-1. The correction term $\lambda^n \varphi$ consists

of time-dependent variable λ^n and spatial dependent vector φ .

The objective function I of the VCA method, which represents the error between the CFD simulations and the observation data, is given by

$$I = \frac{1}{2} \sum_{p=1}^{P} (\Psi_{cal}^{p} - \Psi_{obs}^{p})^{\mathrm{T}} (\Psi_{cal}^{p} - \Psi_{obs}^{p})$$
(2)

where *P* is the number of observation steps. Ψ^{p}_{cal} and

 $\Psi^{p}{}_{obs}$ are the calculation vector and the observation vector at time t_{p} , respectively. ()^T notation denotes the transpose of a vector or matrix.

Based on the comparison of the mass conservation equation and Eq.(1), the correction term of Eq.(1) is assumed to be the source term of the mass conversation equation.

The spatial dependent vector φ is searched by minimize the first-derivative of *I* with respect to φ , which is expressed by

$$\frac{\partial I}{\partial \varphi} = \sum_{p=1}^{P} \frac{\partial \Psi^{p}}{\partial \varphi} \left(\Psi^{p}{}_{cal} - \Psi^{p}{}_{obs} \right)$$
(3)

The spatial dependent vector φ calculated by the steepest descent method is given by

$$\varphi^{k+1} = \varphi^k + \alpha \frac{\partial I}{\partial \varphi}\Big|_{\varphi = \varphi^k}$$
(4)

where *k* is the number of iteration, α is a learning rate which is decided by the changing rate of the spatial dependent vector φ .

Procedures of numerical experiments

In order to estimate the source location and its intensity by the VCA method, the numerical experiments were performed by the following procedures.

(1) The concentration fields were calculated by the CFD simulation with the 'correct' boundary conditions. We call this concentration fields the 'correct' concentration fields. Several concentration data extracted from the 'correct' concentration fields are called as observation datasets. (2) The concentration fields were calculated by the CFD simulation with the 'pseud' boundary conditions, in which there was no contaminant source. We call this concentration fields the 'pseud' concentration fields. In this

case, 'pseud' concentration was zero in all calculated domain.(3) By assimilating "observation datasets" into the 'pseud' concentration fields, the 'pseud' concentration fields were revised by the VCA method.

Calculated domains

The calculated domain including the contaminant storage facility is shown in Fig.1. The size of the domain is $9 \text{ m} \times 5.25 \text{ m} \times 4 \text{ m}$ with the grid resolution of 0.25 m.

It is assumed that the uniform wind speed of 1.0 m/s in the x direction is given and that the size and the intensity of contaminant source is one grid ($0.25 \text{ m} \times 0.25 \text{ m} \times 0.25 \text{ m}$) and 1.0 g/m³/s, respectively.

The flow fields are shown in Fig.2. The correct concentration fields at t=1, 5, 10 and 15sec are shown in Fig.3.



Figure 1. Calculated domain of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m).



Figure 2. The flow fields of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m).



Figure 3. The correct concentration fields of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m)

Observation datasets

Three types of the observation datasets were prepared (Fig 4). (A) 9 observation data which are located to 1 meter behind the contaminant source. (B) 10 observation data which include the above 9 data and 1 observation data which is located to 1 meter ahead the contaminant source. (C) 18 observation data which include the above 9 data and 9 observation data which are located to 1 meter ahead the contaminant source. These observation data is assimilated once per second into the pseud concentration fields from the release of contaminant to 90s.

RESULT

Concentration fields

The VCA method was applied to assimilate the observation datasets into the 'pseud' concentration fields without the contaminant source. At any observation point, the revised concentration could be retrieved within 15% of the correct concentration.

The revised concentration fields using the observation datasets (A), (B) and (C) are shown in Fig. 5, 6 and 7, respectively. The revised concentration fields shown in Fig.5 spread more widely than the correct concentration fields. The revised concentration fields using additionally one downward concentration data shown in Fig.6 were improved compared with Fig.5. The revised concentration fields using additionally

nine downward concentration data shown in Fig.7 became close to the correct concentration fields. The downward concentration was reasonably disappeared compared with Fig.5 and Fig.6.

The accuracy of three numerical experiments was estimated by normalized RMSE (Root Mean Square Error) defined by

$$nRMSE_{upward} = \sqrt{\frac{\frac{1}{M_{upward}}\sum_{j=1}^{M_{upward}} (\psi_{j,true} - \psi_{j,revised})^{2}}{\frac{1}{M_{all}}\sum_{i=1}^{M_{all}} \psi_{i,true}}}$$
(6)
$$nRMSE_{downward} = \sqrt{\frac{\frac{1}{M_{downward}}\sum_{j=1}^{M_{upward}} (\psi_{j,true} - \psi_{j,revised})^{2}}{\frac{1}{M_{all}}\sum_{i=1}^{M_{upward}} \psi_{i,true}}}}$$
(7)

where M_{all} is the number of grids, $\Psi_{i,true}$ and $\Psi_{i,revised}$ are the correct concentration value and the revised concentration value respectively. The time series of *nRMSE* is shown in Fig.8. *nRMSE* of the datasets (A) was the worst among three *nRMSE*. nRMSE of the datasets (B) was less than 0.2. This result suggested that the observation data in the downward side was important in order to improve the pseud concentration fields to the correct concentration fields by the VCA method. *nRMSE* of the datasets (C) showed the moreover improvement due to more observation data in the downward side.

Source location

The results of the source location by the VCA method are shown in Fig.9. The dark red and the light red represent the ranges of 50 % and 90 % of the total source intensity, respectively and the white circle represents the maximum value of the source intensity. The spread in the downward side of source location in the datasets (C) was controlled compared other numerical experiments.

Source intensity

The results of the source intensity by the VCA method are shown in Fig.10. The source intensity estimated from three numerical experiments were stronger than the true source intensity. Though the size of the true source was one grid (0.25 m \times 0.25 m \times 0.25 m), the size of the estimated source spread widely as shown in Fig.9. This is the reason why the source intensity become the overestimation.





Figure 4. Observation grids of x-z cross section (y=3.375m) and x-y cross section (z=1.625m) of datasets (A), datasets (B) and datasets (C).



Figure 5. The revised concentration fields of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m) using datasets (A)

Figure 6. The revised concentration fields of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m) using datasets (B)



Figure 7. The revised concentration fields of (a) x-z cross section (y=3.375m) and (b) x-y cross section (z=1.625m) using datasets (C)



Figure 8. Time series of normalized RMSE between the true concentration fields and the revised concentration fields by the VCA method. (a) Windward side of the contaminant source. (b) Downward domain of the contaminant source.



Figure 9. The estimated source location of x-z cross section (y=3.375m) and x-y cross section (z=1.625m) by using dataset (A), datasets (B) and datasets(C).



Figure 10. True source intensity and the estimated source intensity by using dataset (A), datasets (B) and datasets(C)

CONCLUSION

In this study, the VCA method was applied for the simple steady flow field in order to estimate source intensity and location from the observation datasets, which were extracted from the true concentration fields with the correct boundary conditions.

Adding the observation data in the downward side of the contaminant source, the VCA method was confirmed that the accuracy of the concentration fields, the source intensity and location were improved.

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