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Contaminant source identification based on sensitivity analysis algorithm

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ABSTRACT

Accidental contamination events often threaten people's health and life, and it is necessary to identify a contaminant source rapidly so that prompt actions can be taken. Therefore, it's crucial to develop investigation about identification of sudden contaminant source and prediction of contaminants' harmfulness, which could help to improve the ability of enclosed environments to deal with sudden contaminant. Source location is the key to source identification. In this paper, a discrete concentration stochastic model was set up, moreover, an identification method based on Sensitivity Analysis Algorithm (SAA) was developed to locate a source position and estimate its emitting strength. The proposed method could identify the source position by estimating its initial emission time and approximate strength. Numerical simulations are conducted to identify the position of a source with continuous emission.

KEYWORDS

Source identification;
Concentration prediction;
Sensitivity analysis;
Discretized concentration stochastic model.

INTRODUCTION

Accidental environmental pollutions often occur with the rapid development of society, and environmental protection has become a security issue. This issue is a key for some enclosed spaces, such as manned spacecraft and large aircraft. Once a contamination event happens, location of the source should be identified quickly so that mitigation procedures can be then taken to minimize the impact on the environment. Some sudden air pollution incidents in the cabin have increasingly called our attention along with the prolonging of navigation time[1,2]. Therefore, it is very important to identify a sudden unknown contaminant source.

Researches on contaminant source identification in enclosed spaces have just started recently in other countries. So far, methods widely used include the optimization approach, the analytical approach, the probabilistic approach and the direct approach using CFD reversing the governing equations directly. Qingyan Chen from Purdue University and Zhiqiang Zhai from TianJin University have carried out thorough research to identify a contaminant source in an aircraft cabin by using probabilistic approach combining with direct CFD approach[3-5]. Their researches have provided some thought to identify the source characters. But these developed methods can not predict the source strength dynamically. The above attempts have been promoting the development of source identification.

The primary goal of this research proposes a method to identify the contaminant source. The rest of this article is organized as follows. Section 2 introduces a discretized concentration stochastic model. Section 3 introduces a sensitivity analysis algorithm (SAA) for preliminary analysis on the strength and location of an unknown source. Section 4 contains numerical simulation to demonstrate the method.

DISCRETIZED CONCENTRATION STOCHASTIC MODEL

First we set up a three-dimensional discretized concentration transport model by discretizing the convection-diffusion transport model, then add the stochastic noise term to the model to overcome modeling error caused by fluctuation of air flow or some other factors.

For an incompressible, with the equations of continuity, momentum, energy and mass, the distribution of air flow velocity *u* in enclosed space can be obtained by using SIMPLE algorithm. The transport equation for contaminant concentration *C* can be written as:

In this work, we are assuming that the contaminant undergoes no chemical or physical transformations during its transport. The transport equation for contaminant concentration, *C*, can be written as:

$$\frac{\partial C}{\partial t}+\nabla\left(\boldsymbol{u}C\right)=\nabla\left[\Gamma\cdot\mathbf{grad}(C/\rho)\right]+S \tag{1}$$

where *u* is the bulk air velocity, Γ is the diffusivity, ρ is the density of the fluid and *S* is the function that describes the strength and location of contaminant sources.

Discretizing Eq. (1) using power format based on control volume integration[6,7], the discrete function for any arbitrary point can be written as

$$\begin{aligned}&a_P(i,j,k)C^{t+1}_{i,j,k}-a_E(i,j,k)C^{t+1}_{i+1,j,k}+a_W(i,j,k)C^{t+1}_{i-1,j,k}+a_N(i,j,k)C^{t+1}_{i,j+1,k}+\\&a_S(i,j,k)C^{t+1}_{i,j-1,k}+a_T(i,j,k)C^{t+1}_{i,j+1,k}+a_B(i,j,k)C^{t+1}_{i,j-1,k}=a^0_p(i,j,k)C^{t}_{i,j,k}+S_{i,j,k}\end{aligned} \tag{2}$$

This system of equations for all the points is then represented as a single matrix equation in terms of the state transition matrices A_1 and A_2.

$$\boldsymbol{A_1C^{t+1}=A_2C^t+S} \tag{3}$$

Considering the calculation time, we use the classic Alternating Direction Implicit scheme (ADI)[8]. Then Eq. (3) can be written as Eq. (4)~(6).

$$\begin{aligned}&a^0_p(C^{*}_{i,j,k}-C^{t}_{i,j,k})=\frac{1}{2}[a_EC^{*}_{i+1,j,k}-(a_E+a_W)C^{*}_{i,j,k}+a_WC^{*}_{i-1,j,k}+a_EC^{t}_{i+1,j,k}-(a_E+a_W)C^{t}_{i,j,k}+\\&a_WC^{t}_{i-1,j,k}]+a_NC^{t}_{i,j+1,k}-(a_N+a_S)C^{t}_{i,j,k}+a_SC^{t}_{i,j-1,k}+a_TC^{t}_{i,j,k+1}-(a_T+a_B)C^{t}_{i,j,k}+a_BC^{t}_{i,j,k-1}+b_{i,j,k}\end{aligned} \tag{4}$$

$$\begin{aligned}&a^0_p(C^{**}_{i,j,k}-C^{t}_{i,j,k})=\frac{1}{2}[a_EC^{*}_{i+1,j,k}-(a_E+a_W)C^{*}_{i,j,k}+a_WC^{*}_{i-1,j,k}+a_EC^{t}_{i+1,j,k}-(a_E+a_W)C^{t}_{i,j,k}+a_WC^{t}_{i-1,j,k}]+\frac{1}{2}[a_NC^{**}_{i,j+1,k}\\&-(a_N+a_S)C^{**}_{i,j,k}+a_SC^{**}_{i,j-1,k}+a_NC^{t}_{i,j+1,k}-(a_N+a_S)C^{t}_{i,j,k}+a_SC^{t}_{i,j-1,k}]\backslash+a_TC^{t}_{i,j,k+1}-(a_T+a_B)C^{t}_{i,j,k}+a_BC^{t}_{i,j,k-1}+b_{i,j,k}\end{aligned} \tag{5}$$

$$\begin{aligned}&a^0_p(C^{t+1}_{i,j,k}-C^{t}_{i,j,k})=\frac{1}{2}[a_EC^{*}_{i+1,j,k}-(a_E+a_W)C^{*}_{i,j,k}+a_WC^{*}_{i-1,j,k}+a_EC^{t}_{i+1,j,k}-(a_E+a_W)C^{t}_{i,j,k}+\\&a_WC^{t}_{i-1,j,k}]+\frac{1}{2}[a_NC^{**}_{i,j+1,k}-(a_N+a_S)C^{**}_{i,j,k}+a_SC^{**}_{i,j-1,k}+a_NC^{t}_{i,j+1,k}-(a_N+a_S)C^{t}_{i,j,k}+a_SC^{t}_{i,j-1,k}]\\&+\frac{1}{2}[a_TC^{t+1}_{i,j,k+1}-(a_T+a_B)C^{t+1}_{i,j,k}+a_BC^{t+1}_{i,j,k-1}+a_TC^{t}_{i,j,k+1}-(a_T+a_B)C^{t}_{i,j,k}+a_BC^{t}_{i,j,k-1}]+b_{i,j,k}\end{aligned} \tag{6}$$

Thus, the discretized concentration equations can be expressed as the following equations:

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$$\left(-\frac{A_x}{2}+a_P^0\right)C^* = \left(\frac{A_x}{2}+A_y+A_z+a_p^0\right)C^t+b$$
$$\left(-\frac{A_y}{2}+a_P^0\right)C^{**} = -\frac{A_y}{2}C^t+a_P^0C^* \quad (7)$$
$$\left(-\frac{A_z}{2}+a_P^0\right)C^{t+1} = -\frac{A_z}{2}C^t+a_P^0C^{**}$$

where A_x, A_y and A_z are tridiagonal matrixes. The equations set is then represented as a single matrix equation in terms of the state transition matrices M and N.

$$MC^{t+1}=NC^t+B \quad (8)$$

where

$$C^t=(C_t^{*T},C_t^{**T},C_t^T)^T \quad (9)$$

$$M=\begin{pmatrix} -\frac{A_x}{2}+a_p^0 & 0 & 0 \\ -a_p^0 & -\frac{A_y}{2}+a_p^0 & 0 \\ 0 & -a_p^0 & -\frac{A_z}{2}+a_p^0 \end{pmatrix} \quad (10)$$

$$N=\begin{pmatrix} 0 & 0 & \frac{A_x}{2}+A_y+A_z+a_p^0 \\ 0 & 0 & -\frac{A_y}{2} \\ 0 & 0 & -\frac{A_z}{2} \end{pmatrix} \quad (11)$$

$$B=(b^T\ 0\ 0)^T \quad (12)$$

Assume the system uncertainty caused by the factors such as rounding error as discretizing, fluctuation of air velocity and eddy diffusivity, it is necessary to add a stochastic disturbance ω_1 to overcome the system uncertainty. Thus, the model turns into a new discretized stochastic model:

$$MC^{t+1}=NC^t+B+U_t\omega_1 \quad (13)$$

where U_t represents the stochastic disturbance transition matrix acts upon ω_1, and ω_1 is an uncorrelated Gaussian white sequence with a zero mean and $E[\omega_1\cdot\omega_1^T]=Q$, Q is a diagonal matrix that represents the model noise. A highly accurate model would have low values for its Q; on the other side, a model that does not represent the physical process too accurately would have high values for its Q.

The model involves three kinds of boundary conditions, which are duct in, the wall and duct out.

IDENTIFICATION METHOD BASED SENSITIVITY ANALYSIS

The identification of sudden source characteristics contains two parts, which are location and dynamic emitting strength identification of source. The latter can't be realized without accurate position information of source. Here we locate a sudden source by using a SAA[11]. Meanwhile, this algorithm can give an initial guess for the strength of the unknown source.

We assume that there is an unknown source, which releases CO_2 at a constant value in a short time.

Define the sensitivity coefficient[11]

$$Z=\left(Z_1^T,Z_2^T,\cdots,Z_N^T\right)^T \quad (14)$$

where

$$Z_i=\frac{\partial C}{\partial S_{ui}},\ i=1,2,\ldots,N \quad (15)$$

S_{ui} represents the assumed unknown source at point i; the sensitivity coefficient Z_i is a $1\times N$ vector, which represents how does the source at the i^{th} grid point affect the concentration distribution. And N is the number of grid points.

In order to calculate Z, we multiply Eq.(1) throughout by $\frac{\partial}{\partial S_{ui}}$, then we get

$$\frac{\partial}{\partial S_{ui}}\left[\frac{\partial C}{\partial t}+\nabla(\boldsymbol{u}C)=\nabla[\Gamma\cdot\mathbf{grad}(C/\rho)]+S_u\right] \quad (16)$$

Since S_u is independent of the co-ordinate axes, we can rewrite Eq.(17) as

$$\frac{\partial}{\partial t}\frac{\partial C}{\partial S_{ui}}+\nabla\left(\frac{\boldsymbol{u}\partial C}{\partial S_{ui}}\right)=\nabla\left[\frac{\Gamma}{\rho}\cdot\mathbf{grad}\left(\frac{\partial C}{\partial S_{ui}}\right)\right]+\frac{\partial S_u}{\partial S_{ui}} \quad (17)$$

Replacing Z_i for $\frac{\partial C}{\partial S_{ui}}$ from the definition for the sensitivity coefficient, we get the direct well-posed problem equation

$$\frac{\partial Z_i}{\partial t}+\nabla(\boldsymbol{u}\cdot Z_i)=\nabla[(\Gamma/\rho)\mathbf{grad}Z_i]+I_i \quad (18)$$

where I_i represents the i^{th} column of the identity matrix.

The boundary conditions and the initial conditions will also be divided throughout by $\frac{\partial}{\partial S_{ui}}$ to obtain the initial and boundary conditions for sensitivity problem.

Since the equation structure is unchanged from the original model equation, the same algorithms and numerical techniques can be used in computing the sensitivity matrix. It worth attention that this part of computations can be performed off-line and before the real contaminant source appear, which can save much time for the identification of source characters.

The solution to Eq. (18), $Z(t)$, is a function of time, where the time refers to the time elapsed since the contaminant source occurres. Since only direct information about the concentration at sensor locations having been known, we focus how the source at different location influences the concentration at sensor locations. Therefore, $Z(t)$ can be divided into a usable part $Z_{sensors}$ and a non-usable part $Z_{non\text{-}sensors}$.

$$\mathbf{Z} = [\mathbf{Z}_{sensors}, \mathbf{Z}_{non\text{-}sensors}] \qquad \textbf{(19)}$$

The diagnosis system can detect a sudden source. The time when the sudden source is detected can be written as t_{detect}. In order to identify the source characters more accurately, we make the identification using $Z^c = Z_{sensors|\tau_w = t - t_{detect}}$ at time $t=t_{detect}+\tau_w$, where τ_w is the lag time after the sudden source is detected; Z^c is an $N\times$m matrix; N is the number of grid points; m is the number of sensors. In other words, Z^c_{ij} represents how does the concentration change at the j^{th} sensor location after $t_{detect}+\tau_w$ seconds when the source changes one unit strength at the i^{th} grid point.

However, when a sudden unknown source appeared, the estimated $\hat{y}_i$ will not consistent with the measurement value z_i. $e = (e_1, e_2, \ldots, e_m)$ represents the predicted error at time t, where $e_i = z_i - \hat{y}_i$ represents the predicted error by the i^{th} sensor.

$Z^c_{ij} = \dfrac{\partial C_j}{\partial S_{ui}} = \dfrac{e_j}{\Delta S_{ui}}$, so source strength can be written as $\Delta S_{ui} = e_j / Z^c_{ij}$. Redefine the source strength as

$$STR_{ij} = \frac{e_j}{Z^c_{ij}} \qquad \textbf{(20)}$$

where STR is an $N\times m$ matrix, STR_{ij} represents the source strength estimated by the j^{th} sensor in case that the source is assumed at i^{th} grid point; N is the number of grid points, and m is the number of sensors.

Then the algorithm being used for this estimation is give below:

(1) Note the predicted error e by sensors at $t=t_{detect}+\tau_w$;
(2) Input the sensitivity matrix $Z^c(\tau_w)$;
(3) Calculate the source strength matrix STR using Eq. (20);
(4) Scale each m-dimension line vector using the mean of the strengths within the line vector;
(5) Calculate the standard deviation of the calculated strengths for each m-dimension line vector.
(6) Choose the line with the minimum standard deviation, the point corresponding with this line is the source location.
(7) Calculate the mean of this line vector, which is the source strength.

The identification algorithm based on sensitivity matrix is developed and we can call it SAA. Actually, there may be only part of the sensor predict errors exceed the threshold value at time $t=t_{detect}+\tau_w$. In other words, the sudden unknown source only affect the concentrations at part of the sensor locations, while concentrations at other part of the sensors locations haven't be affected. In this case, the inactive sensors need to be eliminated. Otherwise, it will affect the accuracy of the SAA result. Therefore, the row dimension of STR matrix we used actually is m or less than m.

SIMULATIONS

A space with one inlet and one outlet is used to test the proposed method further. As shown in Figure 1, it is 560 mm long and 360 mm wide. The width of the inlet and the outlet is 20mm. The flow field with 0.5m/s air outlet velocity is shown in Figure 1.

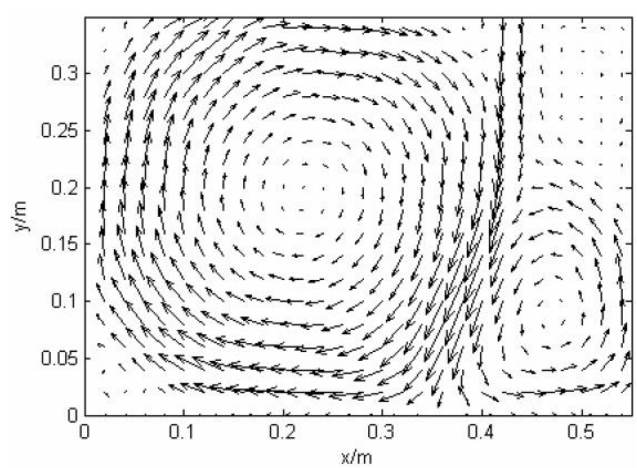

Figure 1 : Air flow field

A mesh consisting of 29×19 nodes is adopted in the simulation, as shown in Figure 2. The sampling

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point or the sensor point is set to be near the outlet at (7, 17). A continuous source is at (16, 22). Its source strength is 10 mg/(m^3·s) and its initial emission time t_e is 50s. The sample time is 1s. The initial concentration C_0=0.05 mg/m^3.

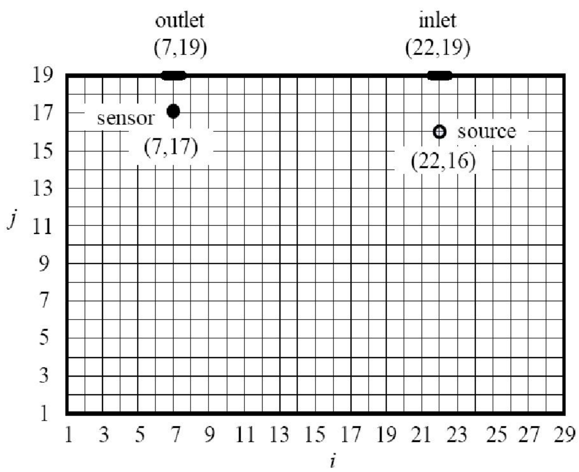

Figure 2 : Air flow space

Figure 3 shows the calculated concentration distribution at time t =55s (5 seconds after the emission of the source).

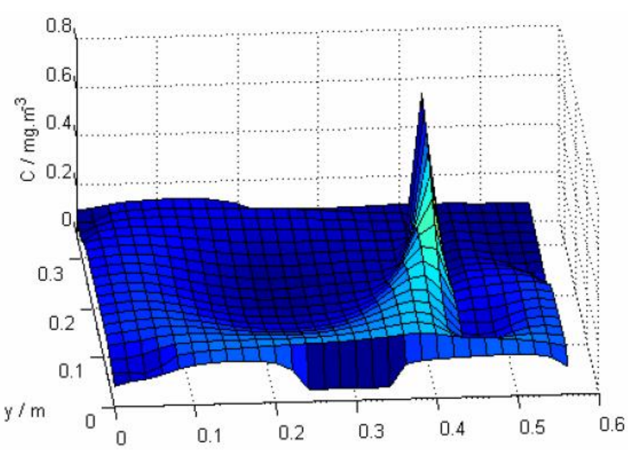

Figure 3 : Concentration distribution at t =55s

Assume we use two sensors with 1 % and 5% measurement errors, respectively. Their measurement ranges are all 1 mg/m^3 range. TABLE 1 gives the source estimation results.

TABLE 1 : Source estimation results

	Sensor error %	t_e s	Location (i, j)	S mg/(m^3·s)
True		50	(22, 16)	10
2	1	55	(22,17)	9.50835
3	5	56	(22,13)	10.1222

From the identification results, we can know that:

(1) The source is estimated near at its true position, (22, 16) by using these two sensors with different measurement error.

(2) Due to the first sensor with lower measurement error, its source identification result is better than the second sensor with higher measurement error.

(3) The sensor error is a key factor for location. The smaller it is, the more accurate the location result is. Therefore, a good location result can be obtained when the measurement noise of the sensor is smaller.

CONCLUSION

Based on a dimensional discretized stochastic model, a source identification method based on SAA was developed by using the sensitivity matrix. In this method, the SAA can locate a source position and estimate its emitting strength preliminary. Simulation results show that, this presented method can identify an unknown source appearing in the enclosed spaces when a high accurate sensor is used. The position and emitting strength can be obtained together as well as the concentration distribution prediction. These researches may make it convenient for occupants to deal with air pollution accidents correctly and quickly.

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