GASEOUS POLLUTENT SOURCE TERM ESTIMATION BASED ON ADJOINT PROBABILITY AND REGULARIZATION METHOD

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Abstract. Fast and accurate identification of source locations and release rates is particularly important for improving indoor air quality and ensuring the safety and health of people. Existing methods based on adjoint probability are difficult to distinguish the release rate of dynamic sources, and optimization algorithms based on regularization are limited to analysing only a small amount of potential pollutant source information. Therefore, this study proposed an algorithm combining adjoint equations and regularization models to identify the location and release intensity of pollutant sources in the entire computational domain of a room. Based on the validated indoor CFD computational model, we first obtained a series of response matrices corresponding to the sensor position by solving the adjoint equation, and then used the regularization method and Bayesian inference to extrapolate the release rate and location of dynamic pollutant source in the room. The results shown that the proposed algorithm is convenient and feasible to identify the location and intensity of the indoor pollutant source. Compared with the real source intensity, the identification of constant source intensity is lower than the error threshold (10%) in 97.4% of the time nodes, and the identification of periodic source is lower than the error threshold (10%) in 95.4% of the time nodes. This research provides a new method and perspective for the estimation of indoor pollutant source information.

1 Introduction

A good indoor environment contributes to people's comfort and work efficiency and, more importantly, reduces the probability of infection from various diseases [1,2]. Therefore, it is very necessary to develop a fast and accurate indoor pollutant source identification strategy.

Kathirgamanathan [3] et al. accurately recover the release history and release rate of full sampled data based on linear least squares regression and Tikhonov regularization. The accuracy of the regularization method for estimating source intensities has been well verified in both 2D and 3D space [4,5]. Liu [6] and Zhuang [7] used regularization method combined with Bayesian probability to successfully locate pollutant sources. However, the above-mentioned studies based on the regularization method need to predict the location of the pollutant source in the room, and the process of obtaining the response factor is cumbersome.

Liu et al. applied the adjoint method to indoor environments, illustrating the method of inverse modeling using the example of air pollution in office spaces and aircraft cabins [8,9].Subsequently, adjoint probabilistic methods have been extensively validated in various contexts. As summarized by Zhai et al. [10], an adjoint probabilistic approach is used to efficiently identify the location of attenuation sources in a building HVAC system. Zhou [11] et al. Use CFD simulations combined with adjoint methods to identify the location of leak sources in an underground tunnel. Although the adjoint probability method can identify the release location of the pollutant source, it cannot estimate the release intensity of the pollutant source.

According to the current research status, this paper combines the regularization method with the adjoint probability method, and validates the method based on the verified CFD case model, so as to apply it to the inversion and identification of true environmental pollutant sources.

2 Methods

When the flow field is fixed, the release intensity q of the source is linearly related to its concentration C distribution, The relationship conforms to the following vector/matrix form:

$$\boldsymbol{C} = \boldsymbol{A}\boldsymbol{q} \tag{1}$$

where the pollutant concentration C can be obtained by arranging the sensors, and the response matrix A is obtained by the adjoint probability method in Section 2.1. However, it is a ill-conditioned problem to judge the release intensity of the pollutant source according to the pollutant concentration information monitored by the sensor. Therefore, we introduce the regularization method to calculate the source intensity in Section 2.2, and use the Bayesian method in Section 2.3 to locate the source.

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https://doi.org/10.1051/e3sconf/202235605048

2.1 Adjoint method for the response matrix calculation

Pudykiewicz [12] introduced the adjoint method into STE for the first time, which only needs to solve the adjoint advection-diffusion equation once for each sensor to obtain the response factor of the entire computational domain. The steady-state flow field in the computational region is simulated using CFD, and the flow field is reversed by importing the UDF. By releasing a pollutant pulse with a time step at the position of the pollutant sensor, the response concentration of the pollutant sensor to the entire space can be obtained by monitoring the response concentration in the domain. The response matrix can be calculated from the MATLAB code.

2.2 Regularization method for source strength determination

The core idea of Tikhonov's regularization method is to introduce a regularization parameter to keep the value of the solution within a certain range, thereby reducing and avoiding the oscillation or divergence of the numerical solution. Eq. (1) can be transformed into a linear least squares optimization function problem as follows:

$$minimize(q) = \|Aq - C\|_2^2 + \lambda^2\|Lq\|_2^2 \qquad (2)$$

where the first term on the right-hand side is the residual parametrization, which represents the square of the second parametrization of the difference vector between the measured concentration C and the calculated concentration; the second term is the regularization term, L is the regularization matrix, and λ is the regularization parameter, which controls the weight of the minimization of the side constraint relative to the minimization of the residual parametrization. The selection of a suitable regularization parameter λ is very important for the accurate derivation of the source intensity q. Compared with other different regularization methods, the GCV method is relatively stable. Therefore, in this paper, the GCV method is used to calculate the regularization parameter λ.

2.3 Bayesian method for source location determination

The Bayesian probability model is used to calculate the unknown probability of the pollutant source. The model determines the maximum possible location of the pollutant source by comparing the matching degree between the monitoring value and the predicted concentration value of the sampling point. The predicted concentration value is calculated by equation (1), according to the monitoring result O, the probability of the source at position Y_k is as follows:

$$P(Y_k|O) = \frac{P(Y_k)L(O|Y_k)}{\sum_{i=1}^{n} L(O|Y_i)P(Y_i)} \qquad (3)$$

where k is the location number of the potential source and $P(Y_k)$ is the prior probability that the source is at location Y_k. If n potential positions have the same probability, $P(Y_k)$ is equal to 1/n. $L(O|Y_k)$ is the likelihood function, which can be obtained based on the Gaussian normal distribution construction[13].

3 Case setup

The validity of the method is verified using a validated 3D model, which is a room with a steady state flow field [14]. The geometry of the three-dimensional ventilation chamber is shown in Figure 1. The dimensions of the ventilation chamber are 5.16 m × 3.65 m × 2.43 m. On the right side of the room there is a supply vent, an exhaust vent in the upper part, two occupants, two computers, two desks, two boxes and six lights. The inlet temperature was 17°C and the airflow velocity was 0.09 m/s. The turbulent kinetic energy k and dissipation rate ε are 1.94e-05 m2/s2 and 2.53e-07 m2/s3. The exhaust is a pressure outlet with a gauge pressure of 0 Pa and the temperature is 26.7°C. This 3D case and experimental data can be found in [14]. The velocity field is calculated by ANSYS FLUENT. The region is divided into 1022665 cells, the governing equations use the standard k- ε model, the numerical method uses the SIMPLE algorithm, and the second-order discrete format for the convection and viscous terms of the governing equations, with a convergence residual of 10−4 for all variables.

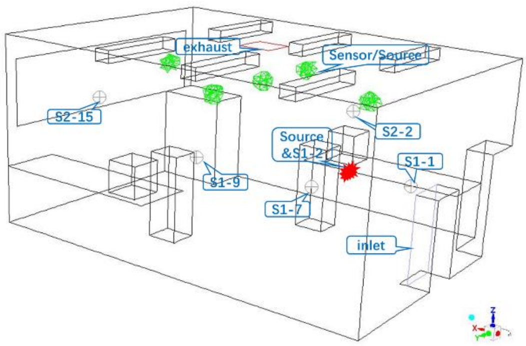


Fig. 1. The office configuration used in the model.

This study uses SF6 as a tracer gas to mimic the spread of contaminants in the room, which was released in two different source forms at the red mark through a porous sphere with a radius of 0.1 m. The forms of pollutant sources include constant source and periodic source, as shown in Figure 2. Five monitoring points were set up at the top of the room to record pollutant concentration information in 2s time steps. In this study, we only used the concentration data in the first 2500 s of the monitoring site to infer the source release history, this information can be used for the verification of the reverse identification of contaminants.

The flow field is reversed using the method described in Section 2.2, and a unit rectangular pulse with a time step is released at the original monitoring point, as shown in Figure 3. Then 30 monitoring points are evenly arranged in the computational domain to collect concentration information for calculating the response factor. Considering that the comparison of 30 monitoring points is too confusing, this study selected 6 special monitoring points (including the real source location) for comparison.

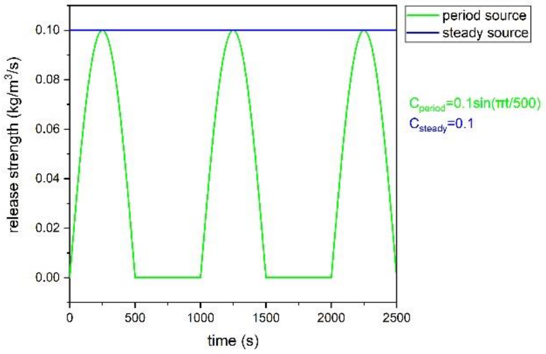


Fig. 2. Form of pollutant source.

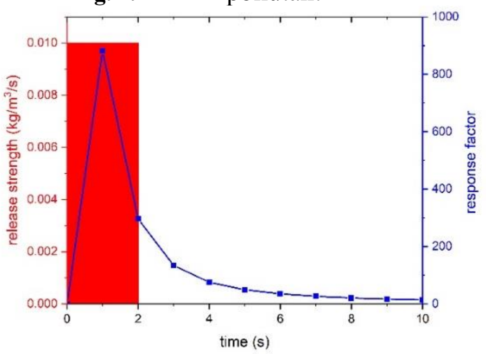


Fig. 3. Rectangular pulse.

4 Results

Since the pollutant concentration information is first monitored by the No. 4 monitoring point, we use the concentration data collected by the No. 4 monitoring point to infer the intensity of the pollutant source, and then use other monitoring points to estimate the location of the pollutant source. Given that it is not intuitive to compare the 30 potential sources together, we select a few more specific locations to compare with the true source locations, as shown in Fig. 1. s1-2 represents the true source locations, s1-1, s1-7, and s2-2 are located around the true source, and s1-9 and s2-15 are relatively far from the true source locations.

The relative error (NME) is introduced to compare the difference between the reverse calculated release rate and the actual source release rate, as follows:

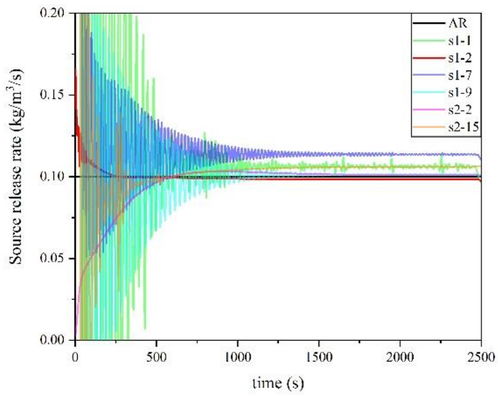
$$NME = \frac{|N_{IR} - N_{AR}|}{N_{AR,peak}} \tag{4}$$

where N_{IR} is the reverse calculated release rate, N_{AR} is the actual release rate. and $N_{AR,peak}$ is the peak release rate of the actual source; in this case, $N_{AR,peak} = 0.1 kg/m^3/s$ .A threshold of 10% relative error was chosen to compare the accuracy of the estimated source intensities at different locations.

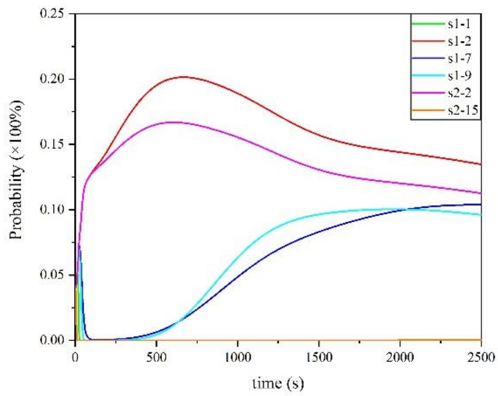
4.1 Steady source

Fig. 4(a) shows the release rate estimates for steady sources using monitoring point 4. It can be seen that in the first 1000s, s1-2 is close to the true source intensity first, while the source intensities at other locations are estimated to have larger fluctuations, or have obvious deviations from the true source. After 1000s, the source intensity estimates stabilize at each location, but it is clear that s1-2 matches the true source more closely, although s1-9 is also close to the true source, but has been fluctuating up and down. Therefore, according to the overall source intensity estimation results, s1-2 is more consistent with the real source intensity, and the number of time nodes less than the relative error threshold accounts for 97.4%, which is a preliminary proof that the method is effective.

Fig. 4(b) shows the estimation of the location of the pollutant source using the data of other monitoring points. It can be seen that s1-2 is obviously more probable than other locations, whether it is s1-1 which is closer to the true location or far from the true location s2-15, the probability quickly dropped to almost 0 at the beginning. Although the probability of other positions does not tend to 0, it is still obviously less probable than s1-2. The results once again confirm that this method is also effective for estimating the position of the source.



(a)



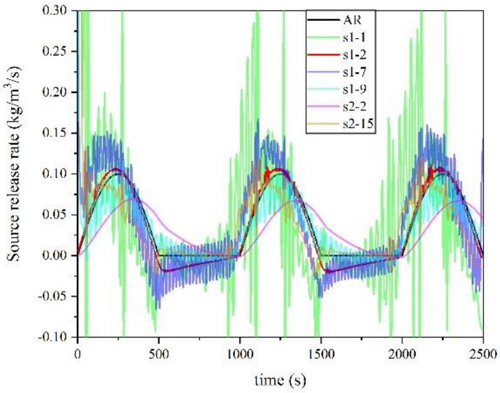
(b)

Fig. 4. STE results for steady source. (a) Pollutant source intensity estimation. (b) Pollutant source location estimation.

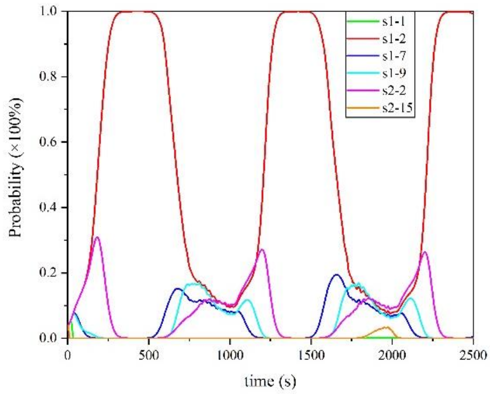
4.2 Period source

Fig. 5(a) presents the release rate estimates for periodic sources using monitoring point 4. It can be seen that the source intensity estimates at all locations exhibit periodic characteristics, but s1-2 is clearly more consistent with the true source waveform, and other locations show more severe vibrations. Compared with the true source, the number of time nodes below the relative error threshold accounts for 95.4%. Therefore, based on the overall analysis results, the method can still accurately calculate the true source intensity.

Fig. 5(b) shows the estimation of the periodic source location using data from other monitoring points. It can be seen that during the period source release, the probability of the s1-2 position is much higher than that of the other positions. During the stop release period, although the probability of s1-2 is smaller, it is still higher than the other positions.



(a)



(b)

Fig. 5. STE results for period source. (a) Pollutant source intensity estimation. (b) Pollutant source location estimation.

5 Conclusion

The accurate location of indoor pollutant sources is of great significance to ensure the health and safety of personnel. In this study, the regularization method is combined with the adjoint probability method to perform reverse identification of indoor pollutant sources. The performance of the proposed method was evaluated by comparing it with the intensity and location of real pollutant sources. It is found that the number of time nodes with relative error of source release rate below the threshold (10%) is 97.4% in the constant source flow field, while the number of time nodes with relative error of source release rate below the threshold (10%) is 95.4% in the steady-state flow field of periodic sources. The method shows superior results in source localization.

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