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Spatial source parameters estimation in urban environment using optimization method combined with adjoint equation simulated via large eddy simulation

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SUMMARY:
Accurate and prompt identification of the location and rate of hazardous gas leakage is essential for ensuring urban air quality and environmental safety. Prior studies have mainly estimated source parameters based on the Reynolds-averaged Navier-Stokes (RANS) model of CFD simulation. However, RANS-based models lack accuracy when predicting complex urban flow compared with large eddy simulation (LES). Although LES has high accuracy, it requires massive computing time. In addition, most studies tend to assume that the coordinate of a certain direction of the source (e.g., the height z) is known and estimate the coordinates of the remaining two directions in the plane where the source is located. However, in many cases, the source may be released at an arbitrary location in space with unknown spatial coordinates. Therefore, based on the LES approach, this paper further develops optimization methods for estimating source parameters by combining adjoint equations. The results indicate that the presented method can promptly and accurately estimate the spatial source parameters under complex urban flow.

Keywords: Source parameters estimation, Large eddy simulation, Optimization method

1. INTRODUCTION

Accurate and prompt estimation of source parameters, such as location and leakage rate, can provide crucial information for controlling contaminants, pollution isolation, ventilation, purification, and emergency evacuation. Source parameters estimation can be achieved using two distinct approaches: using mobile robots or fixed-detector networks (Hutchinson et al, 2017). Estimation relying on fixed-detector networks is a typical ill-posed problem characterized by high nonlinearity, strong dependence on input data, and non-single solutions (Jia and Kikumoto, 2021). Based on the discrepancy between predicted concentrations obtained from the source-detector relationship and measurements obtained from the fixed-detector network, source parameters can be determined using estimating algorithms. However, utilizing CFD simulation based on fixed-detector networks for source parameters estimation is computationally intensive. Therefore, this paper presents a method for source parameter estimation based on fixed-detector networks under complex urban flow, which combines optimization methods with adjoint equations. The presented method can estimate the three-dimensional spatial coordinates and leakage rate of the source based on the LES approach.

2. METHODOLOGY

2.1. Source-detector relationship

The source-detector relationship predicts the expected detector concentrations for a given combination of source parameters. To establish this relationship and derive predicted concentrations, the most straightforward approach is to solve the advection-diffusion equation for each combination of source parameters. However, since the source can be located anywhere in the space, the advection-diffusion equation must be solved N times (N is equal to the number of grids). This approach is computationally intensive. To address this problem, Pudykiewicz (Pudykiewicz, 1998) proposed an alternative method to establish this relationship using the adjoint equation. Analogically, the predicted concentration for each source parameters combination can also be obtained using the following equation: $P_d =< C^*, Q >\equiv \int_0^T dt \int_\Omega (C^* \cdot Q) d\Omega$. The adjoint equation only needs to be solved N' times (N' is equal to the number of detectors) to establish the source-detector relationship. Since N' is much smaller than N, using adjoint equations can substantially reduce computing time.

2.2. Genetic algorithm (GA)

After predicted concentrations are obtained from the source-detector relationship, then combined with detected concentrations, the source parameters can be estimated based on the cost function and using GA. The cost function is based on the form of root mean square error, expressed as: $F = \frac{\sqrt{\sum_{d=1}^{D}(P_d - D_d)^2}}{\sqrt{\sum_{d=1}^{D} {D_d}^2}}$, where D_d is the detected concentration of detector d. In this paper, detected concentrations are synthesized via LES with true source parameters. To ensure that study cases are closer to reality, random Gaussian noise with a standard deviation of $\frac{S_d}{3}$ is added, where S_d is the simulated concentration of detector d resulting from the true source parameters. GA is inspired by the principles of the Darwinian theory of natural evolution and the genetics theory of Mendel. It imitates the stochastic crossover and mutation of chromosomes, where combinations of source parameters with lower cost function values are retained for the next generation, while those with higher values are eliminated (Golberg, 1989).

3. COMPUTATIONAL AND SOLVER SETTINGS

3.1. Research object

To validate the presented method, a three-dimensional dispersion scenario has been designed with a spatial source located on the roof, as shown in Fig. 1. There are 24 detectors in total. The source is located at *x* = 0.79 m, *y* = 0.565 m, *z* = 0.1525 m, and its leakage rate is 1.

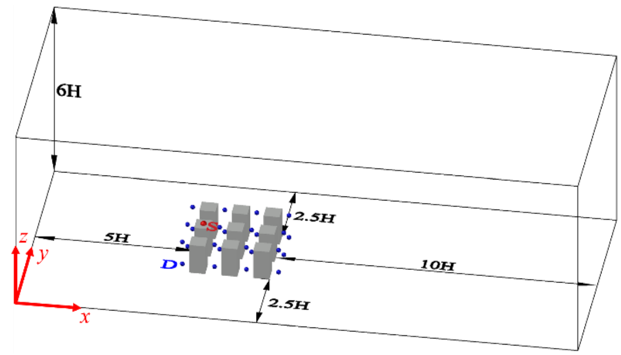
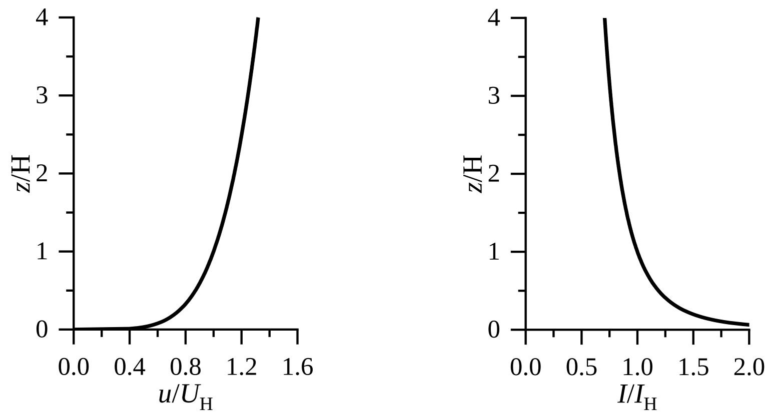


Figure 1. Schematic diagram of the urban environment.

3.2. Boundary conditions and solver settings

The structured grid with a high spatial resolution is adopted. The total number of grid cells is 2,555,136 with densified grids positioned around buildings. The minimum size of the grid is 0.005 m. Numerous studies have confirmed that LES yields more precise results than RANS in simulating flow fields, particularly in the wake region of buildings. Hence, we employed LES approach in this study. The turbulence model is the standard Smagorinsky-Lilly model. The inflow profiles of dimensionless mean streamwise velocity and turbulence intensity are shown in Fig. 2.



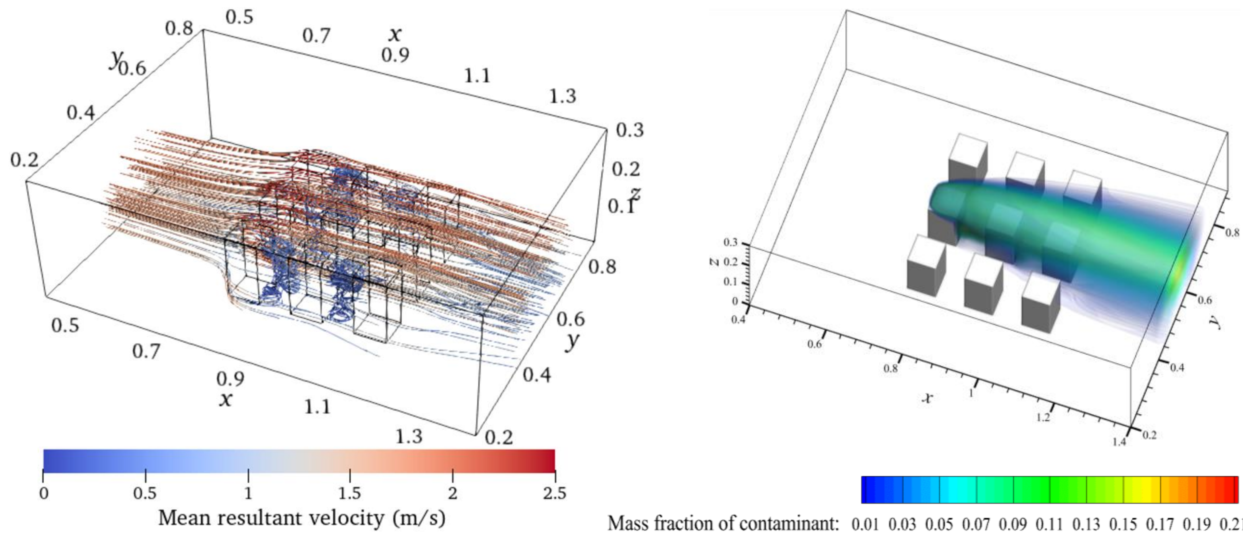
(a) Mean streamwise velocity (b) Turbulence intensity

Figure 2. Dimensionless inflow profiles.

4. RESULTS AND DISCUSSION

4.1. Flow field and concentration field

In Fig. 3 (a), the mean flow field is illustrated. It is apparent that the wind speed is low in many areas, and vortices are formed behind each building due to the combined effects of ventilation and building blockage. Fig. 3 (b) displays the concentration field. The flow field distribution characteristics determine that pollutants tend to accumulate in low wind speed and vortex areas. This accumulation can result in the formation of local optimal areas, which may cause the estimated source parameters to converge to local optimal values, ultimately leading to poor estimation outcomes. Therefore, it is challenging to estimate the source parameters in this scenario.



(a) Streamlines of mean flow field (b) Distribution of concentration field

Figure 3. Distributions of mean flow field and concentration field in urban environment.

4.2. Source parameters estimated results

Due to the randomness of GA, each source parameter is estimated 50 times, and the mean values of these estimations are taken as the final estimated results. The estimated value of x is 0.788 (true value is 0.79), the estimated value of y is 0.575 (true value is 0.565), the estimated value of z is 0.1410 (true value is 0.1525), and the estimated value of the leakage rate q is 1.6733 (true value is 1). All of the estimated results are close to the true values, indicating that the presented method is applicable.

5. CONCLUSIONS

This paper presents a method for estimating source parameters in complex urban flows based on fixed-detector networks. The use of adjoint equations can save significant computational resources and establish an accurate source-detector relationship. By combining this relationship with GA, the proposed method can quickly estimate the source parameters, making it suitable for emergency repairs when hazardous leaks occur.

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