Inverse identification of pollutant sources in 2D street canyons based on real weather conditions

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Abstract
When pollution diffusion occurs in the building environment, timely locating the contaminant source can minimize the damage. Previous studies on source localization have focused on the interior building space without considering the spread of pollutants in street canyons under real weather conditions. A combination of scaled outdoor experiments, adjoint probability method, and Computational Fluid Dynamics (CFD) was used to identify the source location of contaminants in street canyons. Based on existing information, the location of the pollution source can be accurately located in the street canyons. The results of this paper can use the urban scale to provide new ideas for urban layout and pollutant detection.

Highlights
- Application of inverse CFD modeling method in 2D street canyons
- Identify pollution source room locations under real weather conditions
- Identify source room locations by a limited number of pollutant sensors under a scaled outdoor experiment

Introduction
The development of urbanization has negatively influenced human society, such as heat islands, reduction of pollutant dilution, and so on. In the high-density urban environment, the distance between buildings is getting smaller. The distance of pollutant transmission is continuously shortened. It aggravates the pollutant concentration diffusion in the 2D street canyon. The street canyons are composed of two buildings arranged continuously on both sides of a street (Nicholson, 1975). The street canyon is an environment where people have lived for a long time. The problem of pollutant dispersion in the 2D street canyons can threaten human health. It has been reported in many kinds of research that various pollutants in the street canyons, such as traffic exhaust, dust, pollen, airborne viruses, and toxic and odorous emissions, may enter the indoor environment and affect human health (Morawska., 2013). To dilute the dispersion of pollutant concentration in the 2D street canyons, it is crucial to find the location of the pollutant source and control the release strength in the 2D street canyons.

When locating the pollution source in the 2D street canyons, the flow field and concentration field of the pollution source significantly influences the result of the source locating. To obtain the accurate location of the pollution source, a precise velocity field and concentration field are needed to reduce the error of source finding results. Many studies have investigated that the flow field and concentration field of the pollution source in the street canyon may be affected by other factors. Bai (2023) used an outdoor model and machine learning to investigate the factors controlling air pollutant dispersion in street canyons. Zhao (2022) used the CFD method to explore the natural ventilation and pollutant diffusion of different types of building blocks. Dai (2020, 2022) conducted a scaled outdoor experiment to study the interunit dispersion in 2D street canyons based on real weather conditions. The ventilation performance of the source room varies with the location of the room. Lin (2011) conducted wind tunnel experiments to investigate the flow field under different surface heating conditions. The above researches reveal that the flow and concentration field of pollution sources in the street canyon is affected by many factors. Previous studies on source localization have focused on the interior building space without considering the spread of pollutants in street canyons. Studying the inverse identification of pollutant sources in 2D street canyons is essential.

Previous studies on the inverse identification of pollutant sources were conducted in a closed environment and under simulated conditions (Zhang et al., 2007; Hu, 2019; Liu et al., 2007; Sohn et al., 2002). Many researchers cannot focus on conditions based on real weather. Research-based on real weather can more objectively reflect the actual situation. He (2021) conducted a field experiment to investigate the actual changes in urban wind profiles in Hong Kong through Doppler Laser radar. Niahou(2008) measured the temperature and airflow distribution of urban street canyons in hot summer weather.

Previous research has concluded that the inverse identification method of pollutant sources can be applied in the building environment (Hu, 2019; Liu et al., 2007; Sohn et al., 2002; Zhai, 2012). Dai (2023) adopted the Computational Fluid Dynamics (CFD) simulation with the adjoint probability method to obtain the location of the pollutant source. This study aims to find the location of pollutants in the 2D street canyons based on real
weather conditions. Carbon dioxide (CO$_2$) was used as a tracer of indoor pollutants. The paper applied inverse modelling of the source of pollutants in street canyons. The result of this study intends to dilute pollutant dispersion in the 2D street canyons.

**Methods**

**Experiment field design**

The experiment field in this study is located on the southern side of Guangzhou, China (23° 01’N, 113° 24’E). The experiment field is built on a 57.5m × 57.5m concrete foundation and contains more than 2000 concrete models. The dimension of the 2D street canyon is length × width = 44.4m × 12m. The experimental field is composed of 34 composite concrete building models with a length of 12m and four different height-width ratios (the ratio of building height H on both sides of the street to street width W, Aspect Ratio, AR) are 1:1, 1:2, 1:3 and 1:6, respectively. In this paper, the main research object is the 2D street canyon with a height-width ratio of 1:1. A street canyon was built to validate the theory, as shown in Figure 1 (a) and (b). A 10m high wind rod is used to measure the incoming wind speed of outdoor wind entering the experimental site. Specific equipment information can be found in another paper (Dai, 2020).

As shown in Figure 2, Building B was set as the source building. In Figure 2, W represents the windward side, and L represents the leeward side. During the experiment, BW1 and BL2 was set as the source room, and the tracer gas was released continuously for around 30 min.

**CFD method**

The flow field in the computational domain is modeled as a steady-state, three-dimensional Navier-Stokes equation for a confined, incompressible viscous flow of a Newtonian fluid. The concentration field in the computational domain is modeled in a transient process. This paper uses the Renormalization Group (RNG) k-ε model. The Renormalization Group (RNG) k-ε model is derived from a rigorous statistical technique proposed by Yakhot (1986). It is formally similar to the standard k-ε model, but adds the strain-dependent term to the $R_z$ equation, which improves the accuracy of swirling flow.

**Principles of adjoint probability method**

The location probability is the prerequisite for calculating the adjoint location probability.

$$f_x(x_1; t = T; \bar{x}_0) = \frac{C_1}{M_0} = \frac{C(T)}{M_0} \quad (1)$$

where $f_x(x_1; t = T; \bar{x}_0)$ is the forward location probability density at $t = T$, $C_1$ is the pollutant concentration per unit volume at $\bar{x} = \bar{x}_1$, $M_0$ is the total source release mass, $C(\bar{x}, T)$ is the resident concentration distribution of the pollutant at $t = T$ after the release of the point source.

Before establishing the backward location probability, a time parameter $\tau = T - t$ is defined as the backward time, so the location probability density can be expressed as

$$f_x(x; T, \bar{x}) = f_x(x; \tau = 0, \bar{x}_0) = \varphi_x(\bar{x}_0; \tau = T, \bar{x}) \quad (2)$$

where $\varphi_x(\bar{x}_0; \tau = T, \bar{x})$ is defined as backward location probability.

**Backward adjoint probability method**

The adjoint probability is derived from the backward contaminant transport equations (Liu et al., 2007). The adjoint equation can be expressed as:

$$\frac{\partial \varphi}{\partial t} - \frac{\partial \varphi}{\partial x} = -\frac{\partial}{\partial y} \left[ \psi_{ij} \frac{\partial \varphi}{\partial y} \right] + (\psi_{0} \cdot \psi^*) + \frac{\partial h}{\partial \psi} \quad (3)$$

$$\varphi^*(\bar{0}, \bar{0}) = 0 \quad (4)$$
\[
\frac{\partial h}{\partial \mathcal{C}} = \delta(\bar{\mathcal{C}} - \mathcal{C}_w) \cdot \delta(\mathcal{D})
\]

(5)

where \( \varphi^* \) is adjoint (location or travel time) probability, \( \tau \) is the backward time, \( \mathcal{C}_w \) is the place of the measurement. \( -q_0 \) is the outflow rate per unit volume, \( h \) is a function of the state system, \( \mathcal{C} \) is the system state variable, \( \frac{\partial h}{\partial \mathcal{C}} \) is the loaded term specified by (Neupauer et al., 2001), \( \delta(...) \) is the Dirac delta function. By solving Eq. (6), the calculation results of multiple measuring points can be integrated, and the only possible location of the pollutant source can be obtained.

\[
f \left( \mathcal{C}^* ; \cdots ; \mathcal{C}^N ; \tau_0 ; X_1 ; \cdots ; X_N ; \tau_1 ; \cdots ; \tau_N \right) = \frac{f_{\mathcal{M}} \prod_{i=1}^{N} f \left( \mathcal{C}^i ; \tau_0 ; X_i ; \tau_i \right) f_{\mathcal{D}} \left( \mathcal{C}^\mathcal{M} ; X \right) f_{\mathcal{D}} \left( \mathcal{C}^\mathcal{M} ; X \right) dxdM_0}{\int f_{\mathcal{M}} \prod_{i=1}^{N} f \left( \mathcal{C}^i ; \tau_0 ; X_i ; \tau_i \right) f_{\mathcal{D}} \left( \mathcal{C}^\mathcal{M} ; X \right) dxdM_0}
\]

(6)

where \( f_{\mathcal{D}} \left( \mathcal{C}^i ; \tau_0 ; X_i ; \tau_i \right) \) is the SALP of the \( i \)-th measurement; \( \mathcal{C}^i \) is the concentration of the \( i \)-th measurement; \( P \left( \mathcal{C}^i ; \mathcal{M}_0 ; \tau_0 ; X_i ; \tau_i \right) \) is the probability for the measured concentration conditioned on the source mass and source location \( X \).

\[
P \left( \mathcal{C}^i ; \mathcal{M}_0 ; \tau_0 ; X_i ; \tau_i \right) \sim N \left( M_0 \cdot f_{\mathcal{D}} \left( \mathcal{C}^\mathcal{M} ; X \right), \sigma^2 \right)
\]

(7)

where \( \mathcal{C}^i \) is the possible concentration value of the \( i \)-th measurement and \( \sigma^2 \) is the variance for the \( N \) measurements. As concentrations are involved in the calculation, probabilities obtained with Eq. (6) are called conditioned adjoint location probabilities with concentrations and are symbolized as CALP.

**Simulation setting**

According to the real outdoor weather conditions obtained from the experiment, the airflow field of 2D street canyons in the city is simulated numerically in this paper. The results of the numerical simulation are compared with the experimental data to verify the accuracy of the simulation.

The upstream, downstream, and height of the computational domain were 3H, and H was the building height (1.2m) (Ai, 2017), as shown in Figure 3 (a) and (b).

**Boundary condition setting**

The inlet velocity adopted the uniform inlet velocity boundary condition. According to the experimental results, the outdoor wind speed and direction constantly changed during the experimental data. This paper selected the observed data from 2:16:06 p.m. to 2:45:55 p.m. on June 8, 2019, as the entry boundary condition. The experimental data from 2:16:06 p.m. to 2:45:55 p.m. on June 8, 2019, were used for the velocity boundary conditions, as shown in Figure 4.

**Figure 4: Velocity boundary conditions**

During grid independence verification, steady-state velocity fields are used for comparison, and the inlet velocity wind profile uses an exponential function law fitted from experimental data. After fitting the wind speed experimental data from 10 a.m. to 3 p.m. on June 9, 2019, the formula can be expressed as follows:

\[
\frac{U}{U_H} = \left( \frac{Z}{Z_H} \right)^\alpha
\]

(1)

where \( U \) is the wind speed at height \( H \), m/s; \( U_H \) is the wind speed value at the reference height of the street canyon, 2.46m/s; \( Z_H \) is the height of the street canyon, 1.2m; \( \alpha \) is the empirical coefficient, taken as 0.245.
The outdoor wind direction in this period can be approximately seen as blowing vertically to the street canyon buildings. In this paper, the wind speed at 1.2m of the 10m wind pole is selected as the inlet speed. RNG k is still selected for the turbulence model k-ε Model.

\[
k = (U_{\text{ref}} \times T_i)^2 \tag{2}
\]

\[
\varepsilon = \frac{C_{\mu}}{l_i} \frac{3^{1/2}}{3^{3/2}} \tag{3}
\]

where \( C_{\mu} \) is constant, \( C_{\mu} = 0.09 \), \( T_i \) is turbulence intensity, \( l_i = 0.16Re^{-1/8} = 3\% \), \( l_i \) is turbulence characteristic size, \( l_i = 4A_f/L_w = 0.7m \), \( A_f \) is a cross-sectional area of fluid, \( A_f = 0.6m \), \( L_w \) is Wet perimeter length, \( l_w = 0.9m \). The concentration of the source gas is \( 10^6 \) ppm. Monitoring points are set in each room to detect the change in tracer gas concentration in each room and record the concentration data. A threshold of tracer gas concentration value of 10ppm is set in this paper, and exceeding the limit value is regarded as harmful. In the summer experiment (June 8–10, 2019), the tracer gas was released continuously for around 30 minutes, and the flow rate was 1.5 L/min.

**Validation of the CFD method**

**Grid sensitivity test**

Roach (1997) proposed grid convergence index (GCI) to establish grid independence. To verify the independence of the grid, a vertical segment (X=0.6 m, Y=0 m, Z=0-2 m) in the center of the target street canyons was selected for comparative analysis. The corresponding \( U/U_{\text{ref}} \) profiles of the fine grid show 14.6% average deviation from the intermediate grid; the coarse grid’s corresponding deviation is 13.8%. The height-averaged GCI averaged for the Intermediate-fine grids are 1.22% at X=0.6 m, Y=0m. For the intermediate-coarse grids, the value is 0.83%. Since the three grids’ averaged deviations in mean wind speed are less than 25% and their height-averaged GCI values are smaller than 5%. These grids can be used for the CFD simulation. Figure 5 shows the comparison of the results of three different grid systems to predict the dimensionless velocity in the center of the street canyon. The speed predictions of the three different grid systems are very close to each other in the street canyon, and only some areas have deviations. It can be observed from the figure that 7.2 million grid systems overestimate the speed prediction on both lines. From Figure 5, it can be observed that 3.5 million grid systems underestimate the prediction of speed on both line segments. Therefore, in the next steady simulation, 5.6 million grids with the size of 0.005 m near the wall are selected as the basic grid.

**Figure 5:** X=0.6m, Y=0m, Z=0-2 m

**Comparison between results of experiment and simulation**

Figure 6 shows the comparison of experimental and simulated values. The averaged deviation of \( U/U_{\text{ref}} \) between experiment and simulation is 14.12% at X=1.1 m, Y=1.05 m. There is a deviation between the experimental and simulated wind speed results because the outdoor wind direction affects the wind speed. The simulation of wind velocity with the CFD model has the same trend with the experimental data, which indicates the CFD simulation can predict the airflow field of the street canyon.

**Results and discussion**

**Airflow field**

The variation of airflow field in street canyons is a vital factor affecting pollutant dispersion. Figure 7 shows the airflow pattern in the street canyons. The target buildings A, B, and C are selected as examples. The rooms on both sides of the target building have openings and outdoor wind enters the building and create the vortex. After entering the street canyons environment through the top of the building, the outdoor wind flows along the windward side of building B to the bottom of the street and then continues to flow upward at the bottom of the street to the leeward side of building A, forming a clockwise vortex. Part of the outdoor airflow creates vortex in the street canyon, while the other part along the top of the building directly flows into the next street canyon.
Steps to find pollution source

First, this method simulates the forward unsteady flow field in 30 minutes and obtains the final unsteady flow field. Secondly, this method inverses the final flow field. It releases 1 unit of tracer gas carbon dioxide in the monitoring room that exceeds the concentration limit value and obtains SALP1 of the last time step. Thirdly, this method exports SALP1 of all grid nodes in the computing domain, then inverses the flow field at $T = t_3$. It imports from SALP1 of the previous step and solves to obtain SALP2 at $T = t_3$. Fourthly, the method inverses all flow fields and solves SALP. Then it obtains the adjoint probability of the final pollution source. Finally, this method combines the SALP (obtained from multiple monitoring points) and concentration data to get the CALP.

Results of locating pollutant source

Case 1: windward direction

In this study, concentration detection sensors were installed in the center of rooms BW2, BW3, and CL3 to detect the concentration values of these three rooms. The concentration values detected in these three rooms are shown in Table 1. In this study, the concentration values detected in the three rooms were used as important input conditions to conduct inverse identification of pollutant source. The simulated results showed that the location of the pollution source room was BW1, as shown in Figure 8. Meanwhile, the location of the pollution source room in the experiment was also in BW1. Of the three rooms, room BW2 detected a much higher concentration than the other two rooms combined. It can be found that the pollutants in the lower part of the windward room are likely to re-enter the upper room due to the vortex in the street canyon environment.

Case 2: leeward direction

Similarly, concentration detection sensors were installed in the center of rooms BL3, BL4, and AW3 to detect the concentration values of these three rooms. The concentration values detected in these three rooms are shown in Table 2. The concentration values detected in the three rooms were used as important input conditions to conduct inverse identification of pollutant source. The simulated results showed that the location of the pollution source room was BL2, as shown in Figure 9. Meanwhile, the location of the pollution source room in the experiment was also in BL2. The room BL3 and room BL4 detected concentrations exceeding the limit value about 1 minute and 4 minutes after the release of pollutants, respectively. The highest concentration in room BL3 can reach 154.6 ppm, which exceeds the concentration limit by one order of magnitude, indicating that the pollution source in room BL2 has a serious impact on the upper room. As in Case 1, it can be found that the pollutants in the room under the leeward side affected by vortex in the street canyons environment are highly likely to re-enter the upper room.

Conclusions

In this paper, the probability-based inverse modelling method is used to identify pollution sources in 2D street canyons under real weather conditions. The data measured by scaled outdoor experiment are used as the input conditions. Through the analysis of the airflow pattern and the results of source location, the following conclusions can be drawn:

1. By analyzing the airflow field, it can be concluded that the outdoor wind forms a vortex in the street canyons and enters the building interior to form a clockwise vortex. Part of the outdoor airflow creates the vortex in the street canyon, while the other part along the top of the building directly flows into the next street canyon.

2. This paper adopts the data measured by scaled outdoor experiment (concentration value and outdoor wind speed) as the input conditions to locate the pollutant source. The experimental data shows that the pollutant in the lower floor rooms are moved by vortices into the upper rooms. According to the simulation result, the location of pollution source can be accurately found.

Acknowledgement

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References


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Table 1: The concentration of the monitor room (source room is BW1, subtracted background concentration).

<table>
<thead>
<tr>
<th>Room</th>
<th>Over 10ppm time</th>
<th>Concentration value</th>
<th>Maximum concentration value</th>
<th>Final concentration value</th>
</tr>
</thead>
<tbody>
<tr>
<td>BW2</td>
<td>14:18:28</td>
<td>12.8 ppm</td>
<td>39.7 ppm</td>
<td>36.1 ppm</td>
</tr>
<tr>
<td>BW3</td>
<td>14:22:20</td>
<td>10 ppm</td>
<td>16 ppm</td>
<td>12 ppm</td>
</tr>
<tr>
<td>CL3</td>
<td>14:30:58</td>
<td>10 ppm</td>
<td>13 ppm</td>
<td>8 ppm</td>
</tr>
</tbody>
</table>

Table 2: The concentration of the monitor room (source room is BL2, subtracted background concentration).

<table>
<thead>
<tr>
<th>Room</th>
<th>Over 10ppm time</th>
<th>Concentration value</th>
<th>Maximum concentration value</th>
<th>Final concentration value</th>
</tr>
</thead>
<tbody>
<tr>
<td>BL3</td>
<td>15:12:34</td>
<td>16 ppm</td>
<td>154.6 ppm</td>
<td>130 ppm</td>
</tr>
<tr>
<td>BL4</td>
<td>15:15:05</td>
<td>10 ppm</td>
<td>26.8 ppm</td>
<td>21.5 ppm</td>
</tr>
<tr>
<td>AW3</td>
<td>15:18:15</td>
<td>10 ppm</td>
<td>15 ppm</td>
<td>3 ppm</td>
</tr>
</tbody>
</table>