Inverse identification of gaseous pollutant sources in a mixed ventilation room with downwind scheme-based backward modeling

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Abstract. Inverse computational fluid dynamics (CFD) modeling is an effective method to track indoor Pollutant sources. In this paper, heat transfer and instantaneous diffusion of contaminants in the mixed ventilation room have been investigated numerically. On the basis of the numerical simulation of indoor air flows, the reverse time modeling of diffusion-convection contaminant dispersions has been developed with the downwind scheme of the convection term. The program to implement the presented method is written in FORTRAN 90 and applied to the inverse time identification of the pollutant release history and source location. Direct simulation is conducted in the range of, Reynolds number ($2 \times 10^3 \leq \text{Re} \leq 5 \times 10^3$) and Grashof number ($10^6 \leq \text{Gr} \leq 9 \times 10^9$). In addition, the streamfunction and heatfunction are expressed streamlines and heatlines respectively. It is shown that the flow structure, heat transfer level and potential will depend on the interactions of external forced flow and thermal buoyancy driven flows. The numerical results indicated the proposed source identification algorithm is effective and robust in indoor environment.

1. Introduction
With the increasingly prominent problem of environmental pollution, indoor air quality (IAQ) has drawn growing attention. In case pollutants are found in indoor environments, it is vital important to identify the pollutant source so that effective measures can be taken in time. Computational fluid dynamics (CFD) is a powerful tool for simulating airflow and contaminant transport. In general, to obtain the distributions of contaminant concentration, boundary conditions, initial conditions and geometric characteristics of the environment need to be known in advance to solve the governing equations, which was called direct CFD modeling [1-3]. However, inverse CFD modeling aims to find out the location and strength of pollution sources based on the measured results. The inverse time tracing of pollution sources can be classified as an inverse problem in mathematical physics.

Computational instability, as stated by Alifanov [4], is the primary obstacle why inverse solution is not easy to be obtained, namely, inverse CFD modeling is ill-posed. The study of inverse problems exist in different fields, including heat transfer, groundwater transport and indoor contaminant transport, and these inverse modeling can be categorized into analytical [5,6], optimization [7-9], probabilistic [10-12] and direct approach [13-15]. The direct approach was applied to trace pollutant source location, through directly reversing the governing equation of pollutant diffusion. And it will be adopted in this study due to it has less requirement of information about pollutant sources than other methods. The quasi-reversibility (QR) method is the popular direct method recently, and it is to solve...
one that is close to the original equation to ensure the stability of the solution. Based on Q-R method, Skaggs et al. [13] realized the identification of groundwater pollution sources and concluded that Q-R method requires much less computational effort than regularization technique. Zhang [14] applied the QR method to identify the pollution source in the airplane chamber, while the diffusion term in the contaminant dispersion equation were omitted and thermal buoyancy was almost neglected. Also, this QR methodology covering advection-diffusion and thermal buoyancy effects has been adopted to identify the contaminant sources location in the displacement ventilation indoor environment, where the two-dimensional [15] and three-dimensional [16] enclosure have been assumed. Recently, Shi [17] derived the downwind scheme for convection term in the initial concentration equation, and the identification of pollutant sources in a slot ventilated porous enclosure with laminar air flow was realized.

In the present work, the backward time model containing the downwind scheme of the convection term will be applied to the turbulent air flow. Mutual effects of natural convection and forced flows within a two-dimensional mixed ventilation room simultaneously containing thermal and airborne pollutant sources will be researched. Following that, the impacts of pollutant diffusivity and the inflow velocity on the reverse time simulations will be studied.

2. Forward time simulations

2.1. Physical model

As shown in Figure 1, the physical bounded domain under present study is a two-dimensional enclosure with the top air inlet and outlet of same size \( l_{\text{port}} \) respectively on the left and right. It is supposed that the third dimension of the rectangular enclosure is large enough such that fluid flow and mass transfer are of two dimensions. The width and height of the enclosure under investigation is \( W \) and \( H \), respectively (\( W/H=2 \)). A strip heat source \(( L_{\text{HS}}=0.2H \) is centrally located on the ground. In addition, two discrete pollutant sources \(( L_{\text{PS}}=0.1H \) were occurred on the ground on the left and right sides of the vertical centerline severally (the strip distances \( L_{\text{PSR}}=L_{\text{PSL}}=0.5H \) from the vertical centerline).

![Figure 1. Schematic of the ventilated enclosure and coordinate system.](image)

The macroscopic conservation equations based on the above assumptions are the Reynolds-averaged equations for momentum, mass continuity, energy, and species conservation. Then the dimensionless governing equations can be obtained,

\[
\frac{\partial U_j}{\partial X_j} = 0
\]

\[
\frac{\partial U_i U_j}{\partial X_j} = -\frac{\partial P}{\partial X_i} + \frac{\partial}{\partial X_j} \left( \chi_{ij} \frac{\partial U_j}{\partial X_j} \right) + \frac{\partial}{\partial X_j} \left( \chi_{ir} \frac{\partial U_r}{\partial X_r} \right) - \frac{\partial T}{\partial X_i} \frac{\partial T}{\partial X_j} - \tau_{ij} \cdot \textbf{e}_g
\]

(2)
Due to the simulation of turbulent flow, the standard $k - \varepsilon$ model is adopted to investigate the turbulent flows, and two additional turbulence kinetic energy and its dissipation rate equations need to be solved,

$$
\frac{\partial U_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left( x_T \frac{\partial T}{\partial x_j} \right)
$$

$$
\frac{\partial C}{\partial t} + \frac{\partial C U_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left( x_C \frac{\partial C}{\partial x_j} \right)
$$

Where $K$ is the turbulence kinetic energy, $E$ is the dissipation rate of kinetic energy. Then the turbulent eddy viscosity can be written as $\nu_t = C_\mu K^2 / E$, which describe the turbulence intensity and variation.

Figure 2 illustrates a staggered grid system which can be employed to solve the Eqs. (1) - (6) with the finite volume method (FVM). The SIMPLE algorithm was used to solve the original governing differential equation numerically.

For mixed ventilated airflow, the Archimedes number ($Ar = Gr / Re^2$) can represent the relative size of the Reynolds number $Re$ and Grashof number $Gr$. It can also confirm which of the two is dominant, forced convection or natural convection. And the dimensionless forms of the streamfunction ($\psi$) and heatfunction ($\Theta$) can be obtained.

![Streamlines](image1)

![Eddy viscosity](image2)

![Isotherms](image3)

![Heatlines](image4)

**Figure 3.** Steady-state streamlines, turbulent eddy viscosity, isotherms and heatlines for $Re = 5 \times 10^3$, (a) $Gr = 10^6$, (b) $Gr = 2 \times 10^9$, (c) $Gr = 9 \times 10^9$. 
\[
\frac{\partial \psi}{\partial Y} = U, \quad \frac{\partial \psi}{\partial X} = -V, \quad \frac{\partial \Theta}{\partial Y} = \text{RePr} \frac{\partial T}{\partial X} \frac{\partial X}{\partial T}, \quad \frac{\partial \Theta}{\partial Y} = \text{RePr} \frac{\partial T}{\partial X} \frac{\partial X}{\partial T} \quad (7)
\]

2.2. Numerical results of mixed convection

The steady state mixed convection formed in the indoor environment contains forced convection from external airflow and natural convection from thermal buoyancy. The degree of strength of the two will be described by the Reynolds number and Grashof number.

As shown in Figure 3, the Reynolds number remains constant \((\text{Re} = 5 \times 10^3)\), and three situations in which Grashof number \(\text{Gr}\) increases gradually were explored respectively. Firstly, it is obvious from the streamlines that the cross-flow from upper left inlet to upper right outlet was established by the forced flow. And the counterclockwise vortex forms in the central region. On the other hand, In terms of the profiles of heatlines, part of heat is transferred directly from the heat source to the upper right vent, while the rest circulates within the room. As the Grashof number gradually increases from \(10^6\) to \(9 \times 10^9\), the heat transfer path gets thinner and the range of heatlines circulation has been enlarged, which indicate respectively the heat to the outlet is reduced, while growing heat is stuck in the enclosure.

The isotherms are stratified on the right side of the enclosure as the blowing of external airflow and transfer of heat. With the increase of heat source strength and thermal buoyancy, thermal stratification is obvious in the lower area near the heat source and gradually transfers from the right hand side to the left side of the central point of the floor.

3. Backward time simulations

The essence of backward identification of the pollutant source is the solving process of inverse model, in addition to the sensor monitoring, it is more calculated by solving the pollutant transport equation. When the initial concentration field of inversion is obtained, the following governing equation needs to be solved backward in time to reestablish the temporal and spatial distributions of gaseous pollutants,

\[
\frac{\partial C}{\partial t} = \frac{\partial C}{\partial X} \left( \Gamma \frac{\partial C}{\partial X} \right) \quad (8)
\]

Where \(C\) is the pollutant concentration, \(U_j\) is the flow velocity at \(x_j\) direction, \(\Gamma\) is the effective diffusion coefficient \((\Gamma = \frac{1}{\text{RePr}} + \frac{C_{\text{d}} K^2}{\sigma E})\), \(\text{Sc}\) is Schmidt number \((u/D)\).

As to forward simulation, the concentration on some interface depends on upstream nodes, which is the so-called upwind scheme, while for backward simulation it should rely on the downstream nodes, which can be named downwind scheme. For two-dimensional, structured and uniform grid systems (as shown in Figure 2), take the interface \(e\) as an example,

\[
S_e = \begin{cases} 
S_E, U_e > 0 \\
S_p, U_e < 0 
\end{cases} 
\quad (9)
\]

The same way is adopted in other interfaces \((w, n, s)\) and the final discretized formula is obtained for backward simulation,

\[
S_p(t + \Delta t) = \frac{-1 - U_u \Delta X}{\Delta t} + \frac{\Gamma}{\Delta X^2} + \frac{1}{\Delta Y^2} \left( \frac{-1 - V_v \Delta Y}{\Delta t} + \frac{\Gamma}{\Delta Y^2} + \frac{1}{\Delta X^2} \right) \cdot S_W(t + \Delta t) \\
+ \frac{1}{\Delta t} \left( \frac{-1 - V_v \Delta Y}{\Delta X} + \frac{\Gamma}{\Delta X^2} + 2 \frac{1}{\Delta Y^2} \right) \cdot S_E(t + \Delta t) \\
+ \frac{1}{\Delta t} \left( \frac{-1 - U_u \Delta X}{\Delta Y} + \frac{\Gamma}{\Delta Y^2} + 2 \frac{1}{\Delta X^2} \right) \cdot S_S(t + \Delta t)
\]
In order to achieve the computational stability, we can make all the coefficients negative as far as possible. Additionally, the coefficient of $S_p(t+\Delta t)$ should be smaller than -1, the following inequality (11) can be obtained,

$$\frac{1}{\Delta t} \left( \frac{-[U_e,0]+[U_w,0]}{\Delta X} + \frac{-[V_n,0]+[V_s,0]}{\Delta Y} + 2\Gamma \left( \frac{1}{\Delta X^2} + \frac{1}{\Delta Y^2} \right) \right) < -1$$

The inequality (11) is equivalent to the next one,

$$\frac{1}{\Delta t} < -1 - 2\Gamma \left( \frac{1}{\Delta X^2} + \frac{1}{\Delta Y^2} \right) + \left( \frac{-[U_e,0]+[U_w,0]}{\Delta X} + \frac{-[V_n,0]+[V_s,0]}{\Delta Y} \right)$$

For the right part of inequality (12), because the term, $\left( \frac{-[U_e,0]+[U_w,0]}{\Delta X} + \frac{-[V_n,0]+[V_s,0]}{\Delta Y} \right)$, is always positive, the inequality (13) is consequently valid,

$$\Delta t > \left( -1 - 2\Gamma \left( \frac{1}{\Delta X^2} + \frac{1}{\Delta Y^2} \right) \right)^{-1}$$

Thus, the condition of inequality (13) should be satisfied to conduct the right calculations. So the very small time step $\Delta t = 0.001$ is adopted.

![Figure 4](image-url)

**Figure 4.** Effect of Re on backward time simulations with Gr = $10^6$, Sc = 0.6.

(a) Re = $2 \times 10^3$, (b) Re = $5 \times 10^3$, (c) Re = $5 \times 10^4$.

As illustrated in Figures 4-5, reverse time simulation of pollutant dispersion ($t = 50.0 - N \times t$) was investigated under the condition of different Reynolds number and Schmidt number to identify...
pollutant source locations. It can be observed from Figure 4 that particularly accurate source locations were tracked for different Reynolds number. In three cases, with the increase of Reynolds number, the less time it takes, the easier it is to find the pollutant sources. This is in line with that the downwind scheme is more suitable for high Reynolds number in the literature [17].

The effects of Schmidt number on the backward time simulations were shown in Figure 5. Due to the contaminant concentration bounding layer gets thicker with the high mass diffusivity, the pollutant of lower Schmidt number delaminates in the enclosure at $t = 50.0$. With the backward time simulation, perturbation firstly appears around the boundaries, and then the residuals of contaminant concentration gradually converge to the original location of contaminant sources. The results are similar to those in the literature [15], but more accurate than the Q-R method. On the other hand, owing to the thicker bounding layer significantly improves the sensitivity of inverse modeling, the identification of pollutant sources is easier to achieve for the lower Schmidt number airflow.

![Figure 5. Effect of Sc on backward time simulations with Re = 5 × 10^3, Gr = 10^7.](a) Sc = 0.1, (b) Sc = 0.6, and (c) Sc = 2.0.)

### 4. Conclusion

Direct and inverse CFD simulations of mixed ventilation airflow within rectangular enclosure were investigated in this study. Within the mixed ventilation room, steady-state airflow was formed under the combined action of forced convection and natural convection, and then two strip contaminant sources positioned on the floor were assumed to release airborne contaminants. In addition, the backward time model with downwind scheme for convection term has been applied to the turbulent airflow. The numerical results indicated the proposed source identification algorithm is effective and robust in indoor environment.

Enhancing the mass diffusivity and concentration sensitivity of contaminants, including increasing inflow velocity, smaller Schmidt number, will improve the inverse identification of pollutant sources.
Acknowledgements

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