ABSTRACT
Building indoor environment quality (IEQ) has received growing attentions lately because of the extended time people spend indoors and the increasing reports of health problems related to poor indoor environments. Recent alarms to potential terrorist attacks with airborne chemical and biological agents (CBA) have further highlighted the research needs on building vulnerability and protection. To maintain a healthful and safe indoor environment, it is crucial to identifying contaminant source locations, strengths and release histories. Accurate and prompt identification of contaminant sources ensures that the contaminant sources can be quickly removed and contaminated spaces can be effectively isolated and cleaned. This paper proposed a probability concept based inverse modeling method—the adjoint probability method that can identify potential indoor pollutant sources with limited pollutant sensor outputs. The paper introduces the principles of the method and presents the corresponding adjoint equations for computational fluid dynamics (CFD) model. A CFD based adjoint probability inverse modeling algorithm and program have been developed. By using an office building and an aircraft cabin as examples, the study demonstrates the application of the program for identifying indoor airborne pollutant source characteristics (location and release time) with few sensor measurement outputs. The research verifies the feasibility and accuracy of the adjoint probability method for indoor pollutant tracking. The paper indicates the further research directions with the goal of developing an intelligent and integrated building environment management system that can promptly respond to building pollution conditions with effective detection, analysis and control.

KEYWORDS
Indoor air quality, pollutant source identification, CFD, inverse modeling, adjoint method

NO MENC LA TURE
C resident contaminant concentration after a spread time of \( T \).
\( C_0 \) initial concentration
\( C_i \) resident concentration at \( \tilde{x}_i \)
\( \hat{C}_i \) concentration value of the \( i \)th measurement
\( C_i \) corresponding inflow concentration
\( \hat{C} \) possible concentration value of the \( i \)th measurement
\( f_x \) location probability density function
\( g_1, g_2, g_3 \) known functions
\( M_0 \) an assumed mass released from the source
\( M_i \) mass of pollutant trapped in a small finite volume at \( \tilde{x}_i \) after a spread time of \( T \).
\( n_i \) outward unit normal vector in the \( x_i \) direction.
\( N \) number of measurements
\( P \) forward location probability
\( q_i \) inflow (other than advection inflow through boundaries) rate per unit volume,
\( q_o \) outflow (other than advection outflow through boundaries) rate per unit volume
\( S_C \) all other kinds of contaminant sources or sinks in cells
\( S_\theta \) source term
\( t \) time coordinate
\( T \) an assumed spread time
\( \nabla \) velocity vector
\( V_j \) air velocity at \( X_j \) direction
\( \tilde{x} \) location vector of a point in the domain
\( \tilde{x}_i \) an assumed measuring location
\( \tilde{x}_o \) an assumed source location
\( x_i \) measurement location
\( X_j \) \( x, y \) or \( z \) direction
\( \tilde{x}_w \) location where the measurement is made

GREEK SYMBOLS
\( \Delta V_i \) finite volume at \( \tilde{x}_i \)
\( \psi_i \) state sensitivity of resident concentration at \( \tilde{x} \) to the source mass \( M_0 \) at \( \tilde{x}_o \).
\( \tau \)  
backward time  
\( \psi^* \)  
adjoint location probability  
\( \Phi \)  
an air velocity component in a certain direction  
\( \Gamma \)  
diffusion coefficient  
\( \rho \)  
air density  
\( v_{C,j} \)  
effective turbulent diffusion coefficient at \( X_j \) direction  
\( \Gamma_1, \Gamma_2, \Gamma_3 \)  
domain boundaries  
\( \partial h / \partial C \)  
load term  
\( \delta(x) \)  
impulse function  
\( T_r \)  
backward measurement time \((t-T)\)  
\( t_0 \)  
known source release time in the backward time domain  
\( \sigma^2 \)  
variance for the \( N \) measurements

**INTRODUCTION**

Indoor air quality (IAQ) and sick building syndrome (SBS) have received increasing attention over the past few years. Research conducted by various agencies such as the US Environmental Protection Agency (EPA), has shown that the quality of indoor air can be significantly worse than that of the outdoor air. For instance, the air pollution level inside a house can be two to five (and occasionally one hundred) times higher than the outdoor level (EPA 2006). Given the fact that many people spend as much as 90 percent of their time indoors, the health risk due to indoor air pollutants is a critical public health concern. The US EPA ranks poor indoor air quality among the top five environmental risks to public health. In addition, the potential terrorist attacks with chemical and biological agents have become another crucial building safety concern since the September 11 tragedy.

To achieve a healthy and safe indoor environment requires profound knowledge of air movement and contaminant transport in and around buildings, upon which appropriate building environment control strategies can be determined and implemented. In the past decade, a large number of IEQ researches have been conducted, in which computer simulation exhibits its unique role and strong capability due to the high efficiency and flexibility. In particular, the computational fluid dynamics (CFD) method has been widely used for various building IAQ studies (Spengler and Chen 2000). As the most sophisticated transport model, CFD provides the spatial distributions and temporal evolutions of air pressure, velocity, temperature, humidity, contaminant concentrations, and turbulence intensities by numerically solving the conservation equations for mass, momentum, energy, and species concentrations. CFD model can directly predict the fate and transport characteristics of indoor pollutants, which is important for designing appropriate indoor layouts, identifying effective sensor locations, indicating safe rescue paths in emergencies, and determining proper indoor environment control strategies. However, such prediction can be obtained only when the source conditions (e.g., location and intensity) are provided. For many realistic problems, contaminant source conditions are unknown and need be first identified through limited sensor outputs, and then the forward CFD simulation can be conducted to reveal the contaminant release history and predict its development trend with and without proper control measures. Prompt and accurate identification of indoor pollutant sources is also critical for effectively controlling indoor pollution conditions by removing pollutant sources and isolating and cleaning contaminated spaces.

**MODELING**

**PROBABILITY-BASED INVERSE CFD MODELING**

The task of contamination source identification may vary significantly with prior knowledge of pollution conditions. For indoor environment with known contaminant release time, the tracking task is to find the source location and release intensity. The task will become extremely challenging if little or none of prior source information is available. When tracking a pollutant source, the sensor network distribution and sensor performance play an important role, which provides direct consequence indications of potential causes. In reality, diverse sensing systems could be applied. Simple sensors may only provide alarm when a prescribed threshold concentration value is reached such as smoke detectors. Some contaminant sensors may also display current concentration readings while advanced sensors can even record historical values of contaminant concentration in internal or external memories. Different sensing scenarios may lead to different source identification approaches.

This project is to develop a reliable and fast methodology and algorithm that can identify potential indoor contaminant source conditions with limited sensor outputs. As the first step of the whole research, the current study focuses on developing the method to find contaminant source locations with given source release time under different sensing scenarios, which will form the base for further investigation. This paper introduces the principles of the probability-based inverse modeling method and the corresponding equations as well as the CFD based inverse modeling algorithm. It also demonstrates the application of the method for two realistic cases.
Finding contaminant source conditions based on measured concentrations is an inverse problem in that it is the problem of finding unknown causes of known consequences. Liu and Zhai (2006) conducted a thorough literature review on various pollutant inverse modeling methods for both the groundwater and air fields. The review concluded that the adjoint probability method proposed by Neupauer and Wilson (1999 and 2001) for groundwater pollutant source identification is a promising approach for indoor air quality study. The method can identify pollutant source location, flux and release time with little prior information, and the algorithm is faster than others. Although groundwater and air follow the same transport rules, the review also indicated the challenges associated with air applications, which will demand substantial investigation on both mathematical theories and numerical algorithms. This paper presents the fundamentals of the CFD-based adjoint probability method and describes the corresponding probability equations for different sensing scenarios.

**Fundamentals of Adjoint Probability Method**

One of the key concepts of the adjoint probability method is location probability. In a flow domain of interest, if a contaminant parcel is released from a point source at $x = x_0$ and $t=0$, the forward location probability of the parcel is defined as the probability that it reaches some location in the domain at a given time $t=T>0$. Assume the pollution source releases instantaneous contaminants with a mass of $M_0$ into the domain at $t=0$, which spread all over the domain at $t=0$ due to both convection and diffusion flows. If the pollutant mass trapped in a small finite volume $\Delta V_1$ at $x = \bar{x}_1$ at time $t=T$ is $M_1$, the forward location probability at this finite volume $\Delta V_1$ at $t=T$ is

$$P(\Delta V_1 | \bar{x} = \bar{x}_1; t = T, \bar{x}_0) = \frac{M_1}{M_0}$$

(1)

The location probability density function at $t=T$, is then defined as

$$f_s(\bar{x}_s; t = T, \bar{x}_0) = \frac{P(\Delta V_1 | \bar{x} = \bar{x}_1; t = T, \bar{x}_0)}{\Delta V_1}$$

(2)

$$= \frac{M_1}{M_0}$$

where $C_1$ is the resident concentration at $\bar{x} = \bar{x}_1$, defined as a measure of the mass of pollutant per unit volume of flow medium, or a volume-averaged concentration. Generalizing the definition to any location in the domain yields

$$f_s(\bar{x}; t = T, \bar{x}_0) = \frac{C(\bar{x}, T)}{M_0}$$

(3)

where $f_s(\bar{x}; t = T, \bar{x}_0)$ is the forward location probability density at $t=T$, $\bar{x}$ is the arbitrary location vector in the domain, $C(\bar{x}, T)$ is the distribution of resident contaminant concentration at $t=T$ due to the instantaneous release of the point source, $\bar{x}_0$ is the source location, $M_0$ is the total source release mass. For the cases with steady-state velocity field, there is a linear relationship between source release strength and resident concentration, which leads to

$$f_s(\bar{x}; t = T, \bar{x}_0) = \frac{dC(\bar{x}, T)}{dM_0} = \psi(s)(\bar{x}; t = T, \bar{x}_0)$$

(4)

where $\psi(s)(\bar{x}; t = T, \bar{x}_0)$ is the state sensitivity of resident concentration at $\bar{x}$ to the source mass $M_0$ at $\bar{x}_0$.

The forward location probability density function $f_s(\bar{x}; t = T, \bar{x}_0)$ describes the possibility of a contaminant parcel, originating from an instantaneous source at $\bar{x}_0$, to be at an arbitrary $\bar{x}$ after a fixed time $t=T$. From statistics, this forward location probability is equal to the possibility of the parcel found at $\bar{x}$ when $t=0$ to be at source location $\bar{x}_0$ at $t=0$ (or $t=T$ ago if a new backward time sign $t=T-t$ is defined), which is named as backward location probability $f_s^*(\bar{x} = \bar{x}_0; t = T, \bar{x})$. The backward location probability can be determined via

$$f_s^*(\bar{x} = \bar{x}_0; \tau = T, \bar{x}) = \psi_s^*(\bar{x}; \tau = T, \bar{x})$$

(5)

where $\psi_s^*(\bar{x}; \tau = T, \bar{x})$, termed as adjoint location probability, denotes the solution to an adjoint backward equation of the forward contaminant transport equations (Liu and Zhai 2006).

**Standard Backward Probability Equation**

The forward governing equations CFD solves can be written in a general form:

$$\frac{\partial \Phi}{\partial \tau} + (\bar{V} \cdot \nabla) \Phi - \Gamma_s \nabla^2 \Phi = S_\Phi$$

(6)

where $\Phi$ is $V_j$ that stands for the air velocity component in the j direction, is 1 for mass continuity, is $T$ for temperature, is $C$ for species concentration. $\bar{V}$ is velocity vector, $\Gamma_s$ is diffusion coefficient, and $S_\Phi$ is source term. The $\Phi$ can also stand for
turbulence parameters if a turbulence model is used to represent the overall turbulence effect on airflow.

The forward contaminant transport equation of CFD, together with the initial and boundary conditions can be further expressed as

\[
\frac{\partial C}{\partial t} + \mathbf{v}_j \cdot \frac{\partial C}{\partial x_j} = \left( \mathbf{v}_j \cdot \frac{\partial C}{\partial x_j} \right)_L + \left( S_C + q_1 \mathbf{C}_1 - q_0 \mathbf{C} \right)
\]

where \( \rho \) is the air density, \( C \) is the species concentration, \( \mathbf{v}_j \) is the air velocity at \( x_i \) direction, \( \mathbf{v}_j \cdot \mathbf{C}_j \) is the effective turbulent diffusion coefficient for \( C \) at \( x_i \) direction, \( q_0 \) is the outflow (other than advection outflow through boundaries) rate per unit volume, \( q_1 \) is the inflow (other than advection inflow through boundaries) rate per unit volume, \( \mathbf{C}_1 \) is the corresponding inflow concentration, \( S_C \) is all other kinds of contaminant sources or sinks in cells, and \( \left( S_C + q_1 \mathbf{C}_1 - q_0 \mathbf{C} \right) \) is a combined term of all sources or sinks other than advection and dispersion. \( \mathbf{C}_0 \) is the initial concentration, \( g_1, g_2 \) and \( g_3 \) are known functions, \( \Gamma_1, \Gamma_2 \) and \( \Gamma_3 \) are the domain boundaries, and \( n_i \) is the outward unit normal vector in the \( x_i \) direction.

To derive the adjoint equation for the CFD forward contaminant transport equation (7), the sensitivity analysis approach of Sykes et al. (1985) was employed. Liu and Zhai (2006) described the detailed mathematical deduction procedure and provided the CFD-based adjoint equation as

\[
\frac{\partial \psi^*}{\partial \tau} - \frac{\partial \mathbf{v}_j}{\partial x_j} \frac{\partial \psi^*}{\partial x_j} = \left( \frac{\partial \psi^*}{\partial x_j} \right)_L + \left( -q_0 \cdot \psi^* \right) + \frac{\partial h}{\partial C}
\]

\[
\psi^*(x,0) = 0, \quad \psi^*(x,\tau) = 0 \quad \Gamma_1
\]

\[
\left[ \mathbf{v}_j \frac{\partial \psi^*}{\partial x_j} + \psi^* \right] n_i = 0 \quad \Gamma_2
\]

\[
\left[ \mathbf{v}_j \frac{\partial \psi^*}{\partial x_j} \right] n_i = 0 \quad \Gamma_3
\]

where \( \psi^* \) is the adjoint location probability, \( \tau \) is the backward time, \( \mathbf{x}_w \) is the location where the measurement is made, \( \partial h/\partial C \) is the load term, and \( \delta(x) \) is the impulse function which equals 1 when \( x=0 \) otherwise 0. Note that the adjoint of the first-type boundary condition is still first-type (boundary condition on \( \Gamma_1 \)); the adjoint of the second-type boundary condition becomes third-type (boundary condition on \( \Gamma_2 \)); and the adjoint of the third-type boundary condition becomes second-type (boundary condition on \( \Gamma_3 \)).

The initial condition \( \psi^*(\mathbf{x},\tau) = 0 \) implies that the adjoint probability for observed pollutants to be from any potential source location is zero at the backward time \( \tau = 0 \). The boundary conditions constrain the adjoint probabilities at the boundaries. The load term represents a probability source term at the measurement point at \( \tau = 0 \).

To solve Equation (8) requires information of thermo-physical properties of fluid, a steady flow field, sensor location, boundary conditions, and geometric characteristics of the flow domain. The solution provides the backward (and forward) location probability for one sensor observation. Lin (2003) defined this type of backward probability based on one sensor location with no concentration reading as standard backward location probability (SBLP).

The standard backward location probability equation (8) calculates the probability of source location based on one given sensor location and known source release time. A typical example is a smoke sensor in a firing house detecting fire smoke and triggering alarm when the threshold is reached. The SBLP can help locate the fire origin with the sensor location, therefore eliminating or reducing the risk of on-site inspection of firefighters. Apparently, with minimum information (i.e., sensor location), SBLP can only provide a rough estimate for possible source locations that released contaminants reaching the place where the sensor is located.

### Joint Probability Equation for One or Multiple Sensors Detection with Concentration Records

The accuracy of probability prediction can be refined if more contaminant dispersion information can be acquired, such as contaminant concentration. In practice, many contaminant sensors can detect, display and store contaminant concentrations, either the current reading or the entire historical readings. Such quantitative information greatly improves the accuracy and efficiency of the source identification procedure. To incorporate the concentration information into the prediction, Lin (2003) proposed the joint backward location probability for multiple sensor measurements. The joint backward location probability with \( N \) measurements is given by
where \( \mathbf{N} \) is the number of measurements, \( \mathbf{x}_i \), \( \tau_0 \), and \( \hat{C}_i \) are, respectively, the measurement location, the backward measurement time (\( \tau=\tau-t-T \)), and the concentration value of the \( i \)th measurement. \( \tau_0 \) is the known source release time in the backward time domain and \( M_0 \) is the assumed instantaneous source release mass strength. \( f_x(\mathbf{x};\tau_0,\mathbf{x}_i,\tau_i) \) is the SBLP for the \( i \)th observation (without concentration measurement). \( P(\hat{C}_i|M_0,\mathbf{x}_i,\tau_0,\mathbf{x}_i,\tau_i) \) is the probability for the measured concentration conditioned on source mass \( M_0 \) and source location \( \mathbf{x} \). \( P(\hat{C}|M_0,\mathbf{x}_i,\tau_0,\mathbf{x}_i,\tau_i) \) follows a normal distribution as suggested by Neupauer (2002)

\[
P(\hat{C}|M_0,\mathbf{x}_i,\tau_0,\mathbf{x}_i,\tau_i) \sim \mathcal{N}(M_0 \cdot f_x(\mathbf{x};\tau_0,\mathbf{x}_i,\tau_i), \sigma^2_e)
\]

where \( \hat{C}_i \) is the possible concentration value of the \( i \)th measurement and \( \sigma^2_e \) is the variance for the \( \mathbf{N} \) measurements.

In Equation (9), the multiple measurements can be either one-time (static) concentration measures by multiple (or one) sensors or multi-time (dynamic) concentration measures by one (or multiple) sensors. To calculate the conditioned backward location probability (CBLP) with Equation (9) requires first solving the SBLP for each observation location with Equation (8). Figure 1 presents the main algorithm for the probability-based inverse CFD modeling method for identifying contaminant source locations.

**CASE STUDIES**

**Air Contamination in an Office Space**

The paper first demonstrates the application of the algorithm for identifying indoor contaminant source location in a two dimensional office as illustrated in Figure 2. The office is 10m long and 3m high and houses a 70W occupant, a 200W computer, an adiabatic desk, and a large window with incoming heat flux of 100W. The conditioned air was continuously supplied at \( V=0.1m/s \) and \( T=20^\circ C \). A point contaminant source underneath the window released 100 units of contaminant at \( t=0 \).
Air Contamination in a Commercial Aircraft Cabin

The study further applies the algorithm to help identify contaminant source in a commercial aircraft cabin. As shown in Figure 6, the modeled aircraft cabin section is 4.725m wide, 4.1m deep and 2.2m high (the same dimensions as Boeing 767-300). The cabin section has five rows of seats along the length of its axis and each row has seven seats and seven passenger manikins. The aircraft cabin geometries and configurations resembled the physical model built by Sun et al. (2005). In the cabin, conditioned air was supplied from the two slot inlets at the ceiling with a velocity of 2.531m/s and a temperature of 8.3°C. The air was exhausted through two slot outlets located at the side walls near the floor. During the test, the inside wall temperature was kept at 13.9°C. Each manikin consisted of four solid pieces with a total heat generation rate of 75W. The second passenger on the third row was assumed to be the contaminant origin, producing contagious airborne virus from breathing or coughing. Two virus sensors were placed at the same row, which were on the aisle side of the third and fifth passenger’s seats, respectively. Figure 6 illustrates the geometry and configuration of the aircraft cabin CFD model, as well as the locations of the contaminant source and the sensors.

A commercial CFD program was first employed to model the airflow and contaminant concentration distributions in the cabin with given source location and release time. The predicted airflow velocity field and contaminant concentration values at the sensor locations were then used for the inverse modeling demonstration to reversely find the contaminant origin. In the forward CFD simulation, standard k-ε model with wall function (Launder and Spalding 1974) was used for the turbulent flow. It was revealed that a grid number of 1.2×10^5 is appropriate for obtaining reasonably grid-independent solutions for this case, which thus was used for the following simulations.
The forward unsteady pollutant transport simulation predicted the spatial and temporal evolution of the contaminant concentration in the whole space with the given source conditions. Figure 7 presents the contaminant concentration variations at the two sensor locations during the first 100 seconds after the contaminant was released. Apparently, sensor 2 had a much poorer sensing performance than sensor 1 that was located within the same airflow vortex as the contaminant source. The readings of sensor 1 and 2 are, respectively, 1.43 and 0 units/m³ at t=10s. This information was used to verify the inverse modeling algorithm by tracing back and finding the source origin.

![Figure 7 Predicted contaminant concentration variations at the two sensor locations during the first 100 seconds after the contaminant was released in the cabin](image)

The numerical test first used only the information from sensor 1 for the inverse modeling. The simulation successfully located the Y plane (row) of the source origin. Figure 8 shows the predicted source location probability distribution on the correct Y plane (row), which has the peak probability near the actual source location specified in the forward simulation.

![Figure 8 Predicted source location probabilities (%) by the joint probability method with one one-time-reading sensor (sensor 1) for the cabin case](image)

Sensor 2, although did not detect any substantial contaminant concentration, can still contribute to the improvement of the inverse simulation accuracy, as witnessed by the prediction results in Figure 9, where both readings from sensor 1 and 2 at t=10s were used.

![Figure 9 Predicted source location probabilities (%) by the joint probability method with two one-time-reading sensors for the cabin case](image)

CONCLUSIONS

This paper introduced the principles of a probability-based inverse modeling method and developed a CFD-based inverse modeling algorithm that is able to identify pollutant source location with known source release time in enclosed environments. The method and algorithm were demonstrated and verified by two example cases: a two-dimensional office case and a three-dimensional aircraft cabin case, with different sensing scenarios. The numerical experiments verified the feasibility, effectiveness and accuracy of the proposed method for identifying indoor pollutant sources. Further study will be conducted to explore a suitable algorithm that can track indoor pollutant sources with both unknown location and release time. The research will lay a solid ground for developing an intelligent and integrated building environment management system that can promptly respond to building pollution conditions with effective detection, analysis and control.

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