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Probability-based inverse characterization of the instantaneous pollutant source within a ventilation system

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ABSTRACT

Once a biochemical pollutant is deliberately released into a ventilation system, the source information including the releasing time and location need to be determined promptly and accurately. Successful inversion algorithms to identify airborne contaminant source within enclosed spaces were deeply developed by previous studies. Such mathematical algorithms inversely simulate airflow and concentration field with numerous intricate inverse matrixes and spend plenty of time in the simulation process. However, tracking airborne pollutant sources within a ventilation system has a higher requirement on computation time due to the rapid spread of contaminants in high-speed airflow, which imposes a great challenge on model abstraction and method selection. This paper mainly focuses on a specific source identification scenario: characterizing an instantaneous pollutant source within a ventilation system by employing a probability-based inverse model. The mathematical model and the solving process of both forward propagation and backward identification of the source are investigated and proposed. To verify the feasibility of the forward model and to validate the applicability of the proposed inverse modeling, a concentration-measured experiment was conducted in a real-built ventilation system. The measured concentrations are used as model inputs to calculate the unconditional and the conditional backward time probability density function (PDF). Then, the impact of sensor errors, sensor number and the change of the operating status of the ventilation system on the results of source identification are discussed. Finally, the basis and limitations of this work are extensively commented.

1. Introduction

In recent years, terrorists started to use lethal biochemical weapons to attack public buildings and crowded places, which was challenging the safety of our society [1–3]. In the latest case, the central air conditioning system within the Hamburg Airport was chosen as the delivery system for an undefined gas, which caused dozens of people had cough, allergy and other stress responses. In the early events, the nerve agent Sarin was intentionally released into the Tokyo subway in 1995, which killed 12 people and severely injured another 50 victims [4]. Afterwards, terrorists planned to use Sarin gas to assault the European Parliament and kill all 625 parliamentarians. Fortunately, this incident was foiled. In 2001, some anthrax spores letters were transmitted to several office buildings across the United States, which murdered 5 people and infected more than 20 [5,6]. Such terrorist attacks or plans have highlighted the exposure risk of civilians to biochemical pollutants in buildings. In the case of deliberate release of biochemical pollutant, it is crucial to characterize the source location and releasing time promptly and accurately. Compared with the forward pollutant dispersion process based on known source terms and air flow fields within built environments, source identification is backward process. And due to the discrete distribution of limited sensor data and the ill-posed matrix in solving process, the inverse solution of the source term is usually nonexistent [7–11]. However, the regularization method [12] can deal with the ill-posed matrix and stabilize the solution in inversion, making the source term can be mathematically approximated [13–15].

At present, there have been several original studies about the inverse modeling of source identification in the field of building environment. The inversion methods introduced in their works can be mathematically divided into three types: the forward matching method, the backward solving method and the adjoint probabilistic method [16–18].

The forward matching method runs numerous forward simulations to trial all possible sources and searches for the source term that matches the monitored concentration best. Sohn et al. [19,20] integrated the concentration measurements from multiple sensors by Bayesian statistics and calculated the optimum estimation of source information

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Nomenclature

A_i	cross-sectional area of duct i
C_0	concentration of the source released by the TSI 3079, mg/m^3
C_i	contaminant concentration of duct i
C_j^*	contaminant concentration leaving the duct junction j
C_{mk}	aerosols concentration at measuring point k, mg/m^3
$\hat{\boldsymbol{C}}_{\boldsymbol{sk}}^*$	measured concentration vector for sensor nodes
d_i	downstream junctions of duct i
g_τ^*	unconditional backward time PDF
$g_{\hat{C}_{sk}^*}$	normal PDF that describes the random measurement error of sensors
$g_{\tau\|\hat{C}_{sk}^*}$	conditional backward time PDF
G_τ^*	joint backward time PDF for all of the sensor nodes
H	unit of the adjoint state
K	attenuation or reaction coefficient
M_p	total released mass of the contaminant
N	number of duct junctions
PDF	probability density function
t	time
t_f	end time for contaminant transport within the ventilation system
R_s	resident concentration
u_i	upstream junctions of duct i
u_i	air velocity of duct i
V_j	air volumetric rate for the branch at duct junction j
x_i	contaminant dispersion distance along the duct i
x_{sk}	the location for the sensor node k
β	consistent parameter
$\delta(\cdot)$	Dirac delta function for a unit of the adjoint state
ε_x	longitudinal eddy diffusivity
λ	consistent parameter
σ^2	variance of the concentration measurement error
σ_c	standard deviations of calculation errors
τ	backward time
τ_{sk}	backward time at which the concentration is detected at sensor node k
φ_i	adjoint state of the concentration for duct i
φ_j^*	adjoint state of the concentration at the junction j
$\sum_{i\in d_i=j} Q_i$	sum of the air volumetric rate at the downstream end of duct i
$\sum_{i+1\in u_{i+1}=j} Q_{i+1}$	sum of the air volumetric rate at the upstream end of duct $i+1$

by converting the concentration match degree into source probability. The result showed that the estimate method matched the source term well but depended on amount and quality of sensor data and sensor network design. A similar approach was introduced for the optimal design of sensor systems [21–25]. Since the source estimate process regarded the sensor data as model inputs, it was feasible to identify the optimal sensor network and the source term as a whole [20,26]. Cai et al. [26,27] presented an analytical model for rapid identifying releasing locations and emission rates of multiple indoor sources using single or limited number of ideal sensors. Such model combined linear programming model with analytical form of indoor contaminant dispersion to cover a large number of possible releasing scenarios. However, since the pollutant releasing in a building is a random process, storing all possible releasing scenarios in advance to find out the global optimum is sometimes unaffordable in practice [28,29]. Other forward matching methods such as the Markov chain Monte Carlo (MCMC) method, the multi-robot active olfaction method and the artificial neural network (ANN) were investigated to improve identification precision and to reduce computation time [30–33].

The backward solving method for source characterization in a built environment mainly contains the quasi-reversibility (QR) method, the Lagrangian-reversibility (LR) method and the Tikhonov regularization Bayesian method. The QR method coupled with inverse computational fluid dynamics (CFD) modeling was firstly proposed by Zhang and Chen [34] in 2007 to identify a gaseous pollutant source in an enclosed cabin. The numerical stability was improved by their creatively replacing of the second order diffusive term with a fourth order stabilization term in governing equations. Zhang et al. [35] then presented the LR method to locate airborne particulate sources. Such approach tracked the motion of individual particulate in a Lagrangian reference frame with known initial conditions. In the latest progress of backward solving method, Zhang et al. [29] developed an inverse CFD model based on Tikhonov regularization and least-squares optimization to quantify the releasing intensity of a continuously released gaseous contaminant source. Zhang et al. [36] identified the release location, the temporal releasing rate and the sensor alarming time by a united inverse method. To overcome the limitation that current inverse models can identify only single contaminant source, Zhang et al. [28] put forward an inverse method that can accurately determine the locations and intensities of multiple sources releasing same gaseous pollutant. The Tikhonov-based matrix inversion was implemented in this method to obtain the intensities of multiple candidate sources, and the source locations were determined by the Bayesian method.

The adjoint probabilistic method to calculate the backward probabilities of pollutant source location and releasing time was derived first by Neupauer [37–41] and used in groundwater field. Subsequently, the researchers in indoor environmental field introduced the probabilistic method to trace indoor pollutant sources. The pseudo-reversibility (PR) method, which shares similar solving process with the probabilistic method, was proposed by Zhang and Chen [42] and used for identifying sources with single sensor. Soon afterwards, Liu and Zhai [43] coupled the probabilistic algorithm with the multi-zone model and successfully located an instantaneous pollutant source in a multi-zonal office building with known source releasing time. In addition, Liu and Zhai [44,45] derived adjoint equations for CFD and utilized it to predict source location probability within a two-dimensional office space and a three-dimensional aircraft cabin. They then extended the probabilistic method to locate a continuously released source, but the total release mass of the contaminant was needed in advance [46]. The location or travel time probabilities of all potential sources are obtained by calculating the adjoint equation set by one time. The source with the highest location or travel time probabilities denotes the true source [47]. In the newest study, Wang et al. [48] focused on characterizing the airborne pollutant source location in dynamic airflow by solving the time-term-discretization-based adjoint equations.

In real scenarios, the release of indoor airborne contaminants is a complicated process [49,50]. Pollutants can be released anywhere and anytime, which means that they can contaminate the indoor air through many possible airflow channels [51]. In 2011, WikiLeaks revealed a confidential document that terrorists attempted to put cyanide into ventilation systems of public buildings in America. Some researchers [3,52,53] also realized that air duct systems of buildings may serve as an ideal target for bioterrorism. In public buildings with central air-conditioning systems, there are both slow and fast channels for pollutants propagation, which defines two typical scenarios for source characterization. If sources occurred in room spaces, where pollutants diffuse slowly and complexly in the low-speed air velocity field, the inverse CFD modeling [29,34] can locate the sources precisely by solving the governing transport equation for each time step. But it is time-consuming. In case sources occurred in the ventilation system, where the air velocity is high, and pollutants spread fast, the inverse CFD modeling might not be suitable for such scenario because of the time