RECONSTRUCTION OF UNCERTAIN PARAMETERS IN A MULTIZONE MODEL BASED ON CONTAM AND BAYESIAN INFERENCE

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Abstract. The prediction of contaminant distribution in multi-zone environment is critical for ensuring indoor personnel health and making an optimistic ventilation strategy. However, the input of uncertainty parameters (flow coefficients, flow exponents, etc.) has a significant impact on the predicted pollutant concentrations. In this study, we proposed a reconstruction method to achieve parameter estimation for the multi-zone model. MATLAB codes was programmed to call CONTAM engine to accomplish pollutant transport simulation in a multi-zone scaled building model. Then a Bayesian inference algorithm compiled in MATLAB codes was applied to determine the unknown parameters iteratively. Finally, multi-zone scaled experiments with different forms of pollutant sources were employed to validate the reconstruction method. The results showed that the predicted concentrations with the reconstructed parameters agreed well with the measured data in the constant source (CS) experiment. While, for the dynamic source (DS) experiment, the predicted concentrations had some discrepancies with the measured data.

1 Introduction

People spend almost 90% of their time indoors according to statistics [1], and high indoor air quality (IAQ) is of significance to improve human health and life quality. A study by ASHRAE showed that poor indoor air quality led to a series of respiratory illness, e.g., allergy, asthma symptoms and sick building syndrome (SBS) [2]. Recently, the airborne transmission of new coronavirus disease (COVID-2019) has posed considerable threats to the public health globally [3]. Azimi et al. [4] developed a model to speculate the cases on the Diamond Princess Cruise Ship and indicated that the contribution of long-range modes to the infected cases aboard the ship was 35%. Thus, the accurate prediction of airflow and airborne pathogen transmission in multi-zone environments is critical to ensure the health and well-beings for occupants.

Various numerical methods have been proposed for the prediction of indoor contaminant transmission. Most of the above pollutant transport models required input of some immeasurable or uncertain parameters, which could significantly impact the accuracy of simulation. The reconstruction of simulation parameters has been applied in various fields. Sun et al. [5] proposed a method to reconstruct wind field based on Proper Orthogonal Decomposition (POD), Computational Fluid Dynamics (CFD) and sensor measurement data. Vernay et al. [6] developed a data-interpretation framework of multiple CFD simulations combined with measurement data to improve the prediction accuracy of wind field. Brastein et al. [7] used the Profile Likelihood method to diagnose parameter identifiability for grey-box thermal behaviour models. The previous studies demonstrated that the reconstruction of uncertainty parameters could improve the simulation accuracy of the numerical models. However, to our knowledge, few parameter reconstruction methods have been proposed for multi-zone models based on measurement data.

In this study, we proposed a reconstruction method to estimate the uncertainty parameters for the prediction of contaminant transmission in multi-zone environments. The Gibbs sampling algorithm was compiled in MATLAB to call CONTAM engine and determine the uncertainty parameters iteratively. To verify the availability of the proposed reconstruction method, experimental measurement of the uncertainty parameters was carried out.

2 Theoretical methods

The proposed reconstruction method was used to ascertain the uncertain input parameters which are hard to measure for the multi-zone models, e.g., the flow coefficients and the flow exponents. The method consists of following three steps: 1) calling the CONTAM engine in MATLAB, 2) Model selection, 3) Bayesian inference of the uncertainty parameters.

2.1 Calling the CONTAM engine in MATLAB

CONTAM is a widely used multi-zone simulation program for indoor air quality and ventilation analysis. CONTAM version 3.2 was used to simulate the airflow information and pollutant concentrations in this study.
Calling the CONTAM engine in MATLAB was available to directly retrieve the information of airflow and contaminant concentrations without opening the CONTAM interface. The parameter input, result output and data storage for CONTAM were also accomplished through MATLAB. Fig. 1 shows the framework of calling the CONTAM engine in MATLAB. Before calling the CONTAM engine, an existing multi-zone project file (*.prj) including basic project information was loaded. Then a new project file was built with the modification of input parameters in MATLAB. Then, the MATLAB codes executed the CONTAM engine to simulate the new project file iteratively. After the iterative calculation, the output data were stored and exported as the simulation results.

Fig. 1 Framework of calling the CONTAM engine in MATLAB.

2.2 Model selection

In CONTAM, law airflow path model has two general forms and eight deformed forms. In this study, we choose the general form of the power law model in volumetric flow form. The equation can be expressed as \( Q = c \cdot \Delta p^g \), where \( c \) is the flow coefficient, and \( g \) is the flow exponent. These two parameters were reconstructed in this study.

2.3 Bayesian inference of uncertainty parameters

The Bayesian inference has been successfully employed to accomplish the reconstruction of the uncertainty parameters, e.g., source information, Schmidt number and flow parameters in atmospheric environment [8-10]. In this study, the uncertainty parameters of airflow path were reconstructed via Markov Chain Monte Carlo (MCMC) sampling algorithm combined with Bayesian inference, as shown in Fig. 2.

The Bayesian inference can interpret the uncertainty parameter estimation problem through a probabilistic way, which provides the posterior possibility distribution based on prior known information. The posterior probability distributions of uncertainty parameters can be expressed as:

\[
p(X|\mu) = \frac{p(\mu|X)p(X)}{p(\mu)} \propto p(\mu|X) \tag{1}
\]

where \( p(X|\mu) \) is the posterior probability, which quantify the probability of the parameter set \( X \) based on the measured concentration \( \mu \). \( p(\mu|X) \) is the likelihood function, which is the probability of the concentration \( \mu \) given the parameter set \( X \) and usually can be constructed based on the Gaussian normal distribution [11]. \( p(X) \) is the prior probability of the uncertainty parameter set \( X \). In this study, the estimation of an uncertainty parameter set \( X \) in the CONTAM was achieved via using the pollutant concentrations \( \mu \) measured by sensors. The uncertainty parameters of airflow path included flow coefficients \( (c_i, i=1...N) \) and flow exponents \( (n_i, i=1...N) \), where \( i \) is the index for different opening degrees of doors in the multi-zone model. It was presumed that the flow coefficients could be equal to any values within a uniform possible distribution from 0.001 to 0.01 through preliminary experiments, while the flow exponents were also uniformly distributed in the range of 0.5 to 1. Therefore, \( p(X) \) was constant and the \( p(\mu) \) was a normalized constant to compute the posterior distribution.

The algorithm was divided into two step estimations. The preliminary estimation was used to get a rough range for the target parameter, while the refine estimation achieved a more accurate estimation in the rough range. Both the two estimations were based on 1,0000 total samples, and the first 1,500 samples were discarded due to no stable convergence. The remaining 8,500 samples were selected to build the posterior probability distribution of \( p(X|\mu) \).

3 Experimental methods

3.1 Experimental cases

Fig. 3 Multi-zone scaled model: (a) Configuration of the multi-zone model, (b) Full view of the multi-zone model. (Zhuang et al. [12])

Detailed information about the multi-zone scaled model including the air tightness performance can refer to Zhuang et al. [12]. In this study, we conducted the constant source (CS) releasing experiment to reconstruct the uncertainty parameters. Then the dynamics source (DS) releasing experiment was conducted to verify the simulation accuracy with the reconstructed parameters.
The CS experiment released mixed CO$_2$ (0.797% CO$_2$ balanced with N$_2$) in the zone 21 at a rate of 10 L/min until the monitored concentration was stable. In the DS experiment, the releasing source was also located in the zone 21. The source release rate was controlled through a periodic function with a cycle of 100 s. Mixed CO$_2$ (4.99% CO$_2$ balanced with N$_2$) was first released for 50 s at 10 L/min and then stopped for 50 s, continuing for a total of three cycles. In the experiment, we considered the influence of background CO$_2$ and measured its concentration.

In the CONTAM, the boundary conditions for fans and doors were set as the constant volume flow fan model and power law airflow path model, respectively. For the airflow path model, the flow coefficients and flow exponents for the quarter and half opening were correspondingly set as variables of $c_1$, $n_1$, $c_2$, $n_2$ in the reconstruction algorithm. The two concentration values at 140 s and 250 s in the CS experiment were selected as the reconstruction targets.

4 Results and discussion

4.1 Reconstruction of the parameters

Fig. 4 shows the posterior probability distributions of the reconstructed parameters, and the grey shaded areas are the refined subintervals of the last 1500 iteration steps. The refined subintervals of $c_1$, $n_1$, $c_2$, $n_2$ were [0.002518,0.003677], [0.541267,0.597521], [0.003502,0.005699], and [0.56123, 0.639188], respectively. The values of $c_1$, $n_1$, $c_2$, $n_2$ with the highest posterior probability are 0.003239, 0.5661, 0.004947 and 0.6015, respectively.

![Fig. 4 Posterior probability distributions and reconstructed results of the airflow path parameters $c_1$, $n_1$, $c_2$, $n_2$](image)

From Fig. 5, the predicted values based on reconstructed parameters agree well with the sensor monitored values, except for the deviations from $t=5$ s to $t=80$ s. The discrepancies could be attributed to the sensor delay and well mixing hypothesis of the multi-zone model. However, the simulated concentrations based on the measured parameters deviated far from the sensor monitored values. This may be because the uneven distribution of airflow velocity at the cross-section of the door opening and small pressure difference would result in larger fitting errors. In general, the simulated pollutant concentrations with the reconstructed parameters had good accuracy under the CS condition.

As shown in Fig. 6, the simulated concentrations based on the reconstructed parameters and measured parameters were compared with the sensor monitored values in DS experiment. From Fig. 6(a), the predicted concentration with reconstructed parameters is slightly lower than the Sensor A monitored value. While, the predicted concentration with measured parameters is severely overestimated. From Fig. 6(b), the predicted concentration with measured parameters agrees with the Sensor B monitored value better, but the predicted concentration with reconstructed parameters is slightly underestimated. Sensor B was fixed at the exit of the scaled model, and its monitored value was more susceptible to the perturbation from time-varying airflow. In the DS experiment condition, periodically released pollutant sources would cause some certain perturbation to the airflow in the multi-zone model.
5. Conclusions

In this study, a reconstruction method based on the Bayesian inference was proposed to determine the airflow path uncertainty parameters in CONTAM. And the predicted pollutant concentrations with measured uncertain parameters were compared with the concentrations with reconstructed uncertain parameters through the multi-zone scaled experiment. The results showed that the flow coefficient of quarter opening was the most important influencing factor for the pollutant concentration simulation. The simulated pollutant concentrations with the reconstructed parameters agreed well with the measured data in the CS experiment and had some discrepancies in the DS experiment. And the reconstruction-based method performed better than the experiment-based method in determining the uncertainty parameters. The method provided a novel approach for the prediction of contaminant concentration distributions in multi-zone environments.

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