Journal of Hazardous Materials 349 (2018) 68–78

Contents lists available at ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Bayesian source term estimation of atmospheric releases in urban areas using LES approach

Fei Xue[a], Hideki Kikumoto[b], Xiaofeng Li[a,c,*], Ryozo Ooka[b]

[a] Department of Building Science, School of Architecture, Tsinghua University, Beijing, China
[b] Institute of Industrial Science, University of Tokyo, Tokyo, Japan
[c] Beijing Key Lab of Indoor Air Quality Evaluation and Control, Beijing 100084, China

ARTICLE INFO

Keywords:
Source term estimation
Bayesian inference
Large-eddy simulation
Reynolds-averaged Navier-Stokes equations
Urban dispersion

ABSTRACT

The estimation of source information from limited measurements of a sensor network is a challenging inverse problem, which can be viewed as an assimilation process of the observed concentration data and the predicted concentration data. When dealing with releases in built-up areas, the predicted data are generally obtained by the Reynolds-averaged Navier-Stokes (RANS) equations, which yields building-resolving results; however, RANS-based models are outperformed by large-eddy simulation (LES) in the predictions of both airflow and dispersion. Therefore, it is important to explore the possibility of improving the estimation of the source parameters by using the LES approach. In this paper, a novel source term estimation method is proposed based on LES approach using Bayesian inference. The source-receptor relationship is obtained by solving the adjoint equations constructed using the time-averaged flow field simulated by the LES approach based on the gradient diffusion hypothesis. A wind tunnel experiment with a constant point source downwind of a single building model is used to evaluate the performance of the proposed method, which is compared with that of the existing method using a RANS model. The results show that the proposed method reduces the errors of source location and releasing strength by 77% and 28%, respectively.

1. Introduction

Source term estimation (STE) of the releases of hazardous materials into the atmosphere refers to the identification of the source information, e.g., strength and location, based on limited and noisy concentration data. An identification technique can provide the crucial information for emergency preparedness efforts, in case of either accidental or malicious releases, to take appropriate responses to track the unknown sources and to reduce further damage. STE can be considered as an assimilation process of the observed concentration data measured by a sensor network and the predicted concentration data obtained by an atmospheric transport and dispersion model. This process is an ill-posed inverse problem associated with the forward dispersion problem that is characterized by its non-uniqueness and unstable solutions [1].

To solve the inverse problem, various algorithms have been proposed [1,2], among which the optimization method and Bayesian inference are two dominant approaches in STE problem [3,4]. Different STE methods may yield different estimations, a preliminary comparative investigation has been performed by Platt and DeRiggi [5]. The optimization approach aims to minimize a cost function that measures the discrepancy between the observed and predicted concentrations. For different problems of STE, different forms of cost functions have been used, from the simplest form of the classical least squares [6,7], to the more robust ones using regularization [8,9] or renormalization [10,11]. This optimization approach yields point estimates of source parameters without rigorous quantification of their uncertainties.

In contrast, the Bayesian inference, as used in this research, views the STE problems in the probabilistic aspect: every parameter is considered as a random variable with a certain probability distribution instead of a constant. Consequently, the final estimations are also in the form of probability distributions, providing point estimates with associated uncertainty estimations. However, the direct calculation of the joint probability distribution of a set of parameters is a difficult task. Xue et al. [12] decoupled the joint probability distribution into two separate distributions and calculated them deterministically. More generally, stochastic sampling algorithms, e.g., the Markov chain Monte Carlo (MCMC) methods, have been widely used to solve different Bayesian STE problems: single static sources [13–15], multiple static sources [16–18] or mobile sources [19] on flat terrain [20,21] or in built-up areas [22,23].

---

[*] Corresponding author at: Department of Building Science, School of Architecture, Tsinghua University, Beijing, China.
E-mail address: xfli@mail.tsinghua.edu.cn (X. Li).

https://doi.org/10.1016/j.jhazmat.2018.01.050
Received 17 June 2017; Received in revised form 23 January 2018; Accepted 24 January 2018

The STE problem, as mentioned earlier, is an ill-posed inverse problem in the sense that poor model predictions usually lead to large errors in estimations; thus, the accuracy of the transport and dispersion model is critical. On flat terrains, Gaussian dispersion models are generally preferred due to their simplicity and rapid calculations [20,24,25]. However, with respect to urban dispersion, these models fail to characterize the complex turbulent flow caused by buildings and other geometries, thus computational fluid dynamics (CFD) approaches are widely used to reproduce the realistic flow and pollutant dispersion in built-up areas [10,22,26].

In the vast majority of STE investigations performed by using the CFD approach, the Reynolds-averaged Navier-Stokes (RANS) equations modeling is employed to simulate turbulent flow and turbulent passive scalar transport; however, RANS-based models are outperformed by large-eddy simulation (LES) in the predictions of both airflow and scalar transport, especially in the wake region of buildings, where large-scale velocity fluctuations, such as vortex shedding, are dominant [27]. Although better model predictions generally provide better estimations, there are few LES applications in STE investigations [28,29]. Therefore, the objective of this study is to further explore the possibility of using LES approach to improve the estimation of the source parameters.

A direct application of LES approach as RANS models is impractical. In STE, the CFD approaches are used to obtain the airflow and the source-receptor relationship, which is the sensitivity of the concentration at each sensor to a given source location. In general, the airflow is obtained by "forward" simulation and the source-receptor relationship is calculated by solving the adjoint advection-diffusion equations (see Section 3.2) [30], in a form of "backward" simulation. When using RANS models, after the airflow is obtained, the adjoint equations can be easily constructed by reversing the averaged airflow [17,22]. With respect to LES approach, it is still easy to run the forward simulation; however, to run the backward time-stepping simulation using the LES approach, the transient airflow fields of all time steps need to be stored, which requires impractically large size of space considering the small time steps and high grid resolution in the LES approach.

A novel method is proposed in this paper to make LES approach a practical simulation tool in STE using Bayesian inference. To reduce the storage requirement, the adjoint advection-diffusion equations are constructed in a RANS-like structure using the time-averaged flow field simulated by the LES approach based on the gradient diffusion hypothesis. A wind tunnel experiment with a constant point tracer source in the wake region of a single building model is used to evaluate the performance of the proposed method by comparing it with the performance of the existing method using a RANS model.

In Section 2, the STE problem and its solution are formulated using the Bayesian inference. Section 3 describes the calculation method of the source-receptor relationship using the LES approach and the adjoint equations. In Section 4, the experimental and simulation settings of the demonstration case are presented. The results and discussion are provided in Section 5. First, the predicted airflow and concentration fields are compared with the experimental data; then, we present the estimation results obtained by using the proposed method and compare its performance to that of an existing method. The conclusions are described in Section 6.

2. Bayesian inference

Bayesian inference coupled with CFD approach was first used to identify urban releases by Keats et al. [22], who provided the fundamentals of the method, as the flowchart shown in Fig. 1. Following their work, in this paper, the LES approach is employed to improve the accuracy of the estimation results. The proposed method is demonstrated using a basic case of a single point source with a constant releasing strength; however, by combining this with other Bayesian STE methods, it can be generalized to address multiple point sources [16–18] and variable releasing strengths [20,31].

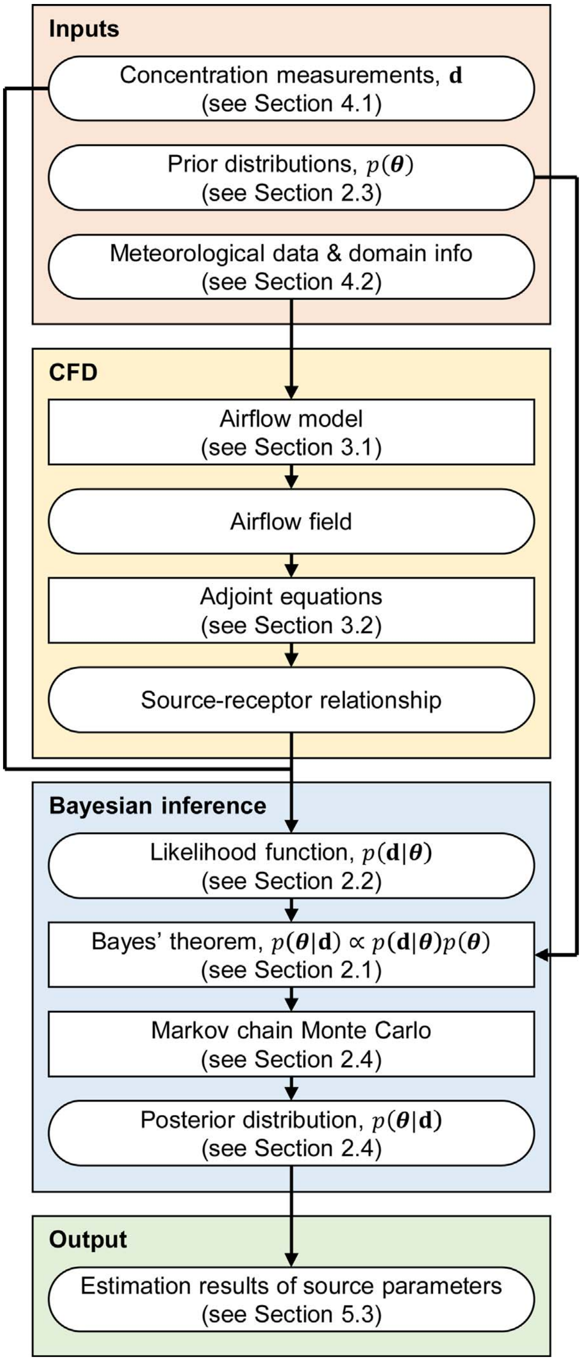

Fig. 1. The source term estimation method using Bayesian inference coupled with CFD.

2.1. Problem formulation

In the Bayesian inference, the STE problems are addressed by using a probabilistic logic. Let $\boldsymbol{\theta}$ denote the set of unknown source parameters, and $\mathbf{d}$ denote the measurement data of a network of sensors. The estimation results can be obtained by calculating the posterior probability based on the Bayes' theorem:

$$p(\theta|\mathbf{d}) = \frac{p(\mathbf{d}|\theta)p(\theta)}{p(\mathbf{d})} \propto p(\mathbf{d}|\theta)p(\theta) \tag{1}$$

where $p(\mathbf{d}|\theta)$ is the likelihood function, $p(\theta)$ is the prior probability which represents all the a priori knowledge about $\boldsymbol{\theta}$, $p(\mathbf{d})$ is the marginal probability which acts as a normalizing factor and does not affect the relative probabilities, and $p(\theta|\mathbf{d})$ is the posterior probability which