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Source estimation methods for atmospheric dispersion

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Abstract

Both forward and backward transport modeling methods are being developed for characterization of sources in atmospheric releases of toxic agents. Forward modeling methods, which describe the atmospheric transport from sources to receptors, use forward-running transport and dispersion models or computational fluid dynamics models which are run many times, and the resulting dispersion field is compared to observations from multiple sensors. Forward modeling methods include Bayesian updating and inference schemes using stochastic Monte Carlo or Markov Chain Monte Carlo sampling techniques. Backward or inverse modeling methods use only one model run in the reverse direction from the receptors to estimate the upwind sources. Inverse modeling methods include adjoint and tangent linear models, Kalman filters, and variational data assimilation, among others.

This survey paper discusses these source estimation methods and lists the key references. The need for assessing uncertainties in the characterization of sources using atmospheric transport and dispersion models is emphasized.
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Keywords: Atmospheric transport and dispersion models; Bayesian updating and inference methods; Inverse modeling; Adjoint and tangent linear models; Kalman filtering; Variational data assimilation

1. Introduction

Atmospheric transport and dispersion (ATD) models are routinely used to assess the impact of emission sources on air quality for varying meteorological conditions. These models are also used at nuclear and chemical plants for emergency response and impact assessments for hazardous substances accidentally released into the atmosphere.

Trajectory models are widely used to establish source–receptor relationships for estimation of atmospheric concentrations or for interpretation of measurements. While forward trajectories describe the paths of the released particles from the source to receptors, backward trajectories from receptors attempt to approximate the particles' paths to the source. Trajectories are less accurate when particles travel in the atmospheric boundary layer because of the effects of turbulence, or when they encounter convective up- and down-drafts (e.g., Stohl et al., 2002).

Both forward and backward modeling methods are being developed to estimate the release rate and duration of chemical, biological, and radiological (CBR) agents in terrorism-related events. Given the meteorology and concentrations observed at several detectors, these methods characterize the source type, and estimate the source strength and location. This survey paper discusses the leading source estimation methods, and lists the relevant key references. These methods are broadly classified as

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forward modeling methods, which model the atmospheric transport from sources to receptors, and backward modeling methods which use one model run in the reverse direction from the receptors to estimate the upwind sources. The importance of assessing various uncertainties in the estimation of sources using ATD models is emphasized.

2. Forward modeling methods

Forward modeling source estimation methods utilize forward-running dispersion models or computational fluid dynamics algorithms. These models are typically run many times over the domain of interest. The predicted concentrations in each run are compared to the observed concentrations and the source conditions are adjusted, using a suitable methodology, until an acceptable level of agreement is obtained. Bayesian updating and inference methods, using stochastic Monte Carlo (MC) or Markov Chain Monte Carlo (MCMC) sampling, are widely used for this adjustment.

2.1. Bayesian updating and inference methods

The basic assumptions and a general derivation of the Bayesian Monte Carlo (BMC) method are given by Patwardhan and Small (1992). BMC approach assumes that the sampled results in a traditional MC analysis correspond to the *prior* distributions for the model parameters and output. Only those MC replications with outputs "consistent" with the observations, defined as falling within an acceptable range of differences, are kept for subsequent analysis. The BMC method refines uncertainty estimates by using a continuous likelihood function to weight the results of individual MC simulations. This likelihood function quantifies the probability of obtaining a specified consistency after accounting for errors in the measurements.

BMC methods have been applied for estimating uncertainties in modeling potential sea-level rise due to climate change (Patwardhan and Small, 1992), modeling water quality (Dilks et al., 1992), assessing environmental health risk (Brand and Small, 1995), and air quality modeling (Bergin and Milford, 2000). Bayesian methodology provides a framework for decoupling the time-consuming ATD model simulations from the interpretation of measurements, while incorporating uncertainty analysis in all steps. For emergency response applications, this permits the ATD model predictions and uncertainty estimates to be computed before a release event, and the sensor data to be interpreted in real time during the event.

Sohn et al. (2002) described the application of the BMC method to rapidly locate and characterize pollutant releases in buildings. Before the release occurs, a suitable ATD model, incorporating probability distributions characterizing the uncertainties in model input parameters, is utilized to build a library of simulations of many hypothetical (but likely) air flow and pollutant dispersion scenarios by applying MC sampling to the uncertain input parameter distributions. During a release event, the algorithm uses a structured probabilistic method, referred to as *BMC updating* or *Bayesian updating*. In this method, application of Bayes' rule (e.g., Gelman et al., 2004, p. 7) allows one to quickly estimate the level of agreement between the data streaming in from the sensors and each realization in the library of simulations, in order to assess the likelihood this realization describes the event in progress. By comparing the relative agreement (indicated by the likelihood estimate), one can determine the best-fitting suite of model inputs and the associated uncertainty. The probability of each model simulation before and after assessing the agreement is referred to as the *prior* and *posterior* probability, respectively.

The posterior probability of the kth MC simulation yielding prediction Y_k given the sensor measurement O, denoted by $p(Y_k|O)$, is calculated from Bayes' rule as

$$p(Y_k|O) = [p(Y_k)\,L(O|Y_k)] \Big/ \sum_{i=1}^{N} p(Y_i)\,L(O|Y_i), \tag{1}$$

where $p(Y_k)$ is the prior probability of the kth MC simulation, $L(O|Y_k)$ is the likelihood of measurement O given model prediction Y_k, and N is the total number of MC simulations. The prior uncertainty of each model input parameter (e.g., source location) and model prediction (e.g., agent concentration in air) is updated according to how well predictions using the prior uncertainty distribution agree with the sensor data. The likelihood function $L(O|Y_k)$ quantifies the error structure of the data. For measurements with uncorrelated normally distributed errors, L is Gaussian:

$$L(O|Y_k) = (\sqrt{(2\pi)}\sigma_e)^{-1} \exp\{-0.5[(O - Y_k)/\sigma_e]^2\}, \tag{2}$$