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Impact of meteorological inflow uncertainty on tracer transport and source estimation in urban atmospheres

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HIGHLIGHTS

- Meteorological inflow uncertainty is quantified for an urban-scale model.
- Uncertainty methods are applied to the Joint Urban tracer release experiment.
- Inflow uncertainty can explain simulated and observed tracer differences.
- Inflow uncertainty effects the ability to invert for an unknown source location.

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ABSTRACT

A computational Bayesian inverse technique is used to quantify the effects of meteorological inflow uncertainty on tracer transport and source estimation in a complex urban environment. We estimate a probability distribution of meteorological inflow by comparing wind observations to Monte Carlo simulations from the Aeolus model. Aeolus is a computational fluid dynamics model that simulates atmospheric and tracer flow around buildings and structures at meter-scale resolution. Uncertainty in the inflow is propagated through forward and backward Lagrangian dispersion calculations to determine the impact on tracer transport and the ability to estimate the release location of an unknown source. Our uncertainty methods are compared against measurements from an intensive observation period during the Joint Urban 2003 tracer release experiment conducted in Oklahoma City. The best estimate of the inflow at 50 m above ground for the selected period has a wind speed and direction of $4.6^{+2.0}_{-2.5}$ m s^{-1} and 158.0^{+16}_{-23}, where the uncertainty is a 95% confidence range. The wind speed values prescribed in previous studies differ from our best estimate by two or more standard deviations. Inflow probabilities are also used to weight backward dispersion plumes and produce a spatial map of likely tracer release locations. For the Oklahoma City case, this map pinpoints the location of the known release to within 20 m. By evaluating the dispersion patterns associated with other likely release locations, we further show that inflow uncertainty can explain the differences between simulated and measured tracer concentrations.

1. Introduction

Urban areas currently support more than half of the world's population and are projected to house two out of every three people by the year 2050 (United Nations, 2014). Accidental or intentional releases of hazardous materials into urban atmospheres can therefore affect the health and well-being of a large number of people and cause serious economic damage. The release of methyl isocyanate in the densely populated city of Bhopal, India in 1984, for example, killed 4 thousand to 20 thousand people, injured half a million, and is regarded as one of the world's worst industrial accidents (Havens et al., 2012). More recently, a train derailment accident in Graniteville, South Carolina in 2005 released 40 tons of chlorine into the environment, which led to 9 fatalities, hundreds of injuries, widespread evacuations, and 30 to 40 million U.S. dollars in economic damage (Buckley et al., 2012).

Atmospheric dispersion models are important tools for assessing and predicting the spread of hazardous materials and contaminants in urban regions, but applying these models in these regions presents a number of challenges. Urban areas have complex features, such as buildings and structures, street canyons, traffic-induced turbulence, and urban heat island effects that affect the

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atmospheric flow and are difficult to represent explicitly in dispersion models (e.g., Britter and Hanna, 2003; Di Sabatino et al., 2003; Kusaka and Kimura, 2004; Hajra et al., 2011). Although computational fluid dynamics (CFD) models can directly simulate the flow and turbulence in the vicinity of buildings, they are computationally prohibitive for most urban applications because meter-scale resolution is needed to capture certain building effects over kilometer-sized urban domains (e.g., Pullen et al., 2005).

Two approximation methods are commonly used to simulate atmospheric flow in urban regions. Large eddy simulations (LES), which are relatively expensive to run, compute turbulent motions directly at larger scales and use parameterizations to estimate the effects of small, subgrid-scale eddies. Models based on the Reynolds-averaged Navier Stokes (RANS) equations, in contrast, are computationally efficient because they compute the flow using suitable averages for both the mean and turbulent motions. For a particular urban dispersion application, the flow generated using LES and RANS will differ, and these differences represent a form of model uncertainty. Likewise, different models make different assumptions about how to represent or parameterize other processes, for example traffic flow, which leads to additional model uncertainty.

In addition to the atmospheric flow, dispersion models require other inputs to realistically simulate the spread of hazardous materials in urban environments. For a specific event, knowledge about the location, timing, magnitude, and chemical properties of the source material are needed. Information about the large scale meteorological inflow conditions at the boundary of an urban area (e.g., the prevailing wind speed and wind direction) also has to be specified to drive the flow within the area. In emergency response situations, predictive simulations can provide advance warning of the transport and extent of plumes and help minimize damage, yet there is often incomplete or limited knowledge about the meteorological inflow and source characteristics. This incompleteness leads to uncertainty that can affect the emergency response (e.g., see Konda et al., 2010). Under these circumstances, there is not usually enough time to collect additional data to constrain all of the inputs, so the existing information needs to be combined with the models and expert judgment to arrive at reasonable estimates of the values of the inputs.

Inverse modeling provides a mathematical framework for determining optimal values of the inputs to an atmospheric dispersion model. Given measurements that can be compared to model outputs, inverse methods solve for the model inputs by minimizing the differences between the simulation outputs and measurements (e.g., see Tarantola, 2004). In addition to the optimal values, some inverse methods (e.g., those based on Bayes' rule) can also provide information about the uncertainty in the model inputs and outputs. For dispersion events, measurements of meteorological variables and atmospheric concentrations in nearby and affected regions are valuable sources of data for constraining the model inputs. This data may constrain the inflow conditions, source characteristics, and potentially other model inputs and parameters.

A variety of inverse methods have been developed for tracer transport and dispersion problems (e.g., Prinn, 2000; Enting, 2000; Giering, 2000; Todling, 2000; Tipping, 2002; Zheng and Chen, 2011). The methods are often used to estimate the magnitude and location of sources (e.g., Chow et al., 2008; Zheng and Chen, 2010), but they can also be used to constrain other inputs. In this study, we use an inverse method to quantify uncertainty in the meteorological inflow at the boundary of an urban region. This uncertainty is propagated through a dispersion model to determine the impact on tracer transport and the ability to estimate the location of a source. The inversion of the inflow is performed and compared against measurements from the Joint Urban 2003 tracer release experiment in Oklahoma City (Allwine and Leach, 2007). Simulations of the urban flow and tracer dispersion are conducted with the Aeolus model (Gowardhan, 2014) using realistic building geometry for Oklahoma City. Aeolus is a building-aware, computationally-efficient CFD and Lagrangian particle dispersion system that simulates atmospheric flow and turbulence in complex, urban areas using LES or RANS.

The effects of meteorological inflow uncertainty on dispersion in urban areas using building-aware models was recently addressed by Rodriguez et al. (2013). The authors quantified the sensitivity of dispersion to inflow direction by developing a plume overlap metric and applying the metric to a variety of urban and building configurations. They found that the sensitivity of the plume depends upon the complexity of the urban features around the source location, with high sensitivity occurring, for example, when the source is surrounded by large buildings and obstacles. Although the main scientific objectives of our report are similar to those in Rodriguez et al. (2013), we use a data-driven Bayesian approach to estimate the uncertainty. As demonstrated below, our approach is arguably better suited for propagating the inflow uncertainty to environmental impacts of hazardous releases.

Our work also follows from related studies that developed and applied Bayesian inversion methods to reconstruct source characteristics and evaluate sensor network designs for source inversions (Chow et al., 2008; Johannesson et al., 2006; Lundquist et al., 2005; Lucas et al., 2015). One important distinction from these studies is our use of backward trajectories (e.g., Stohl, 1998), instead of Bayesian inversion, to infer the source location. Because back trajectories can be computed very quickly, the techniques presented in this manuscript may be used to account for uncertainty in time-critical, emergency response situations. As described in the following sections, the CFD simulations are the most expensive component of our overall analysis and can be pre-computed and stored in a database for a specified urban region (e.g., Oklahoma City). The inversion and uncertainty analysis can be conducted by querying the database, which is a relatively efficient operation. The strategy of using pre-computed CFD simulations for rapid assessments of dispersion in urban areas has been shown to be effective (Boris et al., 2010).

2. Methods

2.1. Overview

The inverse problem for inflow is motivated from a computational black-box perspective by describing the general models and model inputs and outputs used to simulate the transport and dispersion of trace gases in urban atmospheres. Although the discussion is centered around non-reactive trace gases, it can be extended to reactive gases by using models that incorporate processes and parameters for other sources and sinks, such as chemical production and loss, and wet and dry deposition.

The concentration of a trace gas in an urban atmosphere can be expressed, most generally, by

$$\mathbf{y} = F(\vartheta, \mathbf{x}), \tag{1}$$

where F represents a complex computational model that simulates transport and dispersion. As written, this model takes two types of inputs, represented by ϑ and $\mathbf{x}$, and provides an output, $\mathbf{y}$, which corresponds to a vector of trace gas concentrations at different points in space and/or time. The input ϑ is related to the source term, and captures the magnitude, location, and duration of trace gas emissions. The symbol $\mathbf{x}$ represents the atmospheric fluid motion in the urban domain, which occurs through advection,