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Bayesian estimation of airborne fugitive emissions using a Gaussian plume model

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HIGHLIGHTS

- Novel formulation of source inversion as a Bayesian inverse problem.
- Three different models for modelling of prior knowledge.
- Industrial case study of fugitive lead emissions in Trail, BC, Canada.
- Uncertainty propagation study and impact assessment.

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ABSTRACT

A new method is proposed for estimating the rate of fugitive emissions of particulate matter from multiple time-dependent sources via measurements of deposition and concentration. We cast this source inversion problem within the Bayesian framework, and use a forward model based on a Gaussian plume solution. We present three alternate models for constructing the prior distribution on the emission rates as functions of time. Next, we present an industrial case study in which our framework is applied to estimate the rate of fugitive emissions of lead particulates from a smelter in Trail, British Columbia, Canada. The Bayesian framework not only provides an approximate solution to the inverse problem, but also quantifies the uncertainty in the solution. Using this information we perform an uncertainty propagation study in order to assess the impact of the estimated sources on the area surrounding the industrial site.

1. Introduction

Dispersion of airborne pollutants emitted from anthropogenic sources and their effect on the surrounding environment have been a growing source of concern over the past several decades. Both primary polluters and government monitoring agencies dedicate significant resources to tracking and controlling the release of particulate emissions from industrial operations. Atmospheric dispersion modelling, which is the study of mathematical models and numerical algorithms for simulating processes involved in dispersion of pollutants from a known source, is a vital tool for monitoring of existing industrial operations as well as assessing the potential risk and impact of future operations. Many dispersion models address the situation where a pollutant source has already been identified and the source emission rate is known approximately, and many industry standard software packages such as AERMOD (Cimorelli et al., 2005) and CALPUFF (Scire et al., 2000) are already available to solve this problem.

In many practical settings the main problem of interest is not to determine the impact of known sources but rather to solve the

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source identification problem, which refers to determining the emission properties and possibly also locations for a collection of unknown sources. Inverse source identification is particularly prominent in the study of fugitive sources, which are particulate or gaseous emissions that derive from leaks or other unintended releases from building windows or vents, entrainment from debris piles, or operations of trucks and loading equipment. In these situations, it is usually not possible to obtain direct measurements of the fugitive source emissions by installing sensors; this is in contrast with emissions from stacks and exhaust vents where such measurements are routine. Nevertheless, it is often still possible to take *indirect measurements* of fugitive emissions, for example by measuring concentration of a pollutant at a remote location some distance from the source. In this case, the challenge is to estimate the rate of emissions based on indirect measurements, which can be posted as an inverse problem (Isakov, 1990; Kabanikhin, 2011).

Atmospheric dispersion modelling is a well-developed area of research, and for a comprehensive overview we refer the reader to the work of Zlatev (Zlatev and Dimov, 2006) or Dimov et al. (2004). The use of partial differential equation (PDE) models based on the advection-diffusion equation for modelling short-range transport of pollutants dates back to the work of Taylor (1915), Roberts (1924) and Sutton (1932). In simple scenarios involving constant emissions, steady-state transport, point or line sources, or flat topography, it is possible to derive approximate analytical solutions to the governing equations (Arya, 1999; Okamoto et al., 2001; Park and Baik, 2008; Seinfeld and Pandis, 1998). These analytical solutions, referred to collectively as Gaussian plume solutions, have the distinct advantage of being simple and relatively cheap to compute, and consequently form the basis of many standard monitoring tools (including AERMOD and CALPUFF). For more realistic situations where one is interested in incorporating effects such as topographical variations or more complex time-varying wind patterns, the only recourse is to solve the governing PDEs directly, typically using approaches based on finite volume (Hosseini, 2013; Hosseini and Stockie, 2016), finite difference (Lange, 1978; Nikmo et al., 1999) or finite element schemes (Albani et al., 2015).

In comparison with the atmospheric dispersion models just described for solving the forward problem, the source inversion problem has attracted less attention in the literature. The monograph by Vogel (2002) is a notable reference that lays out the general mathematical theory for inverse problems as well as common solution approaches. More specific to the context of atmospheric transport, the work of Rao (2007) and Enting (2002) provides an overview of methods for solving the source inversion problem. Recently, Cantelli et al. (2015) used a genetic algorithm in order to identify multiple sources of pollution at once. Sanfélix et al. (2015) also studied the inversion of fugitive sources by coupling a finite volume solver with an optimization algorithm. Another powerful and promising approach to the solution of inverse problems is based on Bayesian methods, whose mathematical formulation is well-described by Kaipio and Somersalo (2005) and Stuart (2010). Although some attempts have been made to apply Bayesian methods in the context of atmospheric dispersion problems, their application is much less extensive than other approaches. Some examples include Huang et al. (2015) who employ a Bayesian method for identifying the location and emission rate for a single point source by incorporating a Gaussian puff solution, while Keats et al. (2007) use Bayesian inference to identify emissions in a more complex urban environment. In both cases, the authors use an adjoint approach to efficiently solve the advection-diffusion PDE and evaluate the likelihood function using a Markov Chain Monte Carlo algorithm. Senocak et al. (2008) and Wade and Senocak (2013) use Bayesian inference along with a Gaussian plume model in order to reconstruct multiple sources in an atmospheric contamination scenario.

In this paper, we aim to develop an accurate and efficient Bayesian approach for solving the inverse source identification problem. We aim to estimate fugitive particulate emissions from various areas of an industrial site based on measurements of contaminant concentration and particulate mass deposited at a distance from the suspected sources. We consider a scenario wherein material from fugitive sources is dispersed by the wind and then deposited on the ground due to a combination of diffusive transport and gravitational settling. Some sources may reasonably be approximated as constant in time, but we are particularly interested in the study of time-dependent sources arising for example from dust entrained during loading operations that are performed on a rotating shift schedule. In order to monitor emissions in such a scenario, various types of measurements are typically performed at fixed locations in the vicinity of the known or suspected sources. We are particularly interested in two classes of measurements, deriving from either total accumulated deposition of particles over a long time period (on the order of one month) or short-time averaged concentrations (taken over a period of one hour, which can be considered essentially instantaneous in comparison with long-term measurements). We utilize a Gaussian plume model for short-range dispersion of pollutants and incorporate this model within the Bayesian framework for solution of inverse problems. We split the industrial site into a number of areas that are suspected to contain the most important fugitive sources. The Bayesian framework provides a natural setting for estimating emission rates and also quantifying the uncertainty associated with the estimates. This study was motivated by a collaboration with Teck Resources Ltd., in which we studied particulate emissions from a lead-zinc smelter located in Trail, British Columbia, Canada (Hosseini, 2013; Lushi and Stockie, 2010).

In contrast with some other studies, we do not consider the problem of determining either the number or location of sources. Instead, we consider a given number of areas corresponding to suspected fugitive emission sources, and approximate each area source by a single point source located at the area centroid; however, we do allow the emission rate for each source to vary as a continuous function of time. We also incorporate multiple measurement types and develop a unified framework in which the forward model relates the entire measurement data set to the emission rates. The main challenge we encounter is in terms of the low quality of the measured data that derives from two main features: first, the most abundant measurements are from dust-fall jars, which measure only monthly accumulated deposition and so unfortunately provide no information about short-time variations in particulate emission; and second, although we do have access to a few real-time measurement devices, these sensors provide useful data only when the wind blows in the direction linking them to the sources of interest. The main advantage of our Bayesian framework is its ability to obtain a solution even when the measured data is of relatively low quality and the problem is severely underdetermined. Another benefit of our approach is that we obtain an estimate of the accompanying uncertainty in the solution. Finally, we stress that our framework can easily be extended to deal with a general class of atmospheric dispersion problems including applications such as seed or odour dispersal (Bunton et al., 2007; Levin et al., 2003), natural disasters such as volcanic eruptions (Turner and Hurst, 2001), and nuclear or chemical accidents (Miller and Hively, 1987).

The remainder of this article is organized as follows. In Section 2 we present the forward model which is based on a Gaussian plume solution. In Section 3 we develop the Bayesian framework for solving the inverse problem by considering three different instances of the inverse problem corresponding to different models