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An inverse Gaussian plume approach for estimating atmospheric pollutant emissions from multiple point sources

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ABSTRACT

A method is developed for estimating the emission rates of contaminants into the atmosphere from multiple point sources using measurements of particulate material deposited at ground level. The approach is based on a Gaussian plume type solution for the advection–diffusion equation with ground-level deposition and given emission sources. This solution to the forward problem is incorporated into an inverse algorithm for estimating the emission rates by means of a linear least squares approach. The results are validated using measured deposition and meteorological data from a large lead–zinc smelting operation in Trail, British Columbia. The algorithm is demonstrated to be robust and capable of generating reasonably accurate estimates of total contaminant emissions over the relatively short distances of interest in this study.

1. Introduction

Urban air quality is an issue of major concern owing to recent upward trends in population growth and urbanisation and industrialisation around the world. Consequently, there is an increasing need to understand the detailed dynamics governing emission and transport of particulate matter in the atmosphere. Turner (1979) mentions a multitude of possible sources of airborne particles, including those of anthropogenic origin such as industrial complexes and automobiles, as well as natural sources such as dust storms and volcanic eruptions. Recently, there has been a surge of interest in related problems for disaster planning and national security that involve transport of radionucleotides and biological or chemical agents (Settles, 2006).

The physics of particulate transport in the atmosphere are complex, in many cases involving multiple spatial scales (ranging from the particle scale to near-source and long-range effects), multi-physics (coupling mass transport, turbulence, chemistry and wet/dry deposition), and complex geometry (e.g., involving flow over topography or man-made structures). Models for these and other aspects of atmospheric dispersion have a long history dating back to the pioneering studies of turbulent diffusion by Richardson (1920) and Taylor (1922). The bulk of previous work has tackled the *forward problem*, by which we refer to the process of determining downwind contaminant concentrations given source emission rates and meteorological conditions. These forward models are usually based on a solution of the advection–diffusion equation that is obtained through either analytical or numerical means (or a combination of both). The most prevalent approach used in practice, and which is implemented in many industry-standard software packages, employs an approximate analytical solution for point-source emissions known as the "Gaussian plume solution." The one-dimensional plume solution for a single point source was originally derived by Sutton (Sutton, 1932) and has since been extended to higher dimensions, as well as being applied to a variety of other more general situations involving ground-level deposition (Ermak, 1977), multiple sources

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(Calder, 1977), height-dependent wind speed and diffusion coefficients (Liley, 1995; Lin and Hildemann, 1997), and line and area sources, to name just a few. We remark that while a majority of the applications considered to date have involved transport in the atmosphere, the Gaussian plume models just mentioned may also be used to solve other advection–diffusion problems in such diverse areas as population growth (Condie and Bormans, 1997) or water flow in rivers (El Badia et al., 2005) and the subsurface (Kennedy et al., 2005).

Another related stream of research has focused on solving the corresponding *inverse problem*, whereby measurements of particulate concentrations or ground-level depositions are given and the aim is to determine information about the location or efflux rate of contaminant sources. Inverse methods based on Gaussian plume type solutions have been developed by a number of authors in this context including Jeong et al. (2005) and Hogan et al. (2005), while MacKay et al. (2006) developed an alternate solution approach using complex variable theory. Other researchers have applied a more direct computational approach by solving the nonlinear governing equations using methods based on Kalman filtering (Mulholland and Seinfeld, 1995), Lagrangian particles (Seibert and Frank, 2004), Bayesian techniques (Enting, 2002; Goyal et al., 2005), or by integrating the equations backward in time (Seibert and Frank, 2004; Bagtzoglou and Baun, 2005). Several related methods have been developed specifically for handling the added nonlinearities arising from atmospheric chemistry, typically using Newton type iterative methods (Brown, 1993), and sometimes combined with statistical techniques (Houweling et al., 1999). These direct numerical approaches can be very computationally intensive, especially for 3D problems, and so will typically require use of parallel computing resources. Regardless of the numerical method used, the inverse problem is often characterized as ill-conditioned in the sense that small changes in parameters can lead to very large changes in emission estimates; these issues are discussed in much more detail by Enting (2002), Beychok (1999), Atmadja and Bagtzoglou (2001) and Ababou et al. (in press).

The subject of this paper is a lead–zinc smelting operation located in Trail, British Columbia, Canada. We are concerned with the transport of several contaminant species from multiple point sources on the site, and our aim is to develop an inverse algorithm that will determine emission rates based on the Gaussian plume solution of Ermak (1977). The emission sources are not in the usual chimney- or stack-like configuration, and so do not lend themselves easily to direct point-source measurements. Therefore, we have instead made use of "indirect" deposition measurements at a number locations spread around the site. The novelty of this work stems from a combination of factors:

- We make use of real (noisy) meteorological and deposition data, in contrast with some other studies that use synthetic data (Hogan et al., 2005; MacKay et al., 2006).
- Deposition measurements are relatively small in number and represent time-averaged accumulations. This should be compared with some other methods that obtain very high accuracy by using very large numbers of sample points (Jeong et al. 2005). Another example is the work of Hogan et al. (2005), who proposed an iterative method based on the Gaussian plume solution (with constant wind and no deposition) and which exploits the fact that concentration measurements at four locations uniquely determine the location and strength of a single point source. This approach can be very effective when the input data are known very accurately, but it degrades when the data are noisy.
- The emission sources are at known locations, in comparison with some other studies that aim to determine both emission rates and locations (Mulholland and Seinfeld, 1995; Bagtzoglou and Baun, 2005; Brown, 1993).
- We incorporate additional linear constraints on emission rates that are derived from chemical processes within the smelting operation.
- Deposition measurements are taken near ground level and at short distances from the source, which allows us to avoid errors inherent in long-range dispersion estimation and thereby minimize the ill-conditioning of the inverse problem.

Taken together, these factors allow us to develop a robust algorithm that is capable of estimating emission sources with a reasonable degree of accuracy. Other studies have been performed on emissions at the Trail site by Goodarzi et al. (see Goodarzi et al., 2002 and references therein), but they use a much simpler Gaussian plume solution with no deposition and constant wind velocity, as well as validating their results using long-range deposition measurements and different experimental techniques.

We begin in Section 2 by describing the problem under study and developing a detailed list of assumptions underlying the model. In Section 3 we provide details of the Ermak solution to the advection–diffusion equation, and also incorporate multiple sources and a time-varying wind velocity. Section 4 focuses on the inverse problem, deriving the linear equality and inequality constraints and describing the linear least squares solution algorithm. A series of numerical simulations are performed in Section 5, including a study of the sensitivity of the model to changes in parameters and noise in the data. Finally, we conclude with recommendations about the suitability of applying our model to actual environment reporting scenarios, and make suggestions on possible future work on extending our approach in order to improve accuracy and permit application to a wider range of atmospheric dispersion scenarios.

2. Problem description and simplifying assumptions

The motivation for this work was a study of emissions from a number of contaminant sources at a large lead–zinc smelter located in Trail, British Columbia, Canada and operated by Teck Cominco Limited. Our primary aim was to improve the accuracy of airborne emission estimates (especially for zinc) that the Company is required to report annually to Environment Canada's *National Pollutant Release Inventory (NPRI)* (NPRI, 2009). There are some direct measurements of zinc and other contaminants available for certain stack-like emission sources on the smelter site; however, this paper is concerned with other sources that have a configuration very different from the usual stack or chimney (e.g., cooling towers) for which direct measurements are difficult to obtain.

There are four sources on the Trail site that emit zinc (in the form of zinc sulphate, $ZnSO_4$) and these are indicated on the aerial photo in Fig. 1 by the symbol Ss, where $s = 1, 2, 3, 4$. To assist in estimating the level of zinc emissions, the Company performed a series of ground-level measurements of zinc as well as a number of other contaminant species (strontium, sulphur, etc.). The measurements were taken over the two-year span 2001–2002 and consist of one-month accumulations of particulates within dustfall jars or "receptors," which are located at nine separate locations R$r, r = 1, 2, \ldots, 9$ (also indicated in Fig. 1).

Meteorological data is available for the same monthly periods in terms of wind speed and direction averaged over 10-min intervals. The smelter is located in the Columbia River valley which tends to funnel the winds on the site in a specific direction; since the river is located just below the aerial photo in Fig. 1 and runs roughly