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Automated source term and wind parameter estimation for atmospheric transport and dispersion applications

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HIGHLIGHTS

- Methodology for rapid source parameter estimation of hazardous airborne materials releases.
- Computationally efficient algorithm to determine release source parameters and low-level winds.
- Tested in relevant environments and deployed in DoD operational emergency response tools.

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ABSTRACT

Accurate simulations of the atmospheric transport and dispersion (AT&D) of hazardous airborne materials rely heavily on the source term parameters necessary to characterize the initial release and meteorological conditions that drive the downwind dispersion. In many cases the source parameters are not known and consequently based on rudimentary assumptions. This is particularly true of accidental releases and the intentional releases associated with terrorist incidents. When available, meteorological observations are often not representative of the conditions at the location of the release and the use of these non-representative meteorological conditions can result in significant errors in the hazard assessments downwind of the sensors, even when the other source parameters are accurately characterized. Here, we describe a computationally efficient methodology to characterize both the release source parameters and the low-level winds (eg. winds near the surface) required to produce a refined downwind hazard. This methodology, known as the Variational Iterative Refinement Source Term Estimation (STE) Algorithm (VIRSA), consists of a combination of modeling systems. These systems include a back-trajectory based source inversion method, a forward Gaussian puff dispersion model, a variational refinement algorithm that uses both a simple forward AT&D model that is a surrogate for the more complex Gaussian puff model and a formal adjoint of this surrogate model. The back-trajectory based method is used to calculate a "first guess" source estimate based on the available observations of the airborne contaminant plume and atmospheric conditions. The variational refinement algorithm is then used to iteratively refine the first guess STE parameters and meteorological variables. The algorithm has been evaluated across a wide range of scenarios of varying complexity. It has been shown to improve the source parameters for location by several hundred percent (normalized by the distance from source to the closest sampler), and improve mass estimates by several orders of magnitude. Furthermore, it also has the ability to operate in scenarios with inconsistencies between the wind and airborne contaminant sensor observations and adjust the wind to provide a better match between the hazard prediction and the observations.

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1. Introduction

Representative source parameters, in conjunction with atmospheric observations, are key factors in accurately modeling the atmospheric transport and dispersion (AT&D) of hazardous airborne materials released into the atmosphere. In many cases the material source and atmospheric parameters are unknown and consequently based on rudimentary assumptions that lead to errors in the subsequent AT&D simulations. The 2011 incident at the Fukushima Dai-ichi Nuclear Power Plant (FD-NPP) is a recent example where Source Term Estimation (STE) techniques were required to support a disaster response. This disaster had a number of complicating factors: a long duration continuous release of radiation at an unknown rate, multiple intermittent explosive releases of radioactive materials, unknown plume rise, changes in the atmospheric conditions, and disabled observation systems. Collectively these factors limited the ability of emergency response managers to collect the observations necessary to characterize the release and local meteorological conditions. The airborne release source term in conjunction with the local/regional weather conditions were key factors in determining the people who were exposed to radiation, the extent to which they were exposed, and the implications associated with that exposure (Pullen et al., 2013; Bieringer et al., 2013).

The focus of this work is to meet United States (US) Department of Defense (DoD) and Department of Homeland Security (DHS) emergency response modeling needs for situations like the incident at the FD-NPP. The algorithm described in this manuscript is designed to be run on a laptop computer and provide a set of source parameters for a near range release (e.g. within 30–40 km downwind from the release location) from seconds to several minutes after the observations are provided to the algorithm. The technique is suitable for any atmospheric AT&D application where concentration observations and meteorological data are available and one or more of the release source parameters are unknown and an answer is required as soon as possible following the collection of the observations. It can, however, also be used in conjunction with other approaches in more detailed forensic analyses where a STE is required. While the method has been implemented into two US DoD emergency response modeling systems that use the Second Order Closure Integrated PUFF (SCIPUFF) model, we believe the overall approach could relatively easily be adapted for use by other agencies/countries and their respective AT&D models.

In the following section of this manuscript we provide a brief survey of STE methods and how the method described here compares to them. In Section 3 we describe the algorithm and its component models. The system has undergone validation against a variety of data sets and includes data from both field trials and observations generated in a synthetic test environment. In Section 4 we provide some representative performance results from these validation efforts for both the algorithm that has been implemented into the two operational Department of Defense (DoD) emergency response systems, and an enhanced version of the algorithm that is capable of estimating both the source parameters and key meteorological variables. We end with a summary discussion and concluding remarks on the direction of future work in this area.

2. Source term estimation (STE) methods

Sensor data fusion (SDF) and data assimilation are techniques by which observations can be incorporated into a description of an environment using a model that constrains the problem using physical properties and time evolution (Courtier et al., 1994). Here, time varying observations of airborne hazardous materials are fused with available meteorological observations to characterize the release source parameters for these materials. These source parameters are then used to produce a refined hazard assessment or dispersion pattern that best matches the observations. Applying STE methods to real-world scenarios is a challenging technical problem that is complicated by a number of factors. One common factor occurs when the meteorological measurements are not available near the release location. This can lead to inconsistencies between the material and meteorological observations. Releases that involve buoyancy related factors increase the complexity of making the mass estimate due to the relationships between heat flux of the buoyant plume and mass flux in the release. Another complicating factor is associated with scenarios where little is known about the source and there are multiple dimensions in the STE search space. Because there are different combinations of locations, winds, and release times can produce similar concentration observations this introduction of additional search space dimensions makes the STE problem mathematically ill posed.

Backward trajectory or trajectory inversion techniques have been extensively used to address the atmospheric dispersion STE problem (Stohl, 1998; Escudero et al., 2006; Jaffe et al., 1999; Hannan et al., 2000; Flesch et al., 2005; Draxler et al., 2014). Although these techniques are capable of providing reasonable information on source parameters, they have a number critical limitations. First, they assume that the meteorological information are accurate and therefore do not work well in situations where this may not be the case. The simplest backward trajectory methods identify the intersection of relevant variables along the backward trajectory and do not consider how closely a forward model solution matches the observations. More complex backward trajectory approaches involve inverse plume modeling and/or entity backtracking of larger elements that do not ignore diffusion. In these cases, the inverse of the plume model can be loosely considered an adjoint and the solution does seek to match the observations through the dispersion model (Sykes et al., 2008; Annunzio et al., 2012; Draxler et al., 2014). The Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model developed by the National Oceanic and Atmospheric Administration's (NOAA) Air Resources Laboratory (ARL) as well as the inverse version of the Second-order Closure Integrated PUFF (SCIPUFF) model are examples of tools that have STE capabilities that use this approach. Another category of approaches commonly used for STE problems involves the use of evolutionary algorithms. Evolutionary STE algorithms are those that typically follow a set of steps to iteratively evolve a population of one or more trial solutions to identify optimal source parameters. Simulated annealing, Monte Carlo Markov Chain, Bayesian, and Genetic Algorithm methodologies are examples that fall into this category. Thomson et al. (2007), Delle Monache et al. (2008), Shuford et al. (2008), and Brown and Robins (2010) have demonstrated that these approaches can be effective for STE problems using combinations of Monte Carlo and Bayesian methodologies. Similarly, Allen et al. (2006, 2007), Haupt (2005), Haupt et al. (2006, 2007), Long et al. (2010), Cervone and Franeze (2011), Rodriguez et al. (2011), and Schmehl et al. (2012) have shown that Genetic Algorithm approaches can also be used for this application. While evolutionary algorithms provide an effective mechanism for conducting a comprehensive search for optimal CB STE in multidimensional problem, these approaches can be computationally expensive. Furthermore, this computational burden increases significantly as one increases the number observation locations, times, or the dimensionality of the search problem. Given the current computational capabilities of a laptop computer, these methods are typically are not able to provide the rapid response solutions (e.g. within minutes) that are required to characterize the