#### SOURCE INVERSION FOR GROUND-LEVEL LINE SOURCE RELEASES IN STEADY-STATE CONDITIONS

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#### 1. Introduction

The goal of source inversion is the calculation of unknown source parameters from information obtained by a network of gas or particle detectors and meteorological sensors. That is, from a spatial and temporal distribution of concentration and wind measurements source inversion is used to identify the unknown source location, the release amount, perhaps the duration and time of the release, and in some instances the number of sources as well. Source inversion has been used for determining where airborne industrial contaminants originate and could be used by first responders in the case of accidental releases of hazardous materials or for homeland security needs if chemical, biological or radiological agents were deliberately released into the air. Development of robust, accurate, and fast algorithms is important since it could provide critical situational awareness during an event, reduce the population's exposure to dangerous airborne contaminants, lead to better evacuation route planning, and help with the assessment of the magnitude of the clean-up problem.

As part of a national biological agent detection program, the Bio-agent Event Reconstruction Tool (BERT) is used to estimate the magnitude and extent of an airborne biological release based on measurements from wind sensors and biological agent sensors distributed around a city (Brown et al., 2007; Linger et al., 2008). The BERT is used to find potential release areas and eliminate others, and if possible to put upper and lower limits on the amount of material that could have been released. The tool can then be used to predict the potential downwind hazard areas, to compute the total number of persons at risk, and

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to locate hospitals, school, police stations, fire stations and other infrastructure that might be impacted by the release.

The basic components of the BERT system are a diagnostic wind solver, a source inversion model, a segmented Gaussian plume model, a population exposure assessment tool, and a graphical user interface. The tool is built within the ESRI ArcGIS mapping environment so that the user can display wind conditions, sensor measurements and model output on top of topography, street maps, population and other geospatial data of interest. A dedicated server downloads hourly wind measurements for different cities from AIRNOW, MESOWEST and other city-specific servers. The diagnostic wind solver reads in these data and produces a mass consistent interpolated wind field which is afterwards used by the source inversion code. The method used for source inversion, however, only works for point source releases. In this paper, we describe a line source inversion model that is being developed for inclusion into the BERT so that a wider range of problems can be addressed. Preliminary testing of the inversion model using artificial data will be shown as well.

# 2. Background

During the last decade, a large number of research papers in the area of source inversion have been published that describe many different approaches. Most of the source inversion work published-to-date applies to point source releases. The forward dispersion models used range from fast Gaussian plume and puff codes that enable rapid calculations of concentrations and dosages to computational fluid dynamics (CFD) codes that provide more detailed and precise calculations but at the same time are expensive with respect to time and computer resources. Optimization methods like simulated annealing and genetic algorithms have often been used to more rapidly find optimal solutions. Thompson et al. (2007) used a simulated annealing optimization algorithm in combination with a Gaussian plume model to estimate source location and strength in a desert area in order to help find new oil and gas reserves. They also tested the model's performance for different cost functions as well as its sensitivity to randomly introduced noise and offsets to the concentration data. Allen and Haupt (2007) and Allen et al. (2007) used another stochastic optimization approach called genetic algorithms to estimate locations and strengths of multiple sources. The model was successfully applied for estimation of pollution emissions from multiple industrial facilities in urban areas.

One of the popular approaches for source inversion and estimating the probability distributions of source parameter values has been Bayesian inference in combination with Markov Chain Monte Carlo (MCMC), e.g., Keats et al. (2007), Chow et al. (2006), Yee (2007), Senocak et al. (2007). The probability distribution is obtained by running a dispersion model with a series of guesses for the source location and source strength and based on agreement or disagreement with the sensor measurements the new source parameters are either accepted or rejected after comparison with the results from the previous set of source parameters. The advantage of this approach when compared to the previously mentioned optimization methods is that it provides a probability distribution for source parameters instead of giving a single solution.

Pudykiewicz (1998) used the solution of the adjoint tracer transport equation to estimate the source parameters and evaluated the model for use in monitoring of nuclear testing. Yee (2008) developed a system for source inversion when the number of sources is unknown using the reversible-jump MCMC algorithm originally introduced by Green (1995) in the context of a Bayesian model determination problem.

Due to the fast turn-around required for the BERT mission, our team developed a fastrunning source inversion model based on the collector footprint idea. The so-called collector footprint method (Brown et al., 2007; Zajic and Brown, 2008) is fast because the number of plume calculations required to perform is equal to the number of biological agent detectors. In this approach, the analytical concentration equation solution is inverted and instead of solving for a concentration field based on a point source of strength Q, one solves for the Q field based on the sensor concentration. Contours of Q – or upwind collector footprints – are computed for each sensor using a reversed wind field, including those that did not register detections. Potential point source locations and possible release amounts are determined by overlapping contour intervals from hit sensors, and regions are excluded by using the upwind footprints of the null collectors.

# 3. Description of the Line Source Inversion Model

As mentioned earlier, the current source inversion tool in BERT only works for point source releases. Although the collector footprint approach might be adaptable to deal with line sources, it is not Using forward modeling clear if it is possible. approaches with an optimization routine is also possible, but fraught with difficulties due to the unbounded nature of the problem (i.e., many different line source solutions can be hypothesized for a given network of concentration measurements and a given wind field). To make the approach tenable, we make four very simplifying assumptions: 1) the line source is located at ground level; 2) the line source release must be aligned with the road network; 3) the source strength is not allowed to vary over the length of the line source; and 4) the meteorological conditions do not change over the duration of the release. Although these approximations guarantee that we will not find all possible solutions, they are pragmatic choices that will allow us to find a sub-set of likely potential solutions in a reasonable amount of time.

The goal of our work, presented here, is to develop the system for performing line source inversion where the sources coincide with a road network within a given city. Information on the road network is obtained from the Census Bureau's TIGER/Line database which contains the name of the road, the coordinates of starting and ending points of road sections, as well as the speed limit. The source inversion tool reads the road network data in and creates a network of possible line sources where the length of line segments is prescribed by the user. Each line source segments is made up of equidistant point sources where the distance between point sources is defined by the user. The downwind dosage (or concentration) from the line source is obtained by summing up the dosages due to each point source belonging to the line source. As expected, the line source is better approximated with a higher density of points (i.e., a smaller distance between points).

The model reads in wind speed and wind direction information from available sensors and then calculates the wind field using the Barnes Objective Mapping scheme to interpolate nonuniformly spaced wind data. This wind field is then utilized by the segmented Gaussian plume model which then calculates the dosage at each sensor for each line source previously defined. The Gaussian segmented plume model treats dispersion with spatially-varying winds by approximating the plume trajectory as a series of line segments with a Gaussian plume description of the each segment. For each segment a virtual source position is estimated by projecting upwind from the start of the segment. The distance to the virtual position is calculated from the wind speed, cross-wind standard deviation, and vertical standard deviation of the plume concentrations from the end of the previous segment and the wind speed at the start of the new segment. The requirement is that the virtual distance must be chosen so that the centerline concentrations at the end of the previous segment are the same as those of the start of the current segment. Consequently, a virtual distance is chosen so that the product of the wind speed, horizontal standard deviation, and vertical standard deviation at the end of the previous segment is equal to product of those values at the start of the new segment.

The source inversion code performs plume calculations for each line segment created from the imported road network for a source strength of 1 g. For these preliminary tests, the line source length in the source inversion routine was fixed at 2 km in length. In normal practice, the line source length will be allowed to vary over a user-specified range of lengths. The source strength is then normalized by the ratio of the measured and calculated dosages at the sensor with the maximum measured dosage. After dosage values at all sensors are corrected using the same factor, the error of the model with respect to the measurements is estimated using a simple root mean square error defined as:

$$rms = \left(\sum_{i=1}^{n} \left(D_{measured} - D_{mod el}\right)^2\right)^{0.5}$$
(1)

where *n* is the number of sensors that were hit (D>0), while *D*'s are dosages obtained by measurements and plume dispersion calculations.

The non-hit sensors provide information on the plume behavior as well. Each sensor type has a non-zero detection threshold, or a minimum detectable limit. If a postulated line source results in a dosage above the detection threshold at any nonhit sensor, the line source is said to not be possible and is thrown out. In future versions of the code, the source strength Q will be reduced until the dosage is below the detection threshold and then the RMS error metric will be recalculated.

The approach presented here estimates source parameters quickly but it is important to mention that location of possible sources is limited by the road network and currently assumes a steady wind field. Also, the estimation of source strength depends on the ratio of the measured and calculated value at the sensor with the maximum measured value, so the accuracy of a particular sensor will play an important role in source strength estimation. The segmented Gaussian plume model has the advantage of being fast and able to account for spatially-varying winds, but it can be inaccurate, for example, in highly complex terrain, where wind direction varies significantly with height, and under calm wind conditions.

## 4. Testing of the Line Source Inversion Model

#### 4.1 Creation of synthetic collector measurements

As a preliminary step, we have tested the source inversion scheme by creating synthetic detector dosage measurements using the Quick Urban and Industrial Complex (QUIC) plume dispersion model. The QUIC dispersion model is a Lagrangian random-walk code (Williams et al., 2004) that more closely represents reality as compared to the segmented Gaussian plume model used in the source inversion process.

For simplicity, an array of dosage or timeintegrated concentration agent sensors was arbitrarily placed within the existing road network of the city of Miami, FL. The first scenario simulated by QUIC was of a 10 kg release over a line source 2 km in length. The wind profile was set to logarithmic with a wind speed of 3 m/s at 10 m agl, a constant wind direction of 225 degrees, and neutral atmospheric stability. The surface was assumed to be flat with no buildings. Figure 1 shows the locations of the sensors, the major roads in Miami, FL and the location of the line source used for this test Figure 2 shows the dosage field case. calculated using QUIC, with red stars indicating locations of two sensors that detected the release while the remaining sensors were not hit.

The second case was for a straight line source of 8 km in length close to the previously used road segment not coinciding with the road network segments. The amount released (10 kg) and wind conditions were the same as in the first scenario. In this case three sensors were hit, the same two as in the previous case plus the one at the southeast vertex of sensor array (see Fig. 5).

# 4.2 Evaluation Results

For the first case, the best 10 line sources (i.e., those with the smallest RMSE) are shown in Fig. 3. The ten best solutions are found near the actual release location and the release amount ranges from 0.66 to 11 kg (recall that the actual release amount was 10 kg). Table 1 gives the RMSE values and the estimated source strengths for the ten best results. Note that the actual release location, line source ID 2, was only 3<sup>rd</sup> best in terms of RMSE. Figure 4 shows a zoomed in view of the locations of the ten line sources along with their respective ID numbers. The 2<sup>nd</sup> best solution from Table 1 is next to line source ID 2 and since it is slightly closer to the hit sensors its source strength is lower and closer to the actual value. The solution with lowest error was line source ID 19 but its source strength is only 67% of the actual released amount which is expected since this source is much closer to the sensors that detected the agent.

The results for the second case are given in Table 2 and Fig. 5. The locations of the best results are very close to the actual line source and are placed between the source and hit sensors as expected. But analysis of estimated source strength and locations of each listed line source shows that line sources closer to the hit sensors did not always give lower values of source strength as in the previous case. This likely stems from the actual line source being 8 km in length, while the source inversion code fixed the length at 2 km. This peculiarity will be investigated further in future studies.

## 5. Conclusions

A line-source inversion scheme using a segmented Gaussian plume model and a diagnostic wind model was described. The line source inversion problem is ill-posed, i.e., it can have more than one solution. Hence, we made four simplifying assumptions: 1) the line source is located at ground level; 2) the line source release must be aligned with the road network; 3) the source strength is not allowed to vary over the length of the line source; and 4) the meteorological conditions do not change over the duration of the release.

The scheme was tested using synthetic sensor measurements created by the QUIC random-walk transport and dispersion model. For the first scenario the results were very encouraging, although we assumed that we already knew the length of the line source. Numerous line source solutions were found near the actual release location. However, the best solution based on RMSE is much further away from the actual release location as compared to other line source solutions with larger RMSE. This result is to be expected as the segmented Gaussian plume model used in the source inversion scheme describes transport and dispersion differently than the random-walk code used to create the synthetic measurements.

For the second case where we intentionally assumed the wrong line source length and placed the source outside the road network, the model also performed well in locating the line source but gave a broad range of values for the source strength.

Since in real world applications we will not have information on the actual line source length, a module that searches for the optimal line source length will be implemented into the code. Wind variability in time can significantly influence plume transport and dispersion and our plans include adding the capability to account for changing wind direction and wind speed. We will also investigate the performance of the system using different error measures and test the model's sensitivity to introduced sensor noise and bias.

## 6. References

Allen, C. T., and S. E. Haupt, 2007: Source characterization with a genetic algorithm-coupled dispersion-backward model incorporating SCIPUFF. *J. Appl. Meteor.* **41**, 465–479.

Allen, C. T., G. S. Young, and S. E. Haupt, 2007: Improving pollutant source characterization by better estimating wind direction with a genetic algorithm. *Atmos. Environ.*, **41**, 2283–2289.

Brown M. J., M. D. Williams, G. E. Streit, M. Nelson and S. Linger, 2007: An operational Event Reconstruction Tool: Source Inversion for Biological Agent Detectors. *7th Symp. on the Urban Environment, American Meteorological Society, San Diego, CA.* 

Chow, F. K., B. Kosovic, and S. T. Chan, 2006: Source inversion for contaminant plume dispersion in urban environments using buildingresolving simulations. 6th Symp. on the Urban Environment, American Meteorological Society, Atlanta, GA.

Green, P. J., 1995: Reversible-jump Markov chain Monte Carlo computation and Bayesian model determination. *Biometrika*, 82, 711–732.

Keats, A., E. Yee, and F. Lien, 2007: Bayesian inference for source determination with applications to a complex urban environment. *Atmos. Environ.*, **41**, 465–479.

Pardyjak, E.R. and M.J. Brown, 2002: Fast response modeling of a two building urban street canyon. *4th Symp. on the Urban Environment*, May 20-24, 2002, *American Meteorological Society, Norfolk, VA*.

Pudykiewicz J.A., 1998 : Application of adjoint tracer transport equations for evaluating source

parameters *Atmos. Environ.* Vol. 32, No. 17, pp. 3039-3050, 1998

R. (1990),"Bestimmung Röckle, der Stomungsverhaltnisse Bereich komplexer im Bebauungsstrukturen" Ph.D. thesis. Vom Fachbereich Mechanik, Technischen der Hochschule Darmstadt, Germany.

Senocak I., N. W. Hengartner, M. B. Short, and B. W. Daniel 2007: Stochastic event reconstruction of atmospheric contaminant dispersion. *7th Symp. on the Urban Environment, American Meteorological Society, San Diego, CA*.

Thomson, L. C., B. Hirst, G. Gibson, S. Gillespie, P. Jonathan, K. D. Skeldon, and M. J. Padgett, 2007: An improved algorithm for locating a gas source using inverse methods. *Atmos. Environ.*, **41**, 1128–1134.

Williams, M., M. Brown, B. Singh, & D. Boswell, 2004: QUIC-PLUME Theory Guide, LA-UR-04-0561, 22 pp.

Yee E. 2007: Bayesian probabilistic approach for inverse source determination from limited and noisy chemical or biological sensor concentration measurements. *Chemical and Biological Sensing VIII, edited by Augustus W. Fountain III. Proc. Of SPIE Vol.* 6554, 65540W.

Yee E. 2008: Inverse dispersion of an unknown number of contaminant sources, 88<sup>th</sup> AMS Annual Meeting, 15<sup>th</sup> Conf. Appl. Air Poll. Met., January 2008, New Orleans, LA.

Zajic D. and Brown M.J., 2008: Source inversion in cities using the collector footprint methodology, American Meteorological Society, *88<sup>th</sup> AMS Annual Meeting, 15<sup>th</sup> Conf. Appl. Air Poll. Met., January 2008, New Orleans, LA.* 



Figure 1. The major roads of Miami, FL with locations of sensors (red dots), wind direction (green arrow) and location of line source used for QUIC test simulation (open black circle).



Figure 2. The dosage field obtained using QUIC. The red stars denote the two sensors that were hit.



Figure 3. The green ellipse encloses the 10 line sources with lowest RMS error, i.e., the best solutions. The red ellipse indicates two sensors that were hit during QUIC runs.

Source ID	RMS error	Released mass [g]
19	5.16E-05	6658.66
29	5.8E-05	10784.99
2	6.64E-05	11110.74
20	7.36E-05	4644.8
200	7.42E-05	4261.94
21	8.72E-05	3389.62
3	9.43E-05	2700.82
22	9.59E-05	2387.56
89	9.66E-05	657.19
23	9.97E-05	1824.62

Table 1. The ten best solutions showing line source IDs, RMS errors and corresponding source strengths for first test run (see Figure 4 for locations of line sources).



Figure 4. Locations of the ten best-fit line sources listed in Table 1.

Source ID	RMS error	Released mass [g]
23	1.8E-05	5621.79
22	2.04E-05	7356.27
3	2.06E-05	8321.45
51	2.09E-05	3780.65
50	2.13E-05	3579.09
18	2.44E-05	1542.77
17	2.53E-05	30.54
21	4.09E-05	10443.7
20	8.21E-05	14311.01
19	0.000171	20515.86

Table 2. The ten best solutions showing line source IDs, RMS errors and corresponding source strengths for the second case.



Figure 5. Locations of the actual 8k long line source (red line) and the ten best-fit line sources as listed in Table 2 (green lines). The stars show sensors hit during the QUIC forward run.