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# Stochastic Reconstruction of Multiple Source Atmospheric Contaminant Dispersion Events

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## Abstract

Reconstruction of intentional or accidental release of contaminants into the atmosphere using concentration measurements from a sensor network constitutes an inverse problem. An added complexity arises when the contaminant is released from multiple sources. Determining the correct number of sources is critical because an incorrect estimation could mislead and delay response efforts. We present a Bayesian inference method coupled with a composite ranking system to reconstruct multiple source contaminant release events. Our approach uses a multi-source data-driven Gaussian plume model as the forward model to predict the concentrations at sensor locations. Bayesian inference with Markov chain Monte Carlo (MCMC) sampling is then used to infer model parameters within minutes on a conventional processor. The composite ranking system enables the estimation of the number of sources involved in a release event. The ranking formula allows plume model results to be evaluated based on a combination of error (scatter), bias, and correlation components. We use the 2007 FUSION Field Trial concentration data resulting from near-ground-level sources to test the multi-source event reconstruction tool (MERT). We demonstrate successful reconstructions of source parameters, as well as the number of sources involved in a release event with as many as three sources.

*Keywords:*

Event Reconstruction, Bayesian Inference, Source Term Estimation, Gaussian Plume Model

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## 1. Introduction

Environmental awareness plays an important role in public safety, health, and threat mitigation. The release of harmful contaminants into the atmosphere could come by intentional or accidental means, and a quick response is key to limiting possible hazard to the population. Researchers have proposed event reconstruction (ER), also called source-term estimation (STE), methods (Annunzio et al., 2012a; Chow et al., 2008; Keats et al., 2007; Senocak et al., 2008; Stohl et al., 1998) that use contaminant concentration data from a network of well-placed sensors to characterize a dispersion event in terms of its source location

9 and emission rate. STE methods have been studied for many applications including defense  
10 and air quality management (Watson and Chow, 2004).

11 Most ER models adopt an inverse problem methodology along with a forward model  
12 to predict the plume dispersion. In cases where contaminant dispersion takes place over  
13 flat terrain on a scale of several kilometers or less, Gaussian plume models have been an  
14 effective forward model in ER methods (Senocak et al., 2008; Allen et al., 2007). At the  
15 continental scale with variable meteorological conditions, Monache et al. (2008) used the  
16 Lagrangian Operational Dispersion Integrator (LODI) as the forward model in a stochastic  
17 reconstruction method to determine the location of a radioactive release in Algeciras, Spain.  
18 At the urban neighborhood scale, Keats et al. (2007) adopted a computational fluid dynamics  
19 (CFD) model to better capture the effects of complex buildings on contaminant dispersion.

20 Researchers have adopted different methodologies to formulate a STE problem. Both de-  
21 terministic and probabilistic algorithms have been proposed. By and large Bayesian inference  
22 methods form the basis for most of the probabilistic approaches. Johannesson et al. (2004)  
23 presented dynamic Bayesian models using both the well-established Markov chain Monte  
24 Carlo (MCMC) method and the sequential Monte Carlo for target tracking and atmospheric  
25 dispersion event reconstruction problems. Chow et al. (2008) extended the work presented in  
26 Johannesson et al. (2004) to neighborhood scale (building-resolved) atmospheric dispersion  
27 events using CFD models. Keats et al. (2007) combined a Bayesian inference method with  
28 an adjoint approach to reduce the computational time to reconstruct a release event in an  
29 urban environment using CFD based models. Senocak et al. (2008) developed a data-driven  
30 approach within a Bayesian inference framework whereby empirical turbulence diffusion pa-  
31 rameters of the Gaussian plume model are estimated as part of the inverse problem in ad-  
32 dition to characterizing the dispersion event. The practice led to substantial improvements  
33 over the empirically tuned Gaussian plume model.

34 Some researchers have favored a deterministic approach in which an optimization method  
35 is used to solve the inverse problem. Henze et al. (2009) discusses the use of adjoint models  
36 to inversely model  $PM_{2.5}$  (particles with diameter less than  $2.5\mu m$ ) emissions. Akcelik et al.  
37 (2005) describes an optimization method which uses a conjugate gradient method to solve  
38 systems of partial differential equations. This method takes advantage of parallel computing  
39 to improve speed and efficiency of the otherwise lengthy optimizations for single-source event  
40 reconstructions. Another optimization method, proposed by Annunzio et al. (2012b), uses  
41 a Genetic Algorithm (GA) to carry out the optimizations in order to determine the source  
42 location of a single source release.

43 A contaminant dispersion event can involve releases from multiple sources. The source  
44 type may vary (e.g., point, line, area, volume) as well as the source elevation (e.g., ground  
45 level, stack, elevated line from aircraft). The release may also be categorized by the manner in  
46 which it is released, such as instantaneous (puff), continuous, or time-varying. Based on the  
47 methods described in Annunzio et al. (2012b), Annunzio et al. (2012a) introduced the Multi-  
48 Entity Field Approximation (MEFA) method for cases involving one or more ground-level  
49 point sources. With regards to continuous release scenarios, MEFA uses available wind data,  
50 and constrains any multiple releases to fall within a hazard area predicted by calculating the

51 spread far downwind for a single-source plume approximation. MEFA then searches within  
52 this hazard area for the optimal source locations while incrementing the number of possible  
53 sources. A cost function is used in part to determine the number of sources involved in the  
54 dispersion event. Field data is used to show that the method is capable of providing good  
55 approximations for multi-source events.

56 Platt and DeRiggi (2012, 2010) analyzed the blind predictions from STE models provided  
57 by eight different research groups, as applied to the FUSION Field Trials of 2007 (FFT-07)  
58 dataset (Storwold Jr., 2007). The comparative investigation provided useful information as  
59 to how well existing STE models perform relative to other STE models under different release  
60 scenarios. Platt and Deriggi applied a linear regression analysis to determine the significant  
61 factors that affected the reconstruction results obtained from various models. The present  
62 Bayesian inference method (Senocak et al., 2008) with a single-source, continuous release  
63 capability was also a part of the investigation. A subset of the results has revealed the  
64 advantages of a Bayesian inference method over other inverse methods that used the same  
65 forward model (i.e. Gaussian plume model).

66 Reconstruction of a multi-source contaminant release event is more challenging than  
67 reconstruction of a single source event. Yee has shown remarkable success using Bayesian  
68 inference techniques to reconstruct multi-source events with the number of sources unknown  
69 a priori (Yee, 2008, 2012a,b). Yee incorporates the unknown number of sources into the  
70 Bayesian inference framework in a principled fashion, which results in a posterior probability  
71 density for the number of sources. In our approach, we propose an alternative method  
72 to source number quantification by extending the Bayesian inference method presented in  
73 Senocak et al. (2008) to reconstruct contaminant dispersion events from multiple sources  
74 and couple it with a model ranking system. We adopt a data-driven multi-source Gaussian  
75 plume model as the forward model in the Bayesian inference method, and suggest a separate  
76 ranking system to estimate the number of sources involved in a release event. We apply the  
77 combined method to FFT-07 trial cases with up to three sources.

## 78 2. Forward Model

79 We adopt a data-driven Gaussian plume model as the forward model, because it is a  
80 suitable model for short range releases, over flat terrain under steady wind conditions, such  
81 as the FFT-07 trials considered in the present study. It is also computationally inexpensive.  
82 Therefore it can be used rapidly in the sampling process within the Bayesian approach.  
83 We are able to achieve accurate reconstructions in under two minutes on a conventional  
84 workstation with an Intel E8400 3.0 GHZ processor. Speed is an important aspect of STE  
85 when the intended use is first-response. Sophisticated forward models should be preferred  
86 for contaminant dispersion problems where a Gaussian plume model might not be suitable.

87 Stockie (2011) presents a derivation of the Gaussian plume model with single and multiple  
88 contaminant sources. For a single source release, the Gaussian plume model can be written  
89 as follows:

$$C_m(x, y, z) = \frac{Q}{2\pi U \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \times \left\{ \exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right) \right\}, \quad (1)$$

90 where  $C_m$  is the concentration at location  $(x, y, z)$ ,  $Q$  is the rate of emission for the point  
 91 source,  $U$  is the average wind speed, and  $H$  is the height of the release. We set  $z$  to 2m, the  
 92 same height as the samplers used in the FFT-07 field experiments. In the FFT-07 trials, the  
 93 contaminant was released from a near-ground-level source, therefore  $H$  is also set to 2m.  $H$   
 94 can also be set as an unknown and estimated using the Bayesian inference method as was  
 95 shown in Senocak et al. (2008). Additionally, we combine  $\frac{Q}{U}$  into a single parameter. The  
 96 release rate,  $Q$  can then be estimated by calculating an average wind speed from local wind  
 97 measurements at sensor height over the duration of the experiment.

98 We use an open-country Pasquill D type stability (Hanna et al., 1982) to define turbulent  
 99 diffusion parameters  $\sigma_y$  and  $\sigma_z$  as follows:

$$\sigma_y = \zeta_y x (1 + 0.0001x)^{-0.5}, \sigma_z = \zeta_z x (1 + 0.0015x)^{-0.5} \quad (2)$$

100 where  $\sigma_y$  and  $\sigma_z$  are the standard deviations used in Equation 1 for the horizontal and  
 101 vertical plume directions normal to the streamwise plume direction. Here,  $x$  refers to the  
 102 distance along the streamwise plume direction. The parameters  $\zeta_y$  and  $\zeta_z$  are left as unknown  
 103 parameters to be estimated by the Bayesian method, making the forward model a data-driven  
 104 one. The practice results in significantly better estimates for the concentration field (Senocak  
 105 et al., 2008; Senocak, 2010). Data-driven forward modeling gives better predictions than the  
 106 baseline forward model when there are sufficient and reliable sensor data.

### 107 3. Bayesian Inference Method for Multi-Source Release Events

108 The Stochastic Event Reconstruction Tool (SERT) (Senocak et al., 2008) uses Bayesian  
 109 inference to estimate information (i.e., source location, release height, emission rate, wind  
 110 direction and speed) about the dispersion event. In this section, we present the Bayesian  
 111 inference framework in SERT and extend it to multiple source releases. The number of  
 112 sources involved in an event is then estimated separately using a ranking formula.

113 Generally speaking, the inverse problem can be formulated as follows:

$$\mathbf{m} \approx F^{-1}(\mathbf{d}), \quad (3)$$

114 where  $\mathbf{d}$  is a vector of observed concentration values and  $\mathbf{m}$  is a vector of forward model pa-  
 115 rameters to be estimated.  $F$  is the forward model, which is the Gaussian plume model in our  
 116 case. Given the observed data,  $\mathbf{d}$ , our goal is to estimate forward model parameters,  $\mathbf{m}$ . In  
 117 most Bayesian inference methods, Bayes' rule is simplified into the following proportionality:

$$P(\mathbf{m}|\mathbf{d}) \propto L(\mathbf{d}|\mathbf{m})P(\mathbf{m}), \quad (4)$$

118 where  $P(\mathbf{m}|\mathbf{d})$  refers to the posterior probability density of the forward model parameters,  
 119  $L(\mathbf{d}|\mathbf{m})$  is the likelihood function which calculates the likelihood of the observations given the  
 120 model parameters, and  $P(\mathbf{m})$  is the prior probability for the model parameters (Congdon,  
 121 2010).

122 Prior probabilities for model parameters are set based on certain expectations about each  
 123 of the model parameters. All model parameters except  $Q/U$  and  $\sigma^2$  are assigned proper  
 124 uniform prior distributions. The normalized emission rate  $Q/U$  is given a Jeffrey's prior as  
 125 follows:

$$p(Q/U) \propto \frac{1}{Q/U}. \quad (5)$$

126 To avoid division by zero we set a small minimum value for  $Q/U$ .  $Q/U$  is scaled using this  
 127 minimum value to ensure that the maximum prior value is unity.

128 There are sensors capable of detecting trace amounts of a material in the atmosphere.  
 129 But they have their limitations. Sensors can register a nominally zero value when, in fact,  
 130 local concentration level,  $d_i$ , can be non-zero and below the detection threshold of the sensor.  
 131 In such cases, we assign a probability to detecting a zero concentration level as follows:

$$d_i = \begin{cases} 0, & \text{with probability } \exp(-\alpha \cdot \hat{C}_i) \\ \xi_i, & \text{with probability } 1 - \exp(-\alpha \cdot \hat{C}_i) \end{cases} \quad (6)$$

132 where  $\xi_i$  is a concentration measured by a theoretically ideal sensor,  $d_i$  is the concentration  
 133 measured by an actual sensor, and  $\hat{C}_i$  is the concentration predicted by the model at the  
 134 sensor location. Given the model parameters,  $\xi_i$  has a lognormal distribution with the  
 135 following density:

$$p(\xi_i|\mathbf{m}) = \frac{1}{\sqrt{2\pi}\sigma\xi_i} \exp\left(-\frac{1}{2\sigma^2}(\ln \xi_i - \ln \hat{C}_i)^2\right), \quad (7)$$

136 When a sensor makes an observation at the sensor's detection threshold,  $C_{th}$ , we assume  
 137 that it does so with a probability of  $1/2$ . Based on this assumption and Equation 6,  $\alpha$  can  
 138 be computed in the following manner:

$$1 - \exp(-\alpha \cdot C_{th}) = \frac{1}{2} \rightarrow \alpha = \frac{1}{C_{th}} \ln(2). \quad (8)$$

139 Given Equation 6, the conditional likelihood function is written as follows:

$$L(d_i|\mathbf{m}) = \begin{cases} \exp(-\alpha \cdot \hat{C}_i), & \text{if } d_i = 0 \\ \frac{1 - \exp(-\alpha \cdot \hat{C}_i)}{\sqrt{2\pi}\sigma d_i} \exp\left(-\frac{1}{2\sigma^2}(\ln d_i - \ln \hat{C}_i)^2\right), & \text{if } d_i > 0 \end{cases}, \quad (9)$$

140 where  $\sigma^2$ , is the variance, which takes into account modeling and measurement errors cumu-  
 141 latively. We assume that the variance has an inverse gamma prior distribution with hyper

142 parameters  $\alpha = 1.0$  and  $\beta = 1000.0$ .

143 SERT's previous design focused on single source continuous releases. In this study, we  
 144 first modify the forward model to extend SERT to multiple source events. For a multi-  
 145 source plume of a non-reactive and non-buoyant contaminant, the concentration at any  
 146 point  $(x, y, z)$  is the sum of the contributions from each source (Stockie, 2011).

$$C_{total}(x, y, z) = \sum_{s=1}^n C(x'_s, y'_s; Q_s), \quad (10)$$

147 where  $n$  is the number of sources, and  $Q_s$  is the source emission rate. As in Stockie (2011),  
 148 the shifted coordinates,  $x'_s$  and  $y'_s$ , are defined as follows:

$$x'_s = x - X_s, y'_s = y - Y_s, \quad (11)$$

149 where,  $x$  and  $y$  are the Cartesian coordinates,  $X_s$  and  $Y_s$  are the coordinates of source  $s$ .  
 150 The origin is shifted to the source location,  $(X_s, Y_s)$ , and the positive x-direction extends in  
 151 the downwind direction.

152 Next, we introduce additional parameters required by the multi-source model into the  
 153 Bayesian inference framework. Hereinafter we will refer to the multi-source event reconstruc-  
 154 tion tool as MERT. For multiple source releases, we define a reference source, and all other  
 155 sources are defined relative to the reference source based on the distance to the source,  $d$ ,  
 156 and an angle,  $\varphi$ , measured from the global x-axis, as shown in Figure 1. Each source has its  
 157 own emission rate normalized by the mean wind speed,  $\frac{Q}{U}$ . For example, the complete set of  
 158 forward model parameters for a dual source model can then be written as follows:

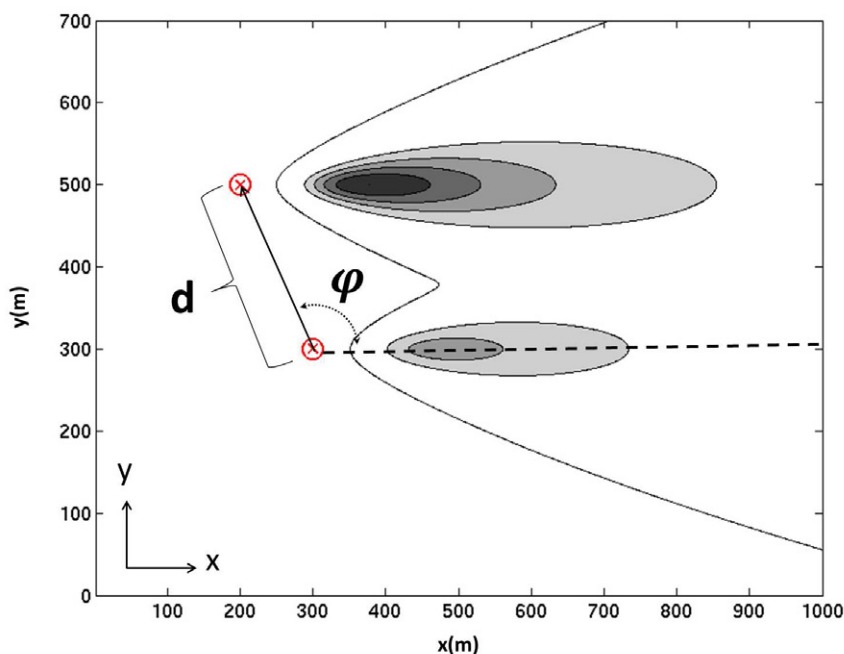
$$\mathbf{m} = \left[ x_{s1}, y_{s1}, \left( \frac{Q}{U} \right), \theta, \zeta_y, \zeta_z, \sigma^2, d_2, \varphi_2, \left( \frac{Q}{U} \right)_2 \right], \quad (12)$$

159 where  $(x_{s1}, y_{s1})$  is the primary source location, and  $\theta$  is the wind direction. We use Markov  
 160 chain Monte Carlo (MCMC) sampling with the Metropolis Algorithm (Metropolis et al.,  
 161 1953) to estimate the posterior distribution of the model parameters. In our approach, the  
 162 candidate state is sampled from a Gaussian distribution centered on the current state.

163 Figure 1 shows a dual source plume with sufficient distance between two sources, such  
 164 that overlap of the plumes does occur downstream and yet the sources are not too close  
 165 together to consider them as a single entity. We assume that the distance between the two  
 166 sources,  $d$ , is relatively small compared to the size of the search region. Therefore, for the  
 167 current study with a sensor grid that covers an area of approximately 500m by 500m with  
 168 50m spacing between sensors, we set an upper limit of 5 times the spacing between sensors  
 169 as the maximum cross-wind distance allowable between sources. If the sources are farther  
 170 apart than this upper limit, they can be treated as individual single-source events in the  
 171 present study. This reasoning also extends to sources that are extremely close to each other  
 172 in the cross-wind direction, such that plumes overlap heavily to behave as a single source  
 173 release. Therefore, a lower limit of one fifth of the spacing between sensors is used, below  
 174 which we assume that plumes overlap and can be considered a single source release.



175 The additional parameters,  $d$  and  $\varphi$ , are used to calculate the location of the second  
 176 source,  $(x_{s2}, y_{s2})$ , relative to the reference source. Equations 13 and 14 show the conversion  
 177 from polar to rectangular coordinates with respect to the location of the primary source. It  
 178 is not necessary to specify a primary source prior to the sampling process, because a source  
 179 location,  $(x_{s1}, y_{s1})$ , is estimated from the MCMC sampling process, which will then serve as  
 180 the reference source for other sources. Note that the other source locations are calculated  
 181 using the estimated parameters  $d$  and  $\varphi$ . The polar configuration allows for additional  
 182 sources to branch off of the primary source.



**Figure 1.** Sample dual source Gaussian plume colored by contaminant concentration at 2m above ground level. Source locations are shown as circles,  $d$  is the distance between sources, and  $\varphi$  is the angle between sources with respect to the positive x-axis.

$$x_{si} = x_{s1} + d_i \cos(\varphi_i) \quad (13)$$

$$y_{si} = y_{s1} + d_i \sin(\varphi_i) \quad (14)$$

183 where  $i = 2, 3, \dots, N$  and  $N$  is the maximum number of possible sources.

#### 184 4. Composite Ranking to Determine the Number of Sources

185 Concentration or dosage of contaminant measured at the sensors can be an outcome  
 186 of releases from single or multiple sources. However, in the ER problem we do not know  
 187 the number of sources involved in a dispersion event, even for a single source release. A  
 188 concentration field resulting from a multiple source release can come close to matching a  
 189 concentration field from a single source with a different emission rate and source location.



190 The Bayesian framework that we presented in the previous section does not provide any  
 191 inference on the number of sources involved in a dispersion event. Therefore, we propose a  
 192 composite ranking approach to estimate the number of sources involved in an event. The  
 193 ranking system is independent of the Bayesian inference to locate the source and emission  
 194 rate. We consider single, dual, and three-source releases, but the overall method is applicable  
 195 to more than three sources. In our approach, we execute MERT for each release possibility  
 196 independently. Once the runs are completed, we extract the most probable value for each of  
 197 the model parameters from the corresponding posterior probability distributions. We then  
 198 run the forward model using the most probable parameters to calculate the concentrations  
 199 at each of the sensor locations. We designate these model concentrations as  $\hat{C}$  and compare  
 200 them to the measured concentrations,  $C$ , for single, dual, and three-source assumptions  
 201 separately using a ranking method.

202 In atmospheric dispersion applications, it is typical to use multiple performance metrics  
 203 to effectively evaluate the predictive capability of a dispersion model. Researchers suggested  
 204 a variety of metrics (Stohl et al., 1998; Pullen et al., 2005; Svensson, 1998; Chang et al., 2003;  
 205 Hanna et al., 1993). We propose a composite ranking model that is inspired by the recent  
 206 Environmental Protection Agency protocol to determine the best performing air quality  
 207 model (EPA, 2012). The literature is mostly in agreement that error (scatter), bias, and  
 208 correlation are important metrics in the evaluation process, all of which are included in some  
 209 form in the global statistics portion of Mosca et al. (1998). Each of these metrics is weighted  
 210 equally in our ranking model to decide whether a specific model achieves better results using  
 211 a single or multiple source setting. We then identify the setting with the higher ranking as  
 212 the release event containing the correct number of sources.

213 Our ranking model has three parts. The first component of the model's rank is the  
 214 FAC2, which is a quantity measuring the fraction of predictions that fall within a factor  
 215 of two of the corresponding observations (Chang et al., 2003), as shown in Equation 15 .  
 216 This operation is performed to obtain a measure of error, or scatter, when comparing the  
 217 observed and predicted values.

$$\text{FAC2} = \text{fraction of data for which } 0.5 \leq \frac{\hat{C}}{C} \leq 2.0, \quad (15)$$

218 where  $C$  is the observed concentration at the sensor and  $\hat{C}$  is the estimated concentration  
 219 calculated by using the most probable parameters, obtained from posterior distributions, in  
 220 the forward model.

221 The next performance metric used in the ranking model is the Fractional Bias (FB). The  
 222 FB is used to indicate a bias towards underprediction or overprediction of concentration  
 223 data by the model. It has been used as a validation parameter for other dispersion models  
 224 and is a robust indicator of model performance (Stohl et al., 1998). The FB ranges from  
 225 -2 (extreme underprediction) to +2 (extreme overprediction), and 0.0 is a perfect score for  
 226 this component. As part of the United States Environmental Protection Agency's (EPA)  
 227 performance evaluation protocol (EPA, 1992), the FB is defined as follows:

$$FB = 2 \left( \frac{\bar{C} - \bar{\hat{C}}}{\bar{C} + \bar{\hat{C}}} \right), \quad (16)$$

where  $\bar{C}$  is the average measured concentration across all sensors, and  $\bar{\hat{C}}$  is the average of the predicted concentrations computed by the model at all sensor locations.

The final component to our ranking model is the Pearson's Correlation Coefficient (R), which contributes a measure of correlation to the ranking model. R ranges from -1.0 to +1.0 with +1.0 corresponding to "perfect positive correlation" (EPA, 2012). An R value close to 0.0 would indicate that the predicted data and the measured data are not related. R is defined as follows:

$$R = \frac{\sum_i (C_i - \bar{C}) \cdot (\hat{C}_i - \bar{\hat{C}})}{\left[ \sqrt{\sum_i (C_i - \bar{C})^2} \right] \left[ \sqrt{\sum_i (\hat{C}_i - \bar{\hat{C}})^2} \right]} \quad (17)$$

The three components described above are combined to form the following ranking model

$$RANK = FAC2 + \left( 1 - \frac{|FB|}{2} \right) + R^2 \quad (18)$$

The ranking model contains a measure of error (scatter), bias, and correlation in a composite fashion. These metrics provide a concise and quantitative description of how well the model performs with a varying number of sources. The composite rank ranges from 0 to 3, with 3 corresponding to a perfect score. The higher the *RANK*, the better the model did at matching the concentration predictions with sensor observations. We use the highest ranking model to make a decision on the correct number of sources involved in the dispersion event.

## 5. Results

In 2007, the Defense Threat Reduction Agency (DTRA) proceeded to address some of the unmet requirements in the current Joint Effects Model (JEM), which is to be used as the standard hazard prediction model at the Department of Defense (Storwold Jr., 2007). One of these requirements was to evaluate source term estimation models used to detect chemical and biological (CB) activity and estimate the characteristics of the source(s) in question. A large data set, FFT-07, was created for the evaluation and improvement of STE algorithms. The FFT-07 database provides detailed meteorological information and trace gas concentration measurements for short range (500m) dispersion experiments. These experiments were performed with single and multiple sources for continuous and puff (instantaneous) releases.

### 5.1. Evaluation with FFT-07 Trials

We use data from Trials 7, 27, 28, and 40 of FFT-07. In trials 27 and 40, there are two sources with different tracer emission rates. Trial 7 is a single source trial that we include

255 in our study to demonstrate that the ranking model will identify the correct number of  
256 source terms, even in a single source case. Trial 28 is a three source case. The true source  
257 locations and emission rates are known from the field data and used to assess the accuracy  
258 of the reconstructed model parameters. In working with the FFT-07 concentration data, we  
259 ignored sensor data that reports an error message for more than 50% of the sampling time.

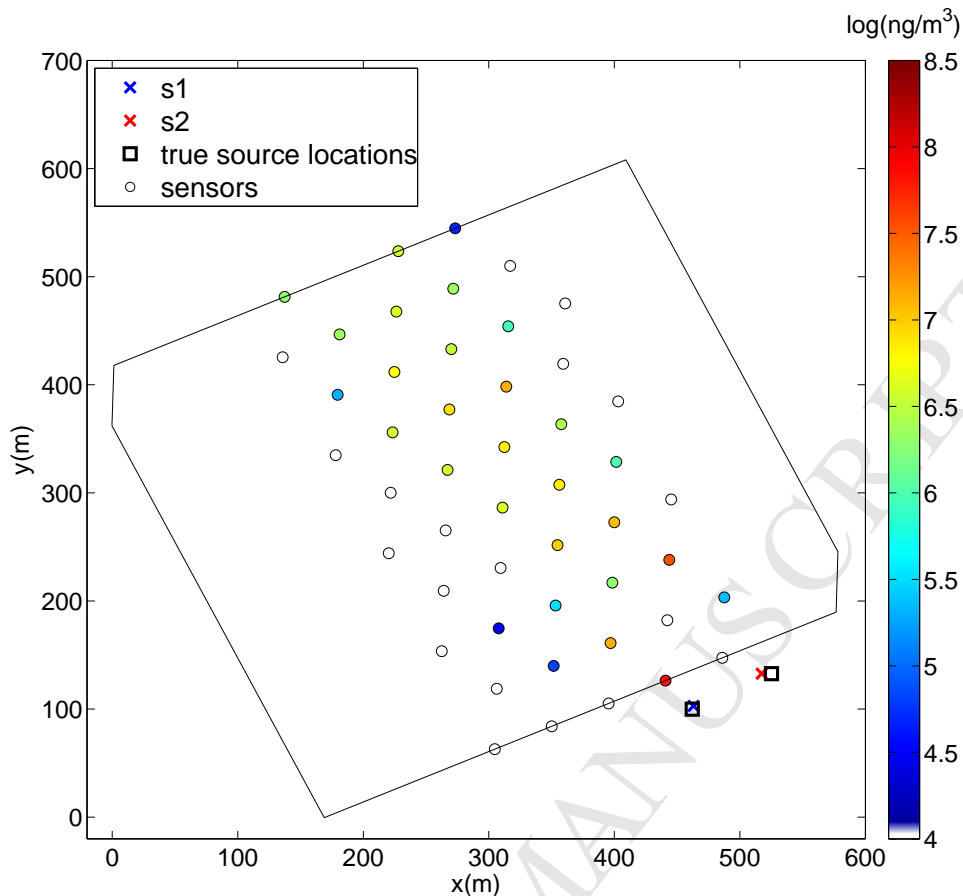
260 In FFT-07, a grid of 100 digital photoionization detectors (digiPID) were spaced evenly  
261 on a square grid at 50m apart and 2m above the ground. A tracer of propylene gas was  
262 released from multiple locations at approximately 2m above ground and at constant flow  
263 rates for approximately 15 minutes per trial. We time-averaged the concentration data from  
264 sensors for the continuous release trials, which are the focus of the present study.

265 FFT-07 Trial 40 had very few poor readings (sensors reporting an error more than 50% of  
266 the time). This abundance of reliable sensor data and fairly uniform wind conditions resulted  
267 in reconstructions of the source locations that are approximately 8 and 6 meters from the  
268 true source locations, as seen in Figure 2. For this case, 48 of the 100 sensors are used in  
269 the estimation. Note that we include all positive reading sensors. Figure 3 shows the tight  
270 posterior distributions for the two source locations in which the true values fall within, or  
271 very close to, the 50% contour line. This inner contour line encompasses 50% of the posterior  
272 samples and the outer contour line includes 90% of the posterior samples. The range of each  
273 cell is normalized in both the horizontal and vertical direction with the limits corresponding  
274 to the minimum and maximum values for each parameter in the posterior samples. The  
275 normalization enables us to assess accuracy in percentage form in a global fashion over the  
276 parameter space. The plots along the diagonal show the marginal distributions of each  
277 parameter. Trial 40 is a good example of successful reconstruction from reliable sensor data.

278 Figure 4 shows a comparison of results from FFT Trial 40, where the left image uses a  
279 single source setting, the middle uses a dual source setting, and the third image uses a three  
280 source setting. The predicted values for the dual source setting (middle) match more closely  
281 to the data measured by the sensors. A perfect match would lie directly on the solid diagonal  
282 line running through the origin. This view of the data allows us to see the difference between  
283 an estimate with a single, dual, an three source setting. It also shows the points which fall  
284 within a factor of two of the observed values (FAC2) as well as the over or underestimation  
285 (Bias). From this figure, we can visually deduce that the dual source setting is most likely  
286 the correct answer, but we need a quantitative measure. Therefore, we proposed a composite  
287 ranking model as described in Section 4.

288 The more reliable the sensor data, the more accurate the reconstruction will be. However,  
289 operational data may be less reliable than desired. Hence we use Trial 27 from the FFT-07  
290 data set, which has much less reliable data than the Trial 40, to test how less reliable or  
291 sparse data affects the reconstruction.

292 Figure 5 shows the layout of the 57 sensors used in Trial 27, as well as the true and  
293 estimated source locations. We observe that the most probable source locations are approx-  
294 imately 15 and 25 meters from the true source locations. The true source locations are  
295 illustrated with squares and the source location estimates with  $\times$ 's. Ideally, the estimates  
296 would fall directly on the true locations (e.g.  $\times$ 's on top of squares). The distances may not



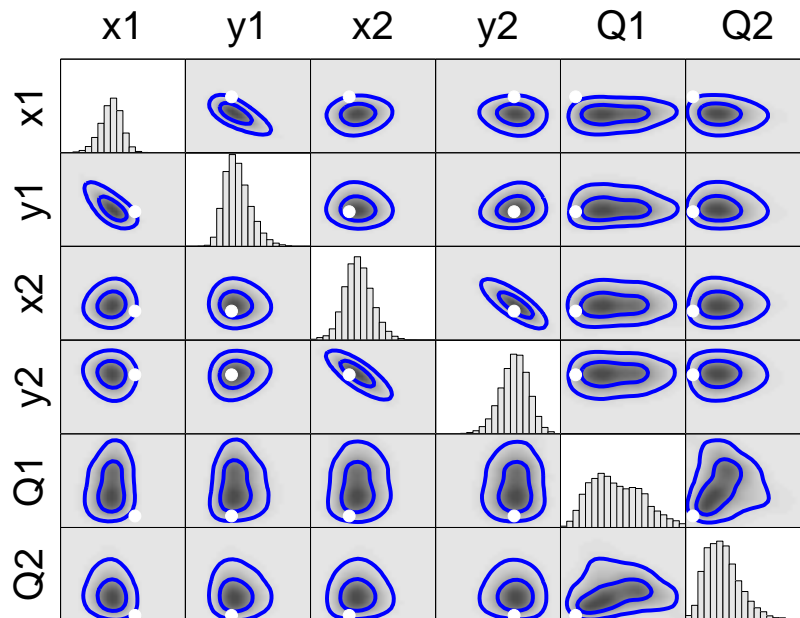
**Figure 2.** FFT-07 Trial 40 source location estimates (s1 and s2) with approximate errors of 8m and 6m. Sensors reporting nominally zero concentration are colored white. Large rotated box is the FFT-07 sensor network boundary.

297 be ideal (and not as small as Trial 40), but can still be very useful from an operational point  
 298 of view since they would at least put any rapid response personnel in close proximity to the  
 299 true locations.

300 FFT-07 Trial 28 is a three-source release event and a similar layout plot can be seen in  
 301 Fig. 6. In this figure we can see that estimated source locations for sources 1 and 3 are fairly  
 302 close to the true values, but the estimated source location for source 2 is approximately 48m  
 303 from the true source location. We do note, however, the estimated sources are in a somewhat  
 304 linear arrangement, as are the true source locations, and they are of approximately correct  
 305 spacing with respect to one another.

### 306 5.2. Composite Ranking Model Results

307 Thus far, we have presented reconstruction of source locations and emission rates for dual  
 308 and three-source releases. We have not made an attempt to estimate the number of sources  
 309 involved in a dispersion event. The composite ranking model that we proposed in Section 4



**Figure 3.** FFT-07 Trial 40 bivariate posterior distributions for location and emission strength. The range of each cell is normalized with respect to the minimum and maximum values for each parameter and distances can be viewed as percent error. The plot is colored by probability density and the darkest regions are the most probable. The outer contour encompasses 90% of the posterior samples and the inner contour includes 50%. White markers represent true values.

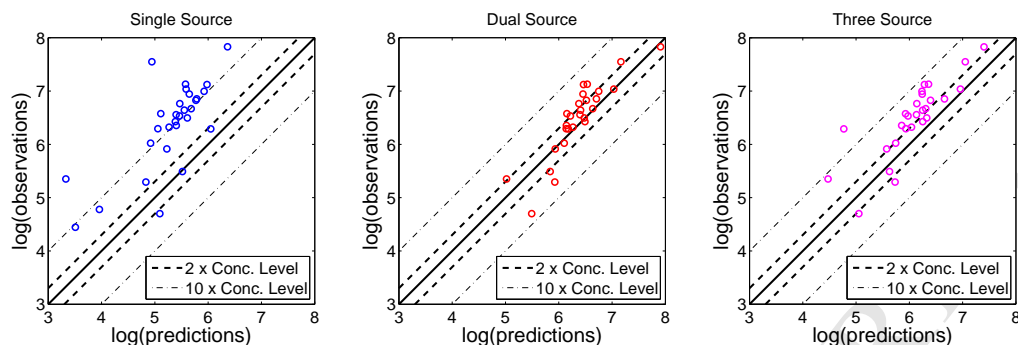
310 enables us to estimate the number of sources. We calculate  $RANK$  using Equation 18. The  
 311 components that make up the  $RANK$  are:  $FAC2$ ,  $FB$ , and  $R$ .

312 Figure 7 shows the composite ranking for all cases in this study, and is colored by con-  
 313 tribution from each component in the rank. A rank of 3.0 corresponds to a perfect score.  
 314 For all the cases tested, the model with the correct number of sources ranked higher. For  
 315 instance, Trial 7 is a single source release, and our ranking model gives the highest score  
 316 to the single source assumption correctly. In all the other cases the correct source-number  
 317 assumption received the highest score, as expected.

## 318 6. Conclusions

319 We have extended a Bayesian inference method to reconstruct single-source contaminant  
 320 release event, SERT, to reconstruct near-ground-level multiple-source release events, MERT.  
 321 We proposed a composite ranking system to identify the number of sources involved in an  
 322 event. The ranking formula is independent of the Bayesian method and can potentially be  
 323 adopted in other event reconstruction methods.

324 We have applied the combined approach to releases from up to three sources, but the  
 325 method can be extended to more than three sources. In the Bayesian framework we used a  
 326 data-driven Gaussian plume model where turbulent diffusion parameters are inferred given  
 327 the concentration data. The practice significantly improves the performance of the standard



**Figure 4.** Observed sensor concentrations for FFT-07 Trial 40 vs. computed sensor concentrations using the most probable model parameters.

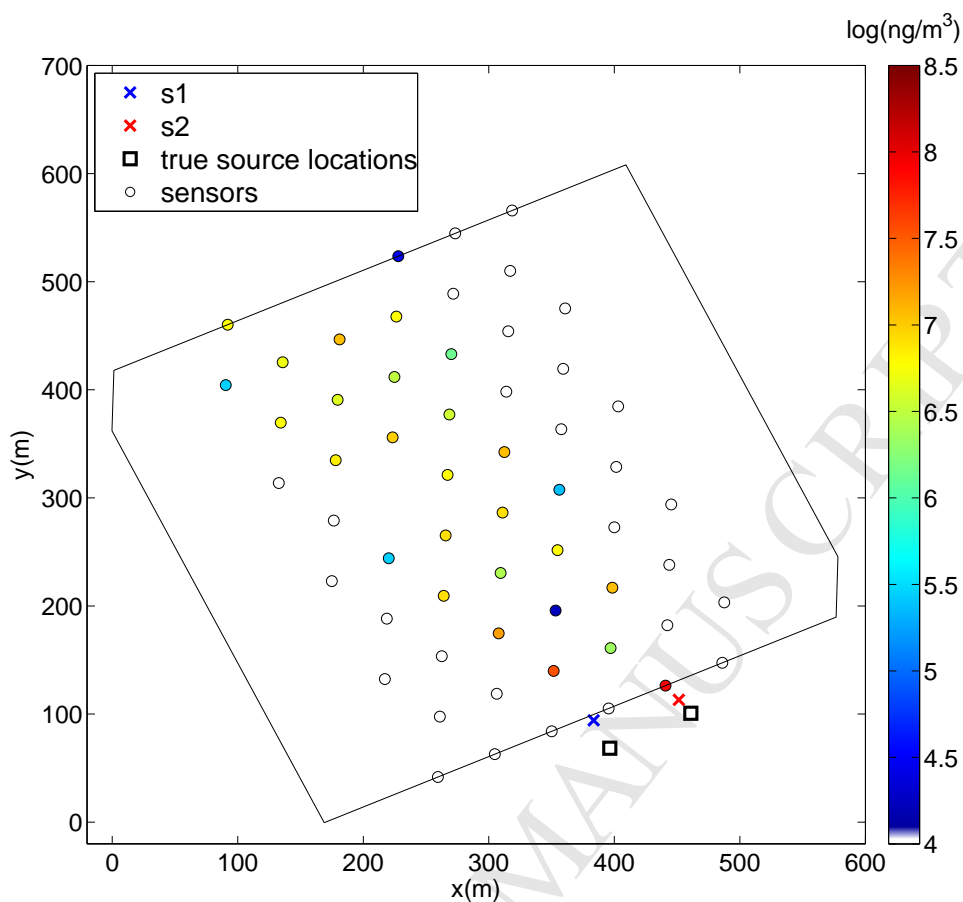
328 Gaussian plume model. However, for complicated dispersion events, sophisticated dispersion  
 329 models should be preferred as the forward model.

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 333 final form of the composite ranking formula.

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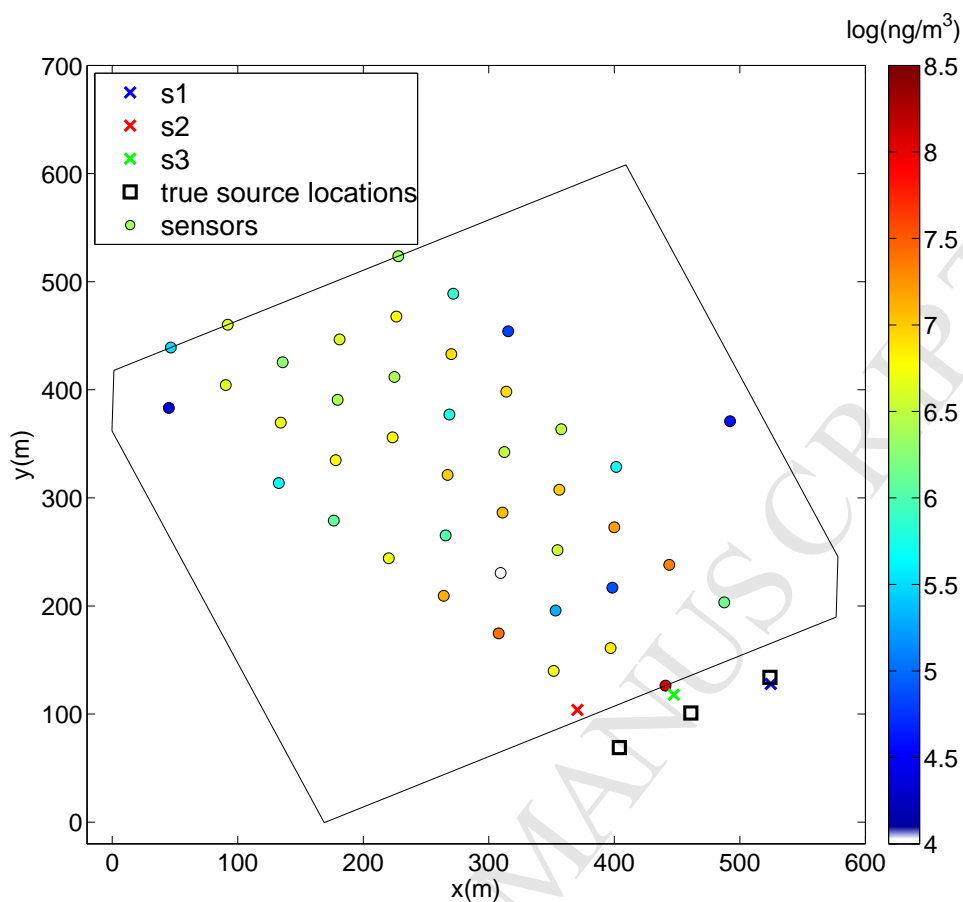
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**Figure 5.** FFT-07 Trial 27 source location estimates (s1 and s2) with approximate errors of 15m and 25m. Sensors reporting nominally zero concentration are colored white. Large rotated box is the FFT-07 sensor network boundary.

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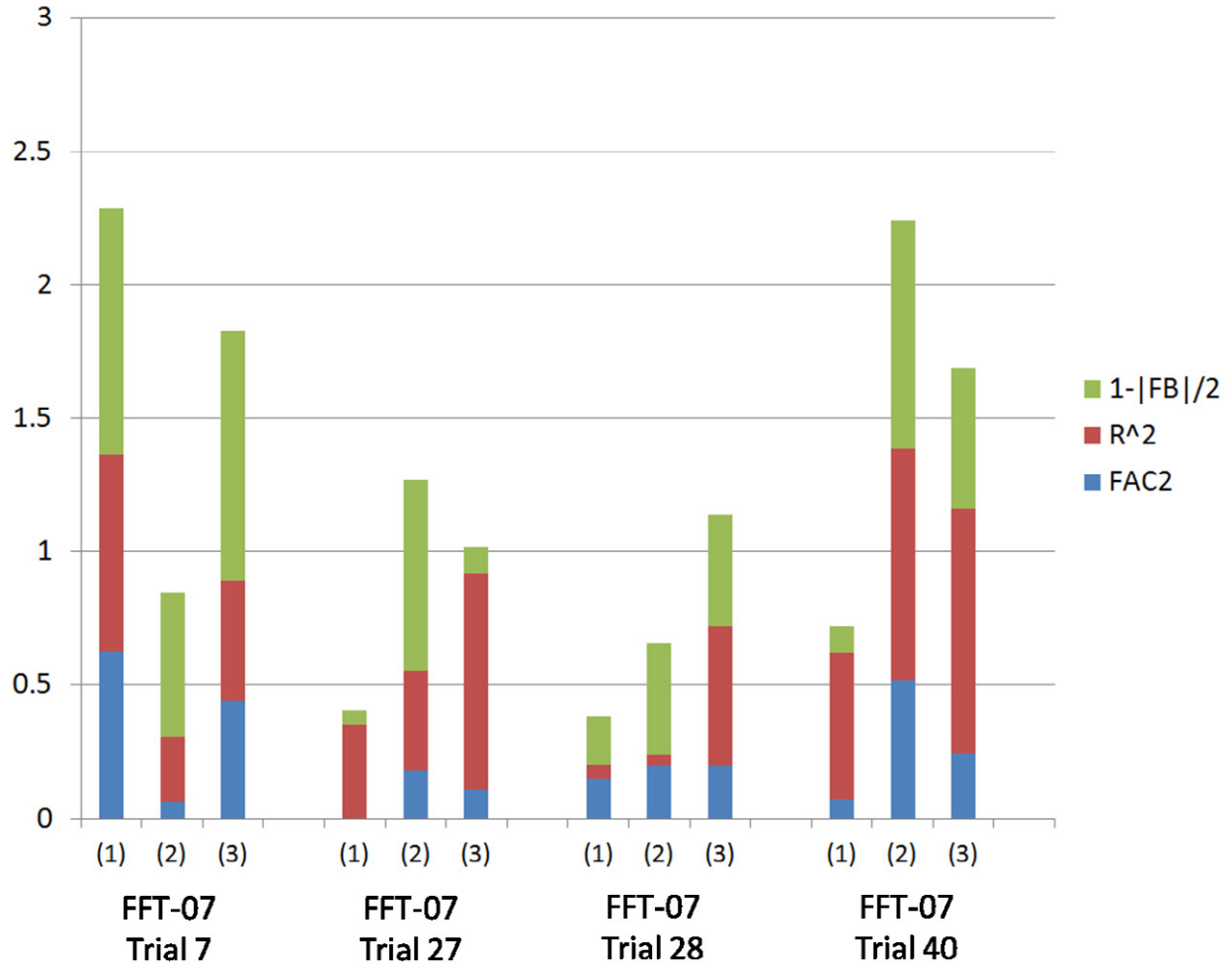




**Figure 6.** FFT-07 Trial 28 source location estimates (s1, s2, and s3) with approximate errors of 7.5m, 21.7m, and 48.3m, respectively. Sensors reporting nominally zero concentration are colored white. Large rotated box is the FFT-07 sensor network boundary.

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**Figure 7.** Ranking for each case tested. Colors correspond to individual rank components (e.g.  $R^2$ , FAC2,  $1 - |FB|/2$ ) as shown in legend. (1),(2),(3) refer to single, dual, and three source settings, respectively. FFT-07 Trials 27 and 40 are truly dual source releases. Trial 7 is a single source release and Trial 28 is a three source release.