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MULTI-SOURCE ATMOSPHERIC DISPERSION EVENT RECONSTRUCTION USING BAYESIAN INFERENCE AND COMPOSITE MODEL RANKING

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1. INTRODUCTION

Public safety, health, and threat mitigation are all of importance to emergency responders in the event of a disaster. Harmful contaminants may be released into the atmosphere intentionally, as in the case of a terrorist attack, or unintentionally due to uncontrollable circumstances, such as accidents or natural disasters. In either case, it is important to have a tool in place to enable first-responders to quickly and accurately determine the source and nature of the release. Source-term estimation (STE) tools have been developed by many researchers [14, 3, 12, 20, 22, 25, 10] The STE methods that have been developed use contaminant concentration data from a carefully-placed network of sensors to re-construct an atmospheric dispersion event in terms of its source(s) and their associated parameters.

Many of these STE methods adopt inverse problem methodology, in which a forward model is specified based on the assumed nature of the release event. These models range in complexity as well as computational intensity. For flat terrain with steady meteorological conditions, it has been shown that a fast-computing Gaussian plume model has been effective for event reconstruction [20, 2]. Other models may be suggested based on the operating conditions and plume assumptions [14, 15].

The STE community has adopted different methodologies. Some researchers prefer a deterministic approach, using adjoint models, genetic algorithms (GA), and other numerical optimization techniques [10, 1, 4, 3]. For instance, the Multi-Entity Field Approximation tool (MEFA), uses a GA to determine a hazard area and a cost function with optimization to infer the number of sources involved in a release event [3].

The second methodology, and the one used in the present study, uses Bayesian inference to take a probabilistic approach to solving the STE problem. Dynamic Bayesian models have been used in conjunction with appropriate forward models to estimate the source-terms involved all the way down to the neighborhood scale [11, 14]. Researchers [25, 26, 27] have used Bayesian inference to characterize release events with multiple sources where the number of sources is unknown a priori. In the present study, an alternative method of source number quantification is proposed by coupling a Stochastic Event Reconstruction Tool (SERT) [20] with a composite model ranking tool. It is important, especially in emergency response efforts, to get a complete picture of the dispersion event, including the number of sources involved, so that decision makers can develop an effective response plan.

Real trial data from the FUSION field trials of 2007 (FFT-07) data set [23] is used to develop and verify the Multi-Source Event Reconstruction Tool (MERT) presented in this study. Researchers [17, 16] have conducted a comparative investigation of STE algorithms based on the FFT-07 data set. In this study, we will use FFT-07 trial data to demonstrate the multi-source reconstruction capabilities of SERT for 1, 2, and 3 source cases, where the number of sources is treated as an unknown parameter in the reconstruction problem.

2. FORWARD MODEL

A data-driven Gaussian plume model [20] is selected as the forward model in the Bayesian inference framework. It is computationally inexpensive and well-suited to the FFT-07 continuous release trials, which are the focus of the present work. The turnaround time for computation is a critical aspect of STE problems when the intended use is emergency response. Any information regarding the event that is quickly discovered can potentially help first-responders first plan and execute their emergency efforts effectively.

Sophisticated forward models are also an option if the release event requires additional capabilities in its forward model. However, for the FFT-07 we found Gaussian plume models to be satisfactory because the experiments were performed over flat terrain and short distances. A complete derivation of the Gaussian plume model can be found in [21] and the concentration at location in Cartesian space, $C_m(x,y,z)$, may be calculated according to the following:

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

where Q is the emission rate, U is the average wind speed, H is the height of the release, $\sigma_y$and $\sigma_z$or the turbulent diffusion parameters in the crosswind and vertical directions, respectively. These turbulent diffusion parameters are driven by the observed data in the sense that the coefficients in the Pasquill stability formulas [8] are determined stochastically within the Bayesian inference method. Pasquill D type stability is assumed and this calculation is shown in Eq. 2.

$$\sigma_y = \zeta_1 x(1+0.0001x)^{-0.5}$$
$$\sigma_z = \zeta_2 x(1+0.0015x)^{-0.5} \quad (2)$$

The coefficients, $\zeta_1$and ζ_2, are the stochastically determined model parameters which make this a data-driven forward model. This data-driven approach to tune diffusion parameters has been shown to substantially improve source-term estimates over the use of empirically determined coefficients [20, 19].

3. BAYESIAN INFERENCE METHOD

An inverse problem can generally be formulated as follows:

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

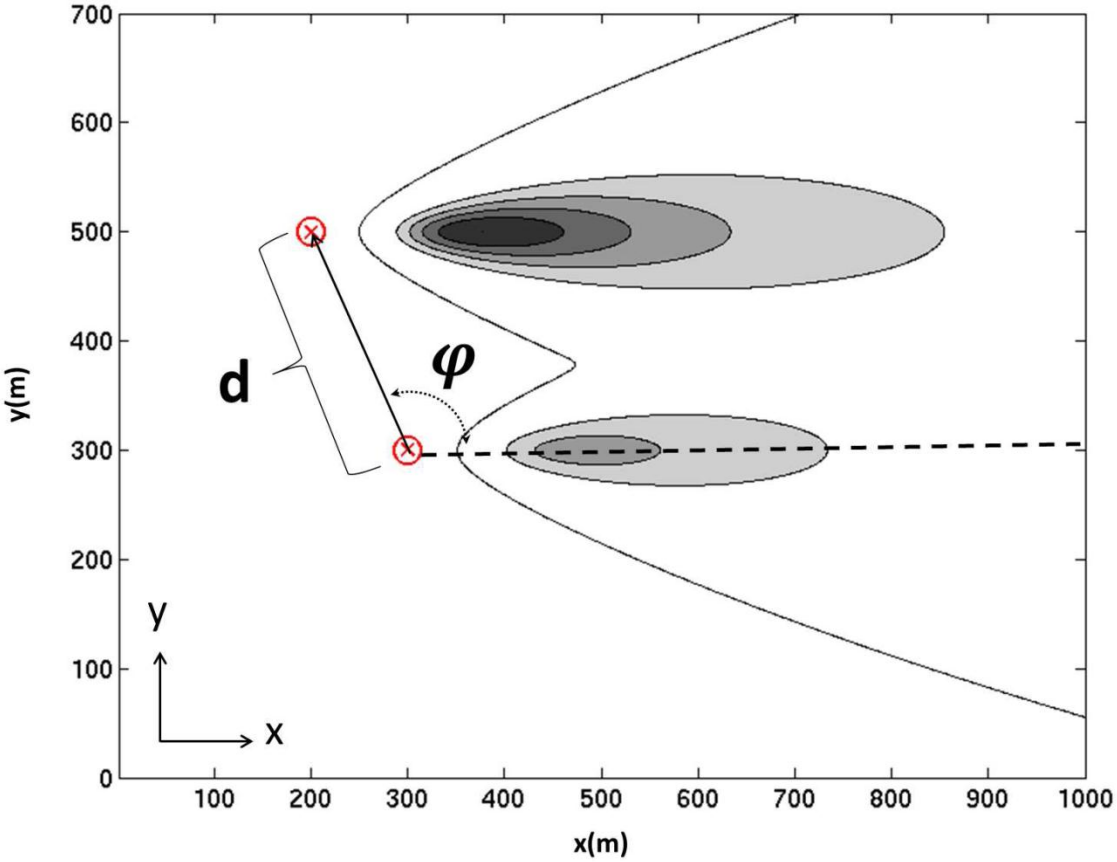
where, $\boldsymbol{d}$ is a vector of observed concentration values and $\boldsymbol{m}$ is a vector of forward model parameters (e.g. location, emission strength, etc.). *F* would correspond to the chosen forward model, in this case, the Gaussian plume model. Most Bayesian inference methods simplify Bayes' rule to the following form [6]:

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

where, $P(\boldsymbol{m}|\boldsymbol{d})$ is the posterior probability density of the forward model parameters, $\boldsymbol{m}$, given the observed concentration values, $\boldsymbol{d}$. $L(\boldsymbol{d}|\boldsymbol{m})$ is the likelihood of the observations, given the set of model parameters and $P(\boldsymbol{m})$ is a set of prior probabilities (one for each parameter). For instance, a dual source release would have the following set of model parameters:

$$\boldsymbol{m} = \left[x_1, y_1, \left(\frac{Q}{U}\right)_1, \theta, \zeta_1, \zeta_2, \sigma^2, d, \varphi, \left(\frac{Q}{U}\right)_2\right] \quad (5)$$

Here, σ^2represents the error variance for the model and measurement errors in a cumulative fashion, and is given an inverse gamma prior distribution with hyperparameters $\alpha = 1.0$ and $\beta = 1000.0$ [20]. The $\frac{Q}{U}$ parameter is the emission rate, normalized by the average wind velocity, and given a Jeffrey's prior [20]. The remaining parameters are given proper uniform priors within maximum and minimum limits. The d and φ parameters are used to define the location of secondary sources. This is depicted in Figure 1 and computed as follows:



$$x_2 = x_1 + d\cos(\varphi)$$
$$y_2 = y_1 + d\sin(\varphi) \quad (6)$$

Our Bayesian inference formulation takes into account the limitations of a sensor. Specifically, a real sensor has a detection threshold if a concentration of contaminant is present at the sensor, but it is below the detection limit such that the sensor cannot detect or quantify the presence of the contaminant. To account for this possibility, a conditional likelihood formula is proposed and detailed in [20]. Markov Chain Monte Carlo (MCMC) via the Metropolis Algorithm [13] is then used to simulate samples from the posterior distribution.

4. COMPOSITE MODEL RANKING TO DETERMINE SOURCE QUANTITY

As stated in the introduction, it is crucial to correctly identify and quantify the number of sources involved in a contaminant release scenario for a number of reasons. The difficulty in this respect is that it is possible to closely match the observed concentrations at the sensor locations with concentrations predicted by a model with an incorrect number of sources. For example, a truly dual source release may deposit certain concentrations across the sensor array, while a single source release, further upwind, may deposit very similar concentrations of material at those locations. Because these are all possible scenarios, it is necessary to have a tool which can correctly quantify the number of sources involved in the release. A composite model ranking tool, inspired by work in [7], uses a variety of metrics to evaluate dispersion model performance as it performs with a varying number of sources. A variety of metrics for model evaluation has been proposed by the research community and it is clear that a measure of error

Figure 1: Sample dual-source plume colored by contaminant concentration at approximately ground-level. The darker contours represent higher concentrations and the source locations are shown as circles. *d* is the distance between sources and φ is the angle between the primary and secondary source.

(scatter), bias, and correlation are all useful metrics for model performance [22, 18, 24, 5, 9]. Three individual metrics are combined to establish a single *RANK* metric in which each component (scatter, bias, and correlation) are weighted equally.

The first component to the *RANK* formula is the *FAC2*, which can be defined as follows:

$$FAC2 = fraction\ of\ data\ for\ which \\ 0.5 \leq \frac{\hat{C}}{C} \leq 2.0 \qquad (7)$$

where $\hat{C}$ is the predicted concentration at a given sensor location and C is the observed concentration at that same location. This metric provides a measure of error or scatter to the composite ranking tool.

The second metric used is the Fractional Bias (FB) which is used to indicate a bias towards under or over-prediction and is calculated as

$$FB = 2\left(\frac{\bar{C} - \bar{\hat{C}}}{\bar{C} + \bar{\hat{C}}}\right) \qquad (8)$$

where $\bar{C}$ is the average observed concentration across all sensors and $\bar{\hat{C}}$ is the average predicted concentration across all sensors. The final component of the composite ranking metric is Pearson's correlation coefficient (*R*), which adds a measure of correlation to the overall ranking method. *R* is calculated as follows:

$$R = \frac{\left(\sum_i (C_i - \bar{C}) \cdot \left(\hat{C}_i - \bar{\hat{C}}\right)\right)}{\left[\sqrt{\sum_i (C_i - \bar{C})^2}\right]\left[\sqrt{\sum_i \left(\hat{C}_i - \bar{\hat{C}}\right)^2}\right]} \qquad (9)$$

The *RANK* metric is then computed in Eq. 10. Each component contributes equally and has a range of 0-1. Therefore, the overall range of *RANK* is 0-3, with 0 being the lowest and 3 being the highest possible score.

$$RANK = FAC2 + \left(1 - \frac{|FB|}{2}\right) + R^2 \qquad (10)$$

The STE algorithm is run separately for single, dual, and three source settings and each run is then ranked. The run with the highest *RANK* is then chosen as the answer with the correct number of sources.

5.1 RESULTS

The FUSION Field Trial 2007 (FFT-07) [23] data set is a set of high resolution continuous and instantaneous tracer release experiments carried out at Dugway Proving Grounds, Utah by the United States Army. This data set was released to STE algorithm developers to explore new methods and improve the abilities of existing algorithms. Details of the field experiments are covered extensively in [23].

We focused on four trials which included one single-source release (Trial 7), two dual-source releases (Trials 27 and 40), and one three-source release (Trial 28). In each of these trials, a propylene tracer was released in a continuous manner for approximately 15 minutes. The plumes traveled past a dense grid of 100 sensors arranged in a rectangle spaced approximately 50m from one another and 2m above ground. The releases were also at a height of 2m. Sensors that reported an error for more than 50% of the sampling time were discarded from the set.

Trial 40, a dual-source release, had good observations with no false readings and equally desirable wind conditions, which were steady and mostly of uniform direction. 48 out of the 100 available sensors were used in the STE, resulting in source location estimate errors of approximately 6 and 8 meters, shown in Figure 3. Additionally, very tight posterior distributions were developed for the model parameters, as seen in Figure 2, where the outer contour line encompasses 90% of the posterior samples and the inner encompasses 50%. The white markers refer to the true values. We see the marginal probabilities for each parameter along the diagonal, which show clear spikes where the most likely solution exists. The cells are normalized with respect to maximum and minimum values for

each parameter and distances may be viewed as percent error. As an example, source 1 is off in the x-direction by approximately 15%. Figure shows a comparison of observed concentrations vs. estimated concentrations at the sensor locations for a single, dual, and three-source estimate for Trial 40. We can see the bias, correlation, and scatter in these plots and note that the dual-source setting appears to be the most likely setting.

Trial 27 is a second dual-source release with a lesser number of reliable sensor data. For this estimation, 57 of the 100 sensors were used and the resulting location errors for source 1 and 2 were 15 and 25 meters, respectively, as shown in Figure 5.

Trial 28 is a three-source release with many sensors reporting error, which makes it a challenge to reconstruct with reasonable accuracy. We can see in Figure 6 that source 1 and 3 estimates are fairly close, but the estimate for source 2 is approximately 48m off. It is noteworthy, however, that the estimates are arranged linearly and spaced approximately correctly when compared to the arrangement of the true sources.

The last trial, Trial 7, is a single source release used to confirm that the ranking algorithm will choose a single source estimate over a dual or three-source estimate. The STE algorithm estimates the source location within 2m for this trial.

5.2 COMPOSITE RANKING RESULTS

Estimates have been achieved, thus far, for single, dual, and three-source settings for each trial. It is now necessary to apply the *RANK* formula to each case to determine which estimate is correct for each individual trial. We refer back to Section 4 for the development of the *RANK* formula and the components included.

Figure 7. shows the composite ranking for each case and is colored by the individual components which make up the *RANK* formula. We remind the readers that the scale is from 0 (worst) to 3 (best) and scores are only relevant within each individual trial. We see that in each case, the setting with the correct number of sources scores the highest, and is therefore chosen as the correct setting.

6. SUMMARY

Single, dual, and three-source tracer experiments from the FFT-07 dataset have been used to test the performance of the presented stochastic multi-source event reconstruction tool (SERT). A composite ranking system has been proposed to quantify the number of sources involved in each release event. Both the STE and *RANK* models perform well in estimating the source parameters and successfully determining the correct number of sources involved in a certain event.

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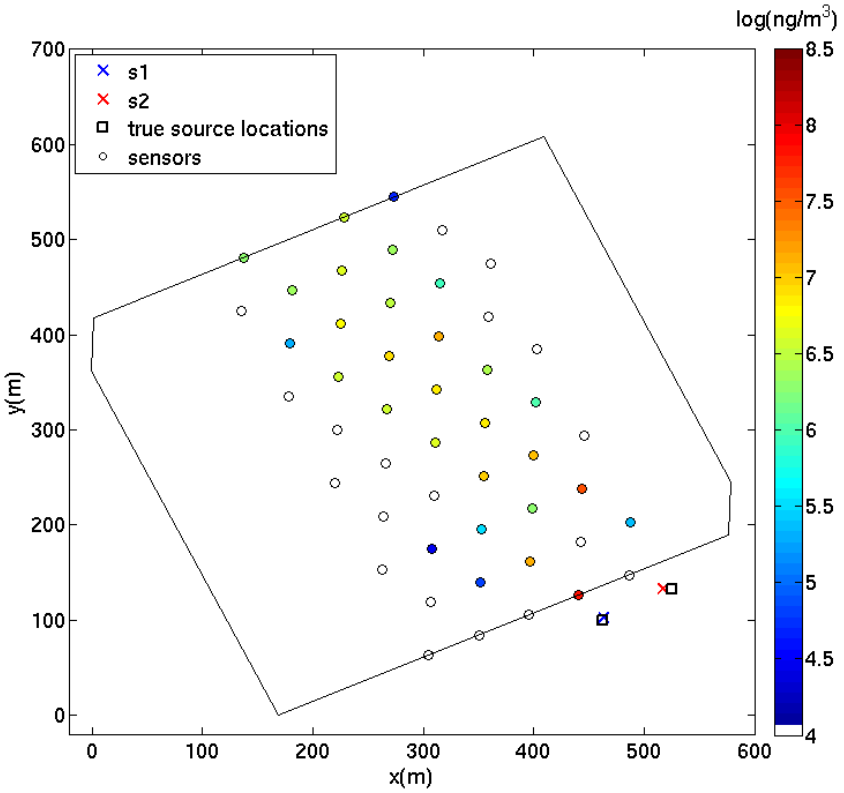

Figure 3: FFT-07 Trial 40 source location estimates (s1 and s2) with errors of 8m and 6m. Magnitudes of concentrations are reported in log(ng/m^3) and zero sensors are colored white.

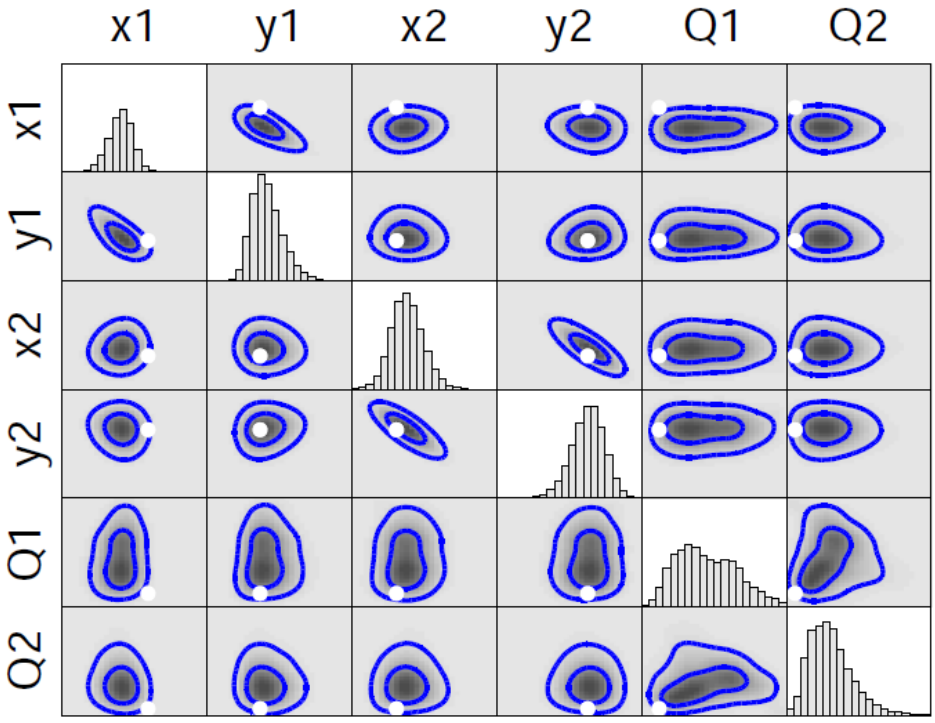

Figure 2: FFT-07 Trial 40 bivariate posterior distributions with marginal distributions along the diagonal. Each cell is normalized with respect to max/min. Outer contour encompasses 90% of samples and inner counter encompasses 50% of posterior samples. White markers represent true values.

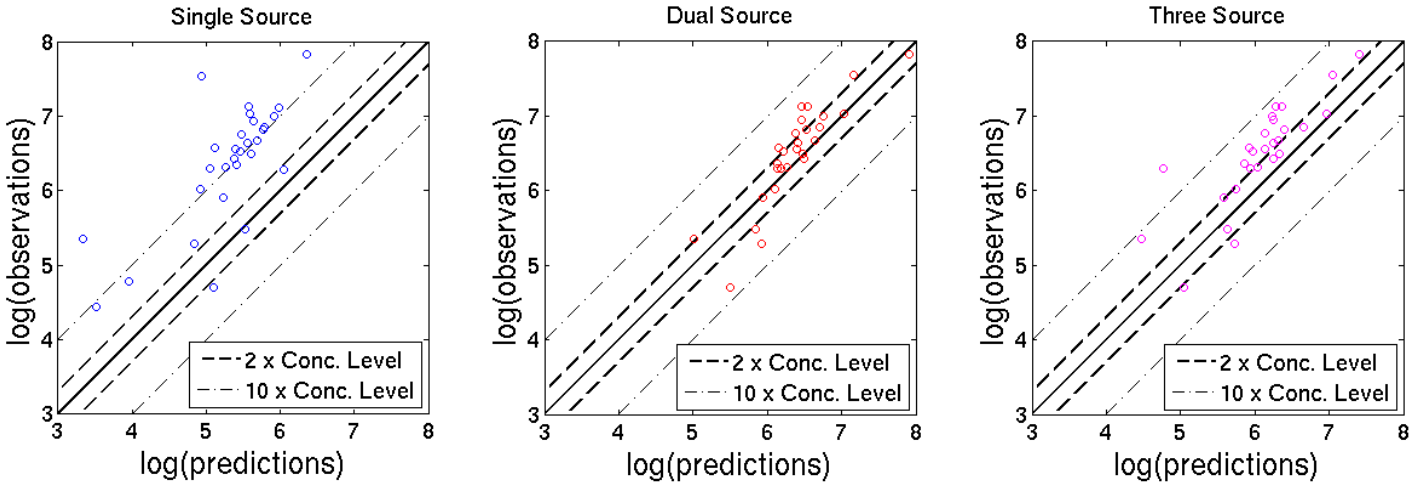

Figure 4: Observed sensor concentrations for FFT-07 Trial 40 vs. computed sensor concentrations for single, dual, and three source settings.

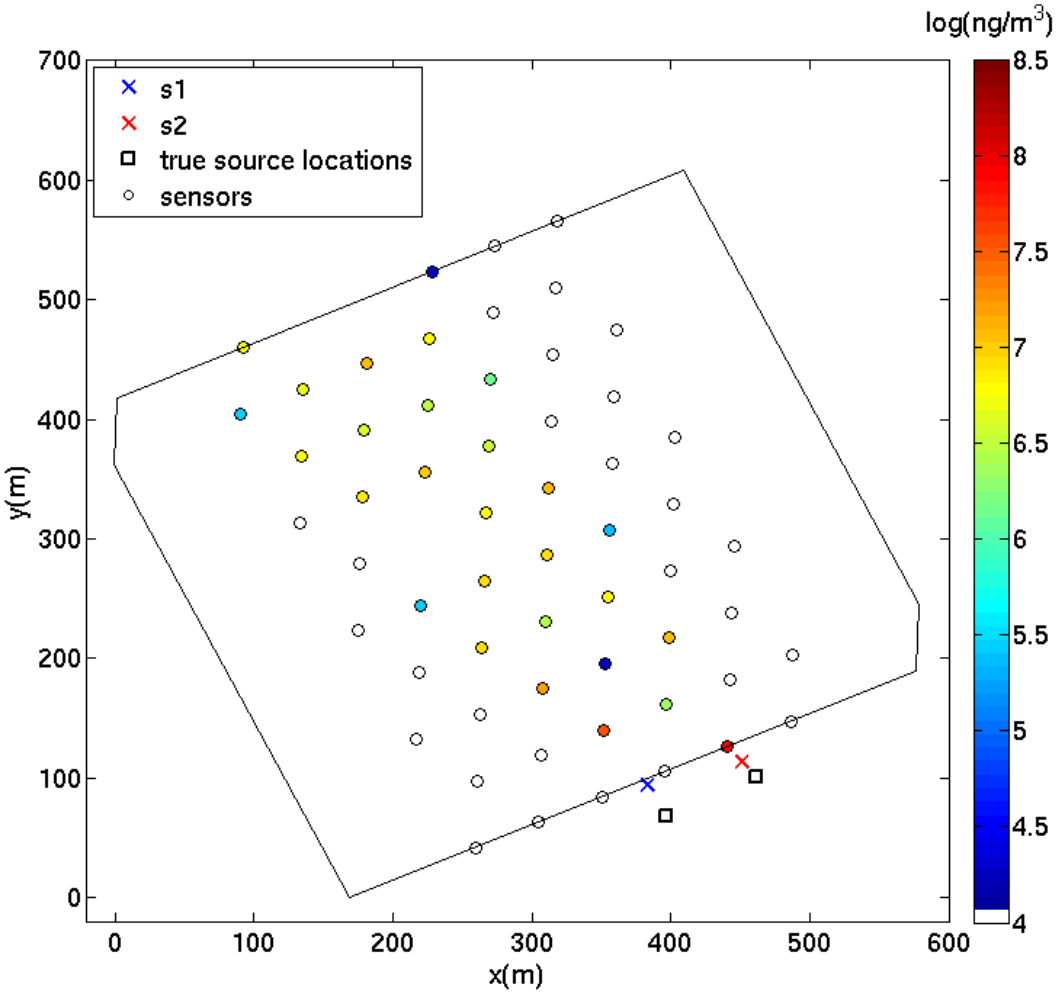

Figure 5: FFT-07 Trial 27 source location estimates (s1 and s2) with errors of 15m and 25m. Magnitudes of concentrations are reported in log(ng/m^3) and zero sensors are colored white.

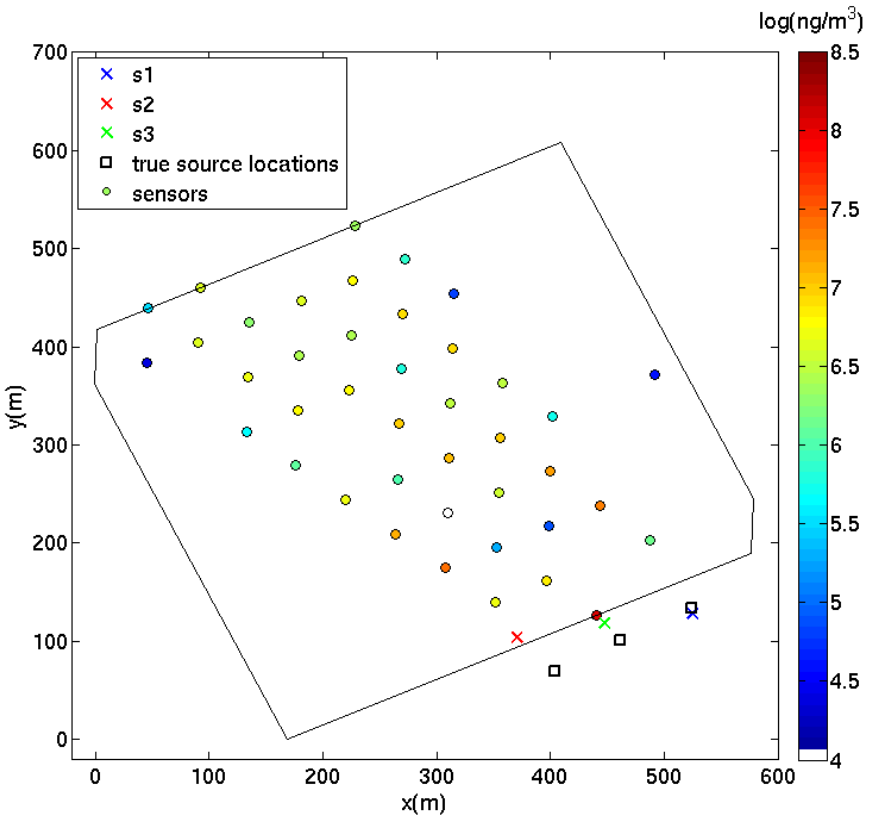

Figure 6: FFT-07 Trial 28 source location estimates (s1 and s2) with errors of 7.5m, 21.7m, and 48.3m. Magnitudes of concentrations are reported in log(ng/m^3) and zero sensors are colored white.

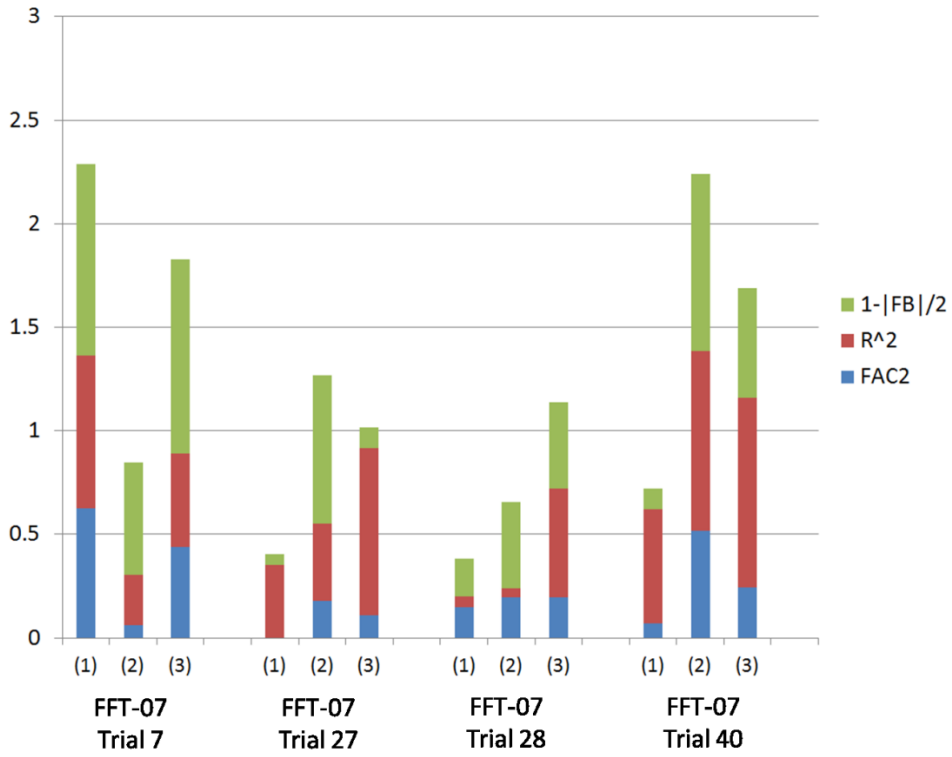

Figure 7: *RANK* for each trial tested. Colors correspond to individual ranking component as shown in legend. Trial 7 is a truly single-source release, Trials 27 and 40 are dual-source, and Trial 28 is a three-source release.