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MODEL UNCERTAINTIES IN BAYESIAN SOURCE LOCALISATION USING THE INVERSE MODELLING TOOL FREAR

Pieter De Meutter[1,2], Andy W. Delcloo[2,3] and Ian Hoffman[4]
[1]SCK CEN (Belgian Nuclear Research Institute), Boeretang 200, Mol, Belgium
[2]Royal Meteorological Institute of Belgium, Ringlaan 3, Brussels, Belgium
[3]Department of Physics and Astronomy, Ghent University, Krijgslaan 281/S9, Gent, Belgium
[4]Radiation Protection Bureau, Health Canada, 775 Brookfield Road, Ottawa, Canada

Abstract: A global network of monitoring stations is set up that can measure tiny concentrations of airborne radioactivity as part of the verification regime of the Comprehensive Nuclear-Test-Ban Treaty. If Treaty-relevant detections are made, inverse atmospheric transport modelling is one of the methods that can be used to determine the source of radioactivity. In order to facilitate the testing of novel developments in inverse modelling, two sets of test cases have been constructed using real-world ^{133}Xe detections associated with routine releases from a former medical isotope production facility. One set consists of 24 cases with 5 days of observations in each case, and another set consists of 8 cases with 15 days of observations in each case. A series of inverse modelling techniques and several sensitivity experiments have been applied to determine the (known) location of the medical isotope production facility. Metrics have been proposed to quantify the quality of the source localisation. From that, it has been found that the Bayesian inference underestimated uncertainties. Here, two approaches are explored to address the issue of underestimating the uncertainty in Bayesian source reconstruction.

Key words: *inverse modelling, ATM, source reconstruction*

INTRODUCTION

Global and regional networks of high-volume air samplers can measure traces of radioactivity in air for the purpose of environmental and treaty monitoring. In the framework of radiation protection and for verifying compliance with the Comprehensive Nuclear-Test-Ban Treaty, it can be of interest to know the origin and release parameters associated to specific detections of radioactivity. For this purpose, the open source inverse modelling tool Forensic Radionuclide Event Analysis and Reconstruction (FREAR) was developed (De Meutter and Hoffman, 2020). The tool makes use of observed airborne activity concentrations and the output of atmospheric transport modelling to determine the unknown source parameters.

INVERSE ATMOSPHERIC TRANSPORT MODELLING

Inverse modelling can formally be written as follows (Seibert, 2000):

$$\boldsymbol{y} = \boldsymbol{M}\boldsymbol{x} + \boldsymbol{\varepsilon} \tag{1}$$

where $\boldsymbol{y}$ is a vector of observations, $\boldsymbol{M}$ is a matrix containing the source-receptor sensitivities obtained from an atmospheric transport model for each geo-temporal release point and associated to each observation. The release at each geo-temporal release point is represented by the vector $\boldsymbol{x}$. Finally, $\boldsymbol{\varepsilon}$ represents the combined model and observation error.

Inverse atmospheric transport modelling involves determining $\boldsymbol{x}$ so that $\boldsymbol{M}\boldsymbol{x}$, the modelled observations, match $\boldsymbol{y}$ taking into account an estimate of the error $\boldsymbol{\varepsilon}$.

TEST CASES

In order to test and validate several inverse modelling approaches, test cases have been identified based on ^{133}Xe measurements at four stations in North America from the International Monitoring System, which is part of the Comprehensive Nuclear-Test-Ban Treaty verification regime. Measurements were selected from 1 September 2014 until 30 December 2014. The vast majority of ^{133}Xe detections at these stations were coming from regulated emissions from Canadian Nuclear Laboratories former medical isotope production facility *CRL* in Chalk River, Ontario, Canada. Therefore, the data offers a good way to test and validate source localisation algorithms as the true source location is known. A series of backward-in-time atmospheric transport modelling calculations have been performed using Flexpart coupled with archived numerical weather prediction data from the European Centre for Medium-range Weather Forecasts. Several source location reconstruction methods available in FREAR were applied to these test cases. For more details, the reader is referred to De Meutter et al. (2024).

One issue that emerged was that the Bayesian source reconstruction at times underestimated the errors. This is illustrated in **Figure 1** (top row, left). The source location posterior probability distribution is very narrow and does not include the true source, CRL. Comparing the observed and modelled activity concentration shows that the uncertainties are underestimating the actual errors (**Figure 1**, top row, right). When using Bayesian inference in FREAR, uncertainties are handled as follows: a multivariate normal likelihood is used and all observations are assumed to have the same relative uncertainty rather than the same absolute uncertainty, otherwise the largest detections would dominate the inference. For instrumental non-detections, the relative uncertainty is multiplied by a multiple of the minimum detectable concentration. The relative uncertainty is not inferred but provided as input. Since the combined model and observation uncertainty is unknown, Yee (2012) introduced an inverse gamma distribution for the uncertainty rather than using a single value. The multivariate normal likelihood is then integrated over all possible values of this uncertainty. As a result, three hyperparameters need to be provided that define the inverse gamma distribution for the uncertainty: s, an estimate for the true relative error, and α and β, scale and shape parameters. The results proved quite robust when increasing s from 0.5 (50% relative uncertainty) to 3 (300% relative uncertainty), with the location of CRL not included in the posterior distribution.

ALTERNATIVE APPROACHES

Here we address the issue of underestimated uncertainty in the Bayesian source location reconstruction. We use the first 15-day test case from De Meutter et al. (2024) with 66 observations, of which 17 detections and 49 instrumental non-detections. Two alternative approaches are tested: a different measurement model and a different likelihood function.

First, a different measurement model (equation 2) is tested following the work of Yee et al. (2014) who introduced multipliers that are allowed to vary between 0.1 and 10 to correct for complex uncertainties in the atmospheric transport and dispersion model. A multiplier m_i is introduced for each observation ($i = 1 \dots N$):

$$y_i = m_i M_{ij} x_j + \varepsilon_i \tag{2}$$

The multipliers are parameters that are inferred during the Bayesian source reconstruction. The total number of inferred parameters becomes 71: the source longitude and latitude, the release amount, the release start and stop times and 66 multipliers.

The second approach involves a different likelihood function: a multivariate normal distribution is taken (Frankemölle et al., 2024), omitting the inverse gamma distribution for the uncertainty. Instead, one value for the uncertainty is introduced for each measurement station, and these are inferred by the Bayesian source reconstruction rather than provided as input. Non-detections are treated in a simplified way by applying a transformation using the minimum detectable concentration as is done for a cost function optimisation approach (see De Meutter et al., 2024). For the uncertainty parameters, a uniform prior is assumed with bounds between 0.5 (50% relative uncertatinty) and 10 (1000% relative uncertainty). The uncertainty is allowed to vary among different measurement stations, which makes sense since the four detectors are part of a sparse network: different measurement stations can experience different weather regimes and are thus subject to different uncertainty regimes. Covariances are currently ignored because it is not trivial to efficiently ensure that the correlation matrix is positive definite during the sampling process. Furthermore, given the sparseness of the network, this is likely a valid assumption. However, it will be assessed in the future how the correlation can efficiently be taken into account. For this case study, there are four different measurement stations, so that the total number of inferred parameters becomes nine: the source longitude and latitude, the release amount, the release start and stop times and four uncertainty parameters.

RESULTS

The results using the multipliers are shown in **Figure 1** (second row). The multipliers succesfully add uncertainty to the posterior as can be seen from the source location probability map, which now includes CRL. The comparison between the observed and modelled activity concentrations show a near perfect match since the multipliers compensate for model error. It also shows that the range of the multipliers (from 0.1 to 10) is sufficiently large for this case. The posterior distribution for the multipliers are shown in **Figure 2**. One can see a clear signal for the detections and a uniform distribution for the non-detections.

The results using the multivariate normal likelihood with inferred uncertainties are shown in **Figure 1** (third row). A wider posterior is obtained for the source location, including the true source location, CRL, and in good agreement with the multiplier method. The match between the observed and modelled activity concentrations is good, with sufficiently large uncertainties. The posterior distributions for the uncertainty parameters are shown in **Figure 3**. For stations RN16 and RN74, the posterior distribution resembles the prior distribution. There were no detections at these stations.

The high inferred relative uncertainty motivated us to perform another Bayesian inference with the default likelihood in FREAR using s = 10. The results are shown in **Figure 1** (bottom row). The resulting probability distribution for the source location is significantly larger than the initial inference using s = 1 and is furthermore in agreement with the results using the multipliers and the inferred uncertainties.

CONCLUSIONS

In order to address the underestimation of uncertainties in the Bayesian source reconstruction in FREAR, three different methods were introduced: the first approach involved the introduction of multipliers into the measurement model following Yee et al. (2014). The second approach involved the inference of the uncertainty in a multivariate normal likelihood with a simplified treatment of instrumental non-detections. The results of the former motivated a third approach which involved using the default likelihood in FREAR with (very) large input uncertainty (s = 10). Three methods have succesfully addressed the underestimation of the uncertainty in the Bayesian source location reconstruction in FREAR. The full set of test cases introduced in De Meutter et al. (2024) will be used in a future study to quantify the performance of these methods in order to select the best method.

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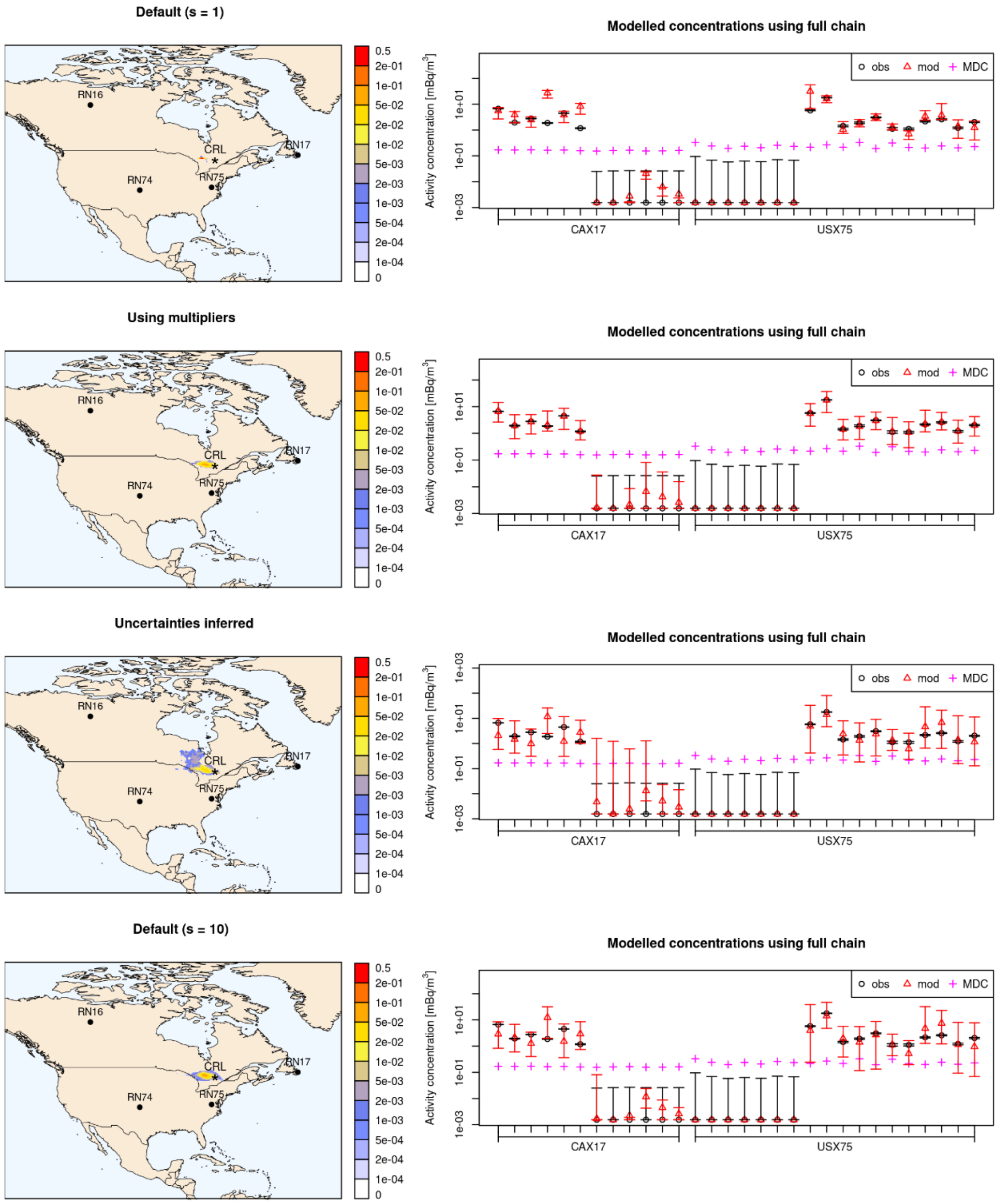

Figure 1. Left column: source location probability map obtained by Bayesian inference for different experiments. Right column: comparison between the observed (black circle) and modelled (red triangle) activity concentrations corresponding to the Bayesian inference for stations RN17 and RN75. The minimum detectable concentration or MDC is also shown (purple '+'-sign).

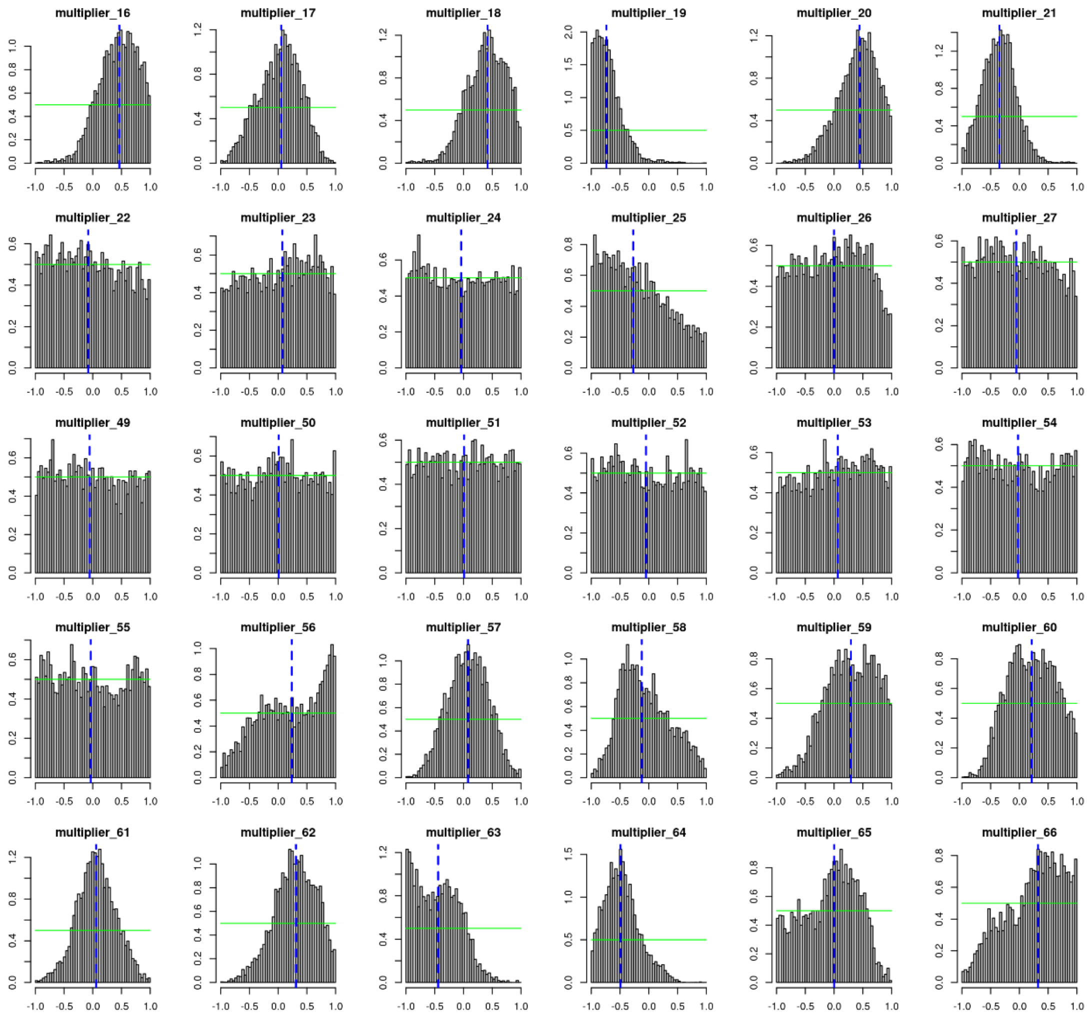

Figure 2. Posterior distribution of the log10 of the multipliers associated to observations at stations RN17 and RN75. The blue vertical line shows the posterior median, while the green horizontal line shows the (uniform) prior distribution.

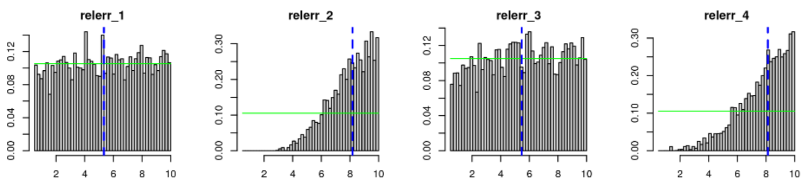

Figure 3. Posterior distribution for the relative uncertainty associated to the four stations: RN16, RN17, RN74 and RN75. The blue vertical line shows the posterior median, while the green horizontal line shows the (uniform) prior distribution.