Source Reconstruction for the ETEX-1 Tracer Release with a Lagrangian Dispersion Model

A contribution to subprojects GLOREAM and GENEMIS

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Introduction

The general aim of our contribution is the development of inverse modelling methods to derive information on emissions from measurements in the regional scale. Our approach has two parts: first, the derivation of a source-receptor matrix (SRM), and second, the inversion to find the emissions that lead to the best fit to the observations and any additional constraints.

Preliminary studies (Seibert, 1997; Seibert, 1999) used simple trajectories to provide a first approximation to the SRM. This approach already yields useful results and can be used instead of more conventional trajectory statistics. However, a real dispersion model (Eulerian or Lagrangian) is needed for an accurate description of the source-receptor matrices. Receptor-oriented Lagrangian models are computationally efficient if the number of receptors (measurements) is less than the number of potential source elements. The usual choice in this case was for a long time the Lagrangian box model. It has the advantage that chemistry can be included, but does not describe transport and dispersion very well (problems related, e.g., to wind shear). As our approach for inversion anyway does not allow for non-linear chemical reactions, a Lagrangian particle dispersion model (LPDM) was an attractive choice as it offers high accuracy though no chemistry is included.

While running the LPDM forward to produce the SRM would have been straightforward, the backward approach we were interested in was new terrain. There is some previous work with backward-running Eulerian as well as Lagrangian models, but it was not yet exploited for the formal determination of a SRM. There is a conceptual problem with running LPDMs backward because the generation of particles in emission areas is not a simply reversible process. The solution found is presented and a first test application, the reconstruction of the ETEX tracer release, is shown.

Method to derive source-receptor matrices with a backward-running LPDM

The elements of the source-receptor matrix M are defined by

$$m_{il} = \partial y_l / \partial x_i$$

where y_l are the ambient concentrations and x_i the source elements. Thus, for a linear source-receptor relationship

$$y_l = \sum_i (m_{il} x_i) \ .$$

In the forward mode, one would do one run for each source element (or treat each source element as a different species) and collect all the relevant ambient concentrations. For the linear case, the ratio of the two would give the SRM elements. It can be shown (details see

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Seibert and Stohl, 2000, and Seibert, 2000) that in the case of the backward-running LPDM the SRM elements are simply equal to the residence time spent in the respective source grid cells by particles released from the receptor.

The key assumptions made to arrive at this result are

1) Only volume sources are considered and no area, line or point sources.

2) Particles carry mixing ratios rather than masses.

The recipe for the SRM determination in the backward mode then is:

- use the same formalism and computer model, but integrate the particle trajectories backward in time, using a negative time step;

- emit a pseudotracer from each measurement site during one measurement interval, with arbitrary (e.g., unit) source strength;

- new interpretation: instead of particle masses, mixing ratios $\chi = c/\rho_{air}$ (in an infinitesimal volume of air) are transported;

- calculate gridded concentrations $\overline{c_i}$ as usual and scale them as follows to obtain the residence times per grid cell $\Delta\tau_i$:

$$\Delta\tau_i = \overline{c}_i \frac{V_i \Delta T}{\mu_{tot}}$$

where V_i is the volume of the grid cell, ΔT the averaging time interval for the output, and μ_{tot} the total emitted mass.

Application to the European tracer experiment ETEX

We are dealing here only with the first of the two releases of a gaseous, nondepositing, inert tracer. The tracer was released from a location in Bretagne, NW France, from 23 Oct 16:00 UTC until 24 Oct 3:50 UTC, 1994 (duration: 7:50 h) at a constant rate of 7.98 g/s. The ambient concentrations were sampled in a network of 168 stations over most of western and central Europe. The sampling resolution was 3 h und its total duration was 90 h (30 samples per station).

The backward simulation was made with FLEXPART[1], a LPDM tested on various tracer experiments (Stohl et al., 1998). It performed well for the ETEX-1 release (correlation coefficient 0.59, fractional bias = 0.01). It was applied with the following specifications:

- Input: ECMWF fields (0.5°, 31 levels, 3 h).

- 30 backward runs (one for each sampling interval)

- 10,000 particles released from each monitoring site

[1] see http://www.forst.tu-muenchen.de/LST/METEOR/stohl/flexpart.html

- each monitoring site was represented by a separate species of the pseudotracer
- the output was sampled in 3 h intervals on a 41x21 grid with 1° resolution, 9 vertical cells (0/75/ 150/300/600/1200/2400/3600/4800/6000 m), 35 time intervals, or with 1 h resolution in 105 intervals.

The SRM thus has (41x21x6x35) x (168x30) = 180,810 x 5740 $\approx 1 \cdot 10^9$ elements. In sparse matrix format, this amounts to approximately 300 MB of data. This matrix is too big for direct evaluation and one of the following simplifications have to be made:

1) Take only lowest layer (or vertical integral), as pseudotracer concentrations are well mixed near the release site.

2) Assume either location as given (sample application: nuclear power plant accident), or release time (sample application: nuclear explosion with core time known from nuclide ratios).

Alternatively, one could start with coarse source resolution and narrow it down iteratively while reducing the domain size.

Results

A useful first visualisation can be obtained by plotting fields that would result if the backward simulation would have been made with releases proportional to the measured concentrations at each receptor. Such plots can be made for each pseudosource (measurement station) separately, or for the sum of all. Plots can show, e.g., horizontal fields at different time interval as in Figure 1 (or a loop over the whole simulation), or the time evolution at the true release site (Figure 2). The fields shown in Figure 1 correspond to classical "trajectory statistics", or the fields presented by Pudykiewicz (1998). It is not yet an inversion, but nice to illustrate the backward simulation. Figure 2 is especially useful to find outliers – measurement sites whose pseudotracer puffs arrive at a completely wrong time at the release location.

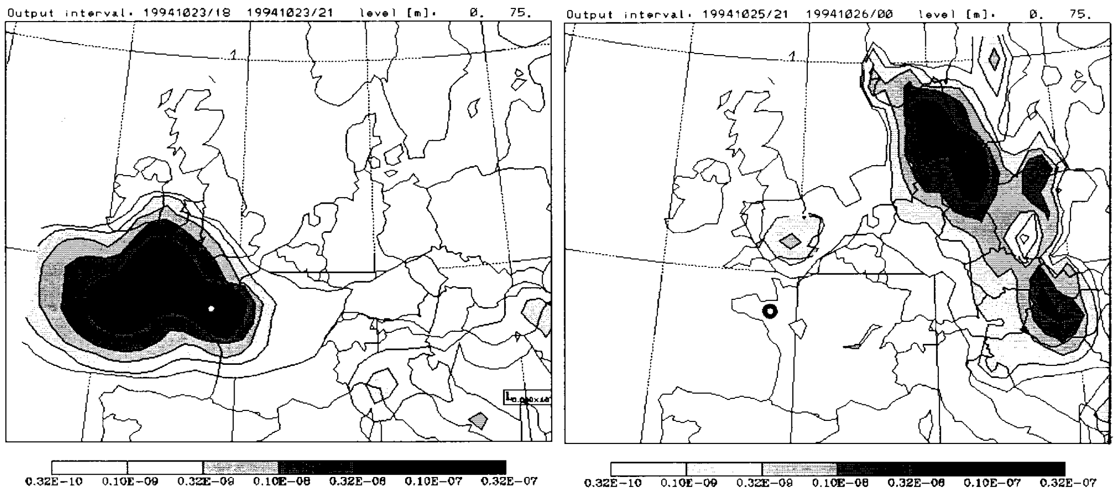

Figure 1. Horizontal distribution of pseudotracer (3 h means) released at the measurements sites proportional to measured tracer concentrations, sum over all sites (logarithmic scale). The real release location is marked by a hollow black dot. Left: situation during the time of the real release (23 Oct, 18-21 UTC); right: situation during a previous stage of the inverse simulation (25 Oct, 21-24 UTC).

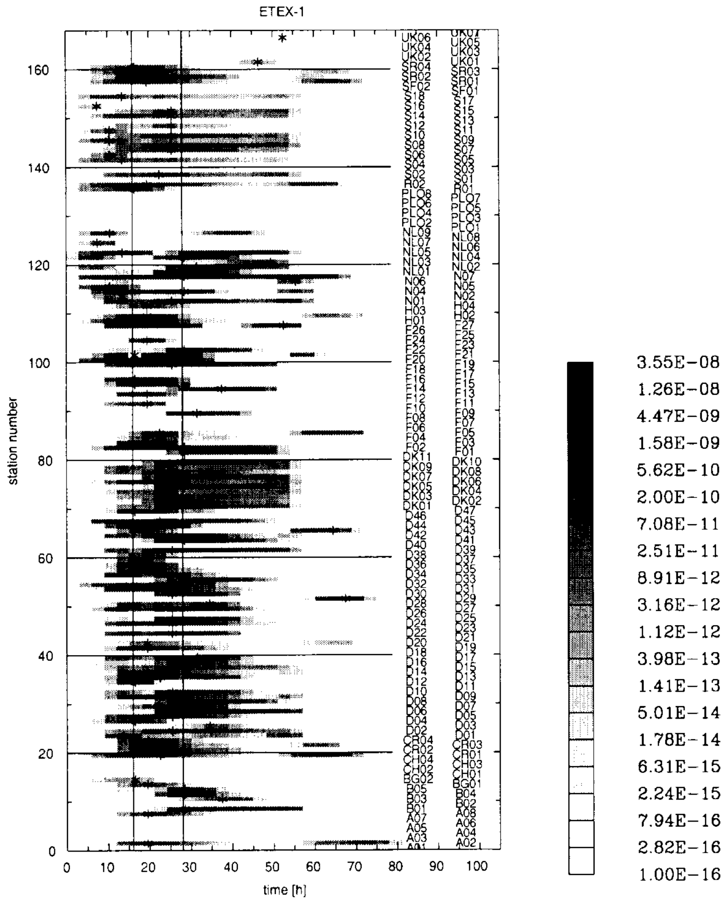

Figure 2. Time series (3 h means) of pseudotracer released at the measurements sites proportional to measured tracer concentrations, sampled at the true release site (logarithmic scale). Each line corresponds to one measurement location (denoted by its ETEX station code) and the sum over all measurement intervals. Asterisks denote the maxima, and vertical lines the begin and end of the real release.

For the inversion, the linear system of equations resulting from the linear source-receptor matrix is solved using a simple regularisation. This regularisation requires that the variance of the solution is small and (optionally) that it is also smooth, meaning that the Laplacian is small. (see Seibert, 1999, for details). The inversion was carried out either for the location of the release with the temporal variation given, or vice versa. It worked well (see Seibert, 2000, for details), though more work is required on the regularisation for point sources and sudden on/off-type sources as well as on the relative weighting of observations.

Conclusions

Backward simulations with LPDMs have been established as a useful tool for source-receptor matrix determination. No code changes are necessary for this application. The inversion of the source-receptor matrix to reconstruct the source location and temporal evolution gives good results for the ETEX case, but some more work on the regularisation should be done for sharply bounded releases. The method appears to be useful for the application to nuclear explosions or nuclear power plant accidents.

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