Inverse Dispersion Modelling as a Tool to Derive Emission Data from Measurements

A contribution to subprojects GLOREAM and GENEMIS-2

Petra Seibert and Helga Kromp-Kolb

Institute of Meteorology and Physics, University of Agricultural Sciences Vienna, Türkenschanzstr. 18, A-1180 Wien, Austria (petra.seibert@boku.ac.at)

Summary

The main achievement of the year was the development of a new method to derive source-receptor matrices from backward runs of a Lagrangian particle dispersion model. As this type of model is more accurate than a Lagrangian box model, it will be used for all our future work. The method has been applied to the first tracer release of the European Tracer Experiment ETEX, and in combination with previously developed inversion methods proved capable of localising the source either in time or in space.

Aim of research

This contribution aims at the development of inverse modelling methods to derive information on emissions from measurements in the regional scale. Such methods shall be applied to suitable data sets and results be compared with conventional emission estimates. In addition, recommendations on the optimum monitoring network design shall be made.

Activities during the year

- A new method has been developed for the derivation of source-receptor matrices from backward simulations with Lagrangian particle dispersion models. The method was used with the model FLEXPART for the first release of the European Tracer Experiment ETEX. The source-receptor matrix was then inverted in a reduced form to derive either the horizontal location or the temporal evolution of the release. The inversion method developed previously (Seibert, 1999) was used.
- Results were presented at the 3rd GLOREAM Workshop (Seibert and Stohl, 2000).
- The precipitation fields from ECMWF and from the ATMES data base (analysed fields from the KNMI) have been merged in preparation for the calculations aimed at reconstructing the source term of the Chernobyl nuclear disaster.
- Contacts were made with the Comprehensive Test Ban Treaty Organisation (Preparatory Commission) in Vienna, and project team members participated in the Working Group B of national technical experts. This organisation, whose task includes the monitoring of the nuclear weapons test ban, is a potential user for the methods developed.

Principal results

It has been shown that a Lagrangian particle dispersion model (LPDM), e.g., the model FLEXPART which is used in the project (Stohl et al., 1998), can be employed in backward mode to derive source-receptor relationships. One just needs to release a unit emission during each measurement interval from each measurement site, trace it back with a negative time step, and evaluate concentrations on the spatio-temporal grid of potential source elements. There is no need to modify the code if the backward time step is already implemented. The only modifications made to FLEXPART were a possibility to switch off the recently introduced density correction (Stohl and Wilson, 1999) because the formulation requires mixing ratios rather than mass concentrations, and some technical changes so that each emission is associated with a separate species which makes the calculations more efficient. The theoretical derivation so far is limited to the case without sinks of the substance under consideration but it should not be too difficult to extend it to cases with sinks that are proportional to the mixing ratio, such as dry and wet deposition or a chemical decay with a rate that is independent of the substance's concentration.

This method is more efficient than forward calculations if the number of potential source elements is larger than the number of measurements. In addition, it is has the advantage that the measurement sites can act as real point sources/receptors, which is neither possible in the forward mode of a LPDM nor in a forward or backward (adjoint) mode of a Eulerian model. This should improve the accuracy.

The method has been successfully applied to the first release of ETEX (see the special issue of *Atmospheric Environment* [Vol. 32, Issue no. 24, 1998] for more background on ETEX). So far, either the temporal evolution of the release has been reconstructed with the location given, or the location was reconstructed with the temporal evolution given. Results are shown in Fig. 1-3.

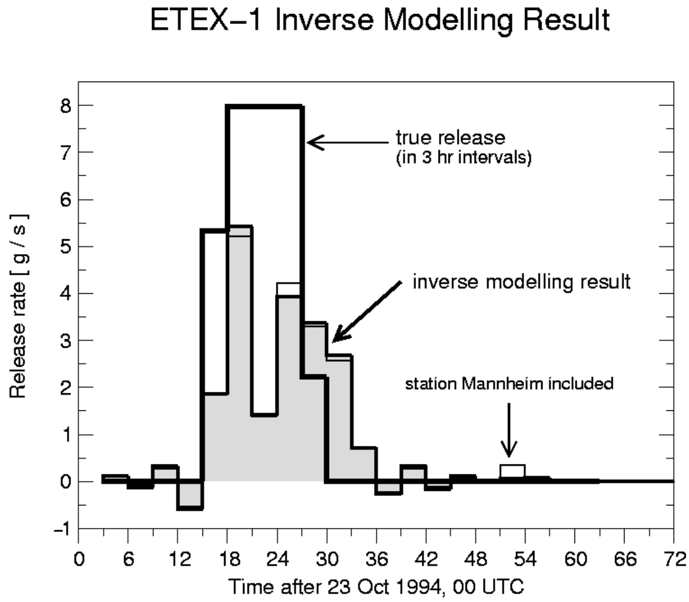

Fig. 1: True and reconstructed temporal evolution of the first ETEX release, based on a 3-hourly source resolution. (Reproduced from Seibert and Stohl, 2000).

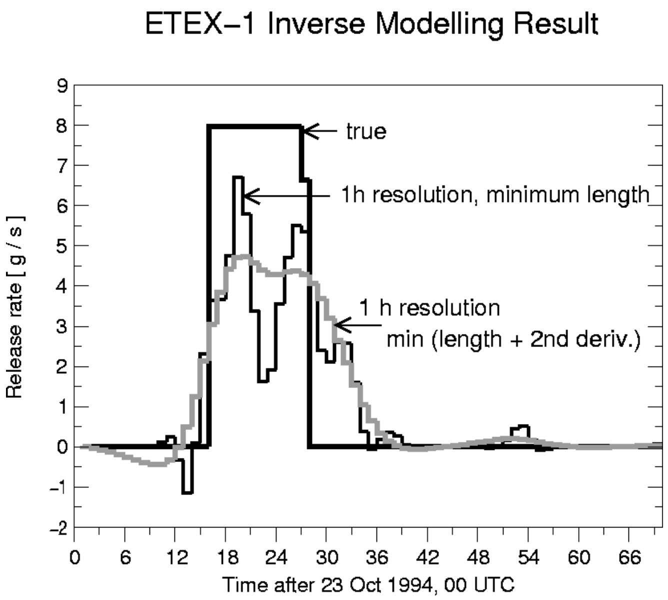

Fig. 2: True and reconstructed temporal evolution of the first ETEX release, based on 1-hourly source resolution, with different types of regularisation used in the inversion. (Reproduced from Seibert, 2000, to be published by Plenum Publishers, New York).

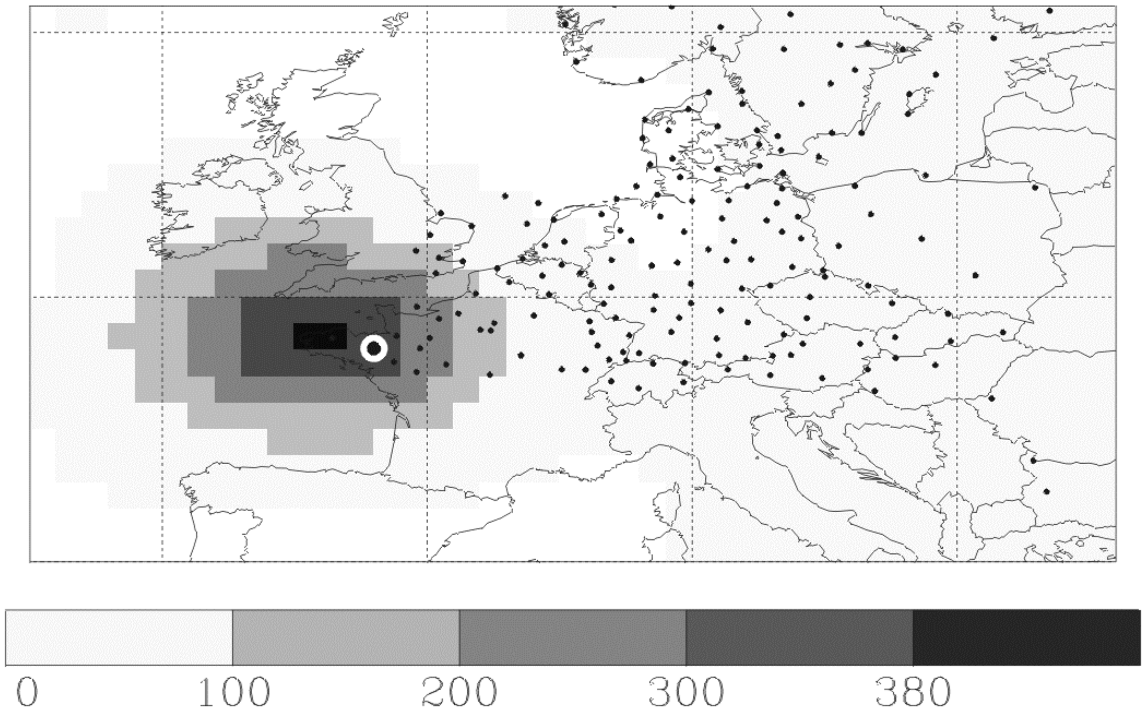

Fig. 3: Reconstruction of the spatial distribution of the first ETEX release, based on a inversion with 1-hourly source resolution, and a regularisation requiring a smooth field. The true source location is marked by a black dot in a white circle, and measurement sites are marked by small black dots. (Reproduced from Seibert, 2000, to be published by Plenum Publishers, New York).

Figures 1 and 2 show that the evolution of the release was reasonably well reconstructed, especially the beginning, whereas the end is not as sharp as it should be. This is probably due to observations remaining longer above the background than explained by the forward simulation. Outliers (e.g., the station Mannheim) can have a visible impact on the result. Moving to a better source resolution (1 h instead of 3 h, Fig. 2 instead of Fig. 1) helps to increase the accuracy (e.g. in terms of bias of the total release amount) but brings a clearer tendency for the reconstructed source to be divided into two separate releases. Applying an additional constraint in the inversion, namely not only minimisation of its variance but also of its roughness (second derivative), yields a rather realistic shape though of course the sudden on/off of the true release cannot be reproduced. This would require a more sophisticated regularisation. This effect is also visible in Figure 3 with the spatial distribution of the reconstructed source. The source is smeared out over several grid elements. However, the maximum comes quite close (about 2 grid cells, or ca. 150 km) to the true source location.

For more information, please check the project web page at
http://boku.ac.at/imp/envmet/ invmod.html

Aim for the coming year

- Expansion of the theoretical basis of source-receptor matrix derivation from particle dispersion models to the case including sinks.
- Refinement of the regularisation schemes, including non-linear schemes to accommodate rectangular and peak-shaped emission patterns.
- Participation in a test for the Comprehensive Test Ban Treaty verification using the radionuclide monitoring network.

- Application to other tracer experiments (CAPTEX, ANATEX) and the release from the Chernobyl nuclear disaster 1986.
- Application to air pollution data.
- All applications shall be carried out with FLEXPART and not with the box model IMPO as originally foreseen.

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References

Seibert, P.; Inverse modelling of sulfur emissions in Europe based on trajectories. *Inverse Methods in Global Biogeochemical Cycles AGU Geophysical Monograph Vol. 114,* eds. P. Kasibhatla et al., (1999) 147-154.

Seibert, P., A. Stohl; Inverse modelling of the ETEX-1 release with a Lagrangian particle model. *Proc. Third GLOREAM Workshop*, Ischia, Italy, Sept. 1999 (2000), in print.

Seibert, P.; Inverse modelling with a Lagrangian particle dispersion model: application to point releases over limited time intervals. *Proc. Millenium International Technical Meeting on Air Pollution Modeling and its Application XIV*, eds. S.-E. Gryning and F.A. Schiermeier, (2000), in print.

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Results of possible policy relevance

A possible area of application arose during the reporting year: the newly developed method would be well suited for finding source areas in the context of the Comprehensive Test Ban Treaty, applying it to the radionuclide monitoring network.

More policy-relevant applications are expected with the work planned for the following year.

Theses

Publications

Seibert, P.; Inverse modelling of sulfur emissions in Europe based on trajectories. *Inverse Methods in Global Biogeochemical Cycles AGU Geophysical Monograph Vol. 114,* eds. P. Kasibhatla et al., (1999) 147-154.

Seibert, P., A. Stohl; Inverse modelling of the ETEX-1 release with a Lagrangian particle model. *Proc. Third GLOREAM Workshop*, Ischia, Italy, Sept. 1999 (2000), in print.

Seibert, P.; Inverse modelling with a Lagrangian particle dispersion model: application to point releases over limited time intervals. *Proc. Millenium International Technical Meeting on Air Pollution Modeling and its Application XIV*, eds. S.-E. Gryning and F.A. Schiermeier, (2000), in print.