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Interactive Comment

Interactive comment on "Adjoint backtracking for the verification of the Comprehensive Test Ban Treaty" *by* J.-P. Issartel and J. Baverel

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General comments

This paper is motivated by the need to derive statements about possible or probable source locations for anomalous radionuclide measurements that may be observed in the global radionuclide measurement network which is under construction for the verification of the Comprehensive Nuclear-Test-Ban Treaty. It introduces the adjoint of a Eulerian transport and diffusion model as a tool to calculate source-receptor matrices (my wording) for these observations in Section 2. Sections 3-5 refer to an event encountered during test measurements at one single station and present methods of various complexity for drawing conclusions on the source based on these measurements (in

Section 5 together with hypothetical other measurements) and the atmospheric transport calculations.

Basically, the paper is scientifically sound; a few problematic issues are addressed in the Specific Comments section. However, the authors appear to be aware only of a small segment of related work that has already been done in the atmospheric science community. The derivation of the adjoint form of the advection-diffusion equation is nothing new (e.g., Elbern and Schmidt, 1999; Kaminski et al., 1999). The methods presented for making inferences on sources are more original, though much more general solutions have been presented, mostly under the heading of "inverse modelling".

Given the fact that simpler methods often do have their justification, e.g., because they are better understandable or involve fewer additonal assumptions, and that the CTBT is a relevant practical problem, I think the paper could be published. To have maximum impact, however, the language which is often unnessarily complicated or speaking more in mathematical than in physical terms, could be improved. Clear definition of terms seems to be an urgent matter for the CTBT atmospheric transport context. Though I am not expecting that it will be solved in this paper, I have included a few hints.

I have had the pleasure to work on atmospheric transport and source location issues in the CTBT context together with Jean-Pierre Issartel and several other colleagues from around the world in an so-called "Ad-hoc Expert Group on Atmospheric Transport Modelling", convened by the Preparatory Commission of the CTBTO, in the first half of 2001. I am surprised that this group and its final report are not mentioned in the paper.

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Specific comments

1. The authors could give a bit more visibility in abstract and introduction to aerosols and their role in the CTBT – there are 80 aerosol stations in addition to the 40 noble gas stations. Even underground tests may vent some iodine, for example.

2. p. 2134, l. 12: The method is not really new, it is made up of known components (adjoint Eulerian transport model, inverse modelling).

3. p. 2134, l. 13: "interpretation of the adjoint transport equation as an inverse transport equation" – what is meant by "inverse transport equation", especially in a turbulent medium? Can one expression be explained by another one whose definition is not really clear? A few lines below, we read "equation which is both adjoint or inverse". This wording is confusing.

4. p. 2134, l. 17-18: "we endeavoured nevertheless ... to establish it on a theoretical basis": There is no lack of theoretical basis in previously published works. A formulation like, for example, "For practical reasons, we include our derivation in Section 2." would be more appropriate.

5. p. 2134, l. 19: The word "retroplume" is used here and elsewhere in the paper. A few people have recently started to use this term (Kalinowski, 2001; Stohl et al., 2002). It is not (yet) an established, well-defined scientific term. I think it was coined on the basis of the visual impression of a plot of the output of a backward-running transport and dispersion model. I suggest that it is used – if deemed necessary at all – with care, and might better be accompanied by a clear definition.

6. p. 2134, l. 24ff.: It might be useful to include more general references about the CTBT and its verification system.

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7. p. 2136 l. 11: Eq. 1 is said to define an exchange rate ϵ, but the its unit is kg^{-1}, so it cannot be a rate which would be something per time.

8. p. 2136 l. 15: "concentration per unit mass of air" – This is normally called a *mass mixing ratio*. It is not so very fortunate to use the symbol c for that, as much more often mass concentration is designated by c. People use also χ, μ or q for the mass mixing ratio.

9. At some locations symbols are introduced without proper explanation of their meaning (may come only much later). Examples are ζ in Eqs. 3 and 4, or μ, u, and y on page 2138.
   Given the fact that units of concentrations, measurements and sources can vary (for example, a source can be expressed as total mass, mass per time, mass per volume, mass per volume and time, or mass mixing ratio change per time, and so on), it would be very helpful if together with a symbol also its unit would be introduced.
   Readability could be improved by keeping the notation as simple as possible, e.g., the position of Freiburg could be designated by x_F (as positions are designated x in this paper) instead of ξ_F (p. 2140). Sources (integral and rates) are denoted q, K, D and σ, which is confusing. Stick to a single symbol and if possible use the `\dot{...}` (temporal derivative) to denote rates.

10. p. 2136, l. 22: What is the difference between σ and q? Why is q dimensionless if it denotes an amount of tracer? Why should the general transport and diffusion equation (2) and its adjoint hold only for a specific value of the tracer released?

11. p. 2137, l. 18-21: This discussion of turbulent diffusion is not sound. Atmospheric turbulence is not "microscopic turbulent motions averaged into a macroscopic diffusion". Turbulent 'diffusion' (a sloppy term by itself) is caused by macroscopic motions, though molecular friction is the final sink of turbulent kinetic energy. The point is rather that atmospheric turbulence, or at least, atmospheric turbulence

as described by K-theory, behaves like Fickian diffusion. The meaning of the last sentence, "The obstacle of an unphysical anti-diffusion, classically restricting backtracking to the Lagrangian investigation of individual backtrajectories, is avoided in this Eulerian approach." is obscure for me, and I am afraid that it may be based on a wrong notion concerning Lagrangian models in backward (adjoint) mode. See also Specific comment # 17.

12. p. 2137, l. 3ff.: The units of σ, π in Eqs. 5 and 6 dont match the previous definition. According to Eqs. 3 and 4, the units of σ, π must be s^{-1}, whereas according to Eqs. 5 and 6 it would be s^{-1} kg^{-1}. The following discussion of these variables and their units, probably aiming at clarifying this seemingly contradicting definitions, is not well understandable. Maybe it is just an English language matter, but at least I could not get the sense.

13. p. 2138 l.15-20: Another example of a complicated, difficult-to-understand wording. It seems to me that it is mainly referring to the textbook fact that only mixing ratios, not mass concentrations, are conservative quantities in atmospheric transport (see also Seibert, 2001).

14. p. 2138 l. 23 - p. 2139 l. 5: It is already well known in the atmospheric science community that the diffusion operator is self-adjoint (e.g., Elbern and Schmidt, 1999). The relevance of the reference to kinetic gas theory is not clear to me.

15. p. 2139, l. 18-24: A clear distinction is lacking between (standard) back trajectories, calculated from the mean wind field, and a backward-running Lagrangian particle dispersion model (LPDM), taking into account also turbulent fluctuations of the wind velocity and possibly other process such as deposition or decay. The output of an LPDM is rarely looked at in the form of particle trajectories, rather as (adjoint) concentrations or as particle positions.

16. p. 2140, l. 1-2: The formulation "It is often considered that, if many backtrajec-

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tories go back to a certain region, then the source is probably there." is rather vague. Of course, if the simulation is sufficiently realistic, the particles of an LPDM (not necessarily the standard back trajectories!) will pass through the source region. However, a localisation of the source amongst all these possible regions is not possible from a single measurement (unless the time of the source is known) and requires some kind of inversion, as the authors discuss later on. The discussion in the next paragraph contributes to my impression that the authors try to construct a wrong view which they ascribe to Lagrangian methods and then prove to be false. I would like to make it clear that source-receptor relationships (my preferred wording which is physically much clearer than "adjoint concentration", which is merely a mathematical tool, or, even worse, than "retroplume", which is more a visual concept) can be calculated by forward or backward (adjoint), Eulerian or Lagrangian methods. If somebody attaches a wrong view to any method (and there is no method which is immune to that), it is their own problem and not a defect of the method.

This unclear language leads to formulations such as "The retroplume establishes a constraint between the position of the source and its intensity." If we substitute s-r relationship instead of *retroplume*, we recognise that the meaning of this sentence is rather trivial.

17. p. 2141, l. 3ff.: My comments to the so-called trajectory calculation are already published on APCD (RC S851).
The authors' response (AC S862) misses the point (to simply leave out the questionable trajectory). They continue to use the terms "Eulerian" and "Lagrangian" in a nonstandard and confusing way. It is not all true that Eulerian calculations must include turbulent diffusion and Lagrangian calculations cannot include it. Both types of models can include that or not. The proper denomination for what Issartel and Beverel call "Lagrangian" would be "(standard/simple) back trajectories".

As for the issue of artificial diffusion in Eulerian models, raised also by Reviewer #1, the authors are simply wrong if they state “Such problems are of course avoided by numerical schemes that have been proposed long ago and are now considered classical (Tiedtke, Bott...).” To my knowledge, Tiedtke has never published an advection scheme (though he is famous for his convection scheme; advection and convection in meteorology denote completely different processes, something that – I admit – is confusing for mathematicians and physicists). And even the best advection schemes just reduce the numerical errors, as confirmed by the authors themselves in their previous answer to Reviewer #1 (AC S849, p. S850). Thus their Eulerian substitute will not match a real trajectory model.

18. p. 2141, l. 16: A source (reference) for these numbers would be desirable.

19. Section 4: As the authors mention, time needs to be descretised in order to solve Eq. 14. It would be desirable to know the time step size used for that purpose, and furthermore it would be very desirable to see the temporal shape of the solution $D(t)$ for some typical locations x.

20. p. 2143, l. 11-13: “when all measurements are from a single station, the same number of local contaminations make up an admissible source” – I don’t understand this phrase. What are “local contaminations”, and to what is “same number” referring to?

21. p. 2144, l. 27: I am not convinced that any nuclear test would “certainly be seen by many stations”.

22. p. 2144/145, 1st paragraph of Section 6: The authors claim that the method that they have presented enables to discern between several local sources (probably from medical or civilian nuclear facilities) and a major release (possibly a nuclear explosion), both affecting several stations. This statement is not sufficiently substantiated, and I doubt it. Already in their Section 5, the authors have shown that

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the actual measurement in Freiburg together with a hypothetical one in Stockholm is compatible with a source around Scotland. Even if the temporal shape of such a source would be too unrealistic, or – especially in the case of more than two stations – indeed no single point would be compatible with all the measurements, there is no way to rule out that one part of the stations was affected by a civilian release while one or more remaining stations still were measuring products of a nuclear explosion. I don't see a way around using nuclide ratios and/or knowledge about civilian sources to discern events they cause from those events that may constitute a violation of the Treaty.

23. p. 2145, l. 2145ff: The authors argue that inversion of the source-receptor matrix together with measurement data as I proposed and tested (Seibert, 2001) should be called a *data assimilation technique* because the system is generally drastically underdetermined. Besides the fact that the underdetermination depends on the details of the setup, the LSEs solved by Issartel and Beverel as indicated in their Eq. 16 are underdetermined as well. Just as I did, they introduce regularisation, obviously to overcome this underdetermination, though they choose not to make that explicit. But the introduction of the condition that the total release should become a minimum is a regularisation method, very similar to the standard Tikhonov regularisation which minimises the sum of squared elements of the source vector instead of the sum of its elements. It assumes as a-priori knowledge that the source should be as small as possible within the bounds allowed by the measurements with their error margins. Of course, this will cause the model estimates for the measurements to have a negative bias and will thus not yield the most probable solution. Furthermore, underdetermination is not the criterion for data assimilation versus inverse modelling. To my understanding, in *data assimilation* the main intention is to reconstruct an *initial condition* at locations and/or for species where there are no measurements, using the information in the measurements together with the information about transport, whereas in

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inverse modelling the intention is to infer information about *sources of trace substances*.

Unfortunately, it seems that the authors have not realised that I did almost the same as they did in their Section 5 when I tried to find the location and the temporal shape of the ETEX-1 release simultaneously from the measurements by trying out each grid as possible source (see Seibert, 2001; Seibert et al., 2002). This is as well a decomposition of a large linear system into a number of smaller ones, each relating to one possible location of a one-grid source. Issartel and Beverel plot resulting total releases, or blank if there is no release compatible with their binary constraint. As already pointed out, I believe that the binary constraint ("hard" bounds for the measurements) is not ideal. In reality, in statistical terms, there is a continuous probability distribution for each measurement. The misfit between modelled and observed concentrations, which I plotted, is therefore a more robust and informative (not just binary) measure of whether a source should be suspected in some place or not. Of course, the amount of the hypothetical release needed in that place to fulfil the measurements is also quite important, but it is a different matter, and should not be calculated with a regularisation that causes strong negative bias (note that – though I did use a different regularisation – I also got a negative bias for the total release).

24. p. 2146, last paragraph: As already explained, I believe that "to confirm that a set of positive measurements is due to several local events" is not possible with purely mathematical methods.

25. p. 2146, l. 9-11: Nonnegativity is not just a "theoretical aim", and the paper quoted by the authors is just one out of many. Already the text book by Menke (1984) includes a section "L_2 problems with inequality constraints", including a sample Fortran programme.

Technical corrections

1. Though abbreviated CTBT, the full name of the Treaty is "Comprehensive *Nuclear*-Test-Ban Treaty" (see CTBTO's web page). This relates to the paper title and the text.

2. Replace dots (.) in units (intended as multiplication sign) by a small space (`\,` or ~ in LaTeX).

3. p. 2135 l. 24: "fourteen Cartesian levels at 32, 150, 360,..., 6000 m above ground or sea level" – What is a "Cartesian level"? A Cartesian co-ordinate system is one with right angles between the co-ordinate surfaces, which is not the case for a terrain-following co-ordinate system. Maybe just drop "Cartesian".

4. p. 2137 l. 22: The wording "Eq. 4 rebuilds a macroscopic history of the air" sounds a litte awkward. What is "history" of air, and how could it be "rebuilt"? "Macroscopic" – everything discussed in this paper is about macroscopic features; maybe "grid-scale" would be more appropriate.

5. I am wondering whether "time Dirac" (p. 2137 l. 5) and "space Dirac" (p. 2141 l. 1) are proper English or a kind of sloppy 'lab (math?) slang'.

6. p. 2142 l. 10: "undergoes the four constraints" replace with "is subject to the four constraints".

7. p. 2142 l. 13: "were possible errors are widely taken into account": Replace by "where possible errors are taken into account with wide margins" or similar, if this is what you mean.

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References

Elbern, H. and H. Schmidt (1999), A four-dimensional variational chemistry data assimilation scheme for Eulerian chemistry transport modeling. J. Geophys. Res. 104(D15), 18583 - 18598.

Kalinowski, M.B. (2001), IDC needs for atmospheric transport modelling and first experiences with the IDC Release 2.1 application software including HYSPLIT, OMEGA, and EDGE. In: Jean, M. and Seibert, P., Informal Workshop on Meteorological Modelling in Support of CTBT Verification, Dec. 2000, Vienna; On-line and on CDROM.,

Kaminski, T., M. Heimann, and R. Giering (1999). A coarse grid three dimensional global inverse model of the atmospheric transport, 1, Adjoint model and Jacobian matrix. J. Geophys. Res., 104(D15):18,535-18,553.

Menke, W. (1984), Geophysical Data Analysis: Discrete Inverse Theory. Academic Press, Orlando, 260 pp.

Seibert, P. (2001), Inverse modelling with a Lagrangian particle dispersion model: Application to point releases over limited time intervals. In: F. Schiermeier & S.-E. Gryning (eds.), Air Pollution Modeling and its Application XIV, pp. 381-390

Seibert, P., Frank, A., Kromp-Kolb, H. (2002): Inverse modelling of atmospheric trace substances on the regional scale with Lagrangian models. In: Pauline Midgley, Markus Reuther, EUROTRAC Symposium 2002, 11-15 March 2002, Garmisch-Partenkirchen; Transport and Chemical Transformation in the Troposphere.

Stohl A., S. Eckhardt, C. Forster, P. James, N. Spichtinger and P. Seibert (2002): A replacement for simple back trajectory calculations in the interpretation of atmospheric trace substance measurements. Atmospheric Environment 36(29), 4635-4648.

Interactive comment on Atmos. Chem. Phys. Discuss., 2, 2133, 2002.