Atmos. Chem. Phys. Discuss., 2, S1003–S1013, 2002
www.atmos-chem-phys.org/acpd/2/S1003/

Atmospheric Chemistry and Physics Discussions

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

J.-P. Issartel and J. Baverel

Received and published: 10 February 2003

We thank the referees for their detailed reading of our paper and for their accurate comments. Referee 1 pointed out in a kindly manner the confusion of some definitions and the unsufficient discussion of some results. We shall try to improve again the intelligibility of our paper according to his advice.

We still have to answer the last comments of Mrs Seibert, referee 2. We are very grateful to her for, despite the fact she is perhaps a bit too personally involved, reading and commenting so abundantly our work, pointing out the weakness of some difficult explanations given too quickly. She has a great practice of adjoint methods and inverse problems and apparently considered our work as a part of this background as suggested by our title 'Adjoint backtracking...'. Our paper is not really about adjoint techniques but about inverse transport shown to be a physical interpretation of adjoint techniques. We shall think of changing the title. Accordingly some of our deductions were mistaken with old and straightforward computational results and our vocabulary was judged confuse. Inverse transport has been defined in hici99 and hois00 from the idea that the air sampled for a tracer measurement existed before being sampled and was transported and scattered in the environment with a concentration homogeneised in the past in a retrograde manner. This is not an adjoint definition. The identification of inverse transport and adjoint transport is unfortunately both intuitive, so that one might think there is no problem at all, and very technical, requiring an accurate quibbling vocabulary precisely as a protection against confusion. In fact we believe the confusion felt in our wording and formulas comes, at least partly, from the nature of things. When preparing this work we always felt that it would be so easy to say wrong things despite, or perhaps because, of a strange combination of good and bad intuitions raised by backtracking. We give three examples of slippery subjects. Firstly diffusion is irreversible but works the same way towards the past as towards the future. Secondly the retroplume is a probability distribution for particles and is a non statistic source-receptor matrix for macroscopic sources. Thirdly we infered that diffusion is self-adjoint, a general result already known in kinetic theory, not to be mistaken with the (not so) obvious computational fact that the Fickian closure is self-adjoint (for an adequate form of the measurement product). Explaining the third point is really a nightmare as most meteorologists think 'Fickian closure' as soon as they hear 'diffusion' and because setting the problem and solving it is mainly a matter of appropriately choosing mathematical conventions. This amounts to using intricate empty-looking tools to solve an unexpected problem. It is nevertheless the price to be paid for a correct comparison of the two natural approaches of backtracking : inverse transport (the idea that the air sampled comes from somewhere) and adjoint transport (the idea that the receptor is influenced by sources). The coincidence of the two intuitions has been seen by ulpi91 (a reference indicated to us by P. Seibert long ago) but these authors did not see the role of conventions so that their explanations are valid only when the density ρ is uniformly constant. We hope with Mrs Seibert that the meteorologists will build a greater familiarity with these topics so that it will be possible to take more liberties with the wording.

The referee kindly reminds we were both involved during the spring 2001 in an Ad-hoc Expert Group on Atmospheric Transport Modelling. This is a nice souvenir for us too and we shall enthusiastically agree her proposal to quote the technical report of the Group ctbt01. We first did not quote it because our ACPD paper is based upon our previous contribution (either not yet quoted) issa00 to the 'Informal Workshop on Meteorological Modelling in Support of CTBT Verification' held in Vienna on 4-6 December 2000.

We now consider the specific comments of referee 2.

specific comment 1 : The definition of inverse transport as regards the aerosols is not as straightforward as that of adjoint transport. We prefer not to raise the problem in this paper.

specific comment 2 : Everything is a combination of older things!

specific comments 3, 4, 5, 10, 12 : Inverse Transport has been previously defined in hois00 referenced in our ACPD paper. Based on this previous work we give a definition of the retroplume by using the notion of 'exchange rate'. This leads to a definition that is very useful but not so intuitive.

Fundamentally a retroplume is defined by considering that the air sampled for a measurement existed before being sampled and was spread among the ambient air with a concentration $C^*(\vec{x}, t)$. Inverse transport merely amounts to calculating $C^*(\vec{x}, t)$ which we call the concentration of the retroplume associated to the measurement. If we are using concentrations per unit mass, the (concentration of the) retroplume C^* defined this way has no dimension : unit mass of air sampled per unit mass of ambient air. Nevertheless the practical use of inverse transport goes through the exchange rate ε which does not depend on a proportionality coefficient on the amount A of air sampled by the detector. Therefore we are using throughout the paper a 'normalised retro-

ACPD

2, S1003–S1013, 2002

Interactive Comment

plume' $c^*(\vec{x},t) = \frac{C^*(\vec{x},t)}{A}$. This normalised retroplume is associated to a dimensionless unit sample: the amount of tracer scattered back in time is a dimensionless unity. The unit of c^* is now the inverse unit mass of air. We shall try to make a clearer distinction between 'retroplume' and 'normalised retroplume' in an improved version of our paper.

The word 'retroplume' is perfectly logical as the retroplume has exactly the same behaviour as a standard plume, except that the time has to be reversed. It is not just a visual impression. The word has been used in the discussions of the CTBT since 1997 and can be found in our contribution issa00 to the Informal workshop of December 2000 (M. Jean and P. Seibert editors of the proceedings), i.e. before the examples quoted by Mrs Seibert. It is to be stressed that the above definition (with or without normalisation) does not rely on any adjoint technique. It is one purpose of the ACPD paper to show that this definition is indeed equivalent to an adjoint definition, and that this equivalence has consequences. It is strange that the referee contests in her sp. com. 4 that there is any 'lack of theoretical basis' while recognising in sp. com. 5 that some authors would have to use the word 'retroplume' as a not well-defined scientific term.

The 'source receptor matrix' of the referee is called a 'Green function' in standard wording of signal theory (this wording is well known of seismologists). The part of the source receptor matrix describing the influence of a given (point-)source over all potential (point-)receptors is, up to a normalizing coefficient, the object known as a 'plume'. We symmetrically call 'retroplume' the part of the Green function describing the influence on a given receptor from all potential sources. The term 'source receptor matrix' has also the drawback to be oriented towards one of many interpretations of the retroplume thus hiding its much more intuitive meaning as a probability distribution for Lagrangian particles. We precisely think that here is an example of the confusion raised by backtracking rather than by our wording. The non-statistic meaning of the retroplume regarding macroscopic sources, simultaneously (as far as we know) clarified by seib00 and issa00, has long suffered confusion due to the statistic meaning

ACPD

2, S1003–S1013, 2002

Interactive Comment

regarding microscopic sources (i.e. particles).

specific comment 7 : The word 'rate', is often used to describe something per unit time. In the use we make of it there is no such idea. We are not native english speakers, but we think that the word 'rate' may be more generally used to designate any proportion.

specific comment 8 : We prefer to go on with the expression 'concentration per unit mass of air' in order to maintain the symmetry of vocabulary between standard plumes and retroplumes and with the letter c, c^* which is used with the same meaning in hois00. A retroplume is indeed defined as the concentration of something, namely the air of the sample. Nevertheless, we shall propose the expression 'mass mixing ratio' between parenthesis for readers that are more familiar with it.

specific comment 9 : Thank you for pointing out some incoherence in the order of definitions. The objects q, K, σ, D correspond to different things that have to be denoted by different symbols. $\sigma(\vec{x}, t)$ is the general form of a source, an amount of tracer per unit mass of volume and per unit time. In our paper it is generally normalised : $\int \sigma d\vec{x} dt = 1$ so that the intensity q of the source and its dispersion are separate problems. q is the intensity of the non normalised real source. When the source is known to be a point, the release of tracer may be described by a rate $D(t)$ which is an amount of tracer per unit time. $K(\vec{x})$ is the minimum amount tracer of acceptable for a source in $\vec{x}$ compatible with a set of measurements. When only one measurement is considered, we use the notation Q instead of K. We shall give more accurate definition of these objects, in particular with respect to normalisation.

specific comments 11, 16 : We use the words 'macroscopic' and 'microscopic' only in order to discriminate between the large scales explicitely resolved and the smallest scale that are not explicitely resolved. In practice, microscopic will mean 'sub-grid scale' which Mrs Seibert understood according to her suggestion of technical correction 4. It is a fact that the investigation of sources has often been proposed through a backward integration of the windfield often considered only close to the ground. Our opinion is that this use of Lagrangian calculations was motivated by the thought that irreversible diffusion could not be taken into account for eulerian calculations. We agree that Mrs Seibert has a different opinion. Nevertheless we do not fully agree her opinion that 'of course, if the simulation is sufficiently realistic, the particles of a Lagrangian Particle Dispersion Model will pass through the source region'. Suppose an important source lies in a region with a weak exchange rate $\varepsilon = 10^{-19}$ kg^{-1}. The probability to find at any given moment a particle transported backward from the detector inside a mesh of 100 km x 100 km x 100 m (roughly 10^{12} kg) around the source is 10^{-19} x $10^{12} = 10^{-7}$.

specific comments 13, 14 : As an illustration of the fact that the self adjoint character of diffusion would be well known in the atmospheric science community the referee quotes the work of elsc99. We found nothing in this reference about the self adjoint character of diffusion. On the contrary, in the forward equation (7) of Elbern and Schmidt diffusion is accounted for by a Fickian closure $-\nabla\ \rho\kappa\ \vec{\nabla}\ \rho c_i$ and in their adjoint equation (8) it becomes $-\frac{1}{\rho}\ \nabla\ \rho\kappa\ \vec{\nabla}\ \delta c_i^*$. This is not the same! The explanation of this difference is given on p. 2138, l. 15-20. The understanding of this point requires a very accurate wording. The concentration c_i used by Elbern and Schmidt is, unlike our c, a concentration of tracer per unit volume. Their adjoint equation (8) is through the simple scalar product $\mu(c_i, \pi) = \int c_i \pi d\vec{x} dt$. As a consequence of this choice, the adjoint variable δc_i^* will be interpreted as a concentration of adjoint tracer per unit mass of ambient air. The difference between standard and adjoint operators is due only to the fact that c_i is per unit volume and δc_i^* per unit mass. This difference would be avoided by using variables $c_i' = \frac{c_i}{\rho}, \delta c_i^*$ both referred to the unit mass of ambient air; these variables are adjoint through the following analytic form of the measurement product : $\mu(c_i', \pi) = \int \rho c_i' \pi d\vec{x} dt$. This problem of an adequate choice of the conventions is very delicate, much attention must be paid to the wording. This is certainly boring but essential for the interpretation of inverse transport.

Nevertheless when saying that diffusion is self adjoint we are not thinking about the

ACPD

2, S1003–S1013, 2002

Interactive Comment

particular Fickian closure used by Elbern and Schmidt and which Mrs Seibert associates to K-theory. Other closures could be proposed. We say that diffusion itself, as defined in fluid mechanics, before any closure operation, is self-adjoint. Accordingly only self-adjoint operators should be proposed as a relevant closure of diffusion. It is perhaps well known that the Fickian closure is self-adjoint (a few calculations are required to see that) but the proposed result is more general. We found an analogous general result only in kinetic theory. The reference mbkk90 is given just because it states very clearly a fact which seems to be known as an evidence by some nuclear physicists. The self-adjoint deep nature of diffusion has also been deduced from physical intuition by ulpi91 but, because of an inappropriate choice of their conventions and scalar product, their result is valid only in a fluid with constant density ρ.

specific comment 15 : The paper is not about models. We do not fully understand the arguments of Mrs Seibert against Eulerian models. They should rather be addressed to the increasing number of scientists building and using them for studying such difficult matters as greenhouse gases or air quality. We think that our use of words Eulerian and Lagrangian is standard. A Eulerian tracer is a continuous tracer described by its concentration at any moment in each fixed position or grid cell. A Lagrangian tracer is a discrete one, the position of each particle being given at each moment.

specific comment 18 : see abhh01 which is not ideal with respect to the accurate numbers.

specific comment 19 : The discretization time step for using the simplex algorithm was one hour. The principle of this method is that only the information about the position of the source is interesting. The rate of release $D(t)$ is positive. The exact shape of D minimising the total release $q = \int D(t)dt$ is not interesting. We never stored it. And anyway, for which supposed position should we? Such more accurate reconstruction of the source term will be considered in a forthcoming paper by means of the method outlined on P. 2145-2146.

ACPD

2, S1003–S1013, 2002

Interactive Comment

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

specific comment 20 : For instance four measurements at station A contaminated by four little releases from a position close to A.

specific comment 21 : See hois00; at northern midlatitudes where industrial Xe133 may be detected, multiple detections of nuclear tests are often probable. But indeed not everywhere as we badly remembered.

specific comments 22, 24 : Mrs. Seibert proposed in December 2000 seib01 to identify an optimum position of the source by minimising a regularised quadratic cost function. This method has two drawbacks. Firstly several positions could often be acceptable for the source, the problem is not to define a best one but to explore all possible hypotheses. Secondly because the best one may fail to be good. As explained in our paper the case should be considered for the operation of the CTBT monitoring network that several local events contaminate almost simultaneously several stations thus conjuring up a nuclear test. Even in that situation a best position will be defined. We say that this situation can be discriminated more carefully in order to see that no position is acceptable for a point source. Mrs. Seibert doubts this and she appropriately notices that sources in Scotland were compatible with the real measurements of Freiburg plus one artificial measurement in Stockholm. We merely forgot to explain that no position is compatible any longer if two zero valued artificial measurements are added in Stockholm just before and just after the positive artificial one thus displaying the rapid evolution tied to a local contamination. In an operational situation, after determining that a set of measurements corresponds to several sources, it is still possible to investigate various selections of stations in order to determine which ones could have seen a test and which other ones were polluted independently. This investigation would usefully complement the observation of nuclide ratios that are different for nuclear tests and civilian releases. It is clear, as emphasized by the referee, that the observation of nuclide ratios cannot be neglected.

specific comment 23 : The discussion is now about a prospective part of our work that shall be illustrated by results in a forthcoming paper. This is a domain where Mrs Seib-

ACPD

2, S1003–S1013, 2002

ert already proposed results seib01 of a great interest as a starting point for further works about, say, data assimilation and inverse methods. We are not saying that her LSE is underdetermined while ours would not be : of course both are. Mrs Seibert argues that her method is equivalent to the one we proposed. We looked carefully and concluded that despite superficial similarities (such as the use of regularisation techniques) the methods are different. Mrs Seibert optimises indeed a vector the dimension of which is the number of grid cells (in space and time) where the widespread source is investigated. The optimisation that we propose (without any result as already reminded) would lead to optimising the coefficients of each retroplume in a linear combination; this makes a vector of dimension the number of measurements.

specific comment 25 : Thank you for insisting about this importance of nonnegativity. We just quoted the references we knew and planned to use.

References

[Arthur et al.(2001)] Arthur, R.J., Bowyer, T.W., Hayes, J.C., Heimbigner, T.R., McIntyre, J.I., Miley, H.S. and Panisko, M.E., Radionuclide measurements for nuclear explosion monitoring, 23rd Seismic Research Review : Worldwide Monitoring of Nuclear Explosions, Jackson Hole, Wyoming, October 2-5, 2001.

[CTBTO/PTS(2001)] CTBTO/PTS, Evaluation of the atmospheric transport modelling tools used at the Provisional Technical Secretariat, Report to the PTS of an Adhoc Expert Group on the evaluation of atmospheric models used at the PTS for radionuclide transport analyses... Preparatory Commission for the Comprehensive Nuclear Test Ban Treaty, Organization, Vienna, report CTBT/EVA/EG-1/1, 73 PP, 2001.

[Elbern and Schmidt(1999)] Elbern, H., Schmidt, H., A four-dimensional variational chemistry data assimilation scheme for Eulerian chemistry transport modelling, J. G.R. 104(D15), 1999.

[Hourdin et al.(1999)] Hourdin, F., Issartel, J.-P., Cabrit, B. and Idelkadi, A., Reciprocity of atmospheric transport of trace species, CRAS, 329, 623-628, 1999.

[Hourdin and Issartel(2000)] Hourdin, F. and Issartel, J.-P., Subsurface nuclear tests monitoring through the CTBT xenon network, Geophysical Research Letters, 27(15), 2245–2248, 2000.

[Issartel et al.(2000)] Issartel, J.-P., Cabrit, B., Idelkadi, A. and Hourdin, F., Localization of sources for events detected during the noble gas equipment test, in Jean and Seibert editors, Informal Workshop on Meteorological Modelling in Support of CTBT Verification, Vienna, December 4-6, 2000.

[McCourt et al.(1990)] McCourt, F.R.W., Beenakker, J.J.M., Köhler, W.E. and Kuščer, I., Nonequilibrium Phenomena in Polyatomic Gases, volume 1, Dilute Gases, International series of monographs on chemistry, 18, Clarendon Press, Oxford, 1990.

[Pudykiewicz(1998)] Pudykiewicz, J., Application of adjoint tracer transport equations for evaluating source parameters, Atmospheric Environment, 32(17), 3039–3050, 1998.

[Seibert(2000)] Seibert, P., Methods for source determination in the context of the CTBT radionuclide monitoring system, in Jean and Seibert editors, Informal Workshop on Meteorological Modelling in Support of CTBT Verification, Vienna, December 4-6, 2000.

[Seibert(2001)] Seibert, P., Inverse modelling with a lagrangian particle dispersion model: application to point releases over limited time intervals, in Gryning and

ACPD

2, S1003–S1013, 2002

Interactive Comment

Schiermeier editors, Air pollution and its application XIV, 381–389, NATO, Kluwer Academic/Plenum Publisher, 2001.

[Stohl et al.(2002)] Stohl, A., Eckhardt, S., Forster, C., James, P., Spichtinger, N. and Seibert, P., A replacement for simple backtrajectory calculations in the interpretation of atmospheric trace substance measurements, Atmospheric Environment, vol. 36 issue 29, October 2002.

[Uliasz and Pielke(1991)] Uliasz, M. and Pielke, R., Application of the receptor oriented approach in mesoscale dispersion modeling, in van Dop and Steyn editors, Air pollution and its application VIII, 399–407, NATO, Plenum Publisher, 1991.

ACPD

2, S1003–S1013, 2002

Interactive Comment