

Interactive comment on “Source-receptor matrix calculation with a Lagrangian particle dispersion model in backward mode” by P. Seibert and A. Frank

P. Seibert and A. Frank

Received and published: 23 October 2003

We are happy that our paper was favourably received by both of the reviewers, and are grateful for their work in evaluating its weaknesses. Below are our answers to the points they have raised (reviewers' comments are *printed in italics*).

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

Review 1

Summary comments

The reviewer seems to regret the ‘intricate accounting detail that tends to obscure the simplicity of the physics’.

We felt that a step-by-step derivation would make the matter better accessible for those not yet acquainted with this methodology. We also believe that it belongs into a paper of this kind. The ‘accounting detail’ for mixing ratio versus mass units at both ends of a simulation is of practical relevance. We have tried to underline the ‘simplicity of the physics’ in a number of places, e.g. in the explanation to Eq. 3 and at the end of Section 2.2. An additional sentence has been inserted into the Abstract.

Specific comments

Can the authors succinctly explain why the backward mode is computationally advantageous (only) if the number of receptors is less than the number of sources?

As written in our paper (p. 4518, l. 10ff), the number of species to be tracked in backward mode is equal to the number of receptors, whereas in forward mode it is equal to the number of sources. The number of species to be tracked can thus be minimised if the backward mode is chosen for the case where the number of receptors is less than the number of sources, and vice versa. If there are just a few area sources and a larger number of point receptors, one may still opt for backward modelling, but in this case for reasons of accuracy and not efficiency. We are making this more clear in the revised version.

It seems to me that the label r^ should appear in the definition appearing immediately*

after eqn (2).

This seems to be a matter of taste. Our idea was that $r(t' = t) = r^*$.

It might be useful to briefly mention why "the approach is based on mass mixing ratios" (p2) and that "particles carry mixing ratios rather than masses" (p4).

On p. 4520, we add "as this is a conservative quantity". On p. 4526, we add: "This is equivalent to the change from $\nabla \cdot \rho \chi \mathbf{v}$ to $\mathbf{v} \cdot \nabla \rho \chi$ between forward and adjoint Eulerian transport models (Elbern and Schmidt, 1999)."

The reference Flesch et al. (1995), given in the context of using backwards Lagrangian models to determine the footprint, and appearing in the left-hand column of page 2, is incorrect: this should be Flesch (1996; Boundary-layer Meteorology, Vol. 78, 399-404).

Flesch's 1996 paper is a small extension of his 1995 paper, so we believe that it is fair to quote primarily the former one.

The convection scheme is interesting and novel. Can the authors explain in more basic terms (than use of the transpose of the redistribution matrix) what is involved in reversing this for the backward scheme?

The following sentences has been added for clarification: "This means that the probability of a particle of having arrived at its present level from another level is considered."

What are the authors meaning when they say, "to convince skeptics" ? To whom is this addressed? Is it necessary to say?

We have met a number of colleagues in the past years who found it quite difficult to accept that it is possible 'to reverse an irreversible process such as turbulent diffusion' (as they initially perceived the procedure). But we have no problem to drop this argument here.

Tests 1 and 2 are rather trivial – I think one can assume the reader will trust that the authors programme is correct. Suppressing those tests will allow space for more

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

explanation of the more interesting tests, especially 4, and the case study (re-emission from contaminated soil due originally to Chernobyl).

Yes, the first two tests are rather trivial – but they helped us to identify a few bugs in the Flexpart programme. As these tests don't appear to be common, and we found them useful, we thought that we would suggest them to others who construct backward or adjoint versions of their models. As there is no page limit in ACP, this should not reduce the space allotted for other tests, and we have – also to respond to other comments of the reviewers – enlarged the respective sections to some extent. One should keep in mind, however, that the Chernobyl application is intended as an illustration only and not as a full study (which had to use a much broader data base and complex methodology).

Figure (2) requires more explanation

We have tried to make the discussion of Figure 2 more clear.

At the base of p9, the authors need to state the obvious, which is not immediately obvious to the reader... why does Fig. 5 indicate the reactor itself is not likely to be the source?

See the answer to the last of the specific comments raised by Reviewer 2.

What is the "NPP site"? (legend of Fig. 5)

NPP is a widely-used abbreviation for nuclear power plant. We have written that out.

Review 2

Main comments

1. *Existing work in micrometeorology disregarded*

We admit that we do not have the same knowledge of the work on footprint determination in micrometeorology as the reviewer. However, contrary to the reviewer's statement, our introduction does mention the (in our opinion) seminal and most important work from this field, the paper by Flesch et al. (1995). We do agree, and we did write that, that a backward Lagrangian particle dispersion model approach has already been developed in this community. We see as main differences (i) that to our knowledge only conservative properties are considered in these models and (ii) this community has a quite different perspective. We have in mind a very general source-receptor relationship for any trace substances (or other quantities that can be described by our Eq. 1) without simplifications such as stationarity, no wash-out etc. (except the non-linear chemistry). The wording 'footprint', though established in the meantime, does not reflect this well. So our wording is not just an arbitrary choice, we believe it does make sense, and it is the established technical term in air pollution science. What we can maybe observe here is how far apart two (quite related!) subfields of atmospheric science have become!

In order to correspond to the comments, we will give more visibility to the achievements in micro- and boundary layer meteorology and add references to Schmid (2002) and Kljun et al. (2002). The paper of Schmid gives a good opportunity to point out the difference between our approach and the micrometeorological one. He wrote (p. 172): "In contrast, the dispersing 'particles' in the backward approach are viewed simply as fluid elements, or parcels, that are not necessarily charged with any scalar mass, but may have varying amounts." This presentation missed the point that there is a well-defined equation for the evolution of the substances represented by such fluid elements (our Eq. 1), and so it is neither realised that mass has to be replaced by mixing ratio nor that effects of linear loss or build-up mechanisms can be included as well. Probably, both effects are not of much interest in micrometeorological applications, so this does not affect the practical validity of the method, but hopefully it makes clear that we are not just applying an already developed methodology on a larger scale. Rather, we have introduced a much more general and well-founded theory. Thus, we would like to

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

continue to call it “new”.

2. Linear processes

a) Well-mixed criterion

The well-mixed criterion by definition can only be applied to conservative properties and thus will not and must not be fulfilled for the mixing ratio of a substance having sources or sinks.

b) Linear chemical reactions?

For a linear chemical reaction, it is sufficient that the reaction rate (as a function of time and space) can be prescribed, e.g. by specifying a climatological distribution of a reaction partner along with the respective rate coefficient. There is no need for a concentration to explicitly appear in our Eq. 1, it can be absorbed into the parameter α . The reviewer is right that if the reaction under consideration would lead to strong depletion of this reaction partner, the linearity would be violated. We don't share the opinion, however, that only trivial cases could be treated by our methodology. Using climatological OH concentrations, for example, is not uncommon, nor is the use of climatological decay or build-up rates for certain substances in cases where a more detailed treatment is not possible. Certainly, this is a major limitation, but it is a limitation our approach shares with all atmospheric transport models not containing a detailed chemistry model (i.e., most LPDMs) and it has nothing to do with our backward mode. Rather, we have demonstrated that all processes that can be treated by a regular LPDM can be included in the backward mode for source-receptor relationship calculation. This and nothing more was our aim, and we don't raise higher claims.

c) Change of physical properties by chemical reactions?

This is a valid comment, and this issue is not limited to chemical reactions, also aerosol dynamics or conversions by radioactive decay of gaseous substances can have such effects. Though not implemented in Flexpart, such changes – except if gravitational

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

settling properties are affected – could be modelled within the given frame of Flexpart and are also covered in principle by our backward approach, as long as the transformation rates are linear and can thus be prescribed. Each computational particle in Flexpart can carry different species, and dry deposition, for example, is changing only the amount of material on the particle affected, not the particle and its movement. Thus there would be no problem to implement transformations between species at prescribed rates. We don't deem this to be of great practical importance and prefer to keep this out of this paper.

Specific comments

c1 $S \leq t'$: I understand that in the author's implementation, time runs backwards (negative time increment). Therefore, and if t' is the variable of the integral and t a specific value, when a particle arrives at time t , any time t' between $t'=0$ and $t'=t$ will be larger (or equal) than t .

This is a misunderstanding. The sign of the time variable has not been redefined in this derivation. The numerical model is integrated with a negative time step. We wrote: "... the same formalism and computer model are applied, but the particle trajectories are integrated backward in time, using a negative time step." This should be clear enough.

if the averaging time exceeds E ': also horizontal homogeneity must be required for what follows.

Why? No horizontal variations are involved, except along the trajectory, which is considered.

due to the limited number of trajectories'. A good reference to kernel methods would be De Haan (1999).

We agree that this is a good reference and add it.

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

do not simulate the effects of convection. This is probably not true for most of Lagrangian models. For example the models of Luhar and Britter (1989), Weil (1994), Rotach et al (1996) etc. do specifically take into account convection.

This is a misunderstanding based on the fact the micrometeorologists have a different idea of 'convection' (process in unstable boundary layer) than people working mainly on larger scales (convective clouds). We clarify that.

Table 2 Number of particles: 1000. This is quite a small number (for a particle model). The authors should comment on this (in connection with the kernel concentration treatment, probably).

There is no turbulence or mean-wind advection in this test. Therefore, a relatively small number of particles is deemed sufficient. The kernel sampling was switched off, as mentioned! For clarity, we introduce '(Therefore we can work with a relative small number of particles.)' into the Section 3.1 (It should be clear enough that in Section 3.2 there is the same situation).

Wet scavenging acts on all particles regardless of their height: a little more information on how this process is parameterized would be desirable.

A little more information is added (and there is the reference to the Flexpart User Guide with its URL).

'appears to be sufficient to explain the observed Caesium.' This statement should be made more precise. Has any (statistical) test been applied in order to support this statement? What is the resolution of the observations, how many data points etc.? [looking at Fig. 4, for many of the days it appears that both forward and backward simulations yield quite a different value than obs +/- error bars]. Similar: column 2: 'Is not likely the source': can the authors be a little more quantitative?

We have taken this comment as a stimulation to do a similar calculation and analysis also for the half-degree grid cell where the Chernobyl power plant is located as the

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

source, and we present these results in addition (forward and backward calculations). The achievable correlation with the observations is worse in that case, supporting the assumption that the contaminated area and not the nuclear power plant itself is the source of the observed caesium. We concede, however, that this conclusion does not have the character of a proof (the whole application is illustratory only, a series study would need to go much more in the depth of various aspects). We modify our wording accordingly.

A further modification, independent of the reviewers' remarks, is made concerning the outlier (observation of October 13th). We now suggest that it may be due to caesium originating from an area to the northwest of Stockholm at distances of less than 100 km which is contaminated in the 40-100 kBq/m² range.

Interactive comment on Atmos. Chem. Phys. Discuss., 3, 4515, 2003.

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper